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

Committee on Future Directions for NSF Advanced Computing Infrastructure
to Support U.S. Science in 2017-2020

Computer Science and Telecommunications Board

Division on Engineering and Physical Sciences

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Committee

- WILLIAM D. GROPP, University of Illinois, Urbana-Champaign, Co-Chair
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- KATHERINE A. YELICK, University of California, Berkeley

Charge

A study committee will **examine anticipated priorities and associated trade-offs for advanced computing** in support of National Science Foundation (NSF)-sponsored science and engineering research. Advanced computing capabilities are used to tackle a rapidly growing range of challenging science and engineering problems, many of which are compute-, communications-, and data-intensive as well. The committee **will consider**:

- The **contribution of high end computing to U.S. leadership and competiveness** in basic science and engineering and the **role that NSF should play in sustaining this leadership**;
- **Expected future national-scale computing needs**: high-end requirements, those arising from the full range of basic science and engineering research supported by NSF, as well as the computing infrastructure needed **to support advances in modeling and simulation as well as data analysis**;
- **Complementarities and trade-offs** that arise among investments in supporting advanced computing ecosystems; software, data, communications;
- The **range of operational models** for delivering computational infrastructure, for basic science and engineering research, and the role of NSF support in these various models; and
- **Expected technical challenges** to affordably delivering the capabilities needed for world-leading scientific and engineering research.

An interim report will identify key issues and discuss potential options. It might contain preliminary findings and early recommendations. A final report will include a **framework for future decision making about NSF's advanced computing strategy and programs.** The framework will address such issues as how to prioritize needs and investments and how to balance competing demands for cyberinfrastructure investments. The report will emphasize identifying issues, explicating options, and articulating trade-offs and general recommendations.

The study will not make recommendations concerning the level of federal funding for computing infrastructure.

Inputs

- Briefings at committee meeting in 2014 and 2015
- SC14 BOF
- Dec 2014 workshop (Mountain View, CA)
- 60 comments, some on behalf of groups or orgs, in response to questions posed in interim report

Reviewers

- Daniel E. Atkins III, University of Michigan
- David A. Bader, Georgia Institute of Technology
- Robert Brammer, Brammer Technology, LLC
- Andrew A. Chien, University of Chicago
- Jeff Dozier, University of California, Santa Barbara
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- Michael L. Klein, Temple University
- David A. Lifka, Cornell University
- Jeremiah P. Ostriker, Columbia University
- Terrence J. Sejnowski, Salk Institute for Biological Studies
- Marc Snir, Argonne National Laboratory
- Warren M. Washington, National Center for Atmospheric Research
- John West, Texas Advanced Computer Center

Some background

- NSF has been very successful at supporting science and engineering through advanced computing
- This success has increased the demand exponentially
- At the same time, the nature of computing is changing in multiple ways
  - Increasing use of data from many sources
  - End of Dennard (frequency) scaling forcing major changes in architecture, in turn requiring investment in new algorithms and software
- Internationally, advanced computing infrastructure recognized as vital to scientific progress

Recommended goals for advanced computing

1. Position the United States for continued leadership in science and engineering
2. Ensure that resources meet community needs
3. Aid the scientific community in keeping up with the revolution in computing, and
4. Sustain the infrastructure for advanced computing

1. POSITION THE UNITED STATES FOR CONTINUED LEADERSHIP IN SCIENCE AND ENGINEERING

Observations about positioning for leadership

- Both large-scale simulation and analysis of massive data revolutionizing many areas of research
  - Rise in volume and diversity of scientific data represents and a significant disruption and opportunity
- Meeting future needs will require systems that support a wide range of advanced computing capabilities, including large-scale high-performance and data-intensive systems
- Increased capability has historically enabled new science. Without continued growth, some research will have difficulty advancing
- Many fields now rely on a greater aggregate amount of computing than a typical university can provide
- “Converged” systems can play a role; more specialized systems may also be needed to meet some requirements

Cloud computing

- Demonstrates value of service model that “democratizes” access
- Not necessarily cost-effective; NSF computing centers already exploit economies of scale and load sharing
- Do not currently support very large, tightly coupled parallel applications
- Positioned today to play a growing role for data-centric applications
  - Especially for innovative software, community data sharing
  - Largest systems at scale larger than any computational science platform
- Rapidly changing; price (cost to NSF) and types of services likely to change
- Cost of commercial cloud could be greatly reduced by reducing or eliminating overhead, bulk purchase by NSF, or partnerships with commercial cloud providers

Recommendation 1 NSF should sustain and seek to grow its investments in advanced computing—to include hardware and services, software and algorithms, and expertise—to ensure that the nation's researchers can continue to work at frontiers of science and engineering.

