Future of Computing:
A BES/ASCR Partnership

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Advanced Scientific Computing Research

- **Background**
- **Near Term**
  - Exascale
- **Longer Term**
  - Quantum Information Systems
  - Neuromorphic

Advanced Scientific Computing Research

Computational and networking capabilities and tools to extent the frontiers of science and technology

- **Exascale:** In partnership with the Department's National Nuclear Security Administration, ASCR is supporting the Exascale Computing Project that is focused on the Research and Development in applications, hardware and software technology needed for a capable exascale system. In the FY2018 budget there are additional facility investments at the ALCF and OLCF to deploy at least one exascale system in 2021 timeframe.

- **Facilities** will deploy a 200 petaflop upgrade at OLCF and continue site preparations for exascale machines and NERSC-9 and prepare for an upgrade of ESnet.

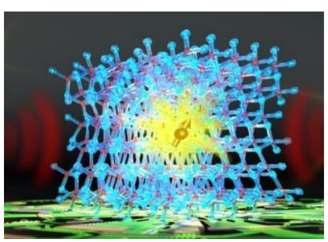
- In FY2017**, SciDAC** is finalizing the recompetition of new institutes and partnerships that span basic science priorities. In FY2018 budget request SciDAC will expanding partnerships in "beyond Moore's law" applications such as quantum information systems.

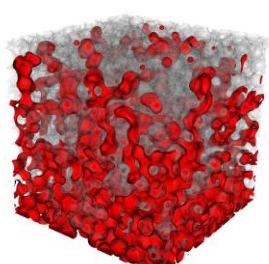
- **Applied Mathematics research** provides the fundamental building blocks (algorithms, mathematical models and methods) for describing complex physical and engineered systems computationally

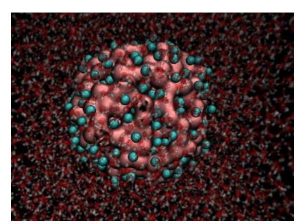
- **Computer Science** has an increased emphasis on data-intensive science challenges and, in collaboration with the SciDAC program, pays particular attention to adaptive algorithms and machine learning, the intersection with exascale, and the collaboration and workflow tools to support the increasing data needs of the DOE scientific user facilities.

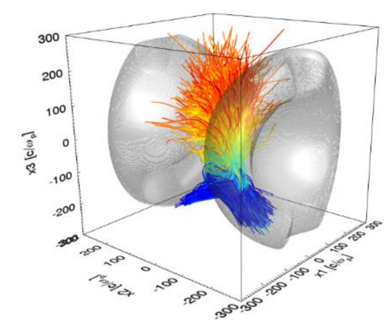
- **SciDAC** and **Research and Evaluation Prototypes** explores technologies "beyond Moore's law including increased investments in quantum applications and testbeds.

- The **Computational Sciences Graduate Fellowship** is funded at $10,000K.









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 ("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.

Current technology is no longer moving in the direction of meeting the growing needs

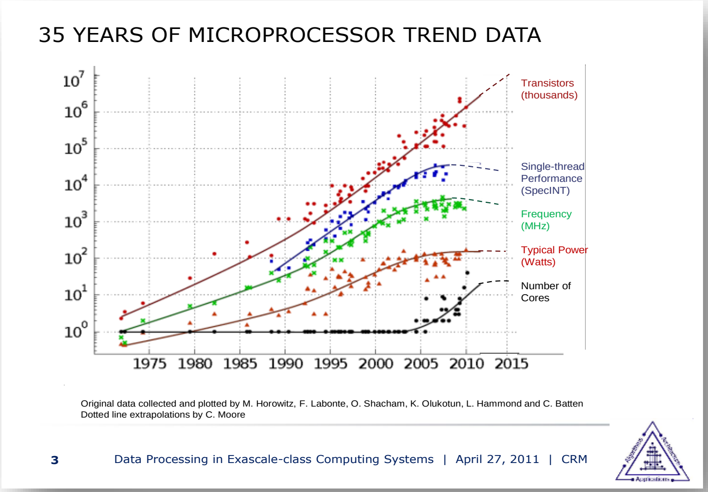
The Problem

- *We are reaching minimum size limits on transistors.*

  Current processors can no longer increase performance by increasing frequency and reducing voltage

  Increasing transistor count (Moore's Law) drives ***apparent*** performance through increasing the number of cores which requires more complex programming

- To minimize energy usage while improving performance industry is migrating from a FLOPS-dominated paradigm to data-movement-dominated paradigm
- Doing nothing will result in decreasing performance for our science codes.
- Consequently, buying off-the-shelf or without deep involvement with application code teams could lead to platforms incapable of scientific at the scale required.

