PANEL

National Strategic Computing Initiative Update

Keith Marzullo
Dean, College of Information Studies
University of Maryland

Supercomputing 2016, Salt Lake City, UT
November 15, 2016
Executive Order Signed July 29, 2015

Enhance U.S. strategic advantage in HPC for economic competitiveness and scientific discovery

• National
  • “Whole of government” approach
  • Public/private partnership with industry and academia

• Strategic
  • Leverage beyond individual programs
  • Long time horizon, at least a decade

• Computing
  • HPC as advanced, capable computing technology
  • Multiple styles of computing and all necessary infrastructure
  • Scope includes everything necessary for a fully integrated capability

• Initiative
  • Above baseline effort
  • Link and lift efforts
NSCI objectives

1. Accelerate delivery of a capable exascale computing system (hardware, software) to deliver approximately 100X the performance of current 10PF systems across a range of applications reflecting government needs.

2. Increase coherence between technology base used for modeling and simulation and that used for data analytic computing.

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

4. 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.

5. Develop an enduring public-private partnership to assure that the benefits are transferred to the U.S. commercial, government, and academic sectors.
The Government’s Role in NSCI

- DOD + DOE
  - Capable exascale program
  - Analytic computing to support missions: science and national security

- NSF
  - Scientific discovery
  - Broader HPC ecosystem
  - Workforce Development

- IARPA + NIST
  - Future computing technologies

- NASA, FBI, NIH, DHS, NOAA
  - Deployment within their mission contexts
Some milestones

- Executive Order 7/29/2015
- Inaugural meeting of NSCI Executive Council 8/26/15
- White House NSCI Workshop 10/20-21/2015
  - Nanoscale-inspired grand challenge announced
- RFI on Science Drivers for Capable Exascale issued 9/15/2015
- Presidents FY 2017 budget: $318M for NSCI activities 2/9/2016
- Second meeting of NSCI Executive Council 3/8/2016
- Strategic Plan Public Report 7/26/2016
- NSCI Anniversary Workshop 7/30/2016
- PCAST Semiconductor Working Group launched 10/31/2016
- Inaugural meeting of Joint Program Office for Strategic Computing (JPO-SC) 11/2016

Visit www.nitrd.gov/nsci to find background information, reports, public events, blog postings, etc. and to subscribe for updates!
Panelists

• Erin Szulman, OSTP
• Steve Binkley, DOE
• Mark Sims, DOD
• Irene Qualters, NSF
• Eric Stahlberg, NIH
The National Strategic Computing Initiative

Erin Szulman
White House Office of Science and Technology Policy
November 2016
History of OSTP

Established by Congress in 1976 to:

• Advise the President and others within the Executive Office of the President on the effects of science and technology on domestic and international affairs.

• Lead interagency efforts to develop and implement sound science and technology policies and budgets.

• Work with the private sector; state, tribal, and local governments; the science and higher education communities; and other nations toward this end.
EXECUTIVE ORDER

CREATING A NATIONAL STRATEGIC COMPUTING INITIATIVE

By the authority vested in me as President by the Constitution and the laws of the United States of America, and to maximize benefits of high-performance computing (HPC) research, development, and deployment, it is hereby ordered as follows:

The NSCI is a whole-of-government effort designed to create a cohesive, multi-agency strategic vision and Federal investment strategy, executed in collaboration with industry and academia, to maximize the benefits of HPC for the United States.
Federal Agency Roles

Lead agencies (DOE, DOD, NSF) are charged with developing and delivering the next generation of integrated HPC capability and will engage in mutually supportive research and development in hardware, software, and workforce to support the objectives of the NSCI.

Foundational R&D agencies (IARPA, NIST) are charged with fundamental scientific discovery work and associated advances in engineering necessary to support the NSCI objectives.

Deployment agencies (NASA, FBI, NIH, DHS, NOAA) will develop mission-based HPC requirements to influence the early stages of design of new HPC systems and will seek viewpoints from the private sector and academia on target HPC requirements.
Related Initiatives

• Materials Genome Initiative
• Advanced Manufacturing Initiatives
• National Nanotechnology Initiative
• The BRAIN Initiative
• Precision Medicine Initiative
• The National Big Data R&D Initiative
White House Workshop on NSCI

Workshop Proceedings now available at the new NSCI webpage:

NSCI webpage
NSCI in the FY 2017 President’s Budget

The 2017 President’s Budget Request was sent to Congress on February 9, 2016. The total funding explicitly allocated to the NSCI was $318 million.

