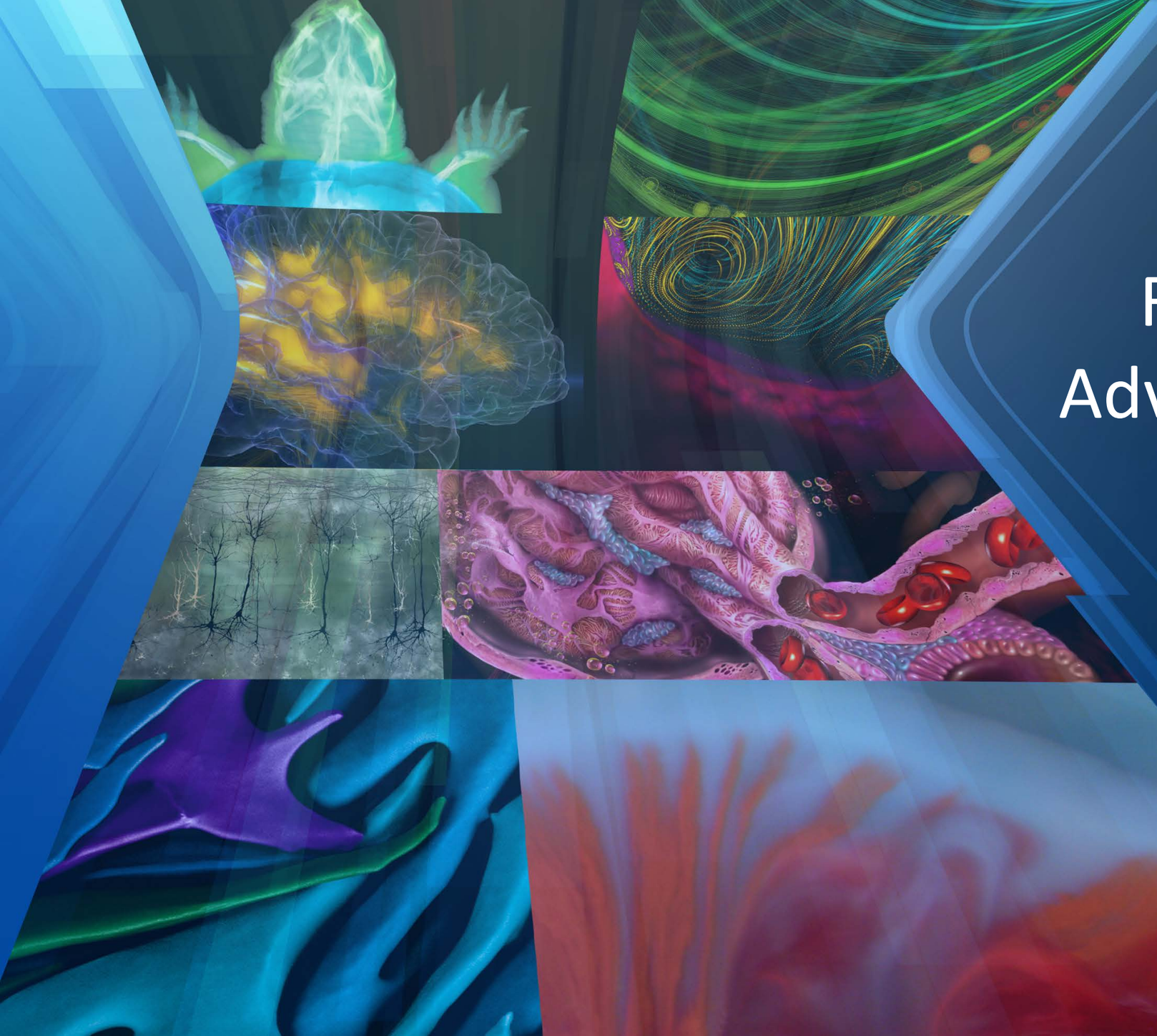


Rocky Mountain Advanced Computing Consortium

Irene Qualters
Division Director, NSF/ACI

August, 2016

Overview

- **Hors D’oeuvres**
- Introduction
- FY 2017 Portfolio
- Beyond FY 2017

NSF investments in shared research cyberinfrastructure enabled LIGO detection of gravitational waves

LIGO relied on advances in computational science, software, hardware, and expert services throughout the research infrastructure.*

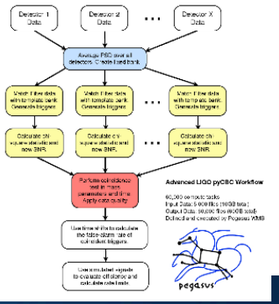
- Access to Large, Diverse and Interoperable CI:
  - Massive, parallel event searches and validation;
  - High performance simulations
  - Open Science Grid (OSG): Comet (SDSC) and Stampede (TACC); Blue Waters PRAC
  - Expertise : XSEDE, TACC, BW
- Computational Science Advances:
  - Numerical relativity and magnetohydrodynamics
  - Visualizations
- Workflow and dataflow: Pegasus and HTCondor
- Networking: upgrades from 10Gbps to 100Gbps WAN

Open Science Grid

Pegasus

XSEDE
Extreme Science and Engineering Discovery Environment

HTCondor
High Throughput Computing



TEXAS ADVANCED COMPUTING CENTER
STAMPEDE

einstein toolkit

*NSF programs: Data Building Blocks (DIBBs), Software Infrastructure (SI2), Campus Cyberinfrastructure Network Infrastructure and Engineering (CC*NIE, DNI), HPC, and others. Many also co-supported by the US. DOE and Int'l Partners

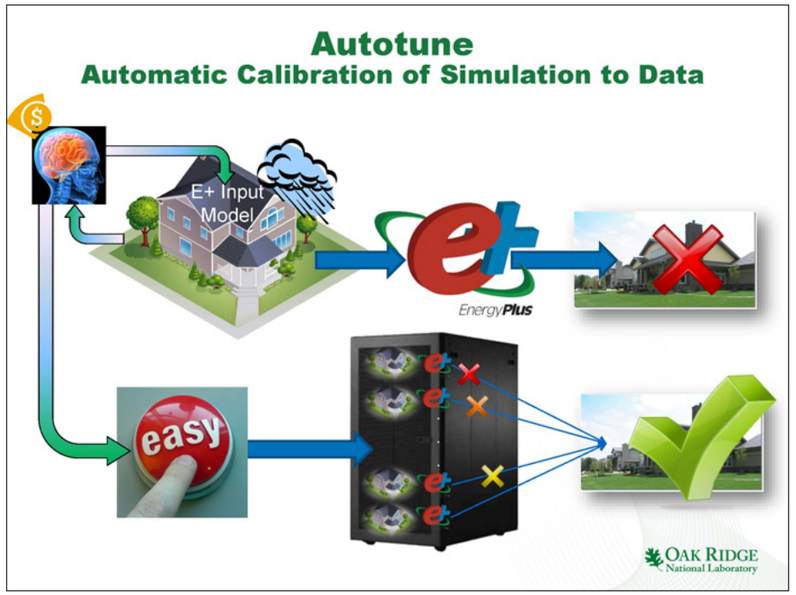
Wrangler/UT Austin (PI Stanzione)

A Transformational Data Intensive Resource for the Open Science Community

The Hobby-Eberly Telescope will collect 200 gigabytes of galaxy spectra data each night for three years, which will be preserved and analyzed on the Wrangler data-intensive supercomputer.

Credit: Ethan Tweedie Photography.

Available to users through XSEDE
Deployed in 2015



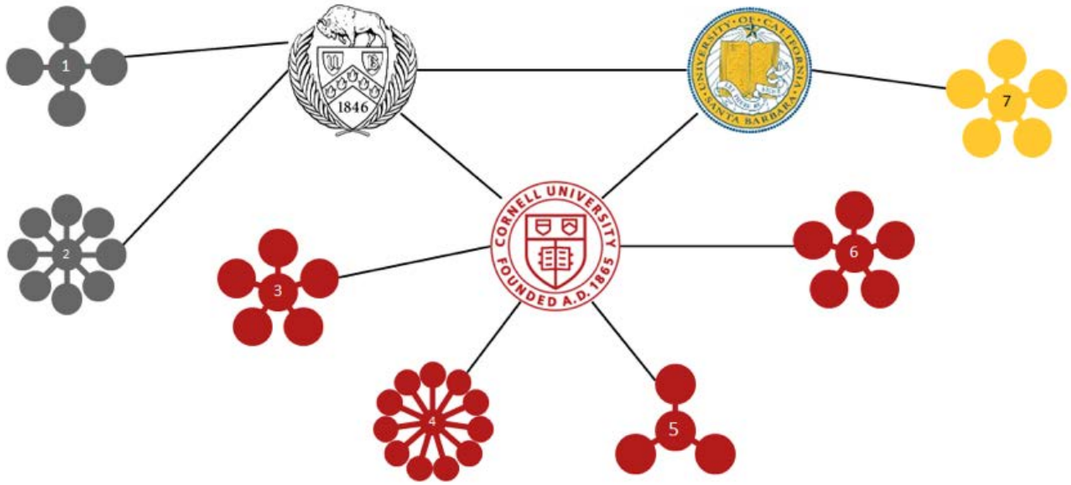
Autotune is a set of automated calibration techniques for tuning residential and commercial building energy efficiency software models (Energy Plus) to match measured data. Credit: Joshua New, ORNL

Aristotle: Federated Cloud

Data Analysis and Management Building Blocks for Multi-Campus

Cornell University/PI Lifka [Award #ACI-1541215]

- Cornell and partners (SUNY Buffalo and UC Santa Barbara) create a federated cloud
- Metric: ‘time to science’
- “Informed Bursting” via *qbets*
  - Private, commercial Clouds



- Includes diverse usage modalities:
  - Seven science use cases
  - An allocation model that provides a fair exchange mechanism between and across multiple institutions
- Explores model for sharing institutional cyberinfrastructure.

