NSF Transforming Science: Blue Waters Emerging Achievements and the Future for Computing Research Infrastructure

CPP Information Item

February 3, 2015

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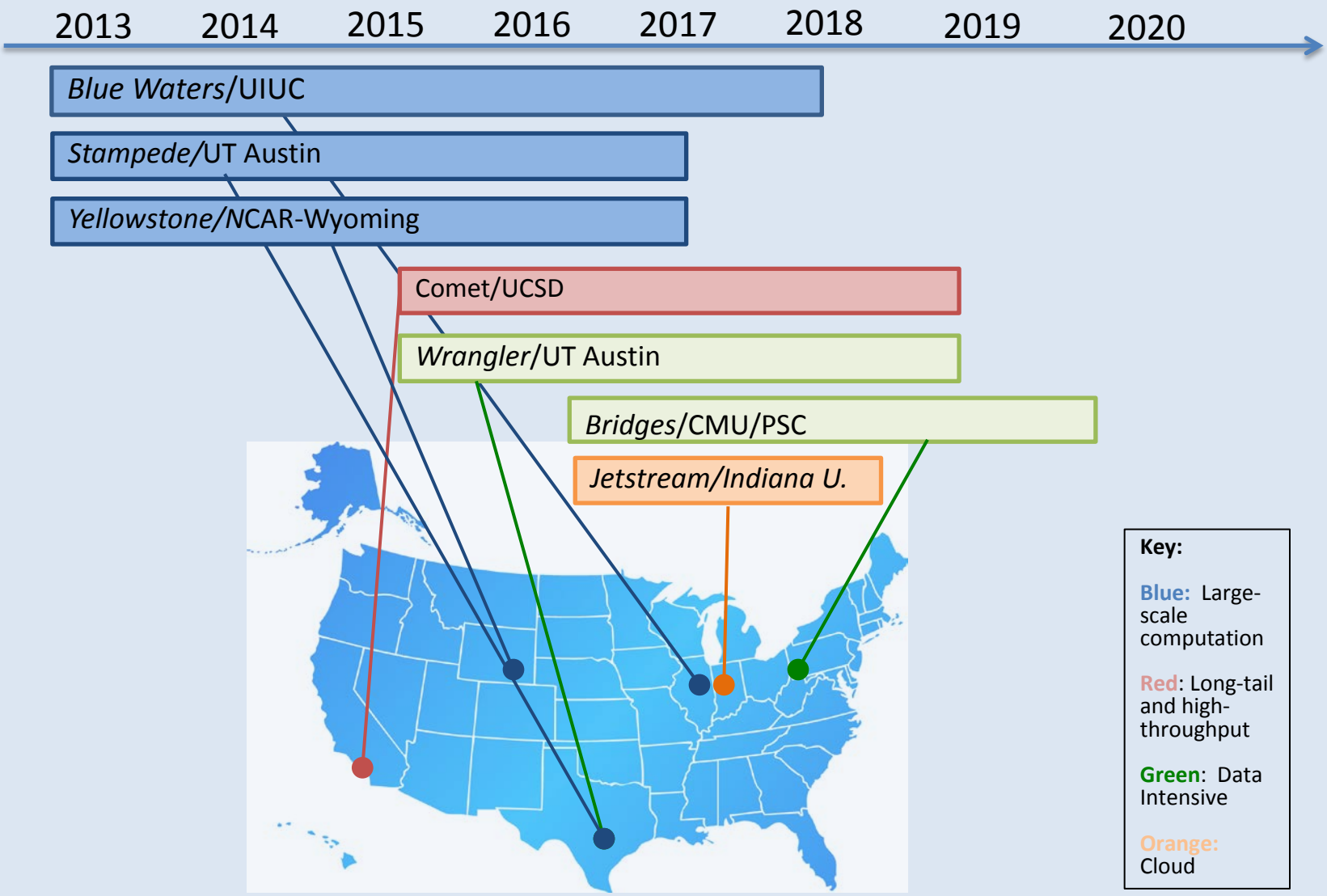
To The Point

- Blue Waters – Emerging Achievements
  - Enabling science not possible otherwise
  - One component in a large, diverse set of investments
- Future for Computing Research Infrastructure
  - Builds on NSF 2012 vision and strategy, planning and input, and partnerships
  - Informed by current scientific directions, community growth in use of current investments, and diverse technological and operational options (e.g., NAS study)
  - Discussion with NSB and community is continuing …

