BEFORE THE UNITED STATES HOUSE OF REPRESENTATIVES

COMMITTEE ON SCIENCE, SPACE, AND TECHNOLOGY

SUBCOMMITTEE ON RESEARCH AND TECHNOLOGY

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Chairwoman Comstock, Ranking Member Lipinski, and members of the Subcommittee, thank you for the opportunity to participate in this important discussion today.

I am currently Director of the National Center for Supercomputing Applications (NCSA) and Founder Professor of Physics and Professor of Astronomy at the University of Illinois. I have previously served as the NSF Assistant Director for Mathematical and Physical Sciences (2009-2012) and Director of NSF's Office of

Cyberinfrastructure (2008-2010). During that period I oversaw in excess of $5 billion in NSF investments in mathematical and physical sciences (including major infrastructure investments such as telescopes, light sources and other Major Research Equipment and Facilities Construction (MREFC) projects) as well as in HPC, Software, Networking, and Data and related education and science application investments. In this context, and of specific relevance to this hearing, I was an initial co-chair in 2011 of the NITRD Senior Steering Group on Big Data under OSTP's Committee on Technology, that led to the March, 2012 Presidential Big Data Initiative. I was also the co-chair of both the Physical Sciences Steering Committee (PSSC) and the Quantum Information Science Interagency Working Group (QIS IWG) under OSTP's Committee on Science, so I am very familiar with the working of the relevant groups. I have also worked in senior science and administrative positions in international research organizations in Germany and Russia, and have served as an advisor to international funding agencies, so I have a good overview of the US role, and its position, in the international context.

Currently, in my role as NCSA Director, I am responsible for an organization that leads the two single largest NSF investments in high-end computing and data analysis and their applications to science and engineering:

- The NSF Blue Waters supercomputer, the most powerful supercomputer in the academic world, is a facility representing over $400 million in combined NSF and Illinois investments, providing unique science capabilities to over a thousand researchers from across the nation, in more than 200 projects, funded separately, across all areas of science, engineering, and industry R&D. Blue Waters enables breakthrough research that requires computing and analysis at scales that simply cannot be done at other NSF-supported computing sites (or nearly any other facility in the nation or the world)[1].
- The XSEDE project, representing more than $130 million in NSF funding over 5 years for services that enable science communities to take advantage of HPC and other computing and data analysis resources at most other NSF-supported advanced computing sites across the nation. The $130 million figure *is only for integrated services to use computing and data facilities that are themselves funded separately* at a half-dozen sites across the country. Likewise, the users of these services have research projects that are funded separately by numerous agencies.

It is important to note that these two computing projects, Blue Waters and XSEDE, support research projects whose research is funded (separately) not only by NSF, but also by many federal agencies. The XSEDE project reported that in its third project year, July 2013 –June 2014, it provided computing services to nearly $800 million dollars worth of federally funded research projects, roughly half of which

[1] A supplemental document describing dozens of research projects carried out on Blue Waters, funded by numerous agencies (e.g., NSF, DOE, NIH, etc.) and also by industry, is provided.

came from NSF, about 18% came from NIH, with DOE, DOD, NASA contributing just under 10% each to this figure. Likewise, Blue Waters supports over $500 million dollars in research by teams funded by many agencies. I will come back to this trend below.

It is also important to note that the NSF XSEDE and Blue Waters facilities are highly oversubscribed, with requests for computing time exceeding what can be accommodated by factors of 4-5x or more. Because all science and engineering research progress is now intricately dependent on computing and data analysis, the pressure from research groups to use these facilities is increasing, while funding for these facilities has been essentially flat (or even slightly declining by some estimates) for more than the last decade. This puts science teams in difficult positions because their funding is independent of being allocated the computing and data analysis resources they need to carry out their research programs.

