

Presentation to BDEC



Division of Advanced Cyberinfrastructure (ACI)
Irene Qualters/Acting Division Director
February 26, 2014

NSF is the only federal agency dedicated to the support of basic research and education across all fields of science and engineering



FY 2014 Budget Appropriation **\$7.2 billion**

Colleges, universities, and other institutions receiving NSF funding **1,895**

Proposals evaluated through a competitive merit review process **48,600**

Competitive awards funded **11,500**

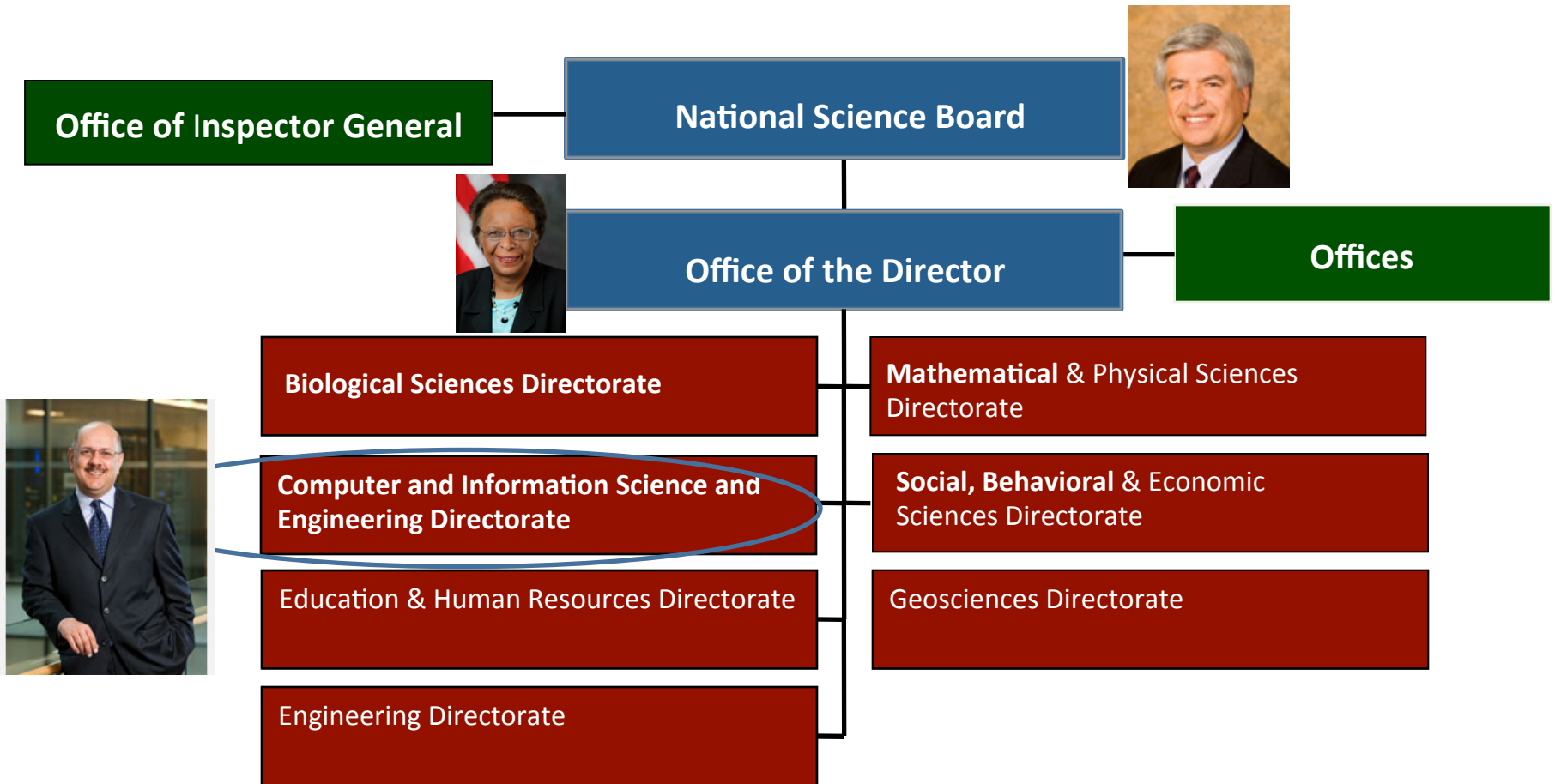
Proposal reviews conducted **236,000**

Estimated number of people NSF supports directly (researchers, postdoctoral fellows, trainees, teachers, and students) **319,000**