NSF-Supported Computational Investments Reflect Increasing National Diversity



Gaining New Insights via Blue Waters

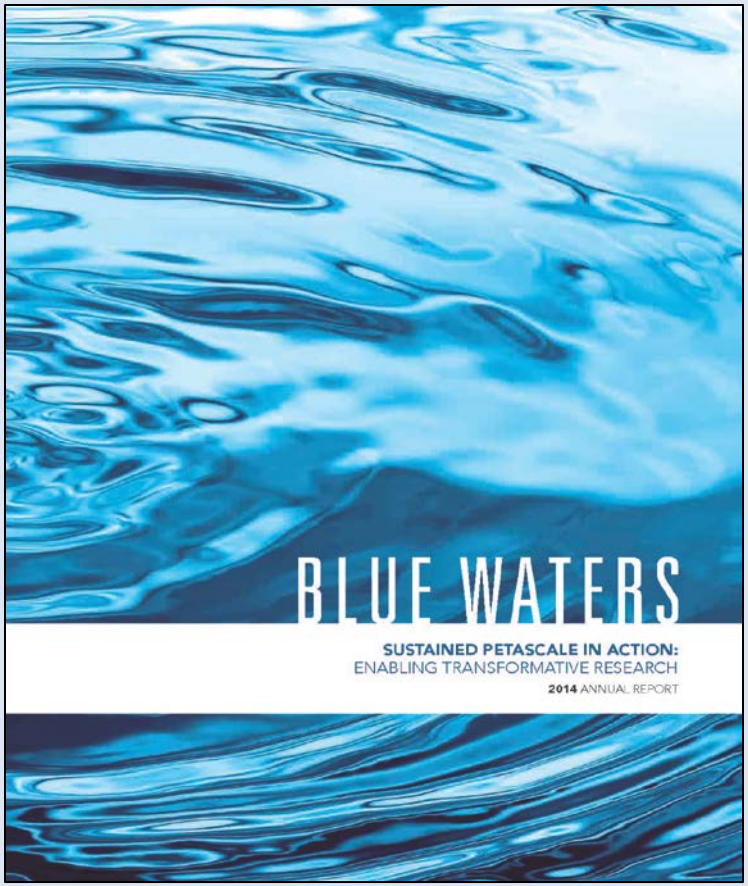
Revealing a protein target to suppress HIV virus and stop the progression of AIDS

- Blue Waters used as a **computational microscope** to determine the precise chemical structure of the HIV capsid
- Project produced the **first-ever atomic-level structure** of a native, mature HIV capsid
- Far beyond the capability of any extant instrument
- Klaus Schulten, UIUC and collaborators at University of Pittsburgh and Vanderbilt University

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

Gaining New Insights via Blue Waters

Enabling science in many disciplines and researchers from many institutions



- **DiMatteo (CMU)** Modeling formation of the first quasars
- **Jordan (USC)** 3-D Physics-based earthquake forecasting models
- **Stein (MSU)** *Ab Initio* models of solar activity
- **Reed (Cornell) & Wood (Princeton)** Advancing space-based earth science using petascale design and management of satellite assets
- **Wuebbles (UIUC)** High-resolution climate simulations

Enabling a 10-year Vision for Computational Science

(0725070) Acquisition Award ($226,551,969) Cooperative Agreement

(1238993) Operations Award ($133,778,949)

October 2007

October 2013

March 2018

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

Operations
System Administration
User Engagement
Education & Outreach

PIs: Kramer, Beldica, Gropp, Hwu

a, Gropp, Bode

Cost sharing: Facilities, Storage, Outreach

Committed partnerships: State, Vendors, Universities, Industry

February 2013 Renewal Resolution: NSB 13-8

December 2014 Review of Progress

80% NSF specified
1% Education and Outreach
< 5% Industry Engagement
5% PI discretion for innovation
2% Great Lakes Consortium (Academic)
7% UIUC

Robust External Review, Significant Progress

"The BW team is to be commended for its singular focus on supporting and enabling breakthrough computational science at such a scale."