As with all major national computing centers, NCSA too is deeply engaged in numerous "big data" projects, illustrating a key point: big data and big computing go hand-in-hand; one is intrinsically integrated with the other. *Hence a third project, an instrument project of the type not mentioned in the PCAST report, needs to be highlighted:*

- NCSA is responsible for producing the data services pipeline for the Large Synoptic Survey Telescope (LSST), under construction for "first light" shortly after the beginning of the next decade. This telescope, funded jointly by NSF and DOE (construction and operating costs for 10 years will well exceed a billion dollars), *will produce roughly as much data each night as the most ambitious previous astronomy survey project did in a decade*. It will observe as many as a million transient events each night. This will be done by collecting enormous amounts of data ---with enormous computing on this data---each night. This will need to be combined with data from other astronomical instruments, and large-scale supercomputer simulations, in order to understand what it and other instruments observe.

Key Trends in Science and Engineering

With this background, I have studied the recent (August 2015) PCAST report on NITRD and spoken to numerous colleagues in relevant research communities and federal agencies, and have several comments and recommendations to make to this subcommittee. But first I would like to focus on critical trends in science, engineering and industrial research, which must be the guiding force for any related federal investments in NIT. Implicit in the above discussion, some trends are critical to the subcommittee's topic of interest:

- While breakthrough research continues to be done by small groups of researchers, increasingly, one finds interdisciplinary teams of researchers, from multiple disciplines, and often funded by multiple agencies, working together on complex problems in science and society (including in industry).

Such problems are beyond the reach of any individual group, discipline, or approach (e.g., theory, computation, experiment, etc.). A recent NRC report entitled "Facilitating Transdisciplinary Integration of Life Sciences, Physical Sciences, Engineering, and Beyond (2014)" speaks to these trends.

- These problems---across all domains---are increasingly computational and data-intensive, often requiring large-scale computing/analysis facilities *and data from experiments, observation systems, and instruments*. The demand is growing rapidly and across all areas. For example, the NSF Directorate for Social, Economic, and Behavioral Sciences (SBE) now uses as much computing time on NSF advanced computing facilities as the (much larger) Mathematical and Physical Sciences Directorate did just a decade ago. *Further, many such problems are beyond the reach of the nation's current computing and data capabilities*, so that one must downscale the problem (to the scale of "toy problems", as described in the PCAST report) to fit available facilities. While insights may be achieved by studying simple versions of real-world problems, the real-world impact may be lost.
- Data has become a de facto currency of research, both enabling quantitative description of research results, and *enabling communication and therefore collaboration between researchers (and the public) at scales never before possible*. The recent discovery of the Higgs boson was possible only because teams of thousands of scientists were able to collaborate via sharing of data collected at the experiment, and by aggregating computing capability across hundreds of sites worldwide.
- New software is needed for researchers to be productive on high-end computing and data systems, and to enable complex problem solving. A recent workshop (October, 2015) sponsored by NITRD "Computational Science & Engineering Software Sustainability and Productivity Challenges" bought together a number of agencies to discuss pressing issues around software requirements, high-productivity software engineering, reproducibility, software maintenance processes, and scalable, reusable, and portable software system architectures.
- Major instruments, such as telescopes, light sources, accelerators, ecological observing systems, highly instrumented and computerized ships, and so on, are required to do scientific research. Outside the scope of the small grants programs that fund many research groups at NSF, DOE and other agencies, these major investments usually take a decade or more to build and easily exceed a billion dollars to construct and operate. *Nowadays, these instruments are fully digital, require hundreds of millions of dollars of investments in computing, data, and networking infrastructure, and serve many communities funded by many agencies.* Both the instruments, and the networks required to transport data to computing facilities and communities that use them, are often neglected in the ecosystem under discussion. This must be addressed (see below).

As is implicit in the above discussion, the problems under study do not respect either disciplinary boundaries or agency boundaries. Federal NIT investments from many agencies must therefore be coherently coordinated if research communities addressing such complex problem to succeed. *NIT systems, including systems such as digital instruments that also serve many communities, must be part of this ecosystem*. The definition of what is an NIT system changes almost as fast as the technology itself, and hence the coordinating process must be nimble and updated frequently. Further, as the computing and data needs of "nontraditional NIT agencies", e.g., NIH, grow rapidly, they may soon find that, due to increasing demand and shortage of supply, they are unable to acquire the resources they need from other agencies, e.g., DOE and NSF, unless sufficient coordination, planning, and shared investments are made across all relevant agencies.