> **Recommendation 1.1** NSF should ensure that adequate advanced computing resources are focused on systems and services that support scientific research. In the future, these requirements will be captured in its roadmaps.
>
> **Recommendation 1.2** Within today's limited budget envelope, this will mean, first and foremost, ensuring that a predominant share of advanced computing investments be focused on production capabilities and that this focus not be diluted by undertaking too many experimental or research activities as part of the Foundation's advanced computing program.
>
> **Recommendation 1.3** NSF should explore partnerships, both strategic and financial, with federal agencies that also provide advanced computing capabilities as well as federal agencies that rely on NSF facilities to provide computing support for their grantees.

Recommendation 2 As it supports the full range of science requirements for advanced computing in the 2017-2020 timeframe, NSF should pay particular attention to providing support for the revolution in data-driven science along with simulation. It should ensure that it can provide unique capabilities to support large-scale simulations and/or data analytics that would otherwise be unavailable to researchers and continue to monitor the cost-effectiveness of commercial cloud services.

3 sub-recommendations

Recommendation 2.1 NSF should integrate support for the revolution in data-driven science into the Foundation’s strategy for advanced computing by (a) requiring most future systems and services and all those that are intended to be general purpose to be more data-capable in both hardware and software and (b) expanding the portfolio of facilities and services optimized for data-intensive as well as numerically-intensive computing, and (c) carefully evaluating inclusion of facilities and services optimized for data-intensive computing in its portfolio of advanced computing services.

Recommendation 2.2 NSF should (a) provide one or more systems for applications that require a single large, tightly-coupled parallel computer and (b) broaden the accessibility and utility of these large-scale platforms by allocating high-throughput as well as high-performance workflows to them.

Recommendation 2.3 NSF should (a) eliminate barriers to cost-effective academic use of the commercial cloud and (b) carefully evaluate the full cost and other attributes (e.g., productivity and match to science workflows) of all services and infrastructure models to determine whether such services can supply resources that meet the science needs of segments of the community in the most effective ways.

“cost-effective academic use of clouds”

- Currently considered a service on which overhead is charged
  - Makes purchase of equipment more attractive to each research group but more expensive in the aggregate for NSF
- Several solutions, including
  - Change overhead rules for cloud services
  - Negotiate directly with cloud provider, provide to grantees

Resources

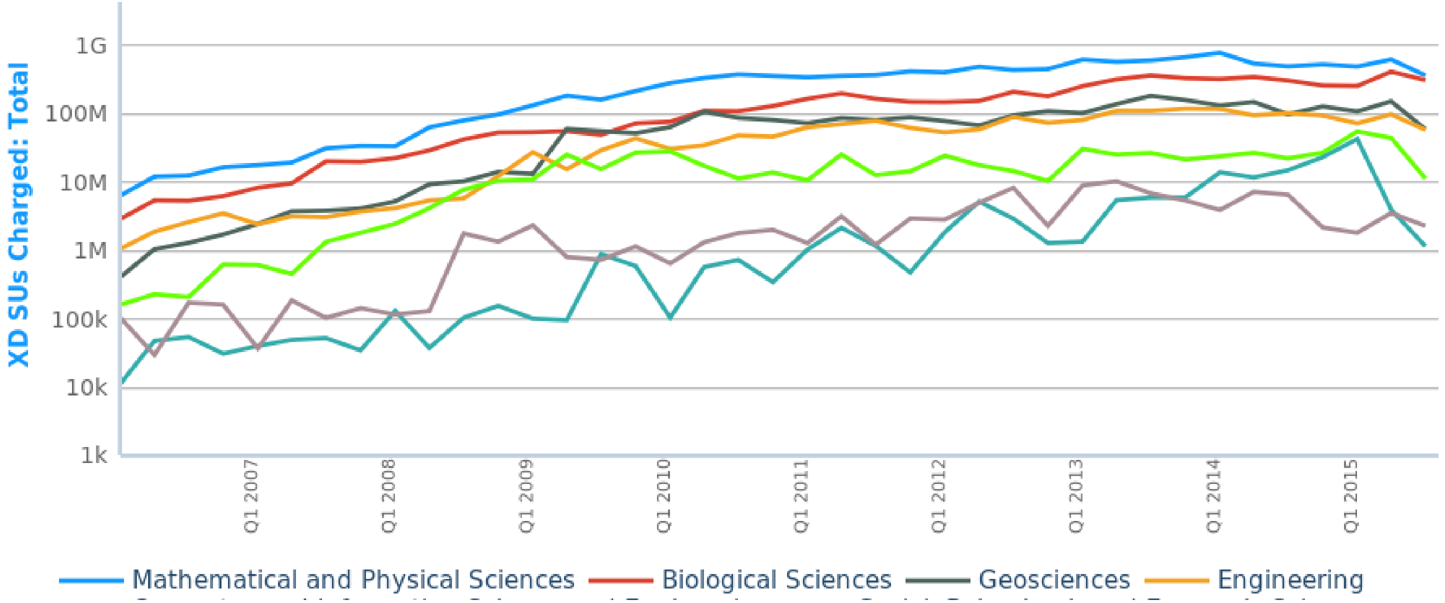
- Maintaining science leadership will be challenging
- Resources for advanced computing inherently limited even as demand is growing
- If NSF cannot increase or better leverage advanced computing resources:
  - Unable to meet future demand
  - Will have to reduce the size of the largest research projects supported by advanced computing