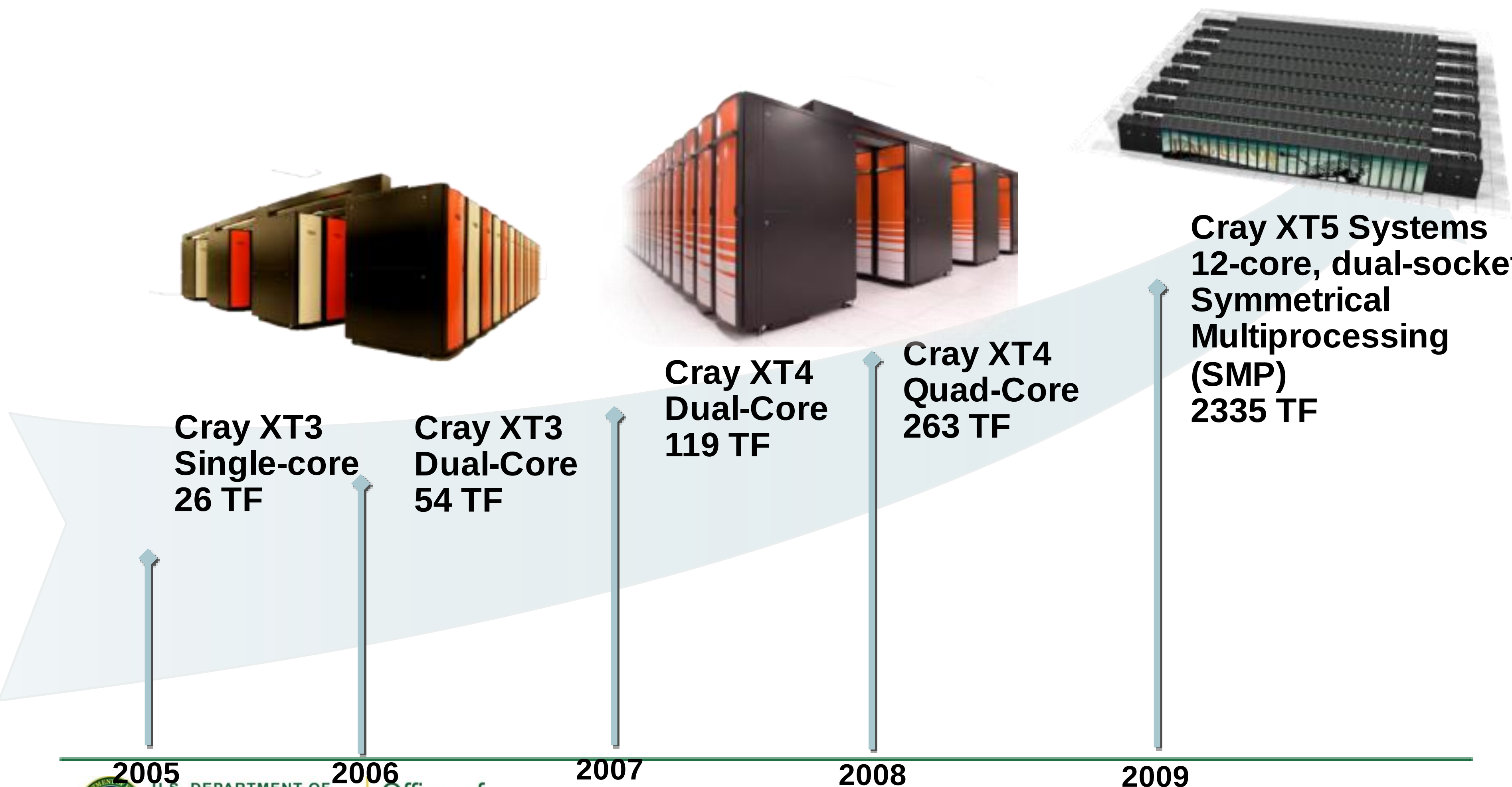


It takes concerted efforts to adapt commodity products to meet scientific code needs!

