# Quantum Computing for Nuclear Physics Workshop
## November 14th , 2017

Ceren Susut, PhD
Advanced Scientific Computing Research
U.S. Department of Energy
Ceren.Susut-Bennett@science.doe.gov

# The DOE Office of Science Research Portfolio

| | |
|---|---|
| Basic Energy Sciences | • **Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels** |
| Advanced Scientific Computing Research | • **Delivering world leading computational and networking capabilities to extend the frontiers of science and technology** |
| Biological and Environmental Research | • **Understanding complex biological, climatic, and environmental systems** |
| Fusion Energy Sciences | • **Building the scientific foundations for a fusion energy source** |
| High Energy Physics | • **Understanding how the universe works at its most fundamental level** |
| Nuclear Physics | • **Discovering, exploring, and understanding all forms of nuclear matter** |

# International Computation in HPC Continues to Intensify

| # | Site | Manufacturer | Computer | Country | Cores | Rmax [Pflops] | Power [MW] |
|---|---|---|---|---|---|---|---|
| 1 | National Supercomputing Center in Wuxi | NRCPC | Sunway TaihuLight<br>NRCPC Sunway SW26010,<br>260C 1.45GHz | China | 10,649,600 | 93.0 | 15.4 |
| 2 | National University of Defense Technology | NUDT | Tianhe-2<br>NUDT TH-IVB-FEP,<br>Xeon 12C 2.2GHz, IntelXeon Phi | China | 3,120,000 | 33.9 | 17.8 |
| 3 | Swiss National Supercomputing Centre (CSCS) | Cray | Piz Daint<br>Cray XC50,<br>Xeon E5 12C 2.6GHz, Aries, NVIDIA Tesla P100 | Switzerland | 361,760 | 19.6 | 2.27 |
| 4 | Japan Agency for Marine Earth-Science and Technology | ExaScaler | Gyoukou<br>ZettaScaler-2.2 HPC System,<br>Xeon D-1571 16C 1.3 GHz, Infiniband EDR, PEZY SC2, 700 MHz | Japan | 19,860,000 | 19.1 | 1.35 |
| 5 | Oak Ridge National Laboratory | Cray | Titan<br>Cray XK7,<br>Opteron 16C 2.2GHz, Gemini, NVIDIA K20x | USA | 560,640 | 17.6 | 8.21 |
| 6 | Lawrence Livermore National Laboratory | IBM | Sequoia<br>BlueGene/Q,<br>Power BQC 16C 1.6GHz, Custom | USA | 1,572,864 | 17.2 | 7.89 |
| 7 | Los Alamos NL / Sandia NL | Cray | Trinity<br>Cray XC40,<br>Intel Xeon Phi 7250 68C 1.4GHz, Aries | USA | 979,968 | 14.1 | 3.84 |
| 8 | Lawrence Berkeley National Laboratory | Cray | Cori<br>Cray XC40,<br>Intel Xeons Phi 7250 68C 1.4 GHz, Aries | USA | 622,336 | 14.0 | 3.94 |
| 9 | JCAHPC Joint Center for Advanced HPC | Fujitsu | Oakforest-PACS<br>PRIMERGY CX1640 M1,<br>Intel Xeons Phi 7250 68C 1.4 GHz, OmniPath | Japan | 556,104 | 13.6 | 2.72 |
| 10 | RIKEN Advanced Institute for Computational Science | Fujitsu | K Computer<br>SPARC64 VIIIfx 2.0GHz,<br>Tofu Interconnect | Japan | 795,024 | 10.5 | 12.7 |

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

## QIS is a thriving area of multidisciplinary science.

- It exploits particular quantum phenomena to measure, process, and transmit information in novel ways that greatly exceed existing capabilities.

## QIS provides a basic foundation for numerous application areas.

- Potential transformative impact on SC grand challenges.

## QIS is at a tipping point.

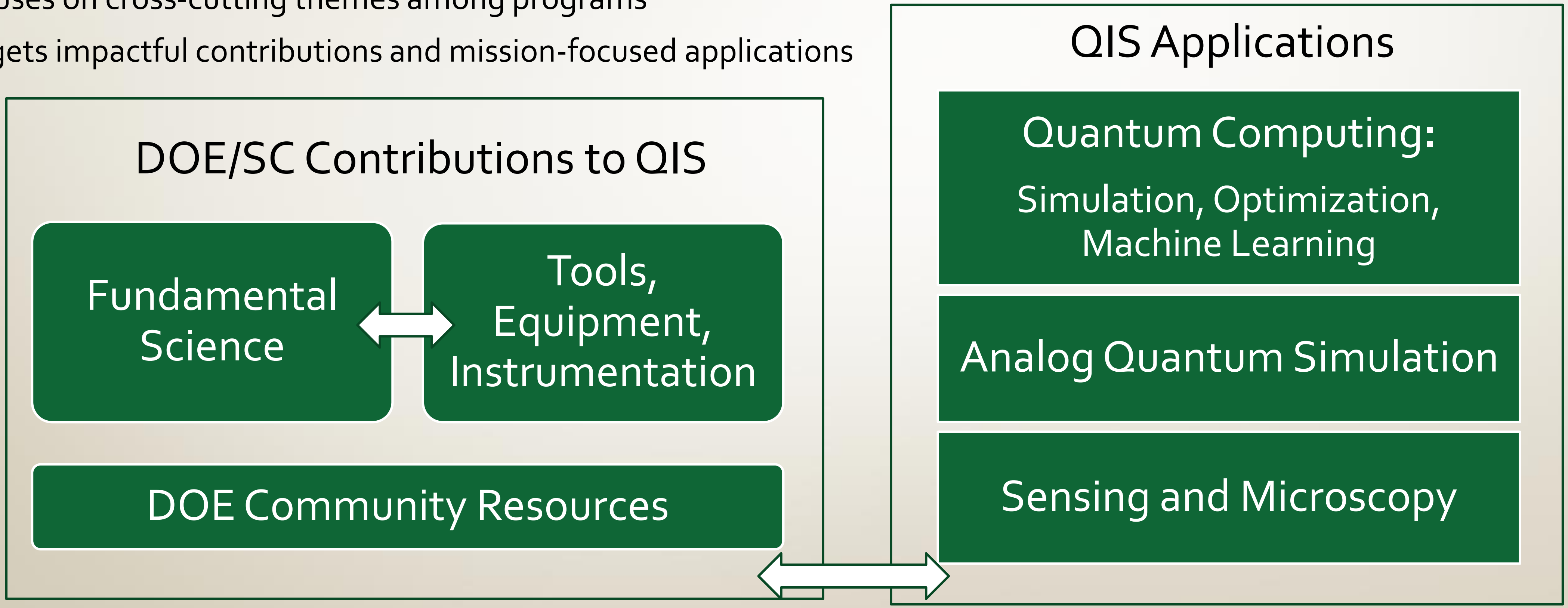
- Major companies are embracing QIS, foreign competition is expanding rapidly.

## Progress in QIS is driven by basic research in physical sciences.

- DOE SC is the Nation's leading supporter of basic research in physical sciences.

# SC's QIS Strategy

- ✓ Builds on community input
- ✓ Highlights DOE/SC's unique strengths
- ✓ Leverages groundwork already established
- ✓ Focuses on cross-cutting themes among programs
- ✓ Targets impactful contributions and mission-focused applications



# SC's QIS Strategy

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## DOE/SC Contributions to QIS

- Fundamental Science ↔ Tools, Equipment, Instrumentation
- DOE Community Resources

## QIS Applications

- Quantum Computing: Simulation, Optimization, Machine Learning
- Analog Quantum Simulation
- Sensing and Microscopy

# Fundamental Science That Advances QIS

| ASCR | BES | HEP | NP |
|---|---|---|---|
| Quantum algorithms; uncertainty quantification and verification & validation methods; software stack; quantum networks | Synthesis, characterization, modeling, and instrumentation to advance quantum chemistry and materials | Black hole physics; quantum gravity and quantum error correction; fundamental aspects of entanglement | Isotopes and trapped ions for quantum devices; lattice quantum chromodynamics |

Quantum Field Theory and Topology

Control of Quantum Phenomena

**SC Unique Strengths**

- Intellectual capital accumulated for more than a half-century
- Successful track record of forming interdisciplinary yet focused science teams for large-scale and long-term investments
- Demonstrated leadership in launching internationally-recognized SC-wide collaborative programs

# Fundamental Science That Advances QIS

We will leverage the groundwork already established in DOE National Labs and the academic groups to maximize SC's impact on QIS. Examples include:


In April 2017, the researchers have successfully run the largest ever simulation of a quantum computer at NERSC, LBNL. The simulation was made possible by the performance boost gained through the use of Roofline model during the optimization process. The Roofline model was developed by SciDAC Institutes; a flagship ASCR program.

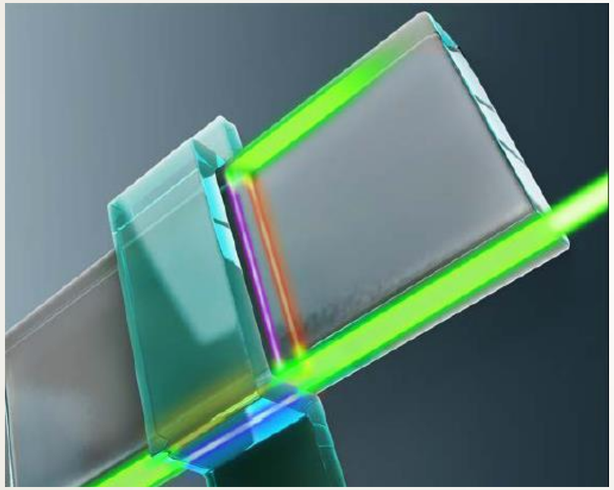
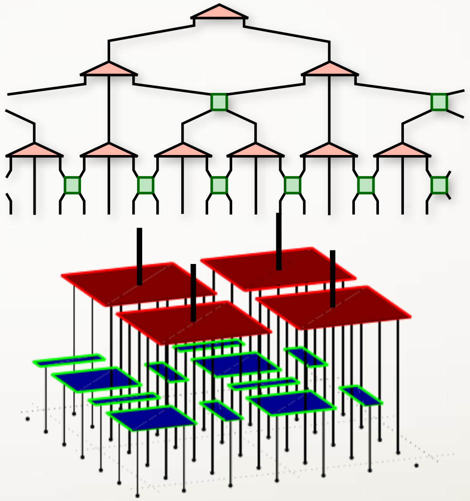
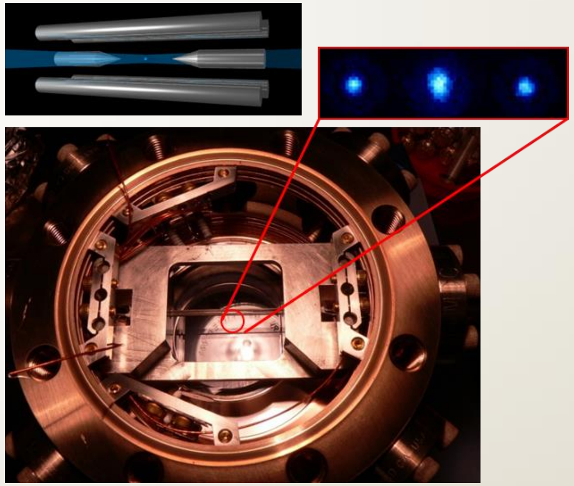


Illustration of a topological insulator with a superconducting layer on top for detection of Majorana fermions (colored lines). Once identified and isolated, Majorana fermions could form the basis of qubits. Electrons (green) travel along the edges of the structure. Supported in part by the BES Energy Frontier Research Center (EFRC) program.



Tensor networks are a key theoretical tool for understanding entanglement, topological order, and other aspects of quantum systems. They comprise a broad family of techniques (2D Multi-scale Entanglement Renormalization Ansatz (MERA) shown here).

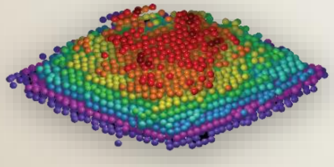


A laser cooled, RF confined ion trap at Argonne National Laboratory: trapped ions can be used as qubits and as quantum simulators.

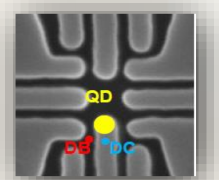
# Fundamental Science That Advances QIS

## Quantum Integration Across Scales

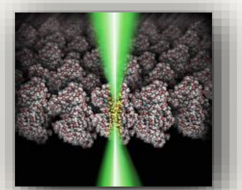
- BES Nanoscale Science Research Centers user facilities are key to the synthesis and characterization of materials and structures from nano-components to prototype-scale quantum systems.
  - Integration and testing couple closely to theory, design, and systems efforts
  - Development and testing of physical models of behavior of quantum devices
  - Co-located with National Lab x-ray, neutron, computing, and microfabrication facilities for understanding and scale-up of quantum structures
  - Next-generation qubits and sensors



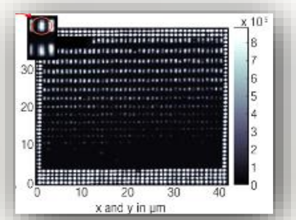
**Sub-atomic Spatial Precision**




**Solid State Artificial Atoms**



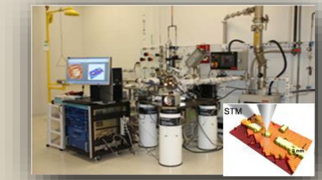
**Single-nm lithography**



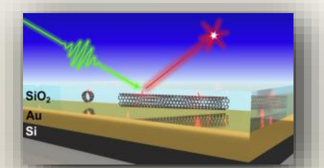

**Entangled Qubit Arrays**

**Quantum-Limited Sensors**

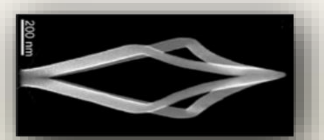
**Quantum Chip Testing**



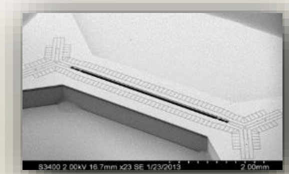

**Atomic Precision Fabrication**




**Single Photon Emitters and Detectors**




**Nanoscale 3D Printing**



**Waveguides, Cavities, Traps**

Nano — Meso — Micro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# Tools, Equipment, Instrumentation

## Quantum Computing Hardware

ASCR's Testbeds Program:
- Research into device architectures and system integration optimized for science applications
- Development of hybrid platforms and quantum/classical coprocessors
- Early access to new quantum computing hardware for the research community

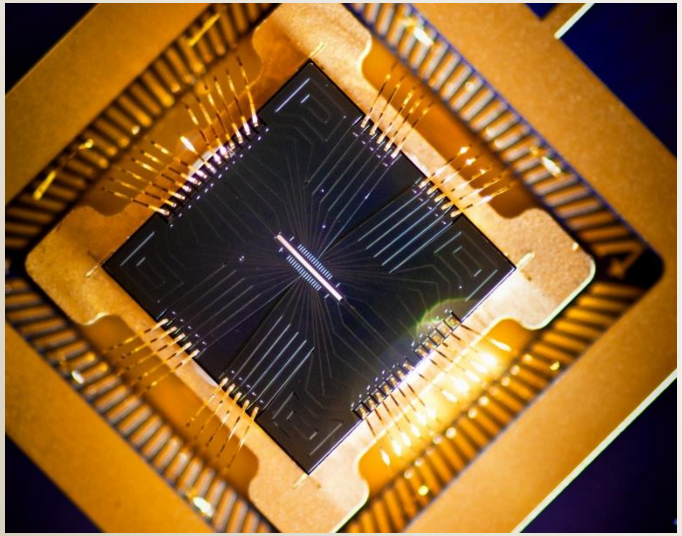
## Tool R&D for QIS

- Extensive nanoscience tools for quantum structure synthesis and integration
- Detectors and metrology
- Quantum sensors enabling precision measurements
- Quantum computational tools
- Superconducting RF cavities, laser cooling, neutral ion traps, spin manipulation technology, and isotope production

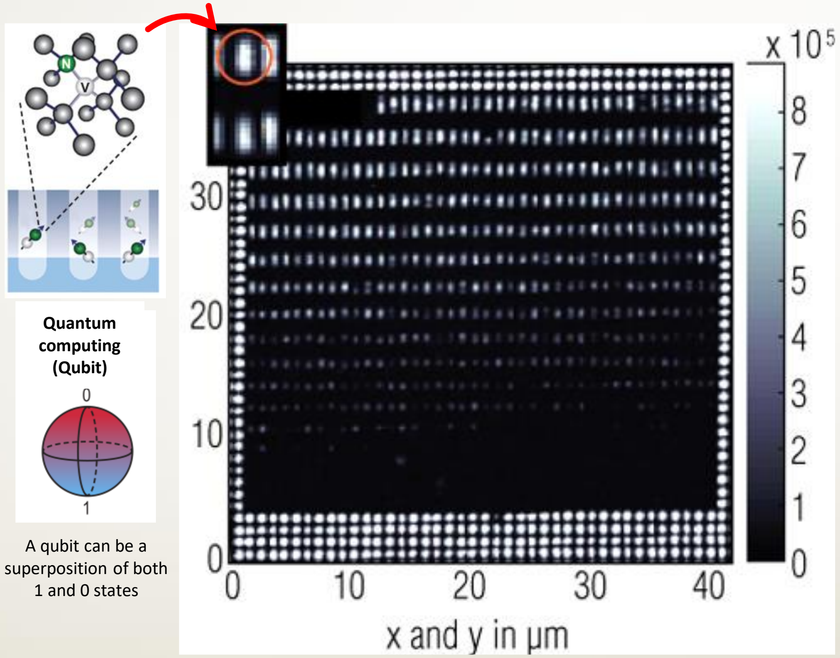
**Key DOE-SC Contributions:**
- Well-established co-design practices in computer hardware development
- Experience in collaborations with industry and core competencies in delivering major projects involving equipment, tools, and instrumentation for discovery and implementation
- Demonstrated success in generating leading scientific tools with and for the international user community

# Tools, Equipment, Instrumentation

DOE SC programs and DOE National Laboratories embody a wealth of knowledge and experience in key technologies to provide mechanisms to enable precision quantum sensors, quantum computing, and development of quantum analog simulators.



*Fabrication of high-performance surface ion trap chips for quantum computation is a unique capability developed at Sandia National Laboratories.*




*(Top left) A graphical representation of nitrogen vacancy (NV) qubits fabricated within diamond. (Right) These NVs were made in precise, dense arrays (μm = micrometers) for future quantum computers. Work performed in part by MIT users at an NSRC.*


*Development of advanced superconducting radio frequency (SRF) cavities (as shown above from FNAL), cryogenics, and other technologies supporting development of qubits, their ensembles, quantum sensors, and quantum controls across DOE National Labs.*

# DOE Community Resources

## World-Class National Laboratory resources

- Advanced fabrication capabilities, (e.g. Microsystems & Engineering Sciences Applications (MESA) facility at SNL)
- Specialized synthesis and characterization capabilities (e.g. Enriched Stable Isotope Prototype production plant)
- Internal research computing capabilities, experimental equipment, and prototypes (e.g. D-Wave)
- Engineered physical spaces (e.g. EM-shielded rooms, low-vibration chambers, deep shafts)

## Focused programs and intellectual property

- Internships and visiting programs for students and faculty
- National Laboratory technical assistance programs
- Access to intellectual property developed at National Laboratories via technology licensing agreements
- Early Career Research Program
- Small Business Innovation Research
- Computational Science Graduate Fellowship

## User Facilities include:

Synchrotron and x-ray free electron laser light sources

Observational and communications networks

Nanoscale Science Research Centers


High Performance Computing and Network

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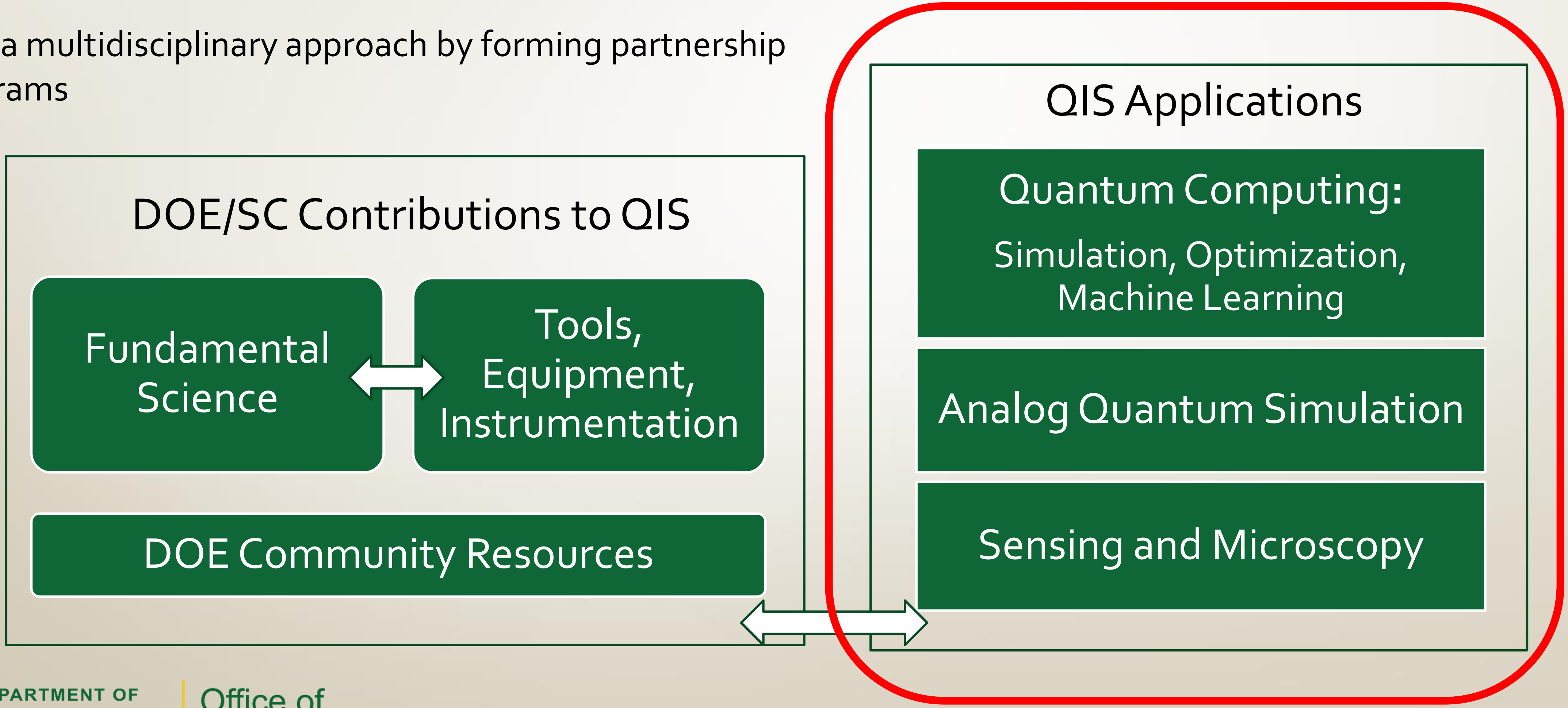
# QIS Applications for DOE/SC Mission

- ✓ Target mission-focused grand challenge problems
- ✓ Application requirements guide DOE/SC contributions to QIS
- ✓ Take a multidisciplinary approach by forming partnership programs



# Quantum Computing Applications for SC Grand Challenges

Simulation of quantum many body systems for materials discovery, chemical processes, and nuclear matter equation of state

Simulations of quantum field theory and quantum dynamics

Machine learning for large data sets and inverse molecular design

Optimization for prediction of biological systems such as protein folding

**Transformative Impact Through Partnership Programs among ASCR, BER, BES, HEP, NP**

Algorithms, Software Tools, and Testbeds

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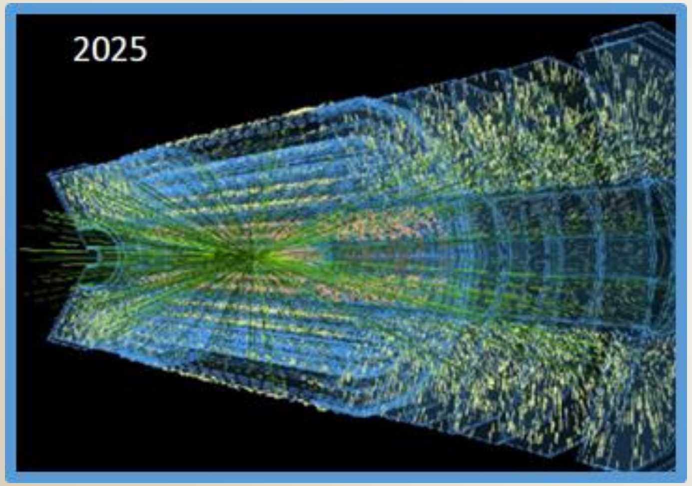
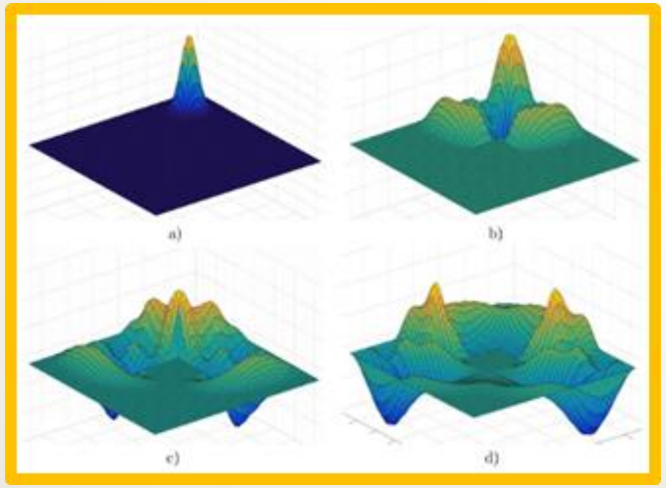
# Some SC Ongoing Efforts on Quantum Computing Applications

## SC Pilot Projects




Quantum annealing for machine learning to separate signal/background in Higgs data from the Large Hadron Collider (*HEP/Caltech-FNAL*)




Simulated particle scattering off a complex boundary condition by quantum algorithms *(HEP-ASCR Pilot/U Maryland)*

## ASCR Programs

**Quantum Algorithm Teams (QATs)**
Aims to stimulate early investigations of quantum simulation and machine learning algorithms by focusing on key topics of research with relevance to problems of interest to SC. In FY17, 3 interdisciplinary teams led by LBNL, ORNL, and SNL were funded.

**Quantum Testbed Pathfinder**
Aims to initiate an exploration of the suitability of various implementations of quantum computing hardware for science applications. In FY17, 2 teams led by LBNL and ORNL were funded.

# Quantum Algorithm Teams (QATs)

**Purpose:** To stimulate early investigations of quantum simulation and machine learning algorithms by focusing on key topics of research with relevance to problems of interest to SC

**Emphasis:** Interdisciplinary teams of QIS experts, applied mathematicians and computer scientists that target specific application areas for quantum computing and analog quantum simulation

**Timeline & Proposals:** A DOE National Laboratory Announcement was issued in May 2017. 13 highly competitive proposals were received in July 2017.

**3 Projects @ Total $4M/year:**

Quantum Algorithms, Mathematics and Compilation Tools for Chemical Sciences. Lead: LBNL (Bert de Jong), Collaborators: ANL (Stefan Wild), Harvard University (Alán Aspuru-Guzik);

Heterogeneous Digital-Analog Quantum Dynamics Simulations. Lead: ORNL (Pavel Lougovski), Collaborator: University of Washington (Martin Savage);

Quantum Algorithms from the Interplay of Simulation, Optimization, and Machine Learning. Lead: SNL (Ojas Parekh), Collaborators: LANL (Rolando Somma), California Institute of Technology (John Preskill), University of Maryland (Andrew Childs), Virginia Commonwealth University (Sevag Gharibian)

# Quantum Testbed Pathfinder

**Purpose:** To provide decision support for future investments in quantum computing (QC) hardware and increase both breadth and depth of expertise in QC hardware in the DOE community

**Emphasis:** Research in the relationship between device architecture and application performance, including development of meaningful metrics for evaluating device performance

**Timeline & Proposals:** A DOE National Laboratory Announcement was issued in June 2017. 6 proposals were received in July 2017.

**2 Awards:**

Advanced Quantum-Enabled Simulation (LBNL, LLNL, UC Berkeley)

Methods and Interfaces for Quantum Acceleration of Scientific Applications (ORNL, IBM, IonQ, Georgia Tech)

# Analog Quantum Simulation

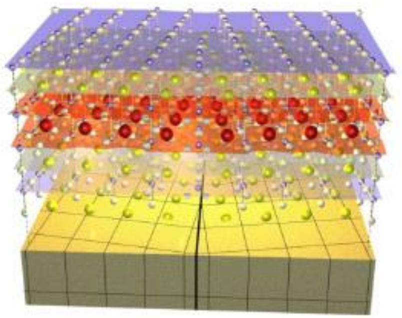
Simulation of many-body systems (e.g. quantum chemistry, physics of neutron stars,…)

**High Impact on Targeted Challenges Through Partnerships Among ASCR, BES, HEP, NP**

Theory, Testbeds, Verification and Validation, Algorithms

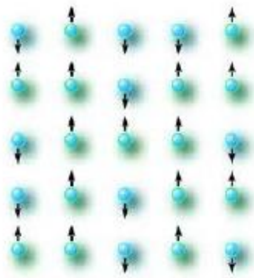
Modeling an experimental system that simulates another quantum physical system

PHYSICAL SYSTEM



(Phenomenological) Hamiltonian

QUANTUM SIMULATOR



Physical Hamiltonian

Example: Hubbard model in 2D: $H = -t\sum_{<ij>,\sigma} c_{i\sigma}^{+} c_{j\sigma} + h.c. + V\sum_i n_{i\uparrow} n_{i\downarrow}$

Offers an approach to problems that are not tractable via classical computing

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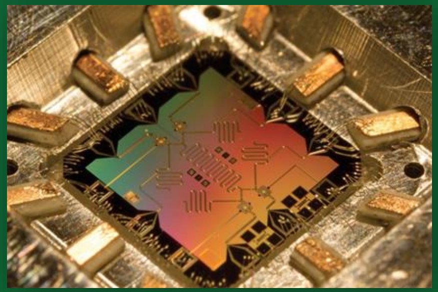
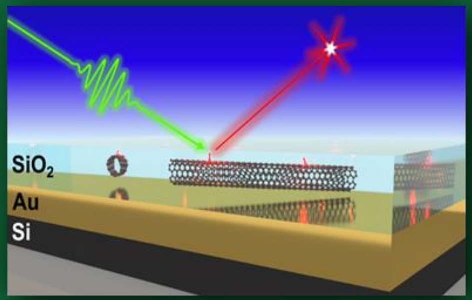
# Sensing and Microscopy



Superconducting qubit sensors for x-ray spectroscopy. As sensors improve, single-photon detection may become possible at far infrared and microwave wavelengths.

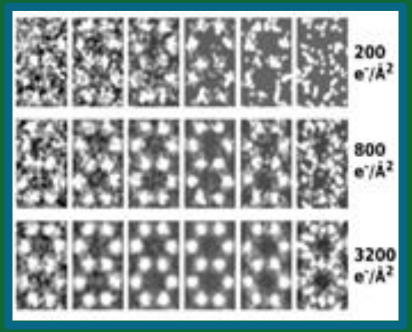
Nanostructured single photon emitters and detectors could be integrated for sensing, communications, and computing systems at room temperature.




## Cross-Cutting Applications in BER, BES, HEP, NP

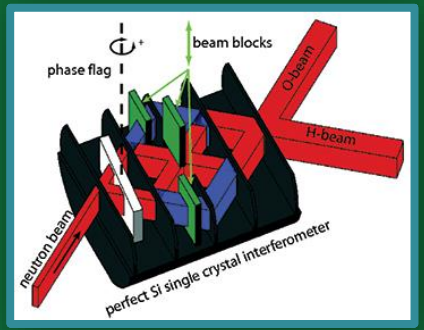
Quantum sensors to perform dynamic, non-invasive visualization of subcellular biological processes

Quantum devices for environmental sensing in field settings for integrating multi-model and multi-scale data (e.g. quantum lidar)




Quantum electron microscope for high resolution at very low doses for imaging of sensitive materials

Single photon detectors can expand the range of discovery for dark universe, non-Newtonian gravity, and new forces.
Quantum error correction reduces noise in matter wave interferometry for such searches.



# SC's QIS Strategy Builds On Community Engagement

- ASCR Quantum Computing Discussion, January 15, 2014, Germantown MD
- LANL Workshop on Materials Opportunities for Quantum Computing, October 7-8, 2014, Los Alamos NM
- ASCR-HEP Study Group: Grand Challenges at the Interface of QIS, Particle Physics, and Computing, December 11, 2014, Germantown MD
- BES-HEP Roundtable: Common Problems in Condensed Matter and High Energy Physics, February 2, 2015, Germantown MD
- ASCR Workshop on Quantum Computing in Scientific Applications, February 17-18, 2015, Bethesda MD
- BES Basic Research Needs on Quantum Materials for Energy Relevant Technology, February 8-10, 2016, Gaithersburg MD
- ASCR-HEP Quantum Sensors at the Intersections of Fundamental Science, QIS & Computing, February 25, 2016, Gaithersburg MD
- Computing Beyond 2025, August 15-16, 2016, Chicago IL
- ASCR Quantum Testbeds Study Group, August 23, 2016, Germantown MD
- The 1st International Workshop on Post-Moore Era Supercomputing (PMES), November 14, 2016, Salt Lake City UT
- LBNL Workshop on Quantum Simulations 101, January 11, 2017, Berkeley CA

# Community Engagement Continues

- ASCR Quantum Testbed Stakeholder Workshop, February 14-17, 2017, Washington DC
- ASCR Extreme Heterogeneity Summit, June 8-9, 2017, Germantown MD
- Workshop on Computational Complexity and High Energy Physics, July 31-August 2, 2017, College Park MD
- BES Roundtable Discussion on Opportunities for Basic Research for Next-Generation Quantum Systems, October 30-31, 2017, Gaithersburg MD
- BES Roundtable Discussion on Opportunities for Quantum Computing in Chemical and Materials Sciences, October 31 – November 1, 2017, Gaithersburg MD
- INT Workshop on Quantum Computing, Seattle, November 14-15, 2017
- The 2nd International Workshop on Post Moore's Era Supercomputing (PMES), November 13, 2017, Denver CO
- FNAL Workshop on Near-term Applications of Quantum Computing for High Energy Physics, December 6-7 2017, Batavia IL
- ANL Workshop on Quantum Sensors for High Energy Physics, December 12-14, 2017, Argonne IL
- NSF/DOE Quantum Science School, 2017-2020
- **DOE/SC co-chairs Quantum Information Science Interagency Working Group**