National Strategic Computing Initiative (NSCI)

NSCI / Joint Program Office
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Irene Qualters (NSF)
Mark Sims (DoD)
October 23, 2017
High Performance Computing (HPC) Technologies
Vital to Economic Prosperity and Scientific Progress

- Finance
- Design and manufacturing
- Weather and climate modeling
- Big Science & Big Data
- Medicine

November 16, 2017
SC17 – ATIP International Workshop
NSCI – Bill Harrod
Opportunities for Government, Academia, and Industry Engagement in HPC

HPC-reliant US economic sectors constitute almost 55% of the GDP

• Three-quarters of the industrial sites said: impact would be "very large" or "somewhat large" on revenues and profits

• More than half described the impact of technology improvement on new jobs, as either "very large" or "somewhat large."

• More than five out of six stated: impact would be "very large" or "somewhat large” on their ability to compete effectively

757 individual sites: 168 provider/academia/government sites and 589 user/industry sites.
Economic Prosperity
Changing Workloads

Factors driving aggressive HPC growth rates across all sectors

• Continued expansion of HPCs into commercial and government modeling and simulation apps
  - Larger problem sizes
  - Higher modeling fidelity
  - More aggressive iteration methods
  - Faster turnaround time

• Expanding volume and diversity of new big data analytics into non-traditional HPC areas
  - Finance & fraud detection
  - Personalized medicine
  - Cyber security sectors
  - Increasing need for real-time big data analysis

• Need for new HPC systems with a broad range of architectures to support AI and deep learning algorithms

• New, rapidly growing opportunities to support migration and expansion of enterprise HPC workloads to cloud-based ecosystems
  - many HPC in-the-cloud operations will be used to augment critical on-premises HPCs capabilities
National Strategic Computing Initiative (NSCI)
Launched in July, 2015

A “Whole of Government” approach, executed in collaboration with industry and academia

NSCI’s Five Objectives

1. Accelerate delivery of a capable exascale computing system delivering approximately 100 times the performance of current systems across a range of applications

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

3. Establish a viable technology path forward for future HPC systems even after the limits of current semiconductor technology are reached (the "post-Moore's Law era")

4. Increase the capacity and capability of an enduring HPC ecosystem

5. Develop an enduring public-private collaboration to ensure that the benefits of the research and development advances are shared among government, industrial, and academic sectors
## NSCI Interagency Coordination and Collaboration
### Agency Roles

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<th>Agency</th>
<th>Lead Agencies</th>
<th>Foundational R&amp;D Agencies</th>
<th>Deployment Agencies</th>
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<tr>
<td>Department of Defense (DOD)</td>
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<td>Department of Energy (DOE)</td>
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<td>ODNI/Intelligence Advanced Research Projects Activity (IARPA)</td>
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<td>National Science Foundation (NSF)</td>
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NSCI Resonates with Administration FY19 R&D Priorities

Among this administration's highest priorities are economic growth and job creation.

- **Prosperity**: Emerging technologies, such as machine learning, and quantum computing, may well have the highest potential to drive the economy and create entirely new industries.

- **Support for Innovative Early-Stage Research**: Funding basic and early-stage applied research that, supplemented by private sector financing of later-stage R&D, can result in the development of transformative commercial products and services.

- **Maximized Interagency Coordination**: R&D priorities require coordinated interagency initiatives.

- **Future-Focused Workforce**: Give priority to policies and actions that place an emphasis on expanding the STEM workforce.

- **Modernized Research Infrastructure**: Maintaining and modernizing research infrastructure is critical to getting the best value out of R&D investment.
Envisioned Results of NSCI

- **New hardware and software** technologies to support next-generation HPC applications and new computing paradigms

- A **robust HPC ecosystem** to support emerging classes of commercial and scientific applications

- A **larger and more skilled HPC workforce** that can take advantage of emerging technologies, including capabilities to support massive-concurrency, data-intensive workflows, tightly-coupled applications, and time-critical responses

- **Economic benefits for companies**—large, medium, and small—that integrate use of HPC tools into their product development and manufacturing cycles

- **Science benefits** across all research enterprise in universities, industries, government, and national laboratories
Related Initiatives in NSCI Interagency Plan

- Materials Genome
- Advanced Manufacturing
- The National Nanotechnology
- The BRAIN
- Precision Medicine
- The National Big Data R&D
- National Photonics

https://www.nitrd.gov/nsci/
Collaboration
2 US Department of Energy organizations
• Office of Science
• National Nuclear Security Administration