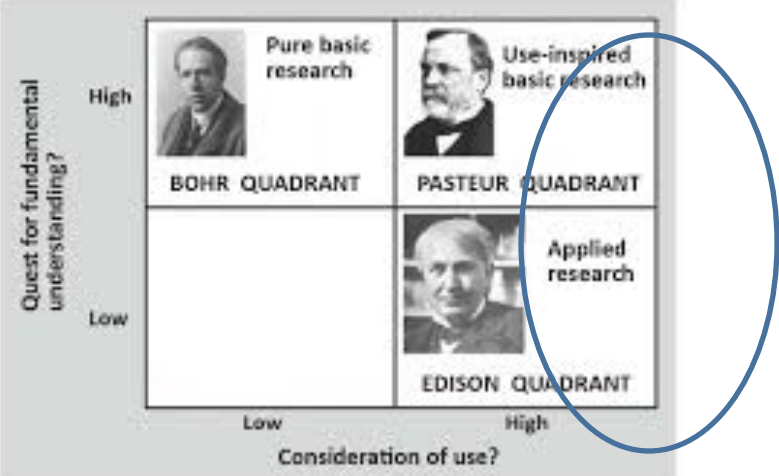
Students supported by NSF Graduate Research Fellowships since 1952 **45,800**



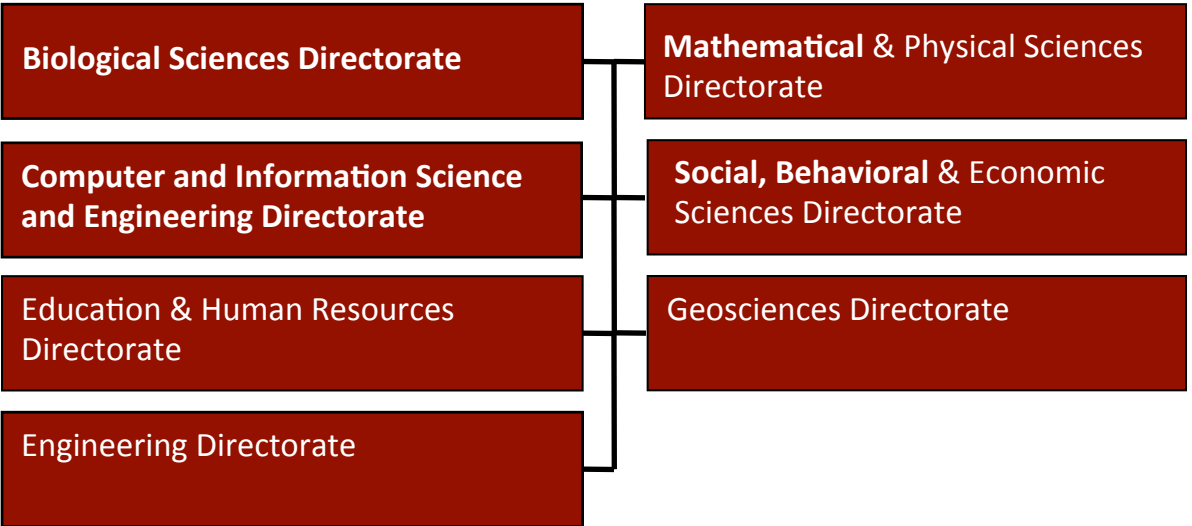
In 2013, NSF's Office of Cyberinfrastructure joined CISE (Computing and Information Science and Engineering) as the division of Advanced Cyberinfrastructure (ACI)



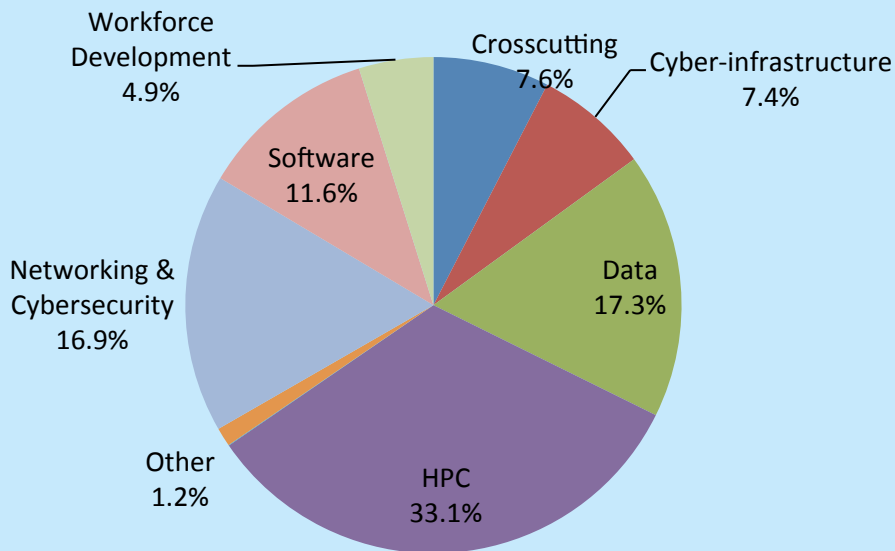
ACI Mission: To support advanced cyberinfrastructure to accelerate discovery and innovation across all disciplines



