SPOTLIGHT

Quantum Information Science and Technology

August 2020

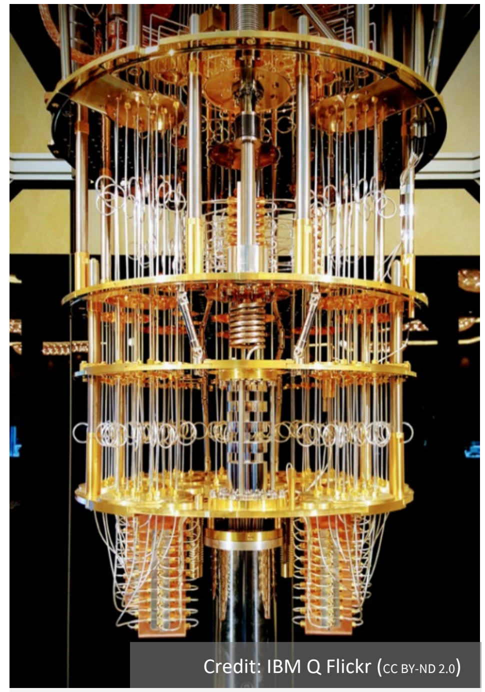
U.S. DEPARTMENT OF ENERGY | *Office of* TECHNOLOGY TRANSITIONS
energy.gov/technologytransitions

Building the Quantum Economy

The term “quantum physics” was coined in 1931 by Max Planck. Since then, quantum physics has significantly enriched our understanding of the atom and transformed modern life—enabling groundbreaking advancements in products like computers, smart phones, and medical devices. Researchers and developers now working in the field of quantum information science and technology (QIST) are leveraging quantum properties and behavior to vastly expand or create entirely new capabilities in computing, sensing, and communications. QIST has the potential to transform our technological landscape through developments such as new sensors for biotechnology and defense; next-generation positioning, navigation, and timing systems; new approaches to understanding materials, chemistry, and even gravity through quantum information theory; novel algorithms for machine learning and optimization; and new cyber security systems including quantum-resistant cryptography.

A robust quantum economy will evolve as these technologies advance and scale up. On the supply side, an economy based around the research and development (R&D), materials, manufacturing, and QIST devices themselves will form. This market is projected to reach $18 billion by 2024.[1] As a result of this development, sectors such as energy, finance, encryption, and many more will be forever changed by QIST advancement.

U.S. stakeholders from academia, industry, and government recognize the need for the United States to cement itself as a technology leader in the coming quantum economy. Our national investments in quantum technology must keep pace with those of other countries to secure a significant share of future markets and the associated economic opportunities.



Credit: IBM Q Flickr (CC BY-ND 2.0)

The End of Moore’s Law

In 1965, Intel co-founder Gordon Moore observed that the number of transistors per square inch in a microchip was doubling each year while costs were cut by half. In the past several decades transistors have become smaller and at the same time computing power has grown, but we are now approaching the physical size limit for transistors. To enable continued growth in computing capability, a fundamentally new way to process information is required, and that’s where quantum computing comes in.

Contents

[1] ResearchandMarkets, *Quantum Technology Market*, researchandmarkets.com/reports/4825350/quantum-technology-market-computing

Sectors of a Quantum Economy

The private and public sectors have invested heavily in building the foundations for our quantum economy. The private sector has seen rapid development in recent years, with over 150 start-ups working in the QIST field.[2] In alignment with national priorities (page 9), the U.S. Department of Energy (DOE) has committed over $1 billion to the advancement of QIST through the establishment of new R&D projects, technology testbeds, and research centers . Within DOE, the Office of Science has launched an initiative to explore four major areas of quantum potential: [3]

- **Computing.** Utilizing the property of entanglement, quantum computers promise an exponential increase in computing power compared to traditional systems.
- **Communication.** QIST can be used in the future to apply secure encryption to communications.
- **Sensing.** Extremely sensitive quantum sensors will vastly improve imaging and broaden applications across disciplines.
- **Foundational Science.** Increased understanding of quantum properties and mechanisms to harness quantum behavior will pave the way toward the applications mentioned above—and more.