Overview

- Hors D’oeuvres
- **Introduction**
- FY 2017 Portfolio
- Beyond FY 2017

NATIONAL SCIENCE FOUNDATION


NATIONAL SCIENCE BOARD (NSB)
Dan E. Arvizu
Chair
Kelvin K. Droegemeier
Vice Chair
703.292.7000

NATIONAL SCIENCE BOARD OFFICE
Michael Van Woert
Executive Officer
703.292.7000

OFFICE OF INSPECTOR GENERAL (OIG)
Allison C. Lerner, Inspector General
703.292.7100

Richard Buckius
Chief Operating Officer

OFFICE OF THE DIRECTOR
703.292.8000

France A. Córdova
Director

Vacant
Deputy Director

OFFICE OF DIVERSITY & INCLUSION (ODI)
Rhonda Davis, Head
703.292.8020

OFFICE OF THE GENERAL COUNSEL (OGC)
Lawrence Rudolph, General Counsel
Peggy Hoyle, Deputy GC
703.292.8060

OFFICE OF INTEGRATIVE ACTIVITIES (OIA)
Suzanne Iacono, Head
703.292.8040

OFFICE OF INTERNATIONAL SCIENCE & ENGINEERING (OISE)
Rebecca Keiser, Head
703.292.8710

OFFICE OF LEGISLATIVE & PUBLIC AFFAIRS (OLPA)
Amanda Greenwell, Head
703.292.8070

DIRECTORATE FOR BIOLOGICAL SCIENCES (BIO)
James L. Olds, Assistant Director
Jane Silverthorne, Deputy AD
703.292.8400

- DIVISION OF BIOLOGICAL INFRASTRUCTURE (DBI)
- DIVISION OF ENVIRONMENTAL BIOLOGY (DEB)
- DIVISION OF INTEGRATIVE ORGANISMAL SYSTEMS (IOS)
- DIVISION OF MOLECULAR & CELLULAR BIOSCIENCES (MCB)
- OFFICE OF EMERGING FRONTIERS (EF)

DIRECTORATE FOR COMPUTER & INFORMATION SCIENCE & ENGINEERING (CISE)
James F. Kurose, Assistant Director
Wendy Blumenthal, Acting Deputy AD
703.292.8900

- DIVISION OF COMPUTER & NETWORK SYSTEMS (CNS)
- DIVISION OF COMPUTING & COMMUNICATION FOUNDATIONS (CCF)
- DIVISION OF ADVANCED CYBERINFRASTRUCTURE (ACI)
- DIVISION OF INFORMATION & INTELLIGENT SYSTEMS (IIS)

DIRECTORATE FOR EDUCATION & HUMAN RESOURCES (EHR)
Joan Ferrini-Mundy, Assistant Director
William (Jim) Lewis, Deputy AD
703.292.8600

- DIVISION OF GRADUATE EDUCATION (DGE)
- DIVISION OF HUMAN RESOURCE DEVELOPMENT (HRD)
- DIVISION OF RESEARCH ON LEARNING IN FORMAL & INFORMAL SETTINGS (DRL)
- DIVISION OF UNDERGRADUATE EDUCATION (DUE)

DIRECTORATE FOR ENGINEERING (ENG)
Pramod P. Khargonekar, Assistant Director
Grace Wang, Deputy AD
703.292.8300

- DIVISION OF CHEMICAL, BIOENGINEERING, ENVIRONMENTAL & TRANSPORT SYSTEMS (CBET)
- DIVISION OF CIVIL, MECHANICAL & MANUFACTURING INNOVATION (CMMI)
- DIVISION OF ELECTRICAL, COMMUNICATIONS & CYBER SYSTEMS (ECCS)
- DIVISION OF ENGINEERING EDUCATION & CENTERS (EEC)
- DIVISION OF INDUSTRIAL INNOVATION & PARTNERSHIPS (IIP)
- OFFICE OF EMERGING FRONTIERS IN RESEARCH & INNOVATION (EFRI)

DIRECTORATE FOR GEOSCIENCES (GEO)
Roger Wakimoto, Assistant Director
Margaret Cavanaugh, Deputy AD
703.292.8500

- DIVISION OF ATMOSPHERIC & GEOSPACE SCIENCES (AGS)
- DIVISION OF EARTH SCIENCES (EAR)
- DIVISION OF OCEAN SCIENCES (OCE)
- DIVISION OF POLAR PROGRAMS (PLR)

DIRECTORATE FOR MATHEMATICAL & PHYSICAL SCIENCES (MPS)
Fleming Crim, Assistant Director
Clifford Gabriel, Acting Deputy AD
703.292.8800

- DIVISION OF ASTRONOMICAL SCIENCES (AST)
- DIVISION OF CHEMISTRY (CHE)
- DIVISION OF MATERIALS RESEARCH (DMR)
- DIVISION OF MATHEMATICAL SCIENCES (DMS)
- DIVISION OF PHYSICS (PHY)
- OFFICE OF MULTIDISCIPLINARY ACTIVITIES (OMA)

DIRECTORATE FOR SOCIAL, BEHAVIORAL, & ECONOMIC SCIENCES (SBE)
Fay L. Cook, Assistant Director
Kathie M. Cragin Henderson, Deputy AD
703.292.8700

- DIVISION OF BEHAVIORAL & COGNITIVE SCIENCES (BCS)
- DIVISION OF SOCIAL & ECONOMIC SCIENCES (SES)
- NATIONAL CENTER FOR SCIENCE AND ENGINEERING STATISTICS (NCSES)

OFFICE OF BUDGET, FINANCE, & AWARD MANAGEMENT (BFA)
Martha A. Rubenstein, Head / Chief Financial Officer
Teresa Grancorvitz, Deputy Head
703.292.8200

- BUDGET DIVISION (BUD)
- DIVISION OF ACQUISITION AND COOPERATIVE SUPPORT (DACS)
- DIVISION OF FINANCIAL MANAGEMENT (DFM)
- DIVISION OF GRANTS & AGREEMENTS (DGA)
- DIVISION OF INSTITUTION & AWARD SUPPORT (DIAS)
- LARGE FACILITIES OFFICE

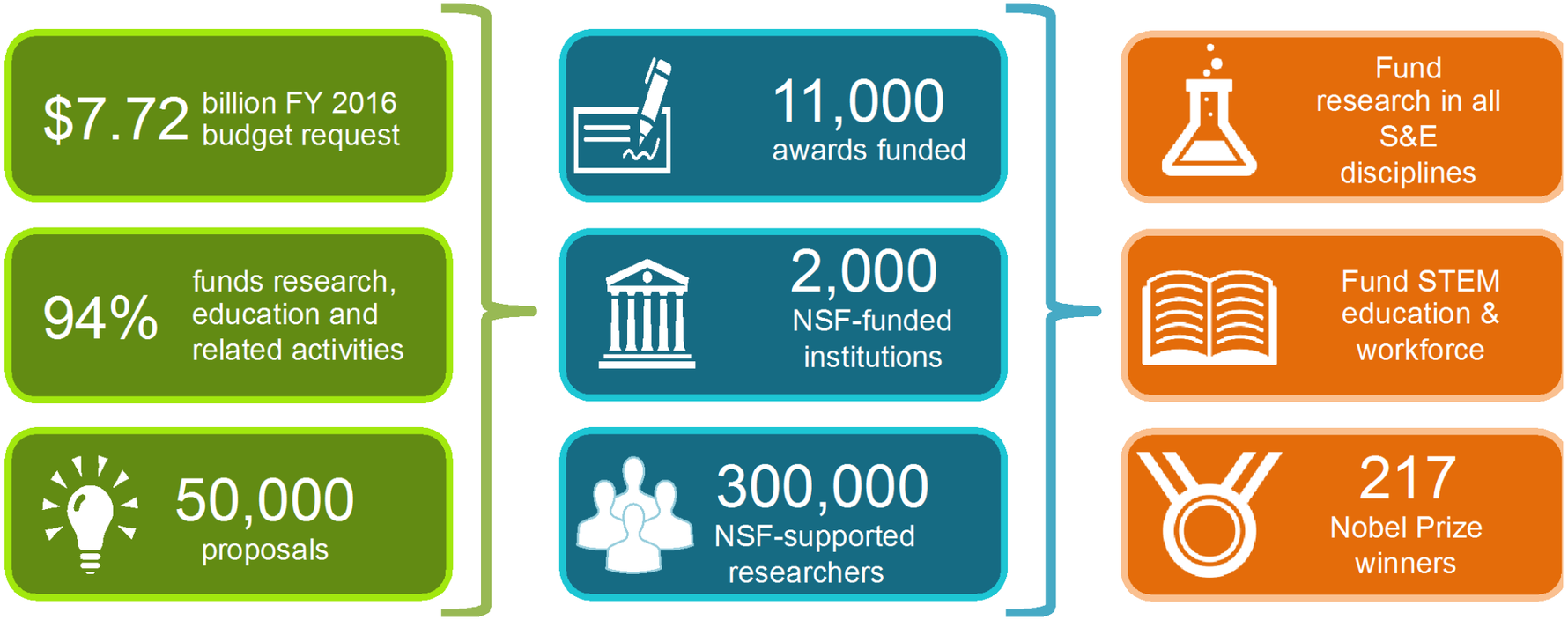
OFFICE OF INFORMATION & RESOURCE MANAGEMENT (OIRM)
Joanne S. Tornow, Head / Chief Human Capital Officer
Donna Bolles, Deputy Office Head
703.292.8100