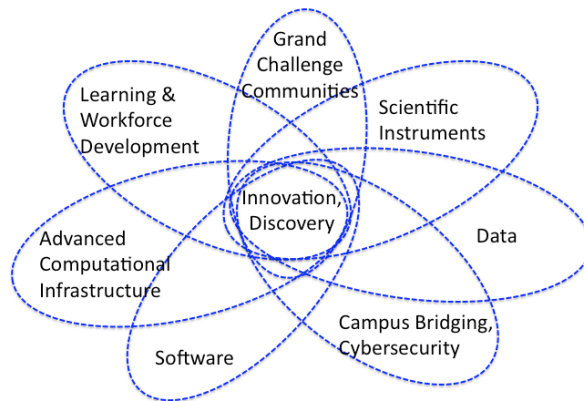
- Use-inspired Cyberinfrastructure
 - Research and Education
 - Science and Engineering
- Inherently multidisciplinary with strong ties to all disciplines/directorates



ACI FY2013 investments reflect a balance across Cyberinfrastructure categories consistent with NSF's CI strategy (CIF21)



CIF21: cyberinfrastructure as an ecological system

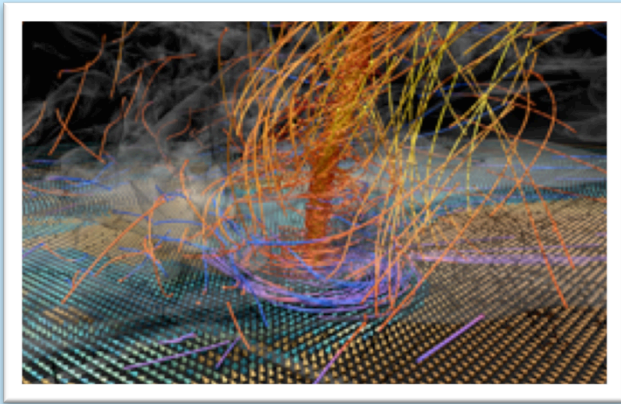


Total ACI FY 2013 funding = \$210,772,572



NSF's computational infrastructure – two key strategies

Vision: Support a comprehensive portfolio of advanced computing infrastructure, programs and other resources to facilitate cutting-edge foundational research in Computational and Data Enabled Science and Engineering (CDS&E) and its applications to all disciplines.



Forecasting Tornadoes: Parallel computing, data mining, and meteorology are being used to determine tornado formation and more reliable tornado forecasting. (Amy McGovern and Kelvin Droegemeier, University of Oklahoma)

- Anticipate and invest in diverse and innovative national scale shared resources, outreach and education complementing campus and other national investments
- Leverage and invest in collaborative flexible “fabrics” dynamically connecting scientific communities with computational resources and services at all scales (campus, regional, national, international)



Advanced Computing Cyberinfrastructure: three major deployments in 2013



Image Credits: NCSA/University of Illinois

Blue Waters, UIUC

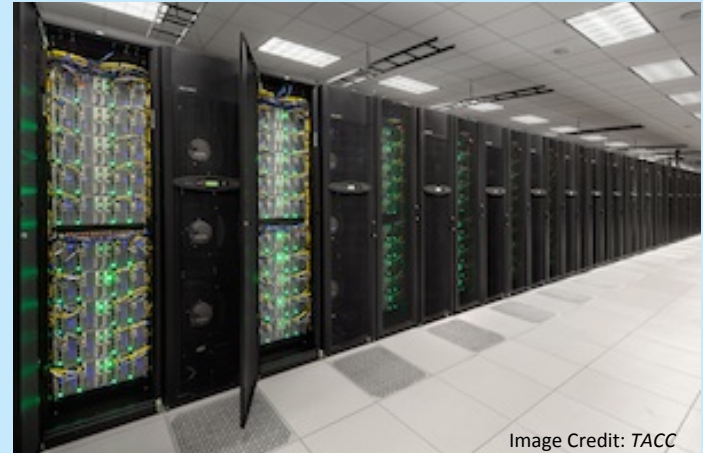


Image Credit: TACC

Stampede, UT Austin



**NCAR/ Wyoming
Supercomputing Center**



Blue Waters: Grand Challenge Computational Science and Engineering through Sustained Petascale Performance

