



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Computing Beyond Moore's Law

Ceren Susut

Advanced Scientific Computing Research

Ceren.Susut-Bennett@science.doe.gov

December 20th, 2016

National Strategic Computing Initiative

July, 2015

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 even after the limits of current semiconductor technology are reached (the "post-Moore's Law era").

(4) Increasing the capacity and capability of an enduring national HPC ecosystem by employing a holistic approach that addresses relevant factors such as networking technology, workflow, downward scaling, foundational algorithms and software, accessibility, 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 United States Government and industrial and academic sectors.



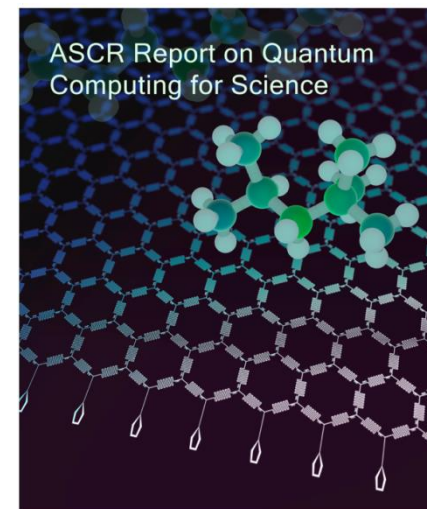
DOE/ASCR Workshop on Quantum Computing in Scientific Applications (Feb 17-18, 2015)

Preceded by Quantum Computing in Scientific Applications Meeting (January 15th, 2014), the workshop explored the following topics:

- **Mission relevance:** What aspects of DOE's science mission are suitable for quantum computing?
- **Impact on Computing:** How will quantum computing improve the properties of the computation with respect to conventional contemporary computational systems?
- **Challenges:** What are the challenges in adopting quantum computing technologies and developing the required infrastructure?

The consensus in the workshop was that quantum computing has reached a level of maturity that warrants considering how it will impact the DOE mission in the near and long term. The report listed the following research opportunities:

- **Quantum Algorithms:** Develop speedups for the fundamental primitives of applied mathematics such as linear algebra, optimization and graph theory.
- **Quantum Simulation:** Solve problems in chemistry, materials science, and nuclear and particle physics by developing and optimizing simulation algorithms.
- **Models of Computation and Programming Environments:** Develop software infrastructure for quantum computation.
- **Co-Design Approach:** Adopt a co-design approach in developing models and algorithms along with prototype quantum computing systems.



<http://science.energy.gov/~/media/ascr/pdf/programdocuments/dcs/ASCRQuantumReport-final.pdf>



Quantum Information Science Interagency Working Group

- **Chartered to:**
 - assess Federal programs in QIS
 - monitor the state of the field
 - provide a forum for interagency coordination and collaboration, and
 - engage in strategic planning of Federal QIS activities and investments
- **Participating agencies: DOC, DOD, DOE, NSF, ODNI, OMB, OSTP**
- **DOE IWG members: Steve Binkley (IWG co-chair), Lali Chatterjee (HEP), Claire Cramer (ASCR, IWG Exec Sec), Dimitri Kusnezov (NNSA)**

2015:

- **NIST-sponsored workshop and RFI to solicit industry views on: R&D opportunities, emerging market areas, barriers to near-term and future applications, workforce needs**

2016:

- **Public report (July)**
- **White House Forum (October)**



QIS IWG: Public Report

Summarized: developments in and impacts of quantum sensing, metrology, communication, simulation, computing, and fundamental QI science

Reviewed: Existing QIS programs at Federal agencies, industry activity, new announcements abroad

Identified Impediments to Progress:

1. Institutional boundaries
2. Education and workforce training
3. Technology and knowledge transfer
4. Materials and fabrication
5. Level and stability of funding

Recommended Path Forward:

1. Stable, sustained, *flexible* core programs
2. Strategic investment in targeted, time-limited programs
3. Continued close monitoring of this rapidly-moving field

https://www.whitehouse.gov/sites/whitehouse.gov/files/images/Quantum_Info_Sci_Report_2016_07_22%20final.pdf





BRIEFING ROOM

ISSUES

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A Nanotechnology-Inspired Grand Challenge for Future Computing

OCTOBER 20, 2015 AT 6:00 AM ET BY LLOYD WHITMAN, RANDY BRYANT, AND TOM KALIL



Summary: Today, the White House is announcing a grand challenge to develop transformational computing capabilities by combining innovations in multiple scientific disciplines.