- DIVISION OF ADMINISTRATIVE SERVICES (DAS)
- DIVISION OF INFORMATION SYSTEMS (DIS)
- DIVISION OF HUMAN RESOURCE MANAGEMENT (HRM)

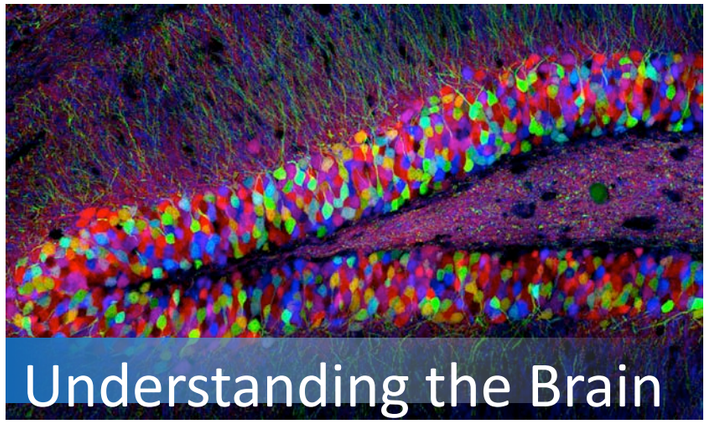
National Science Foundation
4201 Wilson Boulevard
Arlington, Virginia 22230
TEL: 703.292.5111 | FIRS: 800.877.8339 | TDD: 800.281.8749

February 2016

NSF by the Numbers



NSF Addresses National Priorities through Support of Fundamental Research



…..and this requires a highly capable, highly interoperable Research Infrastructure

NSF big ideas for future investment

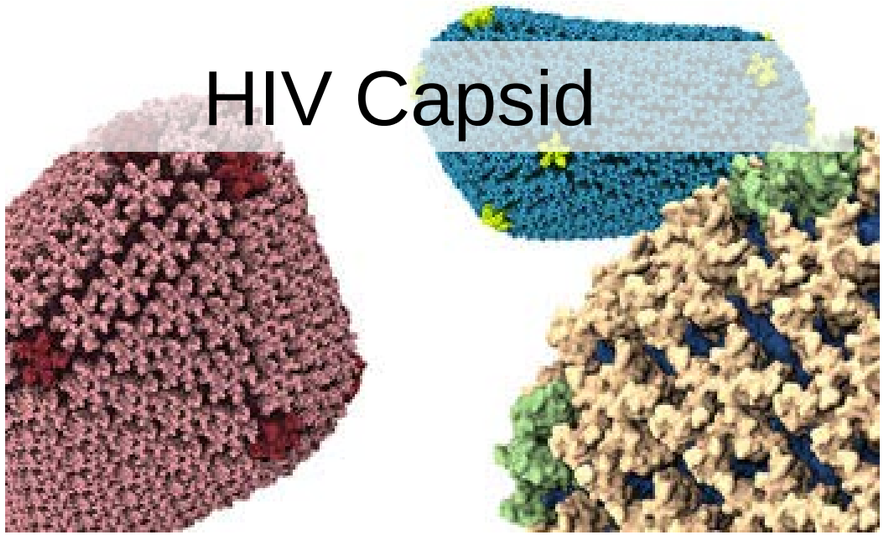
Research Ideas

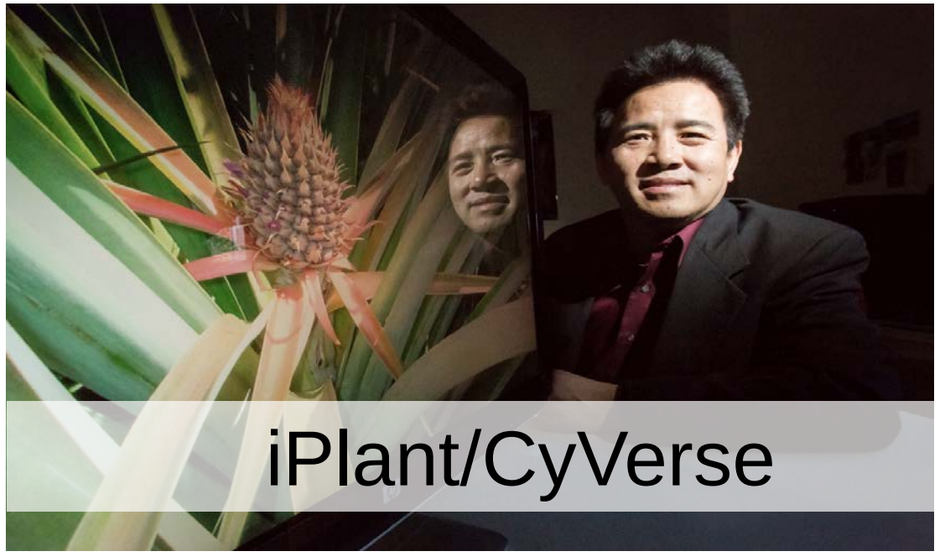
- Harnessing Data for 21st Century Science and Engineering
- Shaping the Human – Technology Frontier
- Understanding the Rules of Life: Predicting Phenotype
- The Quantum Leap: Leading the Next Quantum Revolution
- Navigating the New Arctic
- Windows on the Universe: The Era of Multi-messenger Astrophysics

Process Ideas

- Growing Convergent Research at NSF
- Mid-scale Research Infrastructure
- NSF INCLUDES
- NSF 2050

ACI supported research infrastructure enables discoveries





Overview

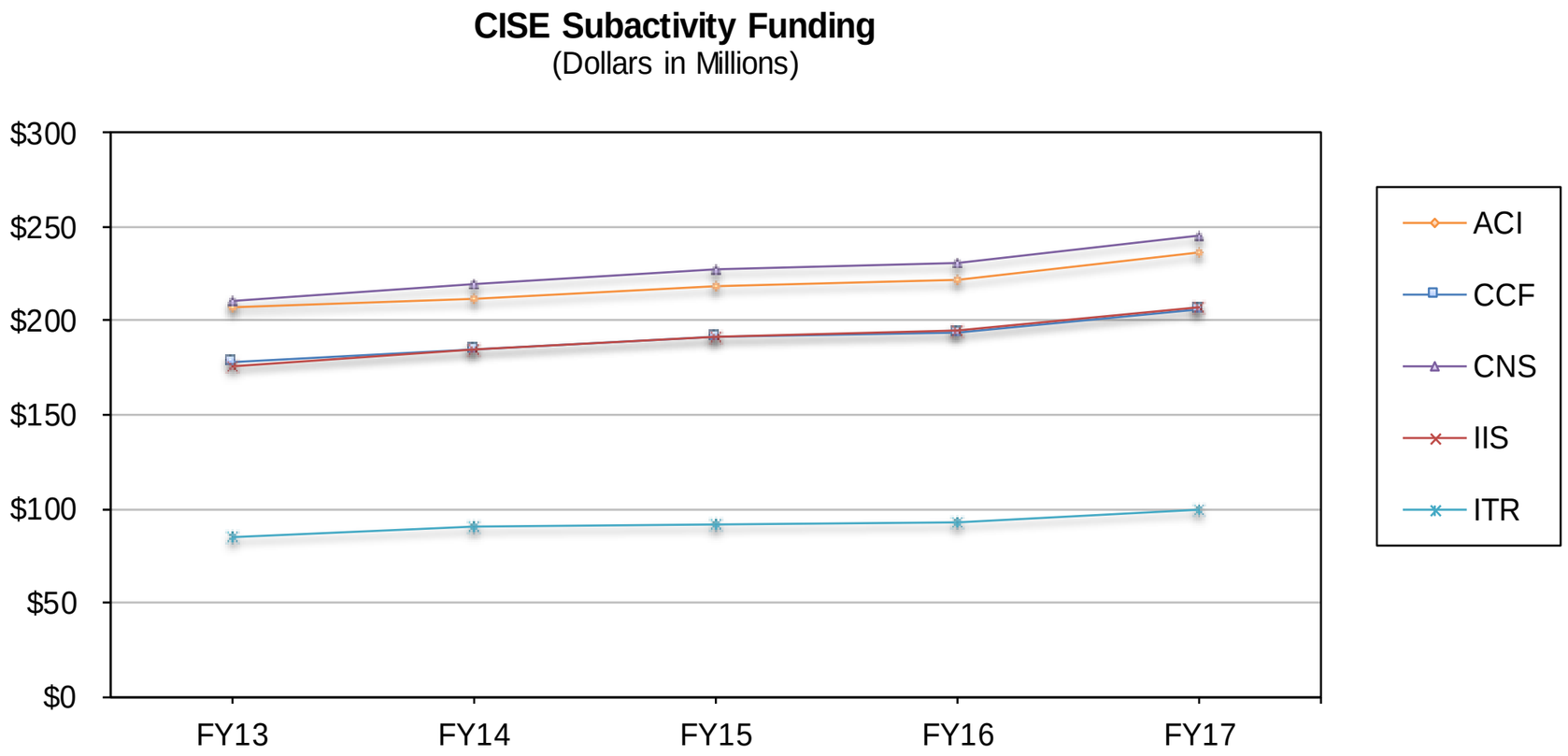
- Hors D’oeuvres
- Introduction
- **FY 2017 Portfolio**
- Beyond FY 2017