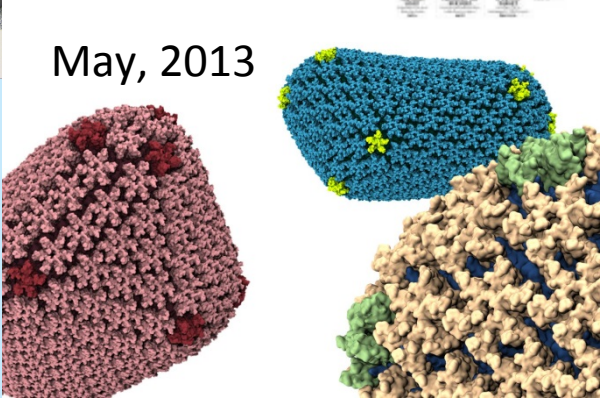
UIUC Data Center



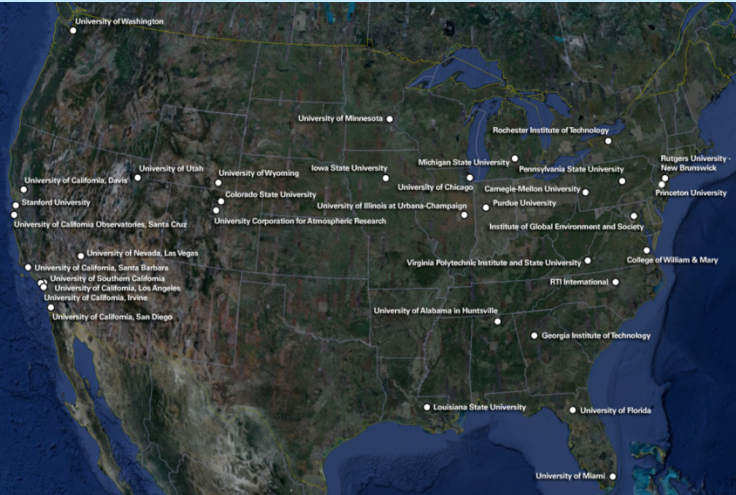
Cray XE6/XK7 accepted December, 2012



May, 2013



Petascale Application Projects



Credit: *Theoretical and Computational Biophysics Group (www.ks.uiuc.edu), Beckman Institute for Advanced Science and Technology, UIUC*



Stampede is both innovative and highly capable, doubling the resource pool for XRAC/XSEDE allocations

A YEAR WITH STAMPEDE

Stampede, one of the most powerful supercomputers in the world for open science research, celebrated its first birthday on January 7, 2014, by completing more than 75,000 years of scientific computations – not bad for a one-year-old. Here are some facts, figures & science highlights that capture the comprehensive impact of the system.

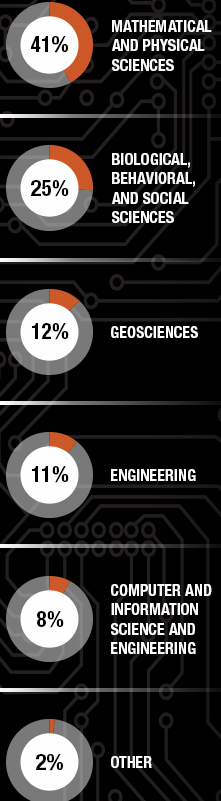
Funded by the National Science Foundation Grant ACI-1134872 and built in partnership with Intel, Dell and Mellanox, Stampede and its academic partners will continue to enable promising computational research in 2014 and beyond.