Blue Waters Symposium 2014

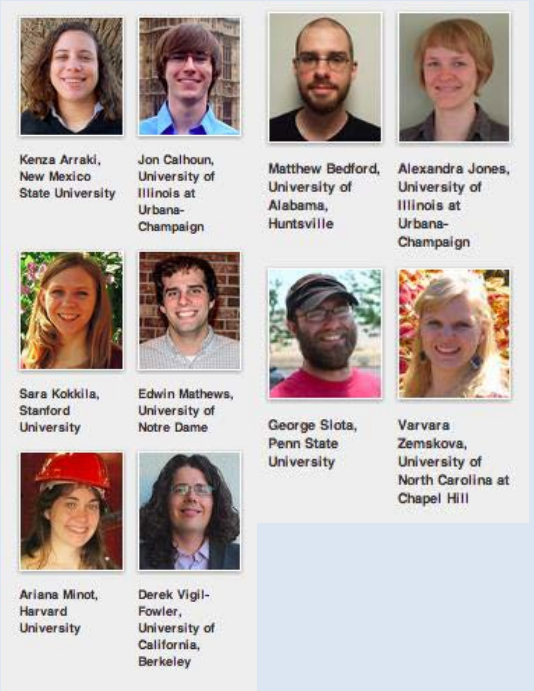
- Enabling transformative scientific research: Goal being achieved
- Broader impacts: Education and outreach programs are diverse and high quality
- System: Effective due to reliability, availability, performance, and security
- Leadership and governance: Stable and effective
- Finances: On schedule, within plan; mature risk management

Recommendations for enhancement made, being addressed

Comprehensive Broader Impacts

Building Community

- Education/Training: 860 participants, 28 institutions
- Blue Waters Industry Projects
  - GE Research, Mayo Clinic, Procter & Gamble,…
- International Collaborations: INRIA, RIKEN
- Blue Waters Interns, Graduate Fellowships & Professorships

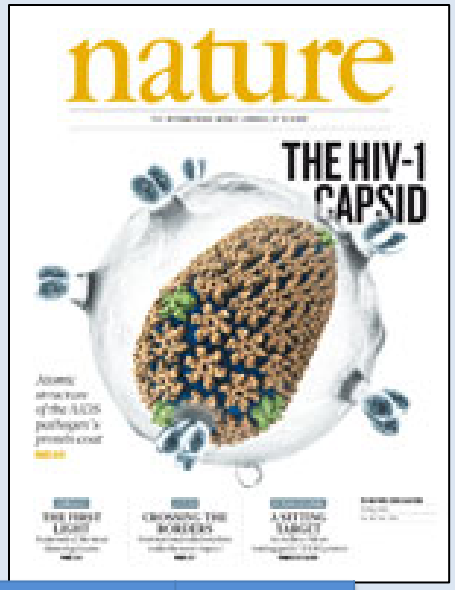


Addressing National Priorities

- U.S. Department of Defense awarded $70 M Grant to UIUC team
  - Grant paves the way for nation's flagship Digital Manufacturing and Design Innovation (DMDI) Institute

Blue Waters: Summary

- Delivering breakthrough science
- First year review shows
  - Project on track
  - Risks under control
- Project oversight continuing



Description of Risk	Risk
Leadership	
Demonstrate scientific value consistent with investment	Decreasing
Position and articulate BW contributions internationally	New, post-review
Position and articulate BW broader impact	New, post-review
Operations	
Reliability and availability of largest NSF system	Decreasing
Security	Continuing
	Decreasing
	Decreasing
storage	Continuing
	Decreasing