FY 2017 Budget Request

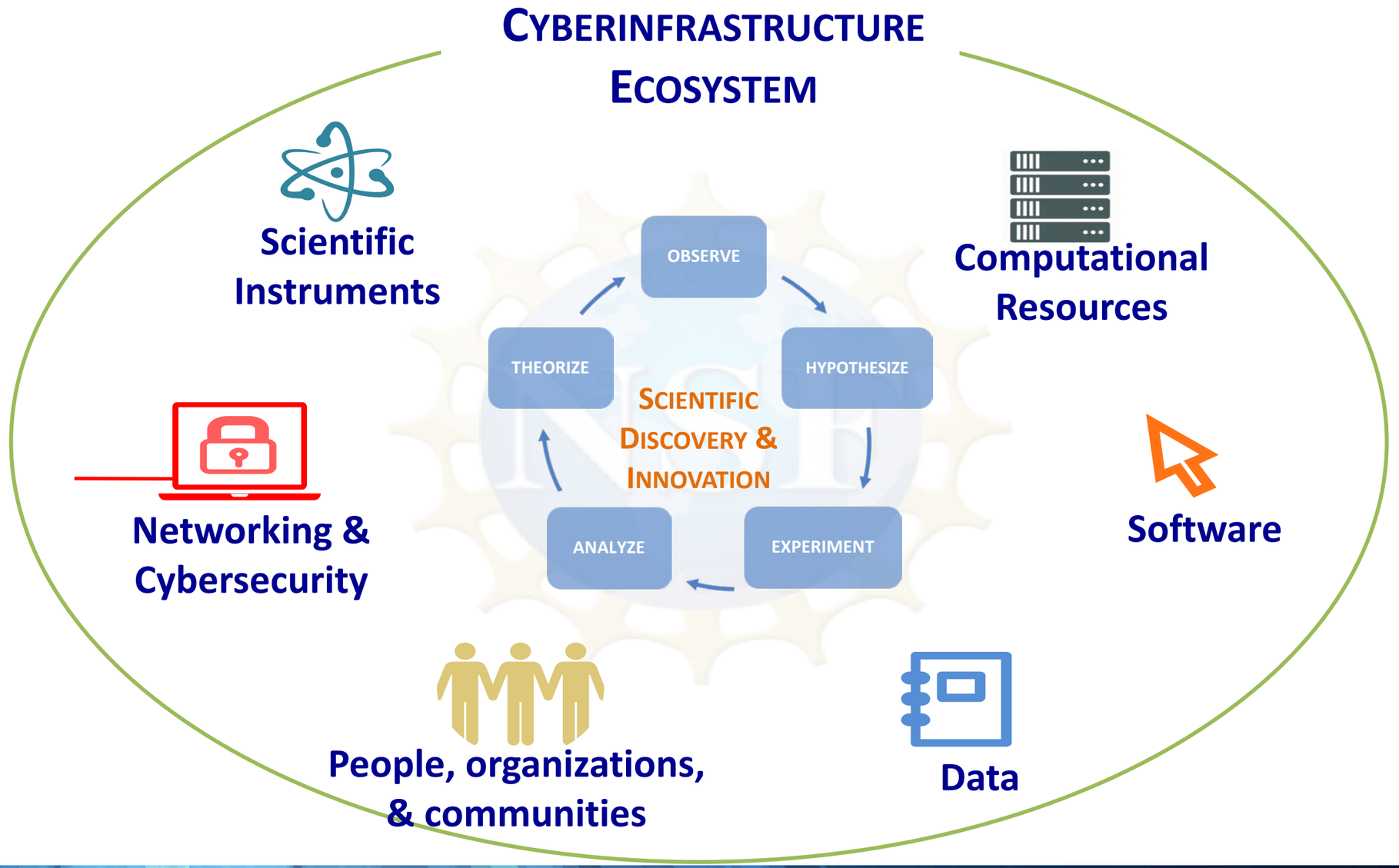
- **NSF**
  - FY 2017 Budget Request: $7,964 Million
  - Increase over FY 2016 Est: $501 Million, +6.7%
- **CISE**
  - FY 2017 Budget Request: $995 Million
  - Comparison to FY 2016 Est: $59 Million, +6.3%
- CISE FY 2017 request is shaped by investments in *core research, education, and infrastructure programs* as well as critical investments *in NSF cross-directorate priorities and programs*.

Growing Division Budgets

Modest, sustained growth across all CISE divisions

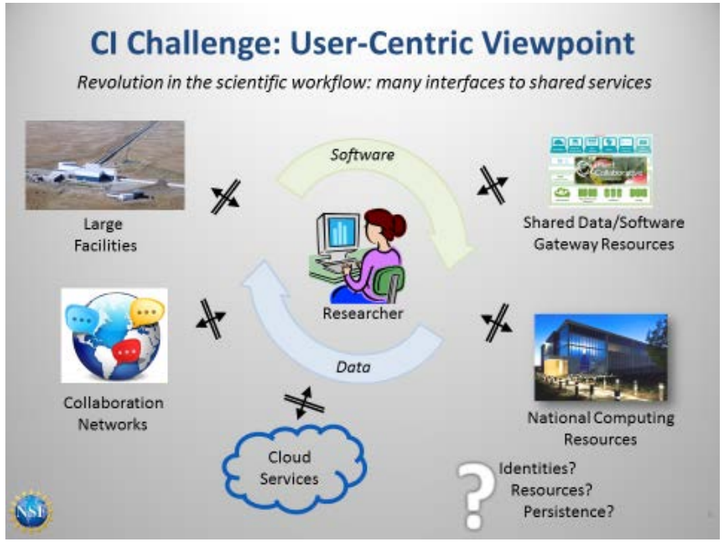


ACI leads an expansive view of research infrastructure driven by research priorities and the scientific process

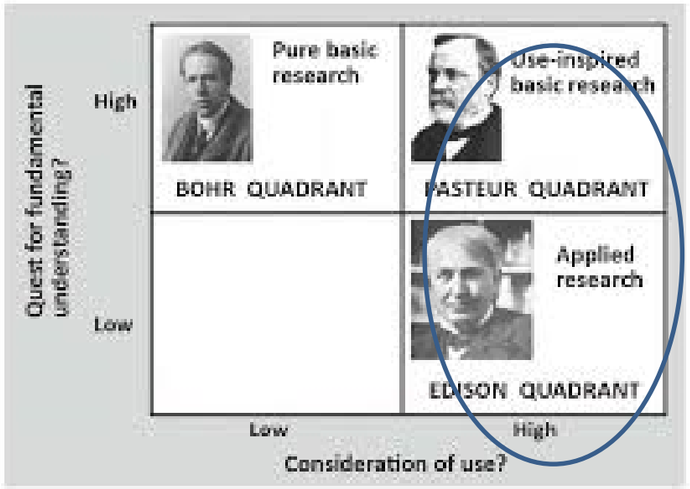


What makes NSF support for Research Cyberinfrastructure unique?