9.6
QUADRILLION
Floating Point Operations per second

WORLD RANKING
7th
MOST POWERFUL
www.top500.org

1247
PROJECTS
2,196,848
COMPLETED JOBS
3400
RESEARCHERS

SCIENCE FIELDS



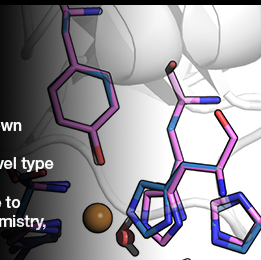
SCIENCE HIGHLIGHTS

Stampede supports the largest number of open science projects in the world across science and engineering domains. Below are three recent highlights:

BIOFUEL PRODUCTION

Researcher: **Gregg Beckham**
National Renewable Energy Laboratory (NREL)

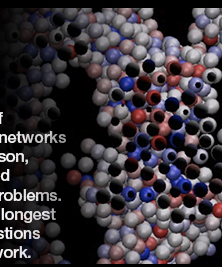
Stampede is helping to determine how enzymes break down cellulose to improve biofuel production. A group of NREL researchers used the supercomputer to predict how a novel type of oxidative enzyme can speed up the process by which cellulose breaks down. The group is also using Stampede to design catalysts for high-temperature deoxygenation chemistry, which is important to convert biomass to fuel.



BIOMEDICINE AND SMART MATERIALS

Researcher: **Roseanna Zia**
Cornell University

Colloidal gels have huge promise in biomedicine. Comprised of microscopic particles suspended in a solvent, these gels form networks of particles that support their weight under gravity. For this reason, these soft solids can be used as injectable pharmaceuticals and artificial tissue scaffolds; however, they are beset by stability problems. Stampede enabled Cornell researchers to conduct the largest, longest simulation of a colloidal gel, which is answering important questions about the structure, dynamics, and stability of the particle network.



SUPERNOVA EXPLOSION

Researcher: **Philipp Mösta and Christian D. Ott**
California Institute of Technology (CalTech)

Using Stampede, astrophysicists succeeded in performing the first fully general-relativistic 3D MHD simulations of progenitor stars that are believed to lead to very energetic, jet-driven supernova explosions. The researchers found that the simulations behave very differently in full unconstrained 3D compared to the same model simulated with imposed symmetries. Stampede's per-core performance pushed these simulations to the limit.



www.tacc.utexas.edu
www.tacc.utexas.edu/stampede
#useTACC #UltimateScienceEnvironment