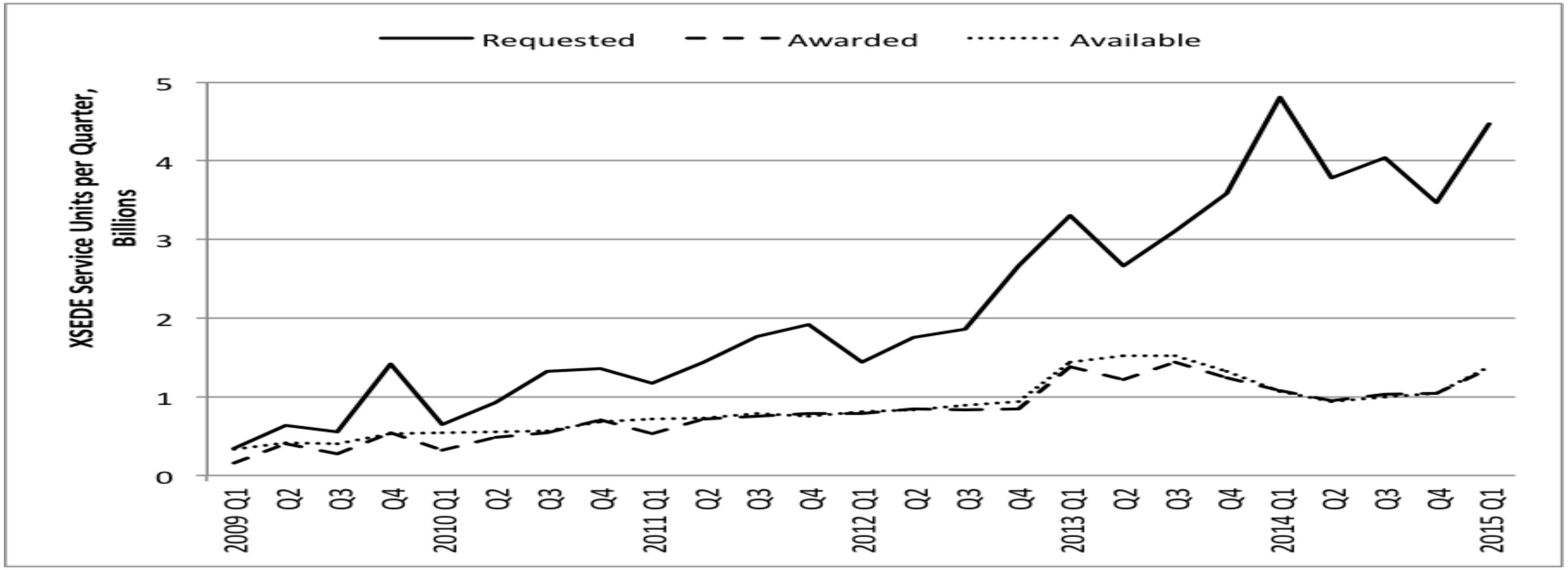
2. ENSURE THAT RESOURCES MEET COMMUNITY NEEDS

Observations about resources and needs

- Demand for advanced computing growing, changing rapidly
- Gap between supply and demand growing
- Overall planning process for advanced computing
  - Not systematic or uniform
  - Not visibly reflected in NSF’s strategic planning
- Ongoing and more regular/structured process would make it possible to:
  - Collect & roll up requirements
  - Prioritize investments based on science and engineering needs
- To be cost-effective, NSF must secure access to capabilities that represent compromises wrt individual applications but reasonably support the overall portfolio
  - Requirements collection and roadmaps will inform decisions

Allocation and request history





No single metric for computers

- Like other major scientific instruments, there is no one metric for capability
  - Telescopes: frequency range, light gathering, even type of radiation (electromagnetic, gravitational)
  - FLOPS or SUs do not capture needs of most users

Recommendation 3 To inform decisions about capabilities planned for 2020 and beyond, NSF should collect community requirements and construct and publish roadmaps to allow the Foundation to set priorities better and make more strategic decisions about advanced computing.