Early Adopters of QIST

Cryptology – Quantum technologies can theoretically provide secure information exchange. Because data in a quantum state changes when it is read, any attempt to intercept information will be immediately detected.

Quantum Chemistry – Quantum systems can exponentially speed up the modeling of molecule-to-molecule interactions. Quantum chemistry will have some of its greatest impacts in fields like drug discovery and material science.

Quantum Sensing – Continued improvements will allow precise detection of magnetic fields, gravitational fields, microwaves, dark matter, and earth tremors, increasing our scientific understanding of the physical world.

Long-term Adopters Within the Quantum Economy

System and Network Optimization (Logistics) – Logistics involves the coordination of complex operations involving people, places, and things. Quantum computing can exponentially improve efforts to optimize logistics.

Grid Interoperability – Use of quantum encryption over long distances is a significant challenge. Solving this issue can ensure that utilities nationwide can securely remain in sync while integrating flow across distributed facilities and devices.

Machine Learning (ML) – ML is a branch of artificial intelligence that enables computers to learn from data to predict outcomes and support decision making. Quantum computing can improve ML by handling increasingly complex datasets.

Financial Models – An increase in computational power will accelerate simulation runs while also allowing financial models to consider more factors. These improvements can improve decision making and reduce overall risk.

Clock and Network Synchronization – While clocks are already remarkably accurate, quantum science can further increase accuracy and drive down costs. Many technologies, like GPS, can benefit from improved clock synchronization.

Environmental Science – Quantum computers can model the climate and enable the discovery of materials and technologies that lower greenhouse gas emissions. In addition, quantum computing can improve weather forecasting.

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[2] "Private/Start Up Companies." Quantum Computing Report. Accessed March 27, 2020. quantumcomputingreport.com/players/privatestartup/
[3] U.S. Department of Energy. "Quantum Information Science." energy.gov/science/initiatives/quantum-information-science

Challenges Facing a Quantum Economy

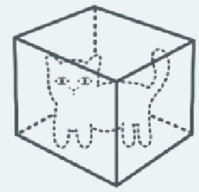
The expected benefits of a robust quantum economy are immense, yet they remain years away. The QIST sector is expected to face major hurdles in four areas, as shown below in different time frames:

Near-Term (1-3 Years)

Gaps in Fundamental Science

Quantum science is still a developing field with existing gaps in knowledge that limit tech-readiness. For example, it is not yet clear which tasks quantum computers will handle better than classical computers. The primitive quantum systems of today need to reduce "noise" in their hardware, scale up, and prove their superiority.

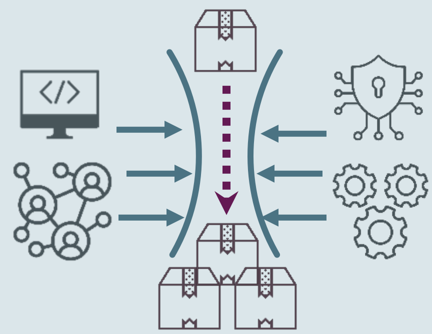
$$i\hbar\frac{\partial}{\,}|\psi(t)\rangle = \widehat{H}|\psi(t)\rangle$$



Mid-Term (3-10 Years)

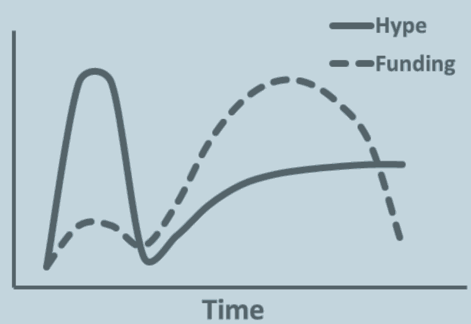
Bottlenecks to Increased Growth

Quantum computers require the development of related software, programming, networking, and security systems, all of which rely on the development of quantum systems. Similarly, scale-up of manufacturing processes is an expected problem as production chains cannot be developed before the technology.