- Research frontiers and communities are vast, dynamic, and multidisciplinary
  - Interoperability critical
  - Deep community engagement essential
  - Dynamic & diverse technology required
  - Fiduciary responsibilities for efficiency and sustainability
- Research (Cyber)infrastructure investments
  - Universities
  - Federal, state and local agencies
  - International funders
  - Private and public entities, profit and non-profit
  - …….and NSF



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



- Coordination role across NF
- Supports Use-inspired Cyberinfrastructure
  - Research and Education
  - Science and Engineering
- Inherently multidisciplinary with strong ties to all disciplines/directorates

Biological Sciences

Computer and Information Science and Engineering

Education & Human Resources

Engineering

Mathematical & Physical Sciences

Social, Behavioral & Economic Sciences

Geosciences

ACI Division Staff

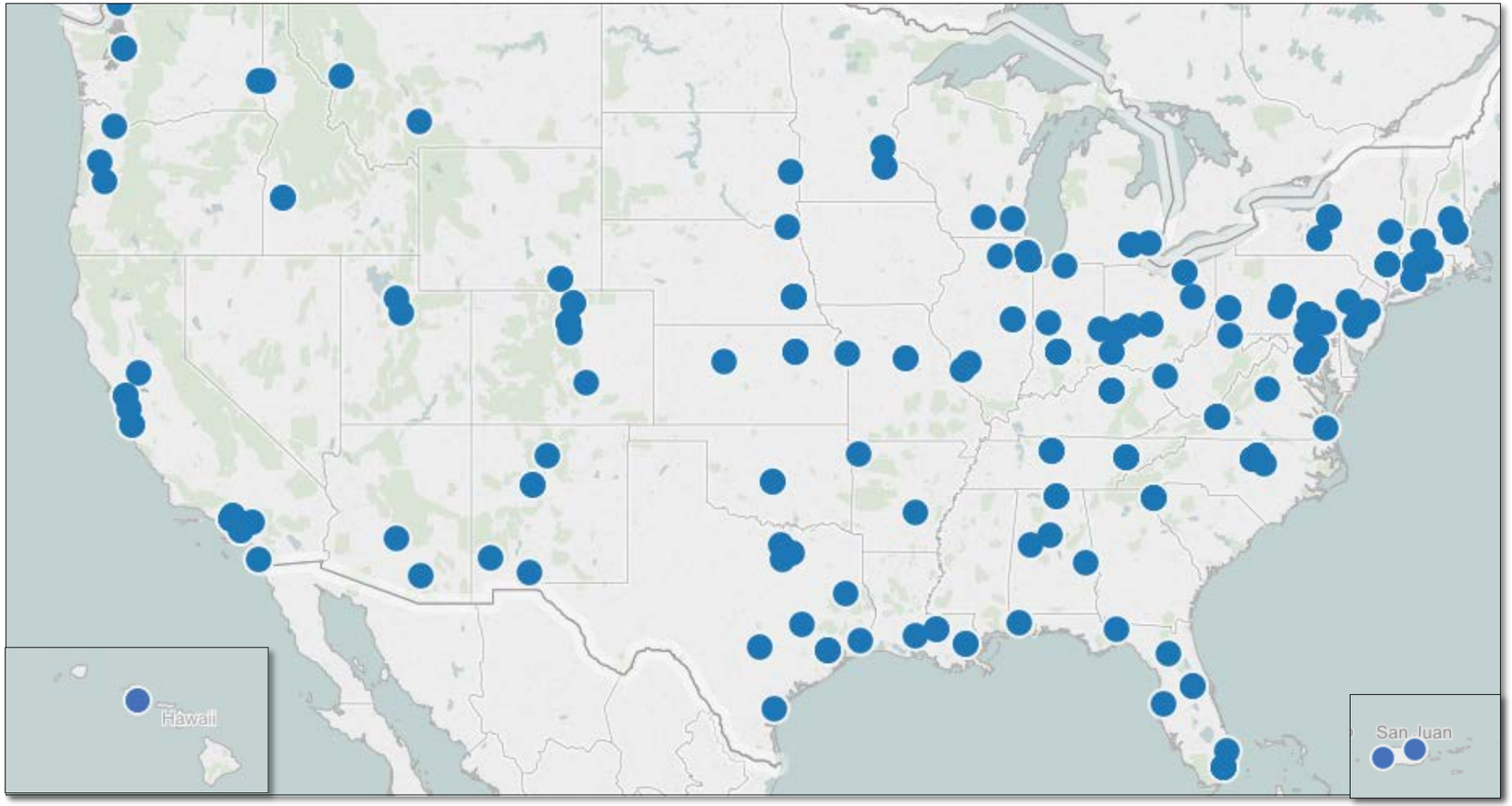
Division of Advanced Cyberinfrastructure (ACI)

Division Director: Irene Qualters
Division Assistant Director: A. Friedlander

Data	R. Chadduck A. Walton
High Performance Computing	R. Chadduck R. Eigenmann E. Walker
Networking/ Cybersecurity	A. Nikolich K. Thompson
Software	**P. Knezek** R.Ramnath **V. Chaudhary**

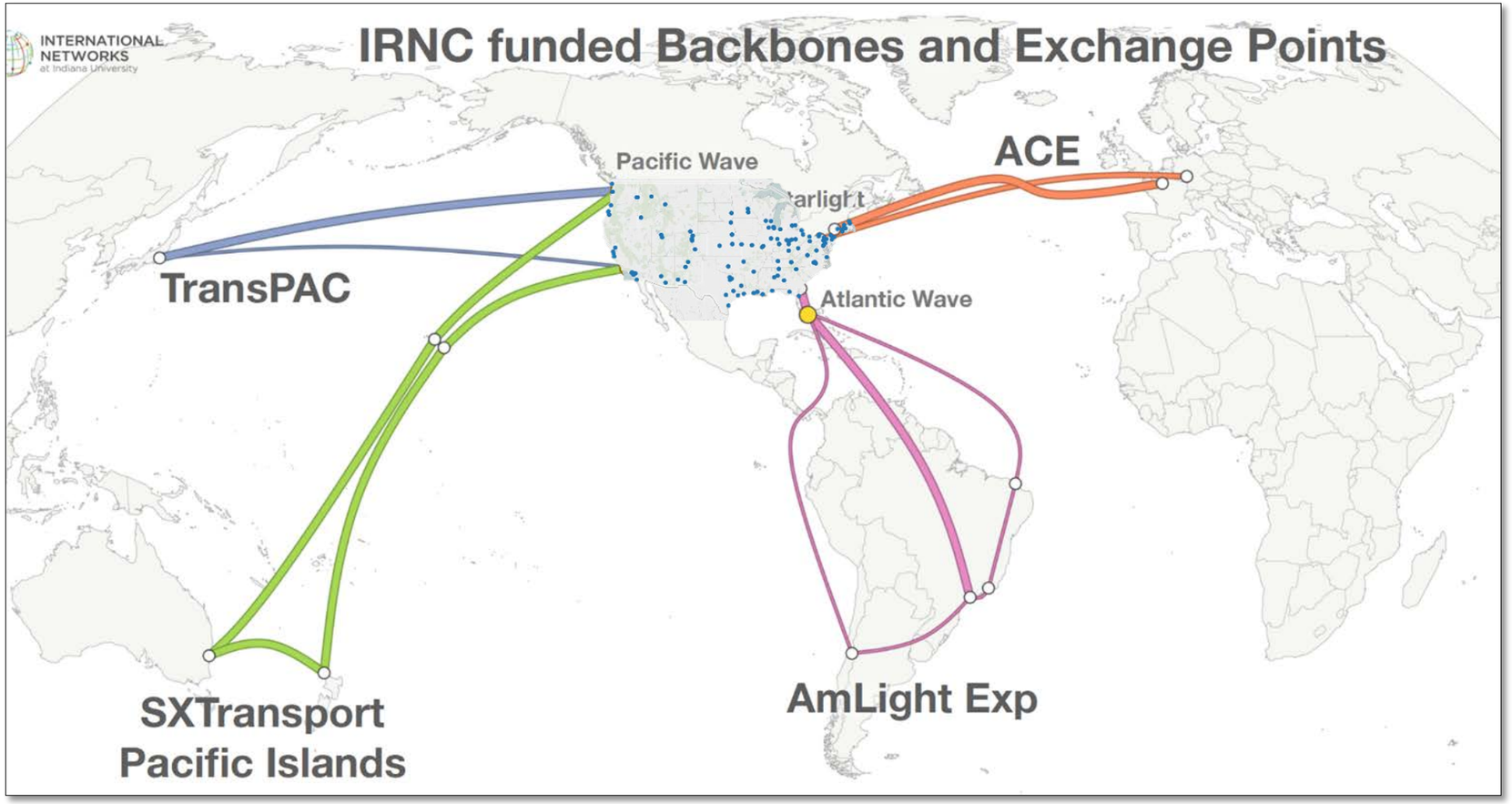
Science Advisor Cross-cutting CI	W. Miller
Learning/ Workforce Development	S. Prasad

Network connections stimulate links across U.S. campuses and facilitate international research coordination