- 4 sub-recommendations

Recommendation 3.1 NSF should inform its strategy and decisions about investment tradeoffs using a requirements analysis that draws on community input, information on requirements contained in research proposals, allocation requests, and Foundation-wide information gathering.

Recommendation 3.2 NSF should construct and periodically update roadmaps for advanced computing that reflect these requirements and anticipated technology trends to help the Foundation set priorities and make more strategic decisions about science and engineering and to enable the researchers that use advanced computing to make plans and set priorities.

Recommendation 3.3 NSF should document and publish on a regular basis the amount and types of advanced computing capabilities that are needed to respond to science and engineering research opportunities.

Recommendation 3.4 NSF should employ this requirements analysis and resulting roadmaps to explore whether there are more opportunities to use shared advanced computing facilities to support individual science programs such as MREFC projects.

Roadmaps

- Reflect visions of communities supported by NSF
  - Both largest users and long tail
- Brief documents with overall strategy, not details
- Look ~5 years ahead with vision ~10 years out
- Purpose:
  - Inform users about future facilities
  - Guide investment; align future procurements and services with requirements
  - Enable more effective partnerships within NSF and with other federal agencies
  - Also, provide ingredients for NSF-wide data plan
  - **Example: 2015 DOE ASCR roadmap**
- Models:
  - Academies astronomy and astrophysics decadal surveys
  - DOE's Particle Physics Project Prioritization Panel
  - But input must be collected from a much wider set of users, and requirements must be aggregated at a much higher level

Part of DOE's Roadmap

System attributes	NERSC Now	OLCF Now	ALCF Now	NERSC Upgrade	OLCF Upgrade	ALCF Upgrades	
Name Planned Installation	**Edison**	**TITAN**	**MIRA**	**Cori** **2016**	**Summit** **2017-2018**	**Theta** **2016**	**Aurora** **2018-2019**
System peak (PF)	2.6	27	10	> 30	150	>8.5	180
Peak Power (MW)	2	9	4.8	< 3.7	10	1.7	13
Total system memory	357 TB	710TB	768TB	~1 PB DDR4 + High Bandwidth Memory (HBM)+1.5PB persistent memory	> 1.74 PB DDR4 + HBM + 2.8 PB persistent memory	>480 TB DDR4 + High Bandwidth Memory (HBM)	> 7 PB High Bandwidth On-Package Memory Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 40	> 3	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Intel Knights Landing Xeon Phi many core CPUs	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	9,300 nodes 1,900 nodes in data partition	~3,500 nodes	>2,500 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	Dual Rail EDR-IB	Aries	2nd Generation Inte Omni-Path Architecture
File System	7.6 PB 168 GB/s, Lustre®	32 PB 1 TB/s, Lustre®	26 PB 300 GB/s GPFS™	28 PB 744 GB/s Lustre®	120 PB 1 TB/s GPFS™	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre®

Japan’s second tier plans

University	2017	2020	2023
Hokkaido	10+PF/s	10+PF/s	50+PF/s
Tohoku	NEC SX-ACE 800TF/s	30+PF/s	30+PF/s
Tsukuba	PostT2k JHPCA 30PF/s	100+PF/s	100+PF/s
Tokyo	Fujitsu FX10 1PF/s	50+PF/s	50+PF/s
Tokyo Tech.	Tsubame 3 20-25 PF/s	Tsubame 4 (100-200 PF/s)	Tsubame 4
Nagoya	Post FX10 upgrade 3 PF/s	50+ PF/s	50+ PF/s
Kyoto	10+PF/s	50+PF/s	50+PF/s
Osaka	NEC SC-ACE 400TF/s	5+PiB/s	5+PiB/s
Kyushu	10+PF/s	10+ PF/s	50+PF/s

Taken from “Japanese “Leading Machine” Candidates Roadmap of the 9 HPCI University Centers”, April 2015. Does not include the “K Computer”

Observations about understanding costs and benefits

- Better information about the relationship among the cost of roadmap choices, requirements, and science benefits would
  - Help inform program managers about the total costs of proposed research
  - Focus researchers’ attention on effective/efficient use of these valuable shared resources

Recommendation 4 NSF should adopt approaches that allow investments in advanced computing hardware acquisition, computing services, data services, expertise, algorithms, and software to be considered in an integrated manner.