Maintenance of Financial Support

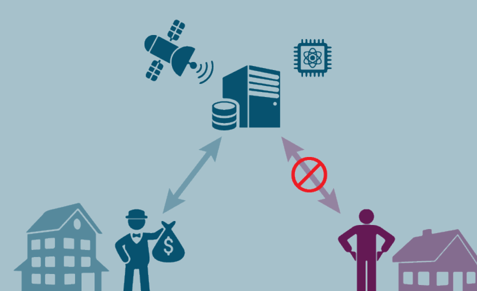
As with any new and developing market, funding levels go through cycles. Upfront hype and public funding often decline into a "valley of death." As time advances, ongoing challenges arise from the uncertainty of government support and hesitance of companies to invest due to a broad landscape of technology choice.



Long-Term (10+ Years)

Long-term Ramifications

Once fully developed, QIST sectors will face several socio-economic and ethical challenges. The complexity and expected cost of systems will mean unequal access by nations and local users. Ethical issues are anticipated as ownership will have to be assigned to the private or public sector, despite funding received from both.

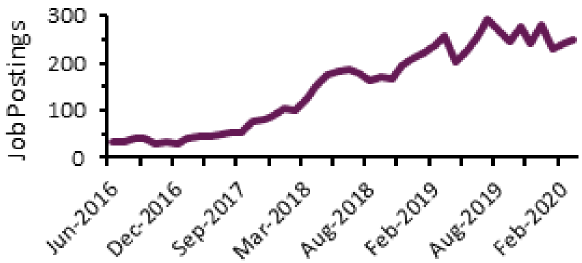


Workforce Development

Workforce is an important consideration in the development of QIST. Current educational systems tend to stress separate academic subjects rather than the multi-disciplinary approach needed to understand and use QIST. The *National Strategic Overview for Quantum Information Science* calls for collaboration among academia, industry, and agencies to promote the development of QIST skill sets.

Current State of Hiring in QIST

The number of new quantum computing jobs has **increased eight-fold** since 2016.[1]



Even with the hiring increase, many companies struggle to find skilled employees.[2]

55% need to provide additional training to new hires

65% find it challenging to hire employees in QIST

DOE's Student Programs:

- Science Undergraduate Laboratory Internships
- Graduate Student Research Program
- Computational Science Graduate Fellowship Program

DOE's National QIS Research Centers:

DOE's Quantum Research Centers are helping to develop the quantum-smart workforce of tomorrow. Through a variety of programs, initiatives, and outreach efforts, each center coordinates with academia, national labs, and industry to educate, train, and engage people at all tiers of the STEM community.

Credit: Andrea Starr | Pacific Northwest National Laboratory

Workforce Development at the DOE National Laboratories

The DOE National Laboratories provide a range of training and education opportunities in science, engineering, and technology. They provide annual programs for over 250,000 K-12 students, 22,000 K-12 educators, 4,000 undergraduates, 3,000 graduate students, and 1,600 postdoctoral researchers. (science.osti.gov/wdts)

The **Northwest Quantum Nexus** works with PNNL to advance QIST training at all levels of education and recently hosted the Northwest Quantum Summit to share views and promote collaboration.

Argonne National Laboratory works in partnership with the **Chicago Quantum Exchange** to facilitate and advance QIS academics at all levels.

The **IBM Q Network** provides training and support to organizations that join the network as a hub, partner, or member. LANL and ORNL are two of the ten existing hubs.

The **Quantum Computing Summer School Fellowship,** hosted by Los Alamos National Laboratory, provides tutorials in quantum computing and mentorship for participating students. Ten to fifteen students are awarded ten-week fellowships to cover expenses.