While the above discussion has been focused on research facing the nation's research communities, similar trends are found in industry. Like many of the nation's HPC centers, NCSA operates a vigorous Private Sector Partner program. Our program has over two-dozen partners who use our facilities and work closely with our expert staff, affiliated faculty and students to improve their methods, products and competiveness. Their needs reflect the same trends described above, and more. They are addressing real-world problems that require realistic, timely real-world solutions that can have tremendous impact on the US economy. For example, one of our private sector partners estimates that a 100PFlop system with appropriate software and algorithms, would enable simulations to improve jet engine efficiency. Merely a 1% improvement would save tens of billions of dollars in the US economy. We have similar discussions with our partners regarding agriculture, energy, transportation and other areas. Hence, while industry requires results sometimes on quarterly time scales, it also requires partnerships with federally funded NIT research on decadal time scales as well.

The need for a National Strategic Computing Initiative

In July 2015, the President issued an Executive Order (EO) that instructed federal agencies to work together in an "all of government", 15-year effort to launch the National Strategic Computing Initiative (NSCI). Within this EO, agencies were given specific roles, for example, NSF, DOE and DOD as "leadership" agencies, with NASA, NOAA, NIH, FBI, DHS singled out as "deployment" agencies that should work with other agencies to develop efforts needed for their missions. The role of industry was also highlighted. Indeed, some of the most articulate members of the small invited panel present at the White House event to unveil the NSCI were from industry.

Of the roles singled out by the EO, the NSF was given the most comprehensive responsibilities, including the central role in scientific discovery advances, a continuing role in leadership in advanced computing, especially the broader HPC ecosystem for scientific discovery, and workforce development. NSF is also leading the efforts to define computing and analysis post Moore's Law. NSF therefore needs to play a special role in the coordination and integration. However, it is neither funded nor staffed adequately to fulfill these roles by itself. It will need help, as will all agencies.

I can say that there was a sense of relief, if not joy, in the broader research and industry communities when this announcement was made. Given the above discussion, it should be clear that the national need for such an effort, cutting across agencies and industry alike, is huge. In order to be effective (to be measured by the impact it has on the research communities that demand it) NSCI will require both:

- Continued and increased investments in the entire NIT ecosystem, which needs to broadened to include major digital instruments and their coordination and integration where warranted with other NIT systems.
- Increased effort and assistance in coordination across agencies, which is often difficult for agencies to do, even when they are in agreement that such coordination is necessary.

A key point implicit in the above is this: *with the vast majority of the research and development activities of our age requiring major developments in computing, networking, and software, not only will more investment in the NIT infrastructure be needed, it must be invested in a more coherent way*. While not lowering the overall investment numbers themselves, a more coherent and coordinated approach will not only better serve the nation's R&D communities, each of which may need access to major HPC facilities, observation systems, and instruments, but it could also lead to savings of individual investments. Considerable synergies could be realized if advanced computing facilities were deeply involved in the planning of construction of major instruments, such as telescopes or light sources, which are themselves highly digital. For example, a recent collaboration between the XSEDE project and NSF's Laser Interferometer Gravitational-Wave Observatory (LIGO) saved an estimated $70 million in computing costs. Even more important, the basic function of these *instruments will require advanced computing, data, and networking services in order to function at all*. In the words of Larry Smarr, "these instruments are more silicon than steel."

The role of NITRD and other groups in coordinating federal investments

Clearly, given the above testimony, federal investments in NIT need to be not only coordinated, but made in the most coherent possible way in order to serve research and industry communities across all areas of science and engineering. The agencies themselves do work earnestly to address some of these issues, and in some cases do an excellent job, especially if the future of a project essential to their research communities requires cooperation, and most critically if it cannot be funded within individual agency budgets.

For example, NSF and DOE have numerous projects that require joint funding, and they have developed mechanisms to accomplish this. For small programs, MOUs may be developed between agencies that are then competed and managed collaboratively. For large construction projects, such as the LSST project described above, the Dark Energy Survey, detectors at the Large Hadron Collider, and others carefully coordinated investments of hundreds of millions of dollars are required. Where appropriate, NSF utilizes its "MREFC" process, while DOE utilized its "CD" process, and a careful and rigorous mapping has been made by the agencies to synchronize them appropriately.

While such deep, joint coordination happens as needed in major construction projects, it rarely happens in the area of NIT (with the exception of the large construction projects that are themselves increasingly NIT projects, e.g., the LSST). The nation's research communities increasingly require this, as evidenced by the figures above, where, e.g., the NSF-funded XSEDE HPC program is used as much by non-NSF funded research groups as it is by NSF-funded groups. The NSCI further requires that agencies work together to address these problems.

NITRD and the NCO have a clear responsibility to play a major role in coordinating federal NIT investments, and they must. In the past, NITRD has not been as effective as it might be in doing so, for many reasons. Agency personnel are very busy, and they have historically served complementary communities, and have a culture of taking care of their own interests and typically a mandate to serve their own missions. When agency investments are tallied up in various "Program Component Areas" (PCAs), these are sometimes done in inconsistent ways.

NITRD has often been an important forum for information sharing, but with little authority or funding of its own, its role in ensuring coherent investments has been limited. Further, it is largely a technology organization, coming under the OSTP Committee on Technology. The underlying trends in science and engineering, as described above, are driven by science communities, coordinated by the OSTP Committee on Science (and I have served on subcommittees for both CoT and CoS). Further, although computing and data analysis technology changes on very short time scales, as noted by the August, 2015 PCAST report, the PCAs have not changed since their inception *twenty years ago* in 1995.

In the recent PCAST review of NITRD, many excellent suggestions were made to address some of these issues, which I believe will go a long way in improving the effectiveness. Among them, specific recommendations to create a more modern set of PCAs, as well as specific recommendations to address the functioning of NCO-guided Groups (e.g., Senior Steering Groups (SSG) and Interagency Working Groups (IWGs)), will be helpful.

However, there are points that do not seem to receive much attention that I would urge to be further considered. Chief among them, I include:

- *Highly compute- and data-intensive instruments should be considered in the portfolio of NIT coordination.* The focus of the PCAST report (and of NITRD itself) is largely and perhaps naturally on NIT itself, defined as it applies to various activities of cybersecurity, high end computing, and so on. This leaves out a most critical aspect of current research trends, namely that major instruments such as light sources, observing systems (e.g., astronomical, ecological, etc), genomic sequencers and accelerators, serve many communities across many disciplines, funded by many agencies, and they are themselves major investments in cyberinfrastructure. These should not be considered as an afterthought but rather as a first class citizen in the NIT portfolio. Each such instrument is typically more expensive than the largest single computing facilities, with computing, networking, and data investments comparable to those at the largest HPC centers, frequently with duplication of many elements. These are not often coordinated with the rest of the ecosystem, but need to be.

- *Coordinating federal investments in NIT need to involve organizations beyond NITRD, including but not limited to, groups under the Committee on Science*. The research communities themselves are driving much of the convergence described above. They cut across disciplines, they are funded by many agencies, and they increasingly are driving the integration of computing, data, networking, and instruments to address their research. Yet these communities are not well-represented by NITRD groups, which come under the Committee on Technology. The Committee on Science represents some of these more effectively. A broader set of organizations must be considered if better coordinated and more coherent NIT investments are to serve research and industry communities.

Finally, if the NSCI is to truly become an initiative that serves the above trends in science, engineering, and industry, not only will additional funding and better coordination be needed to keep the US in the forefront of research and economic competitiveness, but new funding vehicles for large NIT investments, designed to be more deeply coordinated, may also be needed. For example, NSF's MREFC vehicle for funding large facilities and DOE's CD process are used successfully to fund major instruments. One should examine whether such vehicles could be adapted for multi-agency, coordinated, sustained investment in major computing, data, and networking facilities, that typically also have shorter lifecycles, and applied to other agencies, e.g., NASA and NIH, as well.