DOE National Nuclear Security Administration, ($95 million)

• Advanced Simulation and Computing: Activities and research leading to deployment of exascale capability for national security applications in the early 2020’s

DOE Office of Science ($190 million)

• Advanced Scientific Computing Research ($154 million) R&D and design to ultimately achieve capable exascale systems with 1000x performance of current HPC

• Basic Energy Sciences ($26 million): basic research resulting in codes to predictively design functional materials and chemical processes

• Biological and Environmental Research ($10 million): develop science base for increasingly complex climate modeling and data analytic applications

National Science Foundation ($33 million):

• Multi-directorate: Scientific discovery for HPC, HPC for scientific discovery, the broader HPC ecosystem, and workforce development

All of the above is in addition to existing core programs aligned with NSCI goals
One Year Anniversary

• Since the launch of NSCI, Federal agencies have taken important steps to create the foundation for a long-lasting and successful Federal initiative.

• This includes the development and recent release of a Strategic Plan outlining the near-term goals of the Federal partners and opportunities for private sector engagement and leadership.

• In coordination with the Networking and Information Technology Research and Development (NITRD) program, NSCI launched a new website to consolidate and distribute information, news, and opportunities for engagement to the community nationwide www.nitrd.gov/nsci/

• Federal agencies also released a white paper describing the interagency vision for the emerging and innovative solutions needed to realize the Nanotechnology-Inspired Grand Challenge for Future Computing announced in October 2015.
The NSCI agencies published the first NSCI Strategic Plan in July 2016. The Plan identifies the roles assigned to Federal agencies, and highlights ongoing and planned activities that will contribute to NSCI’s goals.

Realizing the vision of the NSCI will demand a fully developed HPC ecosystem that meets the needs of government, industry, and academia.

The Strategic Plan focuses on areas where government engagement is essential in creating the technological capability, computational foundations, and workforce capacity to realize the vision of the NSCI.

The hope is this will be a living document for continuous outreach to industry and academia.
PCAST

• The President’s Council of Advisors on Science and Technology (PCAST) made recommendations dating back to 2010 encouraging the formation of a coordinated program in HPC

• On October 31, 2016, PCAST announced the formation of a new working group focused on strengthening the U.S. semiconductor industry in ways that benefit the nation’s economic and security interests.

• The new PCAST working group will identify the core challenges facing the semiconductor industry at home and abroad and identify major opportunities for sustaining U.S. leadership.

  • Based on its findings, the working group will deliver a set of recommendations on initial actions the Federal government, industry, and academia could pursue to maintain U.S. leadership in this crucial domain.

  • Members include John Holdren, Paul Otellini, Richard Beyer, Wes Bush, Diana Farrell, John Hennessy, Paul Jacobs, Ajit Manocha, Jami Miscik, Craig Mundie, Mike Splinter, and Laura Tyson
Outlook: A Lasting Initiative

• Coordination and collaboration across Federal agencies
  – Agencies have taken initial steps to advance the initiative’s goals in a strongly coordinated fashion
  – NSCI agencies are currently finalizing its governance structure

• Coordination and collaboration with academia and industry
  – There have been numerous NSCI-related workshops and meetings led or sponsored by the Federal agencies with private sector participation.
  – We will continue to ask industry and academia to help us shape and promote follow-on activities.

• Implementation of a long-term strategy for High Performance Computing
  – The President’s FY 2017 budget request and forthcoming strategic plan will be the launching points for sustaining the NSCI across administration boundaries.
National Strategic Computing Initiative

Exascale Computing Project

Presented at the

SC16 Conference

November 15, 2016

J. Stephen Binkley
Deputy Director, Office of Science

www.science.energy.gov
NSCI Strategic Objectives

Executive departments, agencies, and offices participating in the NSCI shall pursue five strategic objectives:

1. Accelerating delivery of a capable exascale computing system that integrates hardware and software capability to deliver approximately 100 times the performance of current 10 petaflop systems across a range of applications representing government needs.

2. Increasing coherence between the technology base used for modeling and simulation and that used for data analytic computing.

3. Establishing over the next 15 years, a viable path forward for future HPC systems in the Post-Moore's-Law Era to advance beyond traditional lithographic scaling of devices.