Execution
800 researchers (22 laboratory and agency partners; 39 universities) engaged in:
• 66 software projects
• 22 science application projects
• 3 national security application projects
• 5 co-design centers
• 6 Vendor partnerships for critical technologies

Goal
Drive pre-exascale science, application development, hardware and software R&D to ensure that the US has a capable exascale ecosystem in 2021

https://www.exascaleproject.org
NSCI: Beyond Moore’s Law
Quantum Computing


- Accelerate “post Moore’s Law”, beyond-CMOS digital computing technology
- Provide potential new computing paradigms
  - Quantum simulators – e.g., for materials properties
  - Quantum computing – e.g., factorization (Shor)
  - Quantum search (Grover)
  - Secure quantum communication

NSF Quantum Science Summer School

- Spin Qubits
- Optical Lattice Quantum Computing
- Superconducting Qubits Theory, Experiment, Quantum Information and Simulation, and 3D Integration
- Trapped Ion Quantum Computing and Information
- Topological Quantum Computing
- Quantum Simulation: Chemistry, Eigenvalue Solver, Optimization

NIST / UMD QuICS Joint Center

- Quantum algorithms
- Quantum complexity theory
- Quantum communication
- Quantum cryptography
- Quantum error correction/fault tolerance
- Implementations of quantum information processing
- Applications of quantum information to physics

Chicago Quantum Exchange
Quantum Information Science

DOE/ASCR Quantum Testbed

- Hardware/software co-design
- Multidisciplinary teams
- Includes:
  - Qubit connectivity schemes
  - Quantum/classical coprocessors
  - Quantum accelerators for traditional HPC
  - Metrics for system evaluation

November 16, 2017
NSCI: Beyond Moore’s Law
Rebooting the IT Revolution

DOE – Big Idea Summit

DARPA - Electronics Resurgence Initiative

Executive Office of the President
President’s Council of Advisors on
Science and Technology

January 2017
EXTRA OR BACKUP SLIDES
References

• FY 2019 Administration Research and Development Budget Priorities
• US Leadership in High Performance Computing
• Worldwide Best Practices in Partnerships between HPC Centers and Industrial Users
• US HPC Centers of Activity
FY16-17: Growing, Diverse Use of HPC for Large-Scale Data Analytic Research (often with Public/Private contribution)

Min Chen, Rice University

Seismic data from 227 earthquakes reveal 3D images. Thanks to the work of NSF-funded researchers and 8 million CPU hours on the Stampede and Lonestar4 supercomputers at the Texas Advanced Computing Center, it’s now possible to take a virtual tour of the Earth’s structures 900 km beneath East Asia.

Artificial Intelligence Beats Top Poker Pros: Libratus, an artificial intelligence developed by Tuomas Sandholm at Carnegie Mellon University, made history by defeating four of the world’s best professional poker players in a marathon 20-day poker competition called “Brains vs. Artificial Intelligence: Upping the Ante”. Libratus’ victory was made possible by the Pittsburgh Supercomputing Center’s Bridges computer, on which the AI computed its strategy before and during the event.

“"The best AI’s ability to do strategic reasoning with imperfect information has now surpassed that of the best humans," Sandholm said. Business negotiation, military strategy, cybersecurity and medical treatment planning could all benefit from automated decision-making using a Libratus-like AI.

Machine Learning to reverse-engineer cellular control networks: Michael Levin, professor of biology at Tufts University and director of the Allen Discovery Center there, Maria Lobikin, a Ph.D. student in his lab, and Daniel Lobo, a former post-doc and now assistant professor of biology and computer science at the University of Maryland, Baltimore County (UMBC), reported results of a study in Scientific Reports in January 2016. They created a tadpole with a form of mixed pigmentation never before seen in nature. The partial conversion of normal pigment cells to a melanoma-like phenotype was predicted by their machine learning code and billions of simulations on Stampede.

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FY2018 Proposed NITRD Budget, $4,789M

The Networking and Information Technology Research and Development Program

Supplement to the President’s Budget

FY2018

October 2017
HPC Collaborations Provide Insights Not Previously Possible

ArcticDEM – Morin (UMn)

- Research and Societal Impact
- Time-dependent, 2m resolution elevation dataset, ~1-2 m vertical accuracy covering 20 million km²
  - Arctic will have higher resolution continuous elevation data than Western US
- Collaborative partnership among agencies, academia, and industry with international. Initiated as part of US Chairmanship of the Arctic Council – Interagency/Public/Private Partnership
  - NGA, NSF, ESRI/AWS and 5 Universities
- Image data from three optical, sub-meter satellites licensed and funded by the National Geospatial-Intelligence Agency (NGA)
- Data analysis on UIUC/Blue Waters over the next 2 years
- Antarctica is next....
- Supported by NSF Awards 1614673, 1542736, 1043681, 1541332, 1559691

- More than 1 million analyses over 2 years
- 452 TB data transferred and analyzed, producing over 280 TB of results

“Blue Waters has exceptional resources and one of the only HPC centers with the capacity to complete this project.”
This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.
Modernizing and Managing Research Infrastructure How do we evolve to a coherent data-intensive software stack that promotes secure access while accommodating disruptive technologies?