The technology problem has solutions, but requires time and resources to implement

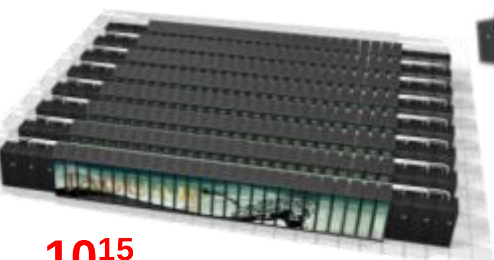
An Illustration

Since clock-rate scaling ended in 2003, HPC performance has been achieved through increased parallelism.



Science requires that we continue to advance computational capability over the next decade on the roadmap to Exascale.

Titan and beyond deliver hierarchical parallelism with very powerful nodes



10^{15}

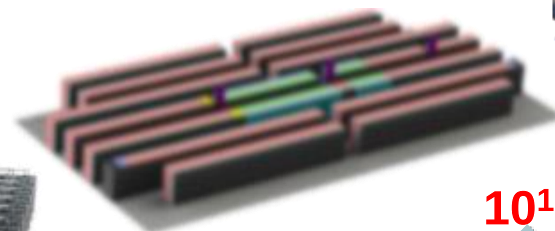
2008

Jaguar 2.3 PF
Cray XT5
18,688 AMD CPUs
7MW

10^{16}

2012

Titan: 27 PF
Cray XK7
18,688 AMD CPUs
18,688 NVIDIA GPUs
9 MW

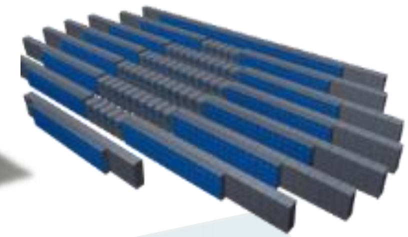


10^{17}

2018

Summit: 200 PF
5-10x Titan on apps
3,400 hybrid nodes with multiple IBM Power 9 CPUs and NVIDIA Volta GPUs
13 MW

CORAL System



10^{18}

2022

OLCF5: 1,000–3,000 PF
5-10x Summit
?????
20-30 MW

Multiple Architectural Choices: Many Core

- **Over 13X Mira's application performance**
- **Over 200 PF peak performance**
  - DGEMM +180PF
  - SGEMM +550PF
- **More than 50,000 nodes with 3rd Generation Intel® Xeon Phi™ processor**
  - Code name Knights Hill, > 60 cores
- **Over 7 PB total system memory**
  - High Bandwidth On-Package Memory, Local Memory, and Persistent Memory
- **~16 MW peak power**

Exascale Computing Project (ECP)

- As part of the National Strategic Computing initiative, ECP was established to accelerate delivery of a **capable exascale** computing system that integrates hardware and software capability to deliver approximately 50 times more performance than today's 20-petaflops machines on mission critical applications.
  - DOE is a lead agency within NSCI, along with DoD and NSF

- Funding in FY2018 President's budget request to deliver at least one exascale system in the 2021-2022 timeframe

- ECP's work encompasses research and development in
  - applications,
  - system software,
  - hardware technologies and architectures

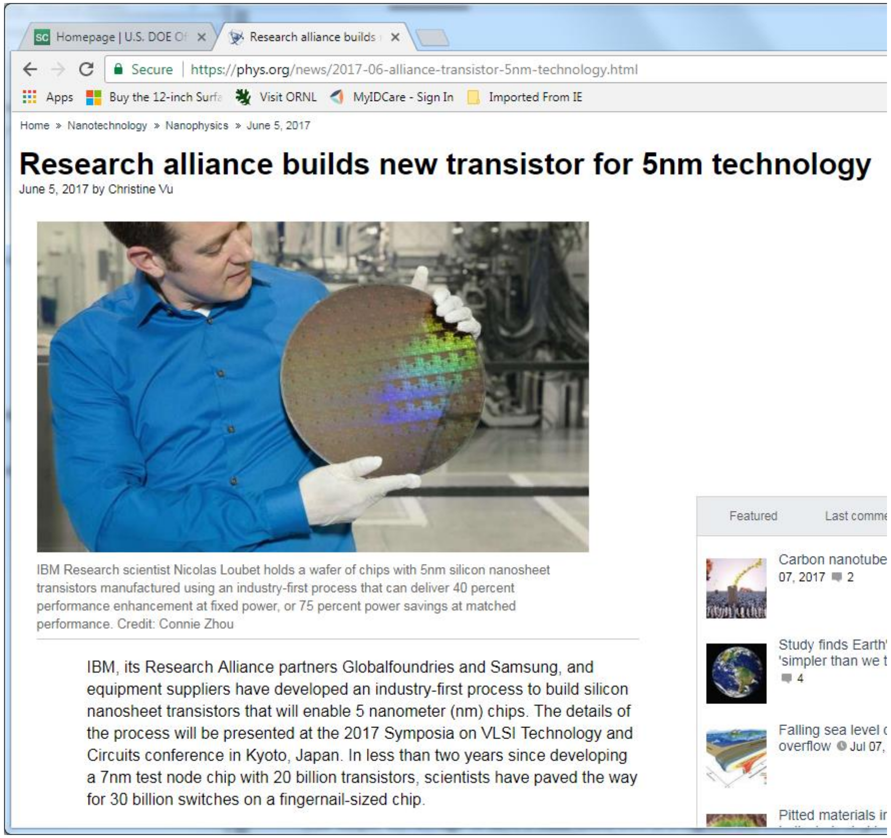
Beyond Exascale….

What will Computers Look Like in the Future?

- Conventional HPC – Extend CMOS/Silicon
- Non-CMOS technology
  - Mimic the Brain – Neuromorphic
  - Mimic Physical Systems – Quantum Information Systems

Future Computing will need a partnership between SC Program Offices, particularly BES for new materials and ASCR for new software and algorithms.

Extending CMOS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Home » Nanotechnology » Nanophysics » June 5, 2017

Research alliance builds new transistor for 5nm technology

June 5, 2017 by Christine Vu

IBM Research scientist Nicolas Loubet holds a wafer of chips with 5nm silicon nanosheet transistors manufactured using an industry-first process that can deliver 40 percent performance enhancement at fixed power, or 75 percent power savings at matched performance. Credit: Connie Zhou

IBM, its Research Alliance partners Globalfoundries and Samsung, and equipment suppliers have developed an industry-first process to build silicon nanosheet transistors that will enable 5 nanometer (nm) chips. The details of the process will be presented at the 2017 Symposia on VLSI Technology and Circuits conference in Kyoto, Japan. In less than two years since developing a 7nm test node chip with 20 billion transistors, scientists have paved the way for 30 billion switches on a fingernail-sized chip.

Featured Last comme
Carbon nanotube 07, 2017 2
Study finds Earth' 'simpler than we t 4
Falling sea level c overflow Jul 07,
Pitted materials ir

"IBM's said it's using a new type of transistor, called **stacked silicon nanosheets**, to pack transistors this closely together. The nanosheet transistor sends electrons through four gates, as opposed to the current-generation FinFET transistor design that sends electrons through three gates. FinFET (short for fin field-effect transistor) began appearing in 22nm and 14nm chips and are expected to continue being used with 7nm chips." June 5, 2017

Non-CMOS: SC Community Engagement

- Computing Beyond 2025, August 15-16, 2016, Chicago.
- ASCR Quantum Testbeds Study Group, August 23rd, 2016, Germantown.
- Neuromorphic Computing– Architectures, Models and Application Workshop, June29-July1, 2016, ORNL
- 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.
- Neuromorphic Computing: From Materials to Systems Architectures Roundtable, October 29-30, 2015, Gaithersburg.
- Quantum Computing in Scientific Applications, Feb 17-18, 2015
- 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.
- Quantum Computing in Scientific Applications Summit, January 15th, 2014

Quantum Information Science (QIS) in the DOE Office of Science

- **Ongoing and anticipated future efforts in QIS differ from earlier applications of quantum mechanics by exploiting uniquely quantum phenomena:**
  - **Superposition** – quantum particles or systems exist across all of their possible states simultaneously, until measured
  - **Entanglement** – a superposition of states of multiple particles in which their properties are correlated, regardless of distance
  - **Squeezing** – a method of improving precision in one variable by permitting large uncertainty in another correlated one, in systems that obey the Heisenberg uncertainty principle
- **Quantum information concepts are proving increasingly important in advancing fundamental understanding in, e.g., the search for dark matter, emergence of spacetime, and the black hole information paradox, as well as in applications including sensing and metrology, communication, simulation, and computing.**
- **SC is uniquely positioned to cover a wide range of QIS activities, with expertise and capabilities in frontier computing, quantum materials, quantum information, control systems, isotopes, and cryogenics. Resources span SC's research and facility portfolio, providing the ability to concentrate efforts and leverage infrastructure via the National Laboratory system and across multiple program offices.**
- **DOE Office of Science (SC) program offices have identified QIS areas in which they have important or unique roles, and bring unusual capabilities to bear.**

SC/ASCR: Beyond Exascale

- Challenge:

  Begin research into computing technologies and associated applied mathematics and computer science to prepare for the generation of scientific computing beyond exascale.

- FY 2017:

  Initiate two activities, predicated on recent community engagement:

  - Establish a the testbed program which will support ASCR, BES, and HEP-based algorithm development activities (Research & Evaluation Prototypes)
  - Continue research into quantum algorithms, focused on areas relevant to SC (Partnerships)

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

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

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


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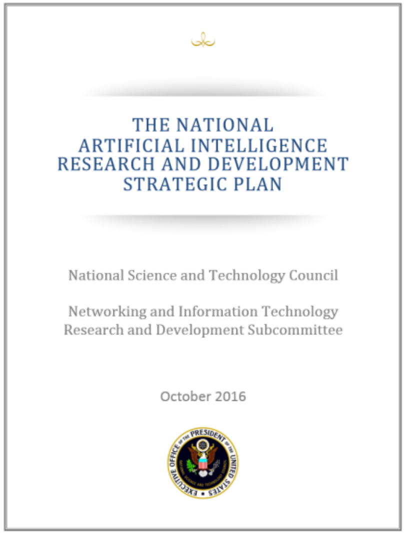
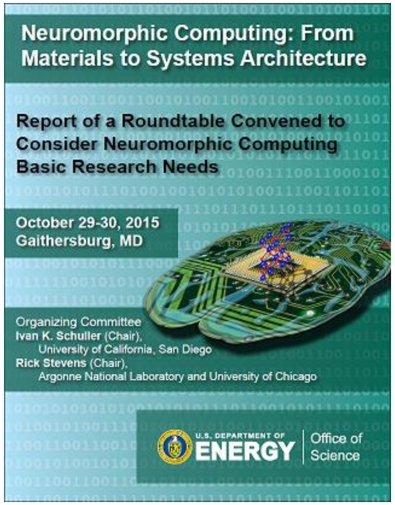
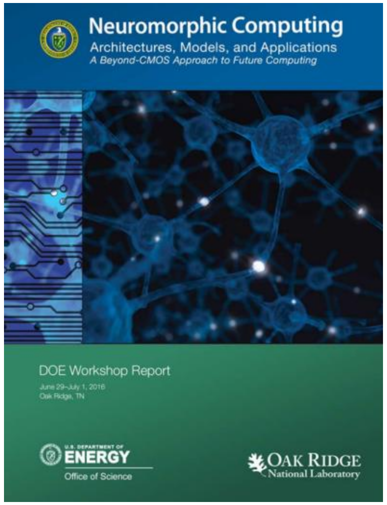

THE NATIONAL ARTIFICIAL INTELLIGENCE RESEARCH AND DEVELOPMENT STRATEGIC PLAN

National Science and Technology Council

Networking and Information Technology Research and Development Subcommittee

October 2016





Backup

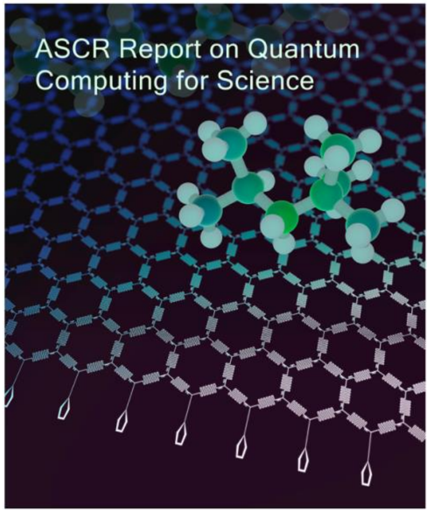
DOE/ASCR Workshop on Quantum Computing in Scientific Applications (Feb 17-18, 2015)

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/docs/ASCRQuantumReport-final.pdf