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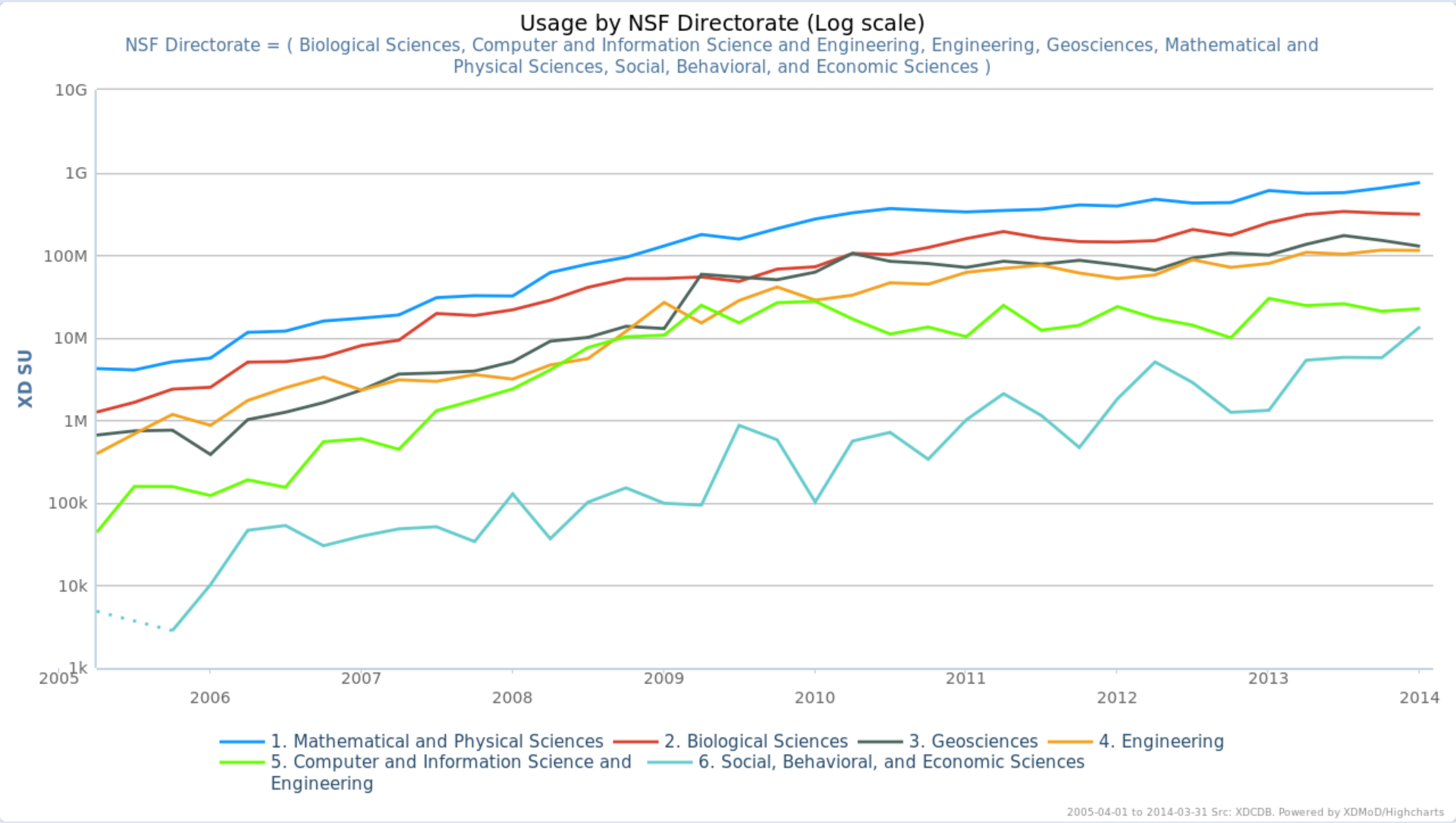
  - Our discussion with NSB and community continues …

Growing Demand

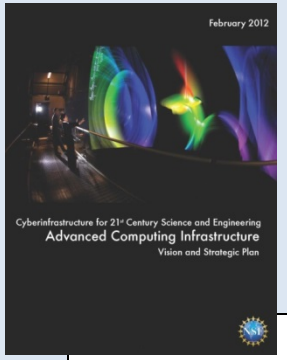
All disciplines are increasing use of national computational resources