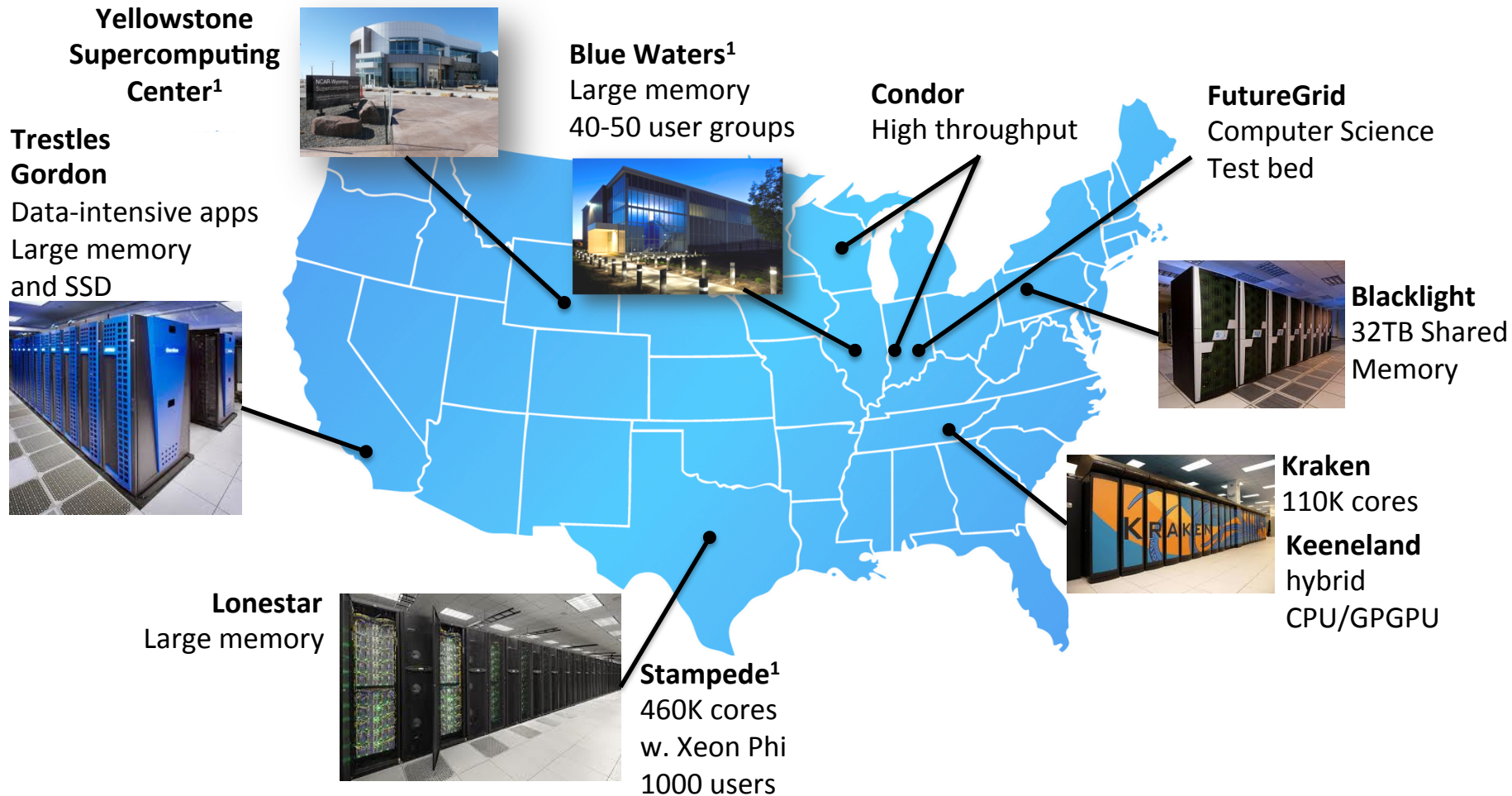


XSEDE

THE UNIVERSITY OF TEXAS
AT AUSTIN



NSF Advanced Computing Infrastructure is increasingly diverse and collaborative



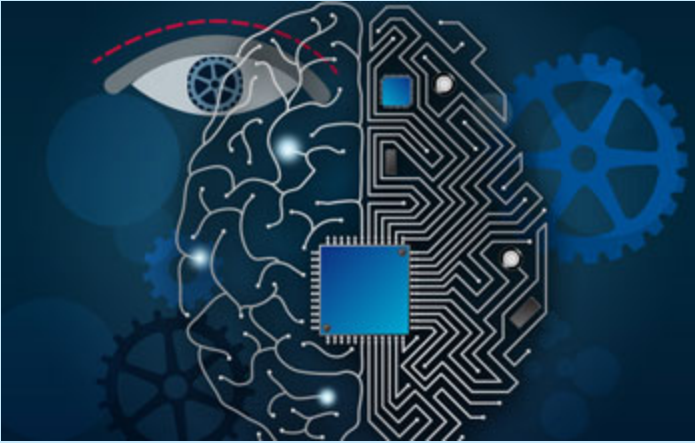
1. Launched in FY 2013

Next steps...

- Resource Solicitations (FY13 & FY14) to expand and diversify the reach of advanced computing
 - High Performance Computing System Acquisition: Building a More Inclusive Computing Environment for Science and Engineering
 - *Wrangler* at TACC: data analysis and management; Hadoop; NAND Flash
 - *Comet* at SDSC: “long tail science”, high throughput; 2 PF; Xeon Phi
 - 1-2 new awards in FY14
 - Deployments in FY15, FY16
- Stampede Upgrade in FY15 of Intel Xeon Phi
- National Academies study: Future Directions for NSF Advanced Computing Infrastructure to support US Science in 2017-2020
 - contribution of high-end computing to U.S leadership/competitiveness in basic S&E and NSF role in sustaining this leadership
 - expected national-scale computing needs, both high-end and in support of full range of S&E
 - complementarities and tradeoffs among investments in computing, software, data, communications
 - range of operational models for delivering ACI for S&E and role of NSF in these models
 - expected technical challenges to affordably delivering the capabilities needed for worldleading S&E