In June, the Office of Science and Technology Policy issued a [Request for Information](#) seeking suggestions for *Nanotechnology-Inspired Grand Challenges for the Next Decade*. After considering over 100 responses, OSTP is excited to announce the following grand challenge that addresses three Administration priorities—the [National Nanotechnology Initiative](#), the [National Strategic Computing Initiative](#) (NSCI), and the [BRAIN initiative](#):

Create a new type of computer that can proactively interpret and learn from data, solve unfamiliar problems using what it has learned, and operate with the energy efficiency of the human brain.

<https://www.whitehouse.gov/blog/2015/10/15/nanotechnology-inspired-grand-challenge-future-computing>



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Grand Challenge Committee - Collaborating Agencies

DOE - *Robinson Pino (co-lead)* DARPA - *Kerry Bernstein*
NSF - *Sankar Basu (co-lead)* NIST - *Curt Richter*
IC - *David Mountain* ARO - *Joe Qiu*

Members sought out participation, ideas, input, feedback, and contributions from home institutions and sister agencies

Objective:

- **Highlight potential areas of Federal R&D focus and investment**
 - Pursue emerging and innovative solutions that will address the Nanotechnology-Inspired Grand Challenge for Future Computing.
- **Describe technical challenges, opportunities, and potential applications**
 - Of interest to the collaborating agencies
 - Serve as a guide for future Federal investments

https://www.nano.gov/sites/default/files/pub_resource/federal-vision-for-nanotech-inspired-future-computing-grand-challenge.pdf



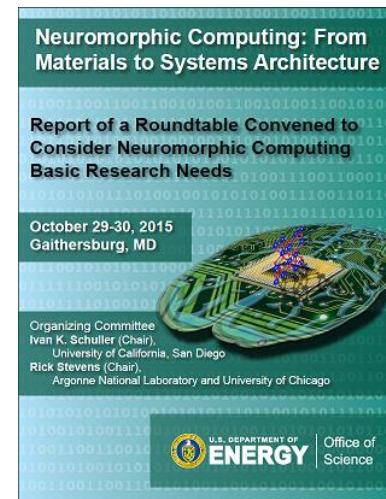
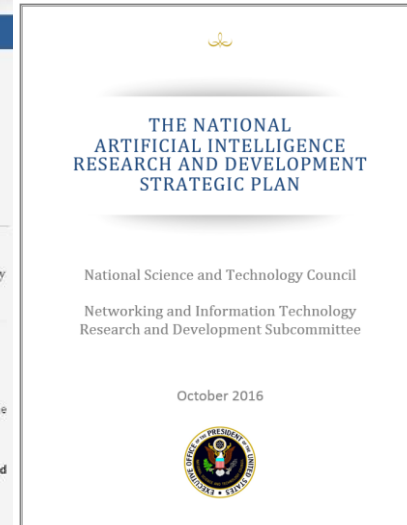
Success = Game-Changing Capabilities

- **Emerging computing architecture platforms, neuromorphic, quantum, ...**
 - Significantly accelerate algorithm performance and concurrency while reducing energy consumption by over six orders of magnitude (from megawatts to watts)
- **Intelligent big data sensors: Autonomous and Reprogrammable**
 - Increased flexibility and communication with other networked nodes while maintaining security and avoiding interference with the things being sensed
- **Machine intelligence for scientific discovery**
 - Enable rapid extreme-scale data analysis and be able to deal with unlabeled data sets
 - Capable of understanding and making sense of results, thereby accelerating innovation
- **Cybersecurity**
 - Prevent/minimize unauthorized access, identify anomalous behavior, ensure data and software code integrity
 - Provide contextual analysis for adversary intent or situational awareness; i.e., deter, detect, protect, and adapt