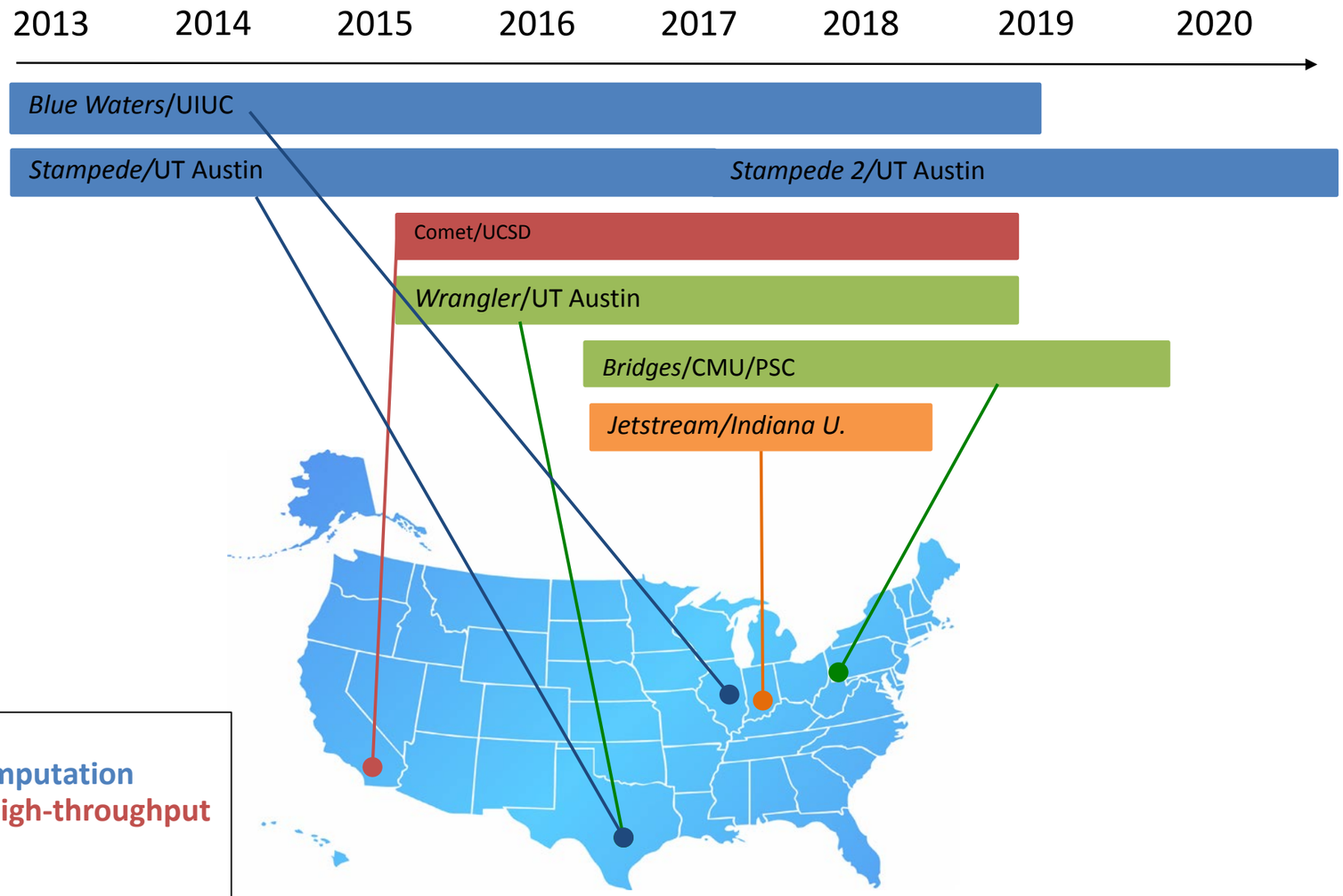
CAMPUS CYBERINFRASTRUCTURE (CC*): Upgrades networking capabilities for >200 campuses

Network connections/exchange points link U.S. campuses and facilitate international research coordination



INTERNATIONAL RESEARCH NETWORK CONNECTIONS (IRNC):
International network services to advance global S&E research and education

A diversity of computational resources complement campus investments and support large scale computing



Legend:
Large-scale computation
Long-tail and high-throughput
Data Intensive
Cloud

XSEDE, OSG, ACI-REF are virtual organizations to connect people, services, and resources

Seamless access to national CI

Training and community building

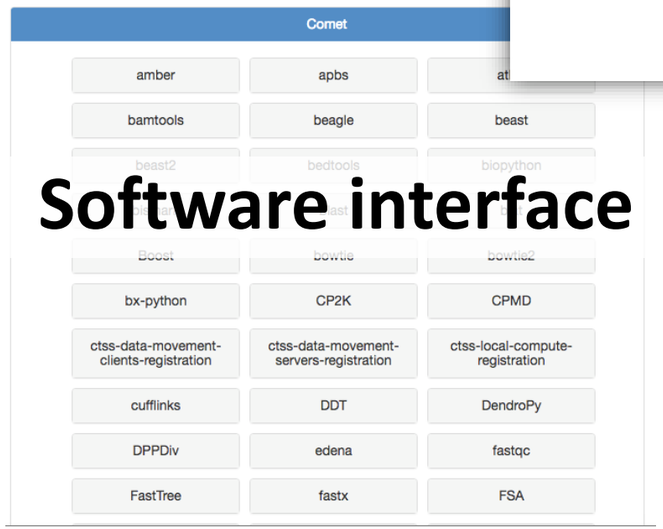
Open Science Grid

XSEDE

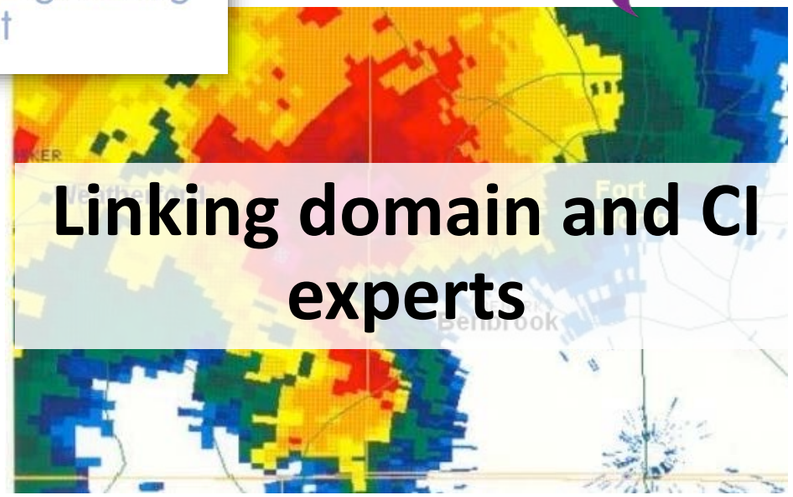
Extreme Science and Engineering Discovery Environment

ACI-REF

Advanced CyberInfrastructure Research & Education Facilitators

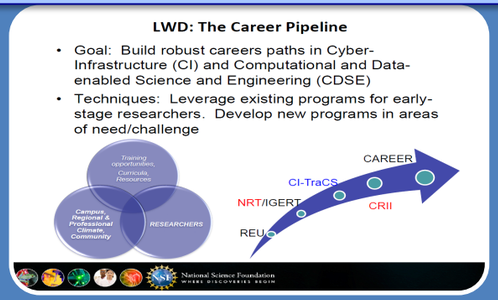


Software interface



Linking domain and CI experts

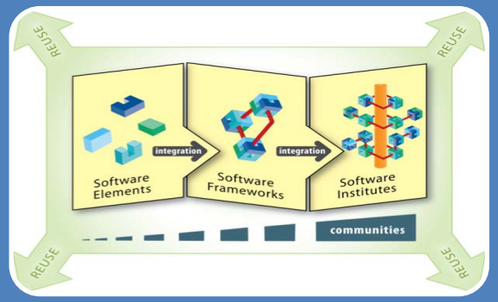
NSF-wide CIF21 Initiative Sunsets in FY17



Learning and Workforce Development for Creators and Users of Research CI

Building robust career paths for CI and Computational and Data Enabled Science and Engineering(CDS&E)

Data Infrastructure Building Blocks ("DIBBs") and Data Science Pilots: Developing communities and infrastructure for using, sharing and reusing research data to advance science and engineering



Software Infrastructure for Sustained Innovation (SI^2):

Transforming innovations in research and education into sustained software resources

Data for Scientific Discovery and Action (D4SDA)

Enabling 21st century science, engineering, and education to move toward effective use of digital data to advance discovery

- Promote foundational research in critical techniques, technologies
- Develop and deploy a model of CI that research communities/institutions can adopt for accessing, using, sharing and reusing data to advance new fundamental research
- Enable/incent science and CI community to address data governance, lifecycle issues, sustainability
- Educate data-savvy workforce of scientists, engineers, educators

National Strategic Computing Initiative (NSCI)

Maximizing HPC benefits for economic competitiveness and scientific discovery:

NSF will play a central role in scientific discovery advances, the broader HPC ecosystem for scientific discovery, and workforce development.

Objectives

- 100x performance increase in HPC simulations
- **Technical synergy in platform for modeling/data analytics**
- **Research into new devices, architectures to scale beyond current limits**
- **Increase capacity and capability of national HPC ecosystem**
- Public/private partnership

NSF Initial Activities

- FY2016: Planning, Coordination, and Community Engagement (NSF-wide)
- FY2017: Pilot Activities
- FY2018+: Full scale Funding

NSF NSCI Investment Areas for 2017

- Low-power computing and future HPC systems in the post-Moore Law device and hardware systems era (28%)
- HPC algorithms and architectures for massive concurrency, energy-efficient computing and system resilience at extreme scale (13%)
- Novel scientific software architectures that are resilient, re-usable, and enduring yet agile (22%)
- Provision of shared infrastructure, workforce development (28%)
- Analyze large complex data sets and assimilate real-time data into models and forecasts (9%)

Overview

- Hors D’oeuvres
- Introduction
- FY 2017 Portfolio
- **Beyond FY 2017**

A vision for research infrastructure

Reusable and agile scientific software with consistent user entrance into an evolving research infrastructure