Dynamic discovery pathways at scale: Architecture view

NERSC Big Data Stack

<table>
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<tr>
<th>Capabilities</th>
<th>Technologies</th>
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<tbody>
<tr>
<td>Data Transfer + Access</td>
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<tr>
<td>Workflows</td>
<td>FireWorks, Swift</td>
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<tr>
<td>Data Management</td>
<td>HDF, mongoDB, MySQL</td>
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<tr>
<td>Data Analytics</td>
<td>Python, Spark, TensorFlow</td>
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<tr>
<td>Data Visualization</td>
<td>Vistr, ParaView</td>
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</tbody>
</table>
Questions:

• How do we replicate, expand, and build upon existing public/private models of collaboration among industry, Labs, Universities and others?

• Software stack:
  • How do we collectively and individually use our strengths to reduce access barriers to all forms of HPC?
  • What steps should be taken to maximize benefits of HPC and cloud in a hybrid ecosystem that allows dynamic and data- and compute-intensive workflows?
  • How do we adapt and adopt software to disruptive technologies?

• What new and existing activities will prepare the computationally literate workforce of the future in industry, universities and government?
National Strategic Computing Initiative (NSCI)

July 29, 2015

**INTENT**

- **National**
  - “Whole-of-government” / “whole-of-Nation” approach
  - Public/private **partnership with industry and academia**

- **Strategic**
  - Leverage beyond individual programs
  - Long time horizon (decade or more)

- **Computing**
  - HPC = **most advanced, capable computing technology available in a given era**
  - Multiple styles of computing / all necessary infrastructure
  - Scope: everything necessary for fully integrated capability
    - Theory and practice, software and hardware

- **Initiative**
  - Above baseline effort
  - Link and lift efforts

**STRATEGIC THEMES**

- Create systems that can apply exaflops of computing power to exabytes of data
- **Keep the U.S. at the forefront of HPC capabilities**
- Improve HPC application developer productivity
- Make HPC readily available
- **Establish hardware technology for future HPC systems**
1. The United States must deploy and apply new HPC technologies broadly for national security, economic competitiveness and scientific discovery.

2. The United States must foster public-private collaboration, relying on the respective strengths of government, industry, and academia to maximize the benefits of HPC.

3. The United States must adopt a whole-of-government approach that draws upon the strengths of and seeks cooperation among all executive departments and agencies with significant expertise or equities in HPC while also collaborating with industry and academia.

4. The United States must develop a comprehensive technical and scientific approach to transition HPC research on hardware, system software, development tools, and applications efficiently into development and, ultimately, operations.
NSCI Agencies

- There are three lead agencies for NSCI: the Department of Energy (DOE), the Department of Defense (DOD), and the National Science Foundation (NSF).
- The Joint Program Office consists of representatives from the NSCI agencies
  - Co-Chairs – Irene Qualters (NSF), Mark Sims (DOD) and Bill Harrod (DOE)
NSCI
Strategic Objectives

• NSCI is a whole-of-Nation effort to sustain and enhance U.S. leadership in high-performance computing (HPC). The NSCI seeks to accomplish five strategic objectives in a government collaboration with industry and academia:
  1. Accelerate the successful deployment and application of capable exascale computing
  2. Ensure that new technologies support coherence in data analytics as well as simulation and modeling
  3. Explore and accelerate new paths for future computing architectures and technologies, including digital computing and alternative computing paradigms
  4. Holistically expand capabilities and capacity of a robust and enduring HPC ecosystem
  5. Establish an enduring public-private collaboration to ensure shared benefit across government, academia, and industry.
High Performance Computing (HPC) Technologies Vital to Economic Prosperity and Scientific Progress

TOP500 Supercomputing List (49th edition, June 2017):
1. China: Sunway Taihu Light
2. China: Tianhe-2
3. Switzerland (CSCS): Upgraded Piz Daint (Cray XC50)
4. US: Oak Ridge Titan
5. ...
6. ...
7. Japan: Oakforest-PACS

Japan plans superefficient supercomputer by 2017
With its next supercomputer, Japan plans to deliver a tenfold increase in computing performance for the same power consumption

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