DOE Office of Science Programmatic Activities

Joint activities by ASCR and BES since launch of Grand Challenge

- Goal and Objectives
 - Evaluate both advanced materials and scientific computing research opportunities to support development of a new paradigm for extreme and self-reconfigurable computing architectures that go beyond Moore's Law and mimic neuro- biological computing architectures
- Why Neuromorphic Computing?
 - Conventional computing fails in some of the most basic tasks that biological systems have mastered such as language and vision *understanding*
 - Cues from biology might lead to fundamental improvements in computational capabilities



ASCR Must Explore “Beyond Moore’s Law” Technologies

Approach:

Advance New Hardware/Software Computing
Paradigms to Glean Unexploited Efficiencies:

- Extending CMOS
- Non-CMOS computing



Quantum Simulation Teams

FY17: Initiate interdisciplinary Quantum Simulation Teams, focused on problems relevant to Office of Science, to begin development and optimization of quantum simulation algorithms.

Goals & Impact:

1. Create and support a robust and versatile set of algorithms.
2. Formulate and inform a quantum basic research agenda in ASCR's applied math and computer science programs.
3. Use quantum testbeds in a co-design fashion, feeding back ideas for improvement.
4. Bring ASCR community's expertise to quantum computing field.
5. Evaluate the efficacy of this funding model for making the resulting tools, methods and resources available to the wider QIS community and expanding the ASCR/SC support in these communities.



Quantum Testbed Program

FY17: ASCR plans a *Quantum Testbed Facility* that will provide the research community with access to early-stage quantum computing devices.

Program goals:

1. Evaluate the utility of quantum computing to advance scientific questions of relevance to DOE
2. To the extent that quantum computing proves valuable for DOE, facilitate the technology development required to provide production-quality quantum computing resources in the post-Exascale timeframe

The facility will:

- Advance quantum computing for science by allowing researchers greater access to early-stage technology
- Lead to insight into how to assemble better systems for quantum computing and simulation
- Adopt the most advanced existing systems of qubits; adapt as technology evolves
- Complement quantum computing investments in NNSA and at other Federal agencies
- Address identified impediments to progress in quantum information science by:
 - Bridging institutional and disciplinary boundaries
 - Training a skilled quantum information workforce
 - Working synergistically with the emerging U.S. quantum computing industry

Developed in response to community input:

1. Significant advances in quantum computing applications will occur when quantum computers are available for researchers to experiment with; significant investment in developing quantum computing hardware will take place when “killer apps” are identified.
2. The DOE labs occupy a niche between universities and industry that can, in principle, play a significant role in advancing quantum information technology.



Neuromorphic Computing

ASCR is actively exploring how neuromorphic computing may address unique challenges for DOE and SC.

- Leverage HPC capabilities for large-scale modeling, simulation, emulation and analysis of the natural analog neuro-biological computing processes that lead to cognitive understanding.
- Identify the appropriate physical platform means by which to deploy an effective neuromorphic computer.
- Prototype promising neuromorphic computing processors.



Community Engagement Continues

Quantum Testbed Stakeholder Workshop:

- identify individual capabilities and interests in quantum computing hardware and its use for science applications
- share best practices for management of collaborative research facilities, including topics such as workforce training and building strong relationships with the research community
- identify technology that will be important for the success of a testbed facility with the goal of advancing quantum computing for scientific applications in the next five years

Agenda to include:

- Presentations outlining DOE lab capabilities
- Breakout discussions on topics including user community development, workforce training, quantum co-design, technical challenges
- Discussion with industry to identify synergistic activities across the national quantum ecosystem

Workshop Dates: Feb. 14-16, 2017

Location: Washington, D.C.

White Papers Due: Jan. 5, 2017

Website: <https://www.ornl.gov/qtsws/default.htm>



Community Engagement Continues

- Computing Beyond 2025, August 15-16, 2016, Chicago.
- ASCR Quantum Testbeds Study Group, August 23rd, 2016, Germantown.
- Quantum Sensors at the Intersections of Fundamental Science, QIS & Computing, February 25th, 2016, Gaithersburg.
- Basic Research Needs on Quantum Materials for Energy Relevant Technology, February 8-10, 2016, Gaithersburg.
- Machine Learning and Understanding for Intelligent Extreme Scale Scientific Computing and Discovery, January 5-7, 2015, Rockville.
- DOE HEP Study Group: Grand Challenges at the Interface of QIS, Particle Physics, and Computing, December 11th, 2014, Germantown.