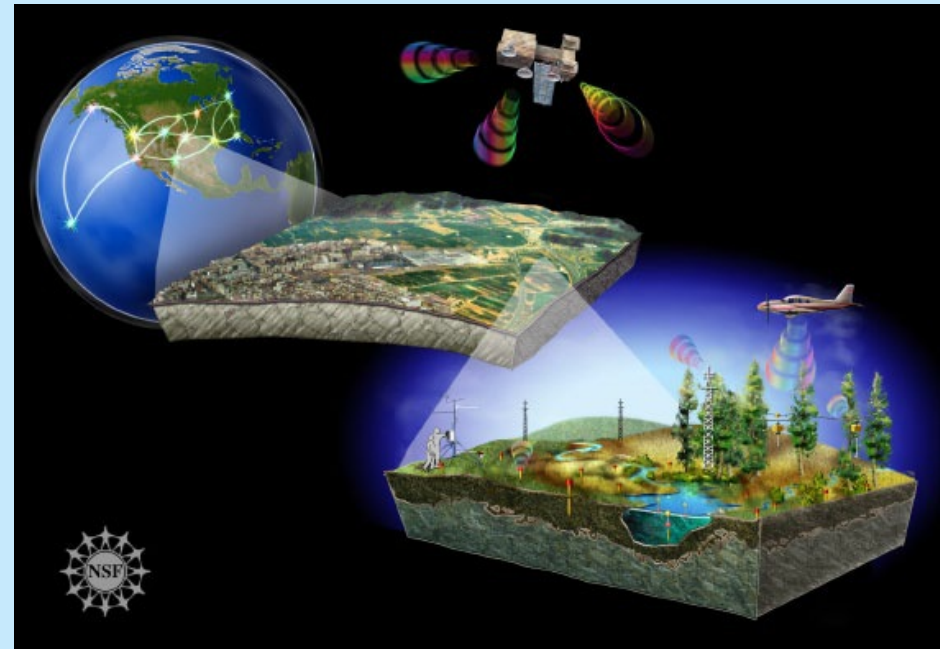
Ubiquity in mobile devices, social networks, sensors and instruments have created a complex data-rich environment ripe for new scientific and engineering advances