- **Recommendation 4.1** NSF should consider requiring that all proposals contain an estimate of the advanced computing resources required to carry out the proposed work and creating a standardized template for collection of the information as one step of potentially many towards more efficient individual and collective use of these finite, expensive, shared resources. (This information would also inform the requirements process.)
- **Recommendation 4.2** NSF should inform users and program managers of the cost of advanced computing allocation requests in dollars to illuminate the total cost and value of proposed research activities.

Why make value of allocations known?

- Goal is to inform decisions
  - A resource that is free is often wasted
  - Can inform choices for code tuning, algorithm development
  - Could pilot project to allow groups to trade resources between software help (tuning, algorithm implementation) and compute cycles
    - Pilot needed to identify unintended consequences
- Not intended for chargeback

3. AID THE COMMUNITY IN KEEPING UP WITH THE REVOLUTION IN COMPUTING

Observations about keeping up with the revolution in computing

- Computer architectures, hardware, program models, are changing rapidly
- Better software tools, technical expertise, and more flexible service models can boost productivity
- Leadership role in defining future advanced capabilities and helping researchers use them effectively will help ensure that:
  - Software and systems remain relevant to science portfolio
  - Researchers are prepared to use current and future capabilities
  - Investments are aligned with future directions

Recommendation 5 NSF should support the development and maintenance of expertise, scientific software, and software tools that are needed to make efficient use of its advanced computing resources.

> **Recommendation 5.1** NSF should continue to develop, sustain and leverage expertise in all programs that supply or use advanced computing to help researchers use today's advanced computing more effectively and prepare for future machine architectures.
>
> **Recommendation 5.2** NSF should explore ways to provision expertise in more effective and scalable ways to enable researchers to make their software more efficient, for instance by making more pervasive XSEDE's practice that permits researchers to request an allocation of staff time along with computer time.
>
> **Recommendation 5.3** NSF should continue to invest in supporting science codes and in continuing to update them to support new systems and incorporate new algorithms, recognizing that this work is not primarily a research activity but rather is support of software infrastructure.

Recommendation 6. NSF should invest modestly to explore next-generation hardware and software technologies to explore new ideas for delivering capabilities that can be used effectively for scientific research, tested, and transitioned into production where successful. Not all communities will be ready to adopt radically new technologies quickly, and NSF should provision advanced computing resources accordingly.

Software is a large part of advanced computing infrastructure

- There is a very large investment in software for computational science
- Much of this will need to be rewritten for the new architectures
- Few groups are ready for this
- Required:
  - New ideas to automate as much as possible
  - Investment in engineering software

4. SUSTAIN THE INFRASTRUCTURE FOR ADVANCED COMPUTING

Observations about sustaining infrastructure

- Expertise and physical infrastructure are essential, long-lived assets
- Recent strategy of acquiring facilities and creating centers relies on:
  - Irregularly scheduled competition among institutions
  - Equipment, facility, and operating cost sharing by states, institutions, and vendors
- Challenges with this approach:
  - Relies on cost sharing that may no longer be viable due to mounting costs and budget pressures
  - Repeated competitions can lead to proposals designed to win a competition rather than maximize scientific returns
  - Most importantly, doesn't provide long-term support needed to develop and retain talent needed to manage systems, support users, and evolve software

Recommendation 7 NSF should manage advanced computing investments in a more predictable and sustainable way.

- **Recommendation 7.1** NSF should consider funding models for advanced computing facilities that emphasize continuity of support.
- **Recommendation 7.2** NSF should explore and possibly pilot the use of a special account (such as that used for MREFC) to support large-scale advanced computing facilities.
- **Recommendation 7.3** NSF should consider longer-term commitments to center-like entities that can provide advanced computing resources and the expertise to use them effectively in the scientific community.
- **Recommendation 7.4** NSF should establish regular processes for rigorous review of these center-like entities and not just their individual procurements.

Managing advanced computing investments in a more predictable and sustainable way

- Benefits researchers currently supported by NSF’s advanced computing programs
- Creates opportunities to apply expertise more broadly within NSF, such as for large scale science projects with large, long-term needs
- Creates new opportunities to address long-term data storage, preservation, and curation challenges