Continuing Community Engagement

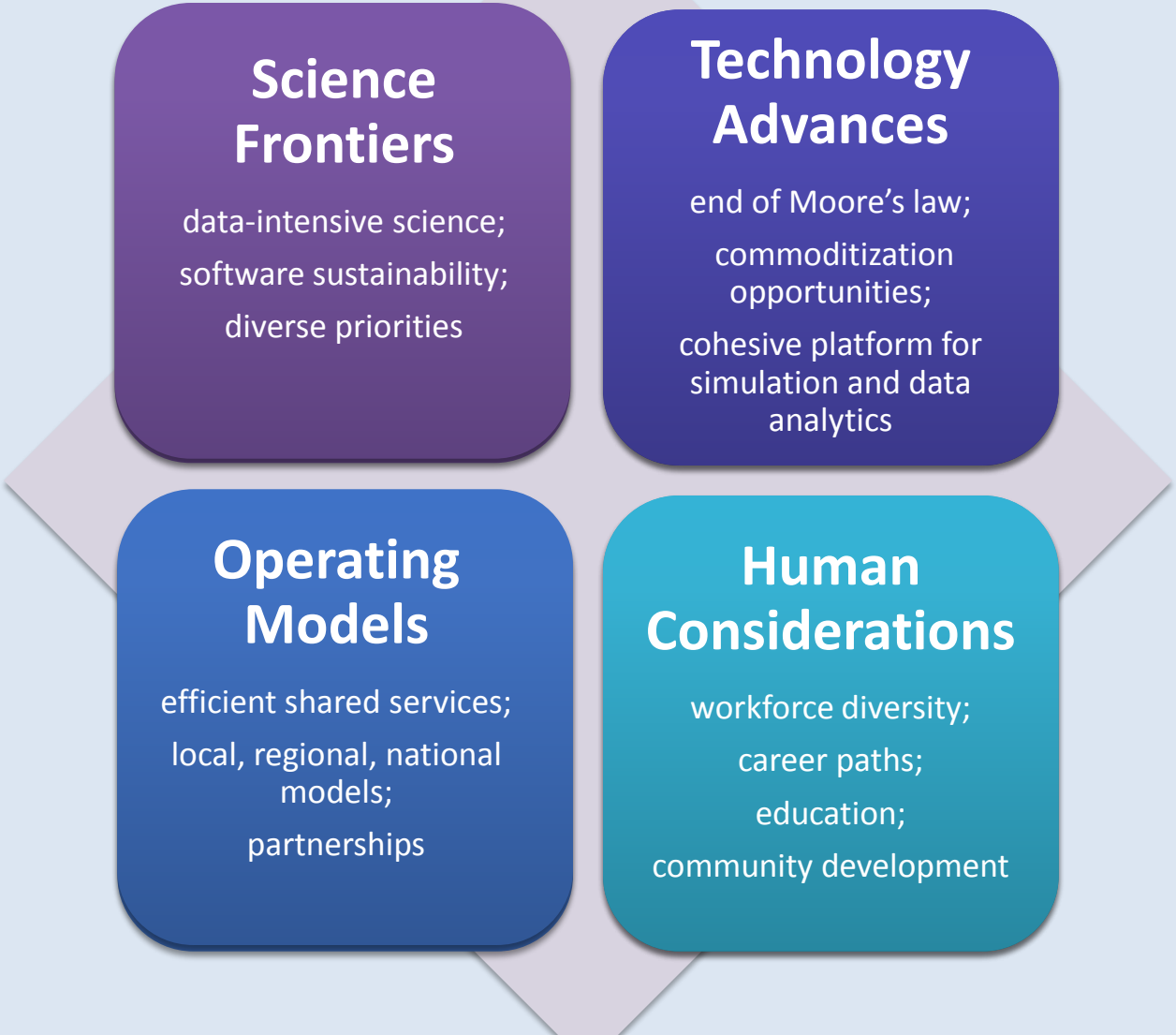
Accelerating Science into the Future during a Period of Transition

- **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)
  - Interim Report (Oct 2014), Final Report (Summer 2015)
- **OSTP-led interagency strategic initiative**
  - Motivation: HPC essential to U.S. security, economic competitiveness, and scientific discovery



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

Optimizing NSF's Role in an Evolving Research Infrastructure Ecosystem



Summary: Moving Forward

- Our CI investments are yielding scientific breakthroughs
- Ongoing community engagements (NAS, Advisory Committee for Cyber-infrastructure) will help to inform future strategic directions
- Optimizing these opportunities will maintain leadership in pushing the frontiers in all areas of science and engineering

Appendix

Blue Waters Risks: Decreasing with Experience

Description of Risk	Risk
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Demonstrate scientific value consistent with investment	Decreasing
Position and articulate BW contributions internationally	New, post-review
Position and articulate BW broader impact	New, post-review
Operations	
Reliability and availability of largest NSF system	Decreasing
Security	Continuing
Staffing	Decreasing
Financial	
Power and cooling costs	Decreasing
Annual costs and rate of growth for storage	Continuing
WAN upgrade	Decreasing