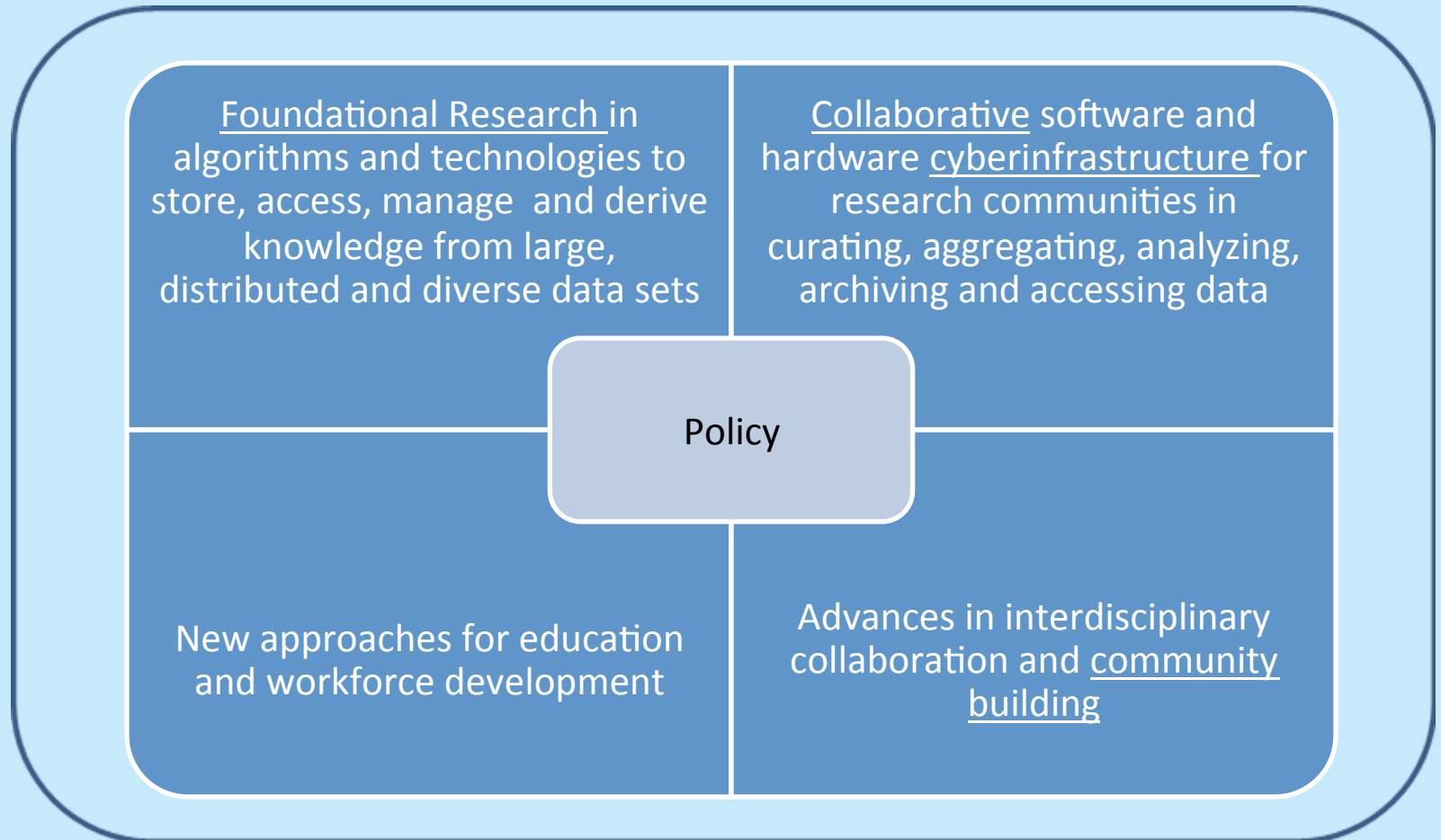
Credit: *Christine Daniloff/MIT*

An artist's conception of the National Ecological Observatory Network (NEON) depicting its distributed sensor networks, experiments and aerial and satellite remote sensing capabilities, all linked via cyberinfrastructure into a single, scalable, integrated research platform for conducting continental-scale ecological research. NEON is one of several National Science Foundation Earth-observing systems.

Credit: *Nicolle Rager Fuller, National Science Foundation*



NSF Data Investment Framework



ACI Data Activities within this Framework

- **Developing data-focused CI usable by multiple scientific disciplines**
- **Addressing problems common to various communities**
- **Being responsive to differing scientific requirements & priorities**
- **Programmatic activities**
 - **Data Infrastructure Building Blocks (DIBBs)** – data-focused CI “building blocks” enabling science & engineering research;
 - **EarthCube** - engagements of multiple earth-centered science communities with each other and with technologists to create integrated geosciences focused infrastructure;
 - **DataWay** - focus on “science pull,” creation of integrated data management structures for science-driven research;
 - **BigData** - Core Techniques & Technologies;
 - **DataNet** - portfolio of 5 early implementations and proof-of-concept” data projects offering suites of tools and other capabilities;
 - **Research Data Alliance** - multi-national communities combining to accelerate data-driven innovations and discoveries;



Networking and Cybersecurity – major network upgrades begun and continuing

- CC-NIE (Campus Cyberinfrastructure – Network Infrastructure and Engineering):

- 43 awards made in FY 2013
- FY2014 solicitation

- IRNC (International R&E Network Connections)

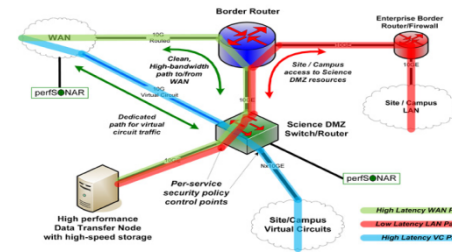
- 100Gbps experimental awards, partners in Europe and Brazil
- FY14 solicitation

- Cybersecurity

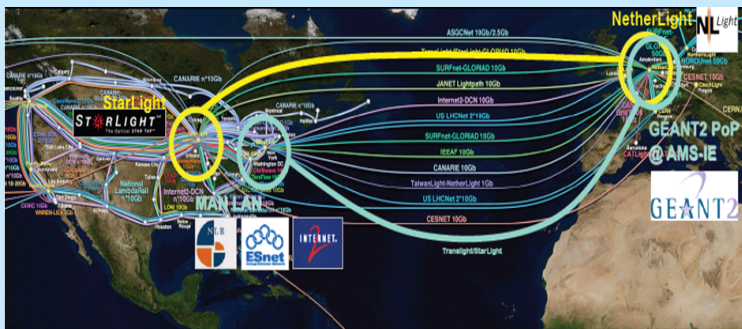
- Continued participation in SaTC w/ Transition-to-Practice support

Simple Science DMZ Diagram

A simple Science DMZ has several essential components. These include dedicated access to high-performance wide area networks and advanced services infrastructures, high-performance network equipment, and dedicated science network resources such as Data Transfer Nodes. A notional diagram of a simple Science DMZ showing these components, along with data paths, is shown below.



The essential components and a simple architecture for a Science DMZ are shown in the Figure above. The Data Transfer Node (DTN) is connected directly to a high-performance Science DMZ switch or router, which is connected directly to the border router. The DTN's job is to efficiently and effectively move science data to and from remote sites and facilities, and everything in the Science DMZ is aimed at this goal. The security policy enforcement for the DTN is done using access control lists on the Science DMZ switch or router, not on a separate firewall.





Thank you!