CYBERINFRASTRUCTURE ECOSYSTEM

Large facilities, instruments

National and local computing, data resources

Software

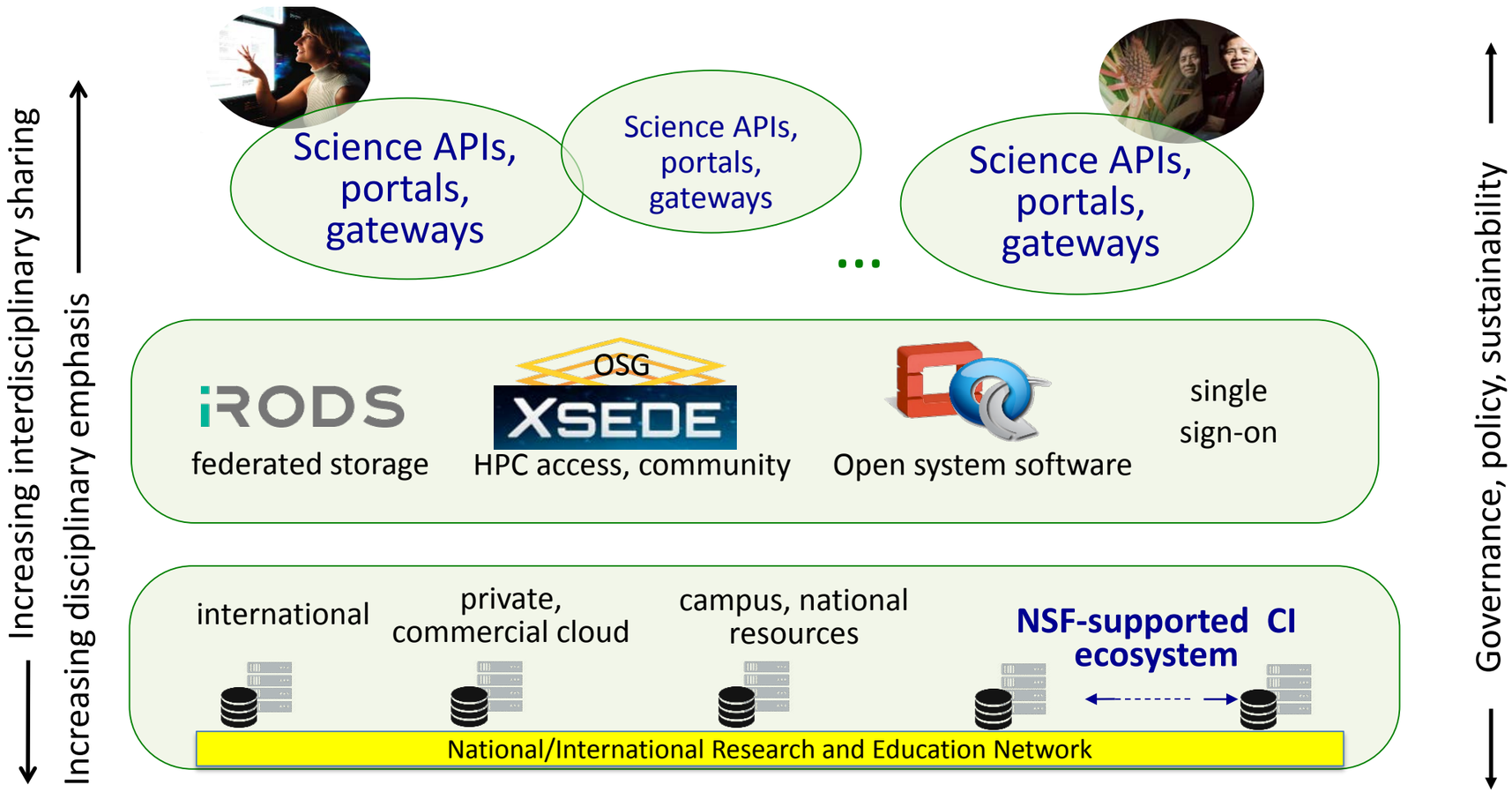
Data

Secure, Collaboration networks

Community portals and software

A vision for research cyberinfrastructure

A national research CI architecture



Looking forward

Critical support for the most demanding science projects

10 years, $300M

2007 — 2013 — 2019

R & D
Pilot System Delivery
System Deployment, Early Operations
Algorithm Improvement & Optimization
Education & Outreach

Operations
System Administration
User Engagement
Education & Outreach

Future Vision, Ongoing Community Discussion

Image courtesy of NCSA at the University of Illinois

Blue Waters

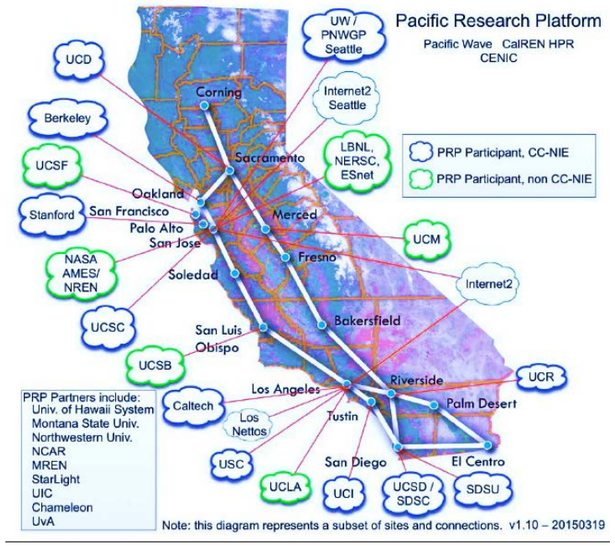
Looking forward

Exploring the cutting edge of next-generation research CI

Data Infrastructure Building Blocks (DIBBs)

Data-centric CI capabilities to accelerate interdisciplinary research

Award:Pacific Research Platform/UCSD/PI Smarr

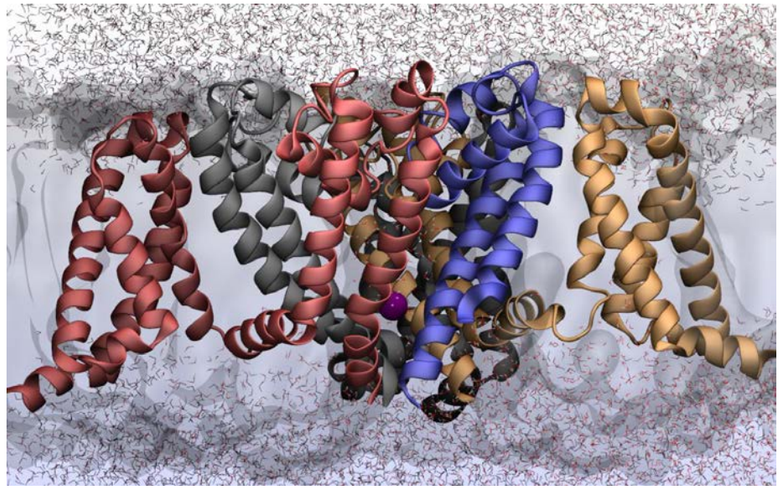


Science-driven, high-capacity, multi-campus data sharing

Software Infrastructure for Sustained Innovation (SI^2)

Accelerating and sustaining software as CI

Award: Molecular Science Software Institute/ Virginia Tech and partners/PI Crawford



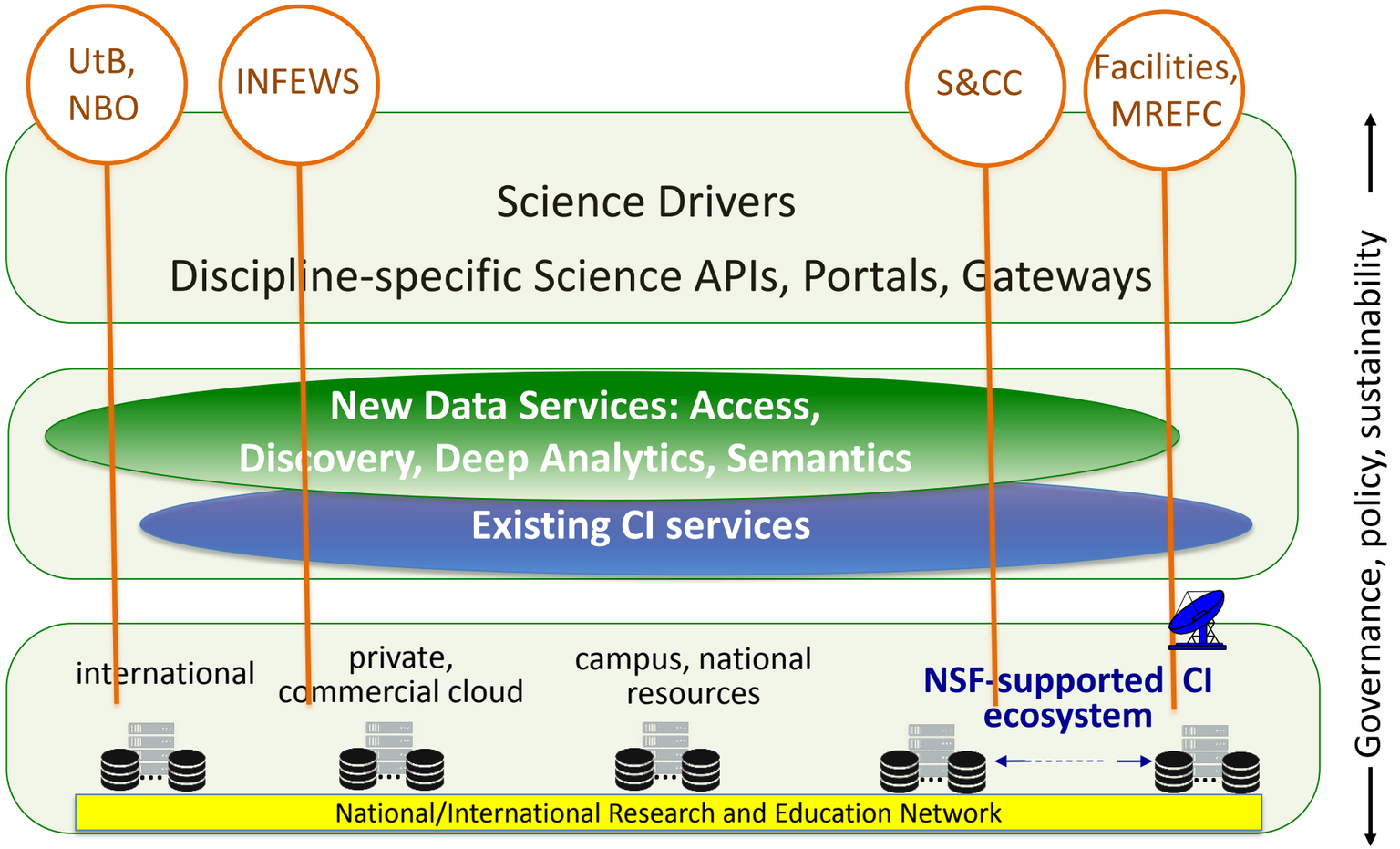
MolSSI: advanced simulations of ion channels in all atom detail on millisecond timescales

Credit: *Matthew Harrigan and Vijay S. Pande, Stanford University*

A vision for research cyberinfrastructure

Architecting a national research infrastructure

Enabling and accelerating science drivers, including NSF initiatives & facilities



ACI LWD Support: Training and Robust Career Paths

Cyber Scientists to explore new CI capabilities

Expert Staff to develop and sustain new capabilities

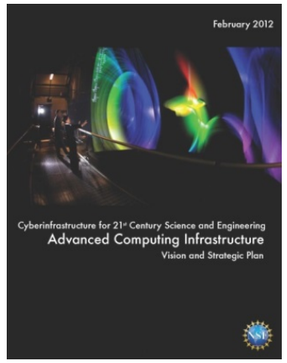
Computational and Data Scientists to expand frontiers using new methods, algorithms and capabilities

ACI

Community input critical to NSF CI planning

Accelerating Science into the Future

- **NSF Advanced Computing Infrastructure for 21st Century Science and Engineering: Vision and Strategic Plan (Feb 2012)**
  - Position, support spectrum of NSF-funded communities at cutting edge of advanced computing technologies, hardware, software, services
- **Future Directions of NSF Advanced Computational Infrastructure to Support US Science in 2017 – 2022**
  - National Academy of Sciences (NAS) Final Report (2016)
  - http://www.nap.edu/catalog/21886/future-directions-for-nsf-advanced-computing-infrastructure-to-support-us-science-and-engineering-in-2017-2020
- **NSCI website**
  - Workshops, RFIs, Reports, Plan
  - http://nsf.gov/cise/nsci/
- **NSF Advisory Committee on Cyberinfrastructure (ACCI)**
  - Co-chairs: Thom Dunning, Victoria Stodden
  - Working Groups: LWD, Data, Software
  - http://www.nsf.gov/cise/aci/advisory.jsp



Final report Co-chairs:
W. Gropp/UIUC
R. Harrison/Stony Brook

Looking forward: Future Directions for *NSF Advanced Computing Infrastructure* to Support U.S. Science and Engineering in 2017-2020

The National Academies of
SCIENCES · ENGINEERING · MEDICINE

GOALS	RECOMMENDATIONS
LEADERSHIP. Position US for continued leadership in science and engineering	1,2
MEETING NEEDS. Ensure that resources meet community needs	3,4
ON THE CUTTING EDGE. Aid community in keeping up with computing revolution	5,6
SUSTAINABILITY. Sustain infrastructure for advanced computing	7

Thanks!

Credits

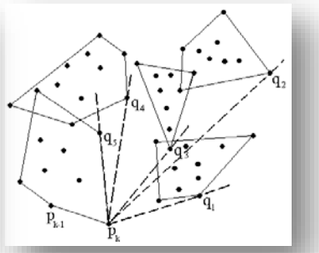
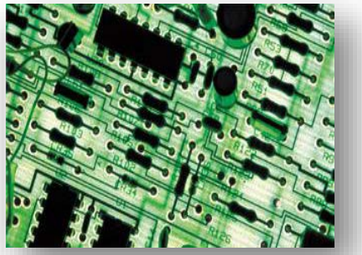
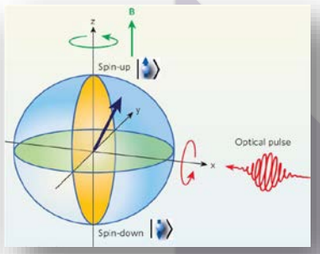
- Copyrighted material used under Fair Use. If you are the copyright holder and believe your material has been used unfairly, or if you have any suggestions, feedback, or support, please contact: ciseitsupport@nsf.gov.

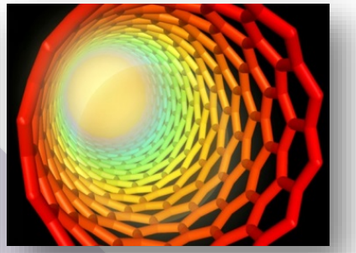
- Except where otherwise indicated, permission is granted to copy, distribute, and/or modify all images in this document under the terms of the GNU Free Documentation license, Version 1.2 or any later version published by the Free Software Foundation; with no Invariant Sections, no Front-Cover Texts, and no Back-Cover Texts. A copy of the license is included in the section entitled “GNU Free Documentation license” at http://commons.wikimedia.org/wiki/Commons:GNU_Free_Documentation_License.

- The inclusion of a logo does not express or imply the endorsement by NSF of the entities' products, services, or enterprises.

NSCI Objective 3

Establish, over the next 15 years, a viable path forward for future HPC systems in the post Moore's Law era



Happening now

- Multi-core and many-core processors
- Domain-specific integrated circuits
- Energy-aware computing
- Hierarchical memories
- High-speed Interconnects

Longer term

- Usable parallelism, concurrency, and scalability
- Resiliency at scale
- Decreased power consumption
- Architectures that reduce data movement
- New materials (e.g., carbon nano-tubes, graphene-based devices)
- Non-charge transfer devices (e.g., electron spin)
- Bio, nano, and quantum devices

NSF Role: Support foundational research

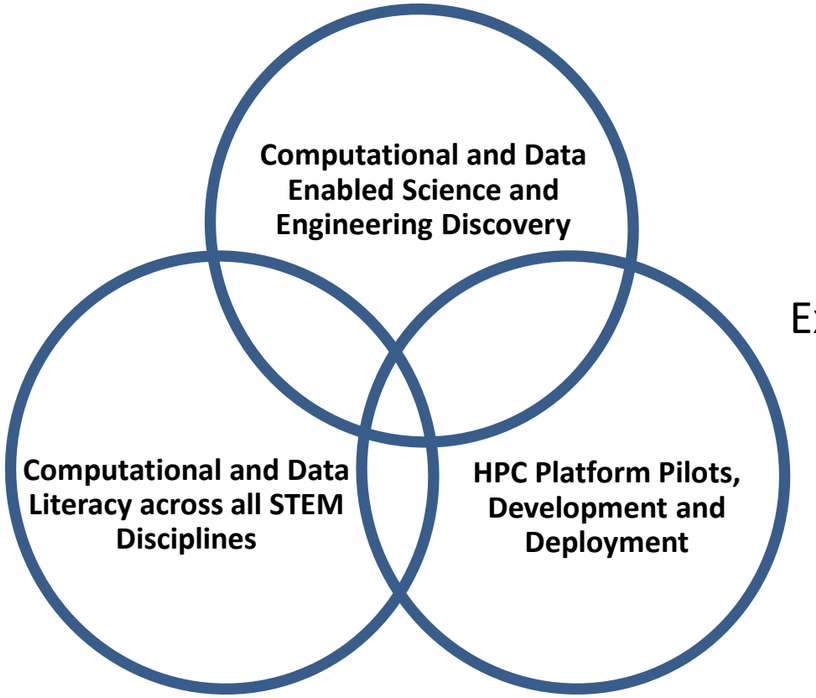
Leadership by CISE, ENG, MPS, and BIO

Build on existing interagency and industry partnerships

NSCI Objectives 2 and 4

Increase synergy between technology base used for modeling and simulation and that used for data analytic computing

Increase the capacity and capability of an enduring national HPC ecosystem, employing a holistic approach … networking, workflow, downward scaling, foundational algorithms and software, and workforce development.



NSF Role: Accelerate scientific discovery advances
Participation by all NSF directorates/disciplines
Expand international, interagency, public sector, and industry collaborations

Emphasis on re-use, agility, interoperability, sustainability