4. Increasing the capacity and capability of an enduring national HPC ecosystem, employing a holistic approach that addresses relevant factors such as networking technology, workflow, downward scaling, foundational algorithms and software, and workforce development.

5. Developing an enduring public-private collaboration to ensure that the benefits of the research and development advances are, to the greatest extent, shared between the U.S. commercial, government, and academic sectors.
Background

• The DOE exascale effort has been underway since 2009, a partnership between Office of Science (SC) and NNSA
  – Exascale was identified as an objective in the National Strategic Computing Initiative (NSCI) Executive Order in 2015
  – In FY 2016, the Exascale Computing Project (ECP) was established to manage the research, development, and implementation of capable exascale systems by 2023

• Exascale development is following DOE project management practices

• The Mission Need Statement was jointly approved by the Office of Science and NNSA on April 14, 2016

• Critical Decision-0, Approve Mission Need, was approved by the DOE Deputy Secretary on July 28, 2016, with a cost range of $3.1 Billion - $5.1 Billion
The ECP Four Focus Areas – A Decadal Approach

- **Application Development** – deliver a suite of broad and varied ECP applications ready for execution on exascale systems.

- **Software Technology** – enhance system software and tools to meet the needs of exascale applications and to use exascale systems efficiently.

- **Hardware Technology** – support supercomputer vendors to perform R&D for hardware technologies and architecture designs for exascale systems.

- **Exascale Systems** – support testbeds, advanced system engineering development (NRE) by the vendors, incremental site preparation, and cost of system expansion needed to acquire capable exascale systems.
Exascale Applications Under Development

**National Security**
- 3 New Technology Integrated Design and Safety Codes

**Energy Security**
- Turbine Wind Plant Efficiency
- Design/Simulation of Small Modular Reactors
- Nuclear Fission and Fusion Reactor Materials Design
- Subsurface Use for Carbon Capture, Petro Extraction, Waste Disposal
- High-Efficiency, Low-Emission Combustion Engine and Gas Turbine Design
- Carbon Capture and Sequestration Scaleup
- Biofuel Catalyst Design
- Reliable and Efficient Planning of the Power Grid

**Economic Security**
- Additive Manufacturing of Qualifiable Metal Parts
- Deep Learning and Simulation for Precision Medicine for Cancer
- Urban Planning
- Earthquake Hazard and Risk Assessment

**Scientific Discovery**
- Cosmological Probe of the Standard Model of Particle Physics
- Validate Fundamental Standard Model Laws of Nature
- Plasma Wakefield Accelerator Design
- Light Source-Enabled Analysis of Protein and Molecular Structure and Design
- Find, Predict, and Control Materials and Properties
- Whole-Device Modeling of Magnetic Fusion Plasma Confinement
- Materials Sci (Exascale) Community Codes
- Chemical Sci (Exascale) Community Codes
- Climate Model (Exascale) Community Codes
- Demystify Origin of Chemical Elements (S)

**Climate and Environmental Science**
- Accurate Regional Impact Assessment of Climate Change
- Stress-Resistant Crop Analysis and Catalytic Conversion of Biomass-Derived Alcohols
- Metagenomics for Analysis of Biogeochemical Cycles, Climate Change, Environ Remediation (S)
ECP is a Collaboration Among Six DOE Labs

- ECP project draws from the Nation’s 6 premier computing national laboratories
  - Argonne, Los Alamos, Berkeley Lab, Livermore Lab, Oak Ridge, Sandia

- Project team has decades of experience with deployment of the first system of a new generation of HPC systems

- Leadership team expertise spans all ECP activity areas

- Collaboration, expertise, and experience with high performance computing is critical to project success
Exascale Project Timeline

DOE Milestones

- **CD-0**: Application Development
- **CD-1/3a**: Software Technology
- **CD-2/3b**: Hardware Technology
- **CD-4**: Testbeds & Prototypes

Timeline:
- **2016**: CORAL 180-200 PF
- **2017**: APEX 90-120 PF
- **2022**: CORAL 2 ~600PF
- **2023**: System Build NRE
- **2024**: Site Prep
- **2025**: System expansion
- **2026**: Exascale Systems

FY: 2016-2026

U.S. DEPARTMENT OF ENERGY
Office of Science

National Nuclear Security Administration