The **Quantum Fundamentals, Architecture, and Machines (Q-Farm)**, located at Stanford University, works with SLAC to develop QIST curricula for undergraduate and graduate students, offering fellowships, and hosting research seminars in which students, faculty, and visitors can share their work.

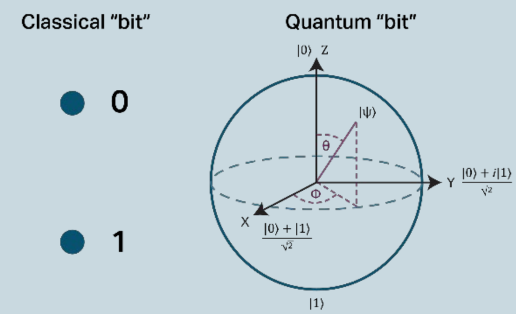
[1] Doug Finke, Managing Editor of The Quantum Computing Report. April 20, 2020.
[2] U.S. Department of Energy. "Building the Quantum Workforce." energy.gov/articles/building-quantum-workforce-0

State of Quantum Computing

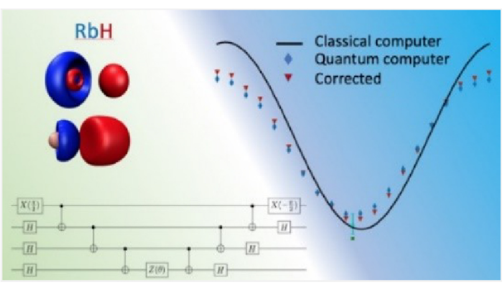
Quantum computing uses the laws of quantum mechanics and quantum behavior to solve problems that cannot realistically be solved using classical computers. Achieving and validating this computing capability will establish “quantum advantage.” The prospect of quantum advantage motivates many organizations to pursue “universal quantum computing,” in which large fault-tolerant quantum computers or hybrid classical/quantum computers will be built and deployed for a wide range of computational tasks. Although the full extent of quantum computing applications is not yet known, the capability will lead to significant advances in medicine, materials development, and national security. Quantum computing is also associated with significant risk; for instance, quantum computers can decipher classically encrypted information, suggesting that the race for quantum capabilities is vital to the privacy of information and our national security.

The Basic Unit of Quantum Computing: The Qubit

While classical computers use bits, a basic unit that has a value of 0 or 1, quantum computers use quantum bits, or qubits. Qubits can exist as multiple states at once, not just 0 or 1. The number of qubits needed varies greatly with the function and type of quantum computer.

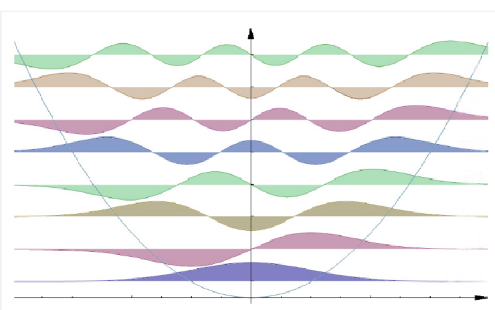


Quantum Simulation Advanced modeling



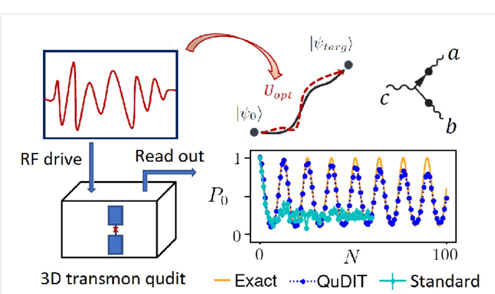
At **Oak Ridge National Lab,** researchers successfully modeled alkali hydride molecules to set a key benchmark for ***modeling chemistry*** on a quantum computer. Calculating the bound state of these molecules is a relatively simple problem for classical computers, but this work will increase understanding of which challenging chemistry problems are best suited to the unique architecture of quantum computing systems.

Picture: molecular orbitals used, schematic of quantum circuit, and results.



At **Fermilab,** researchers in high-energy physics discovered a way to simulate interactions between fermions (particles that are the building blocks of matter) and bosons (force particles that tug on fermions). The binary state of fermions is easy to simulate with qubits, but ***bosons*** can be in any number of occupancy states at once, potentially requiring millions of qubits. Fermilab used harmonic oscillation to represent boson states, exponentially reducing the number of qubits needed.

Picture: wave functions that describe the harmonic oscillator motion.



At **Lawrence Livermore National Laboratory**, researchers discovered and demonstrated an efficient approach for simulating the dynamics of nonlinear three-wave interactions. Simulating these nonlinear processes is an essential part of ***modeling fluids, plasmas, and laser-plasma interactions***. The novel approach used optimized control pulse engineering to improve the achievable gate depth and the overall simulation time by more than an order of magnitude compared to other state-of-the-art approaches to quantum computing.

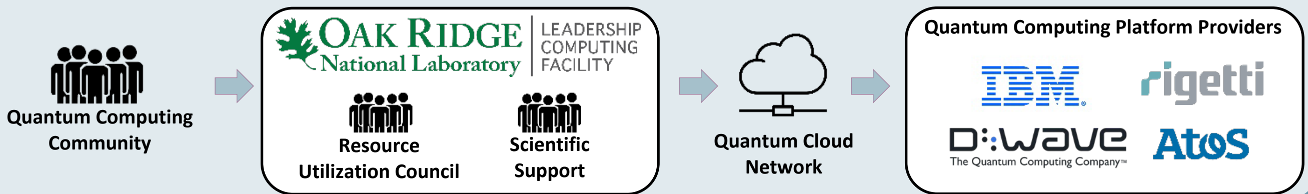
Picture: schematics and results of computing three-wave coupling on quantum hardware.

Different Types of Quantum Computers Available for Use

DOE and its National Labs are leveraging recent progress in QIST, their unique computational resources, and technical expertise to further develop quantum communications, quantum sensing, and other applications. Quantum technologies vary widely, and researchers need broad access to various types—as some are better suited to certain types of challenges. Applications of quantum technologies span diverse purposes, from multi-factor optimization to quantum simulators for developing and testing code.

OLCF Quantum Computer User Program at Oak Ridge National Laboratory

The OLCF Quantum Computing User Program is a DOE user program that enables the public to access quantum computers for testing and evaluation. The program currently supports over 130 users from across industry, academia, and the national laboratories. The growing inventory of available quantum computing systems include devices from IBM, D-Wave, Rigetti, and Atos, which are being used to enable the scientific discovery necessary to support the DOE's mission. olcf.ornl.gov/tag/quantum-computing/

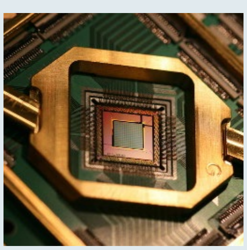


Credit: IBM Q Flickr (CC BY-ND 2.0)

IBM Q Network

The IBM Q Network is a community of Fortune 500 companies, academic institutions, startups, and national research laboratories working with IBM to advance quantum computing. The network provides access to a broad suite of IBM quantum computing systems, development opportunities, and technical support. IBM's technology is a general-purpose, gated system of superconducting qubits. LANL and ORNL (under the OLCF umbrella) operate as IBM Q Hubs or centers for quantum education and research. The IBM Q Network also includes ***Argonne National Lab, Brookhaven National Laboratory, Fermi National Accelerator Laboratory, and Lawrence Berkeley National Laboratory.***

D-Wave Quantum Annealing Computer



Oak Ridge National Laboratory and ***Los Alamos National Laboratory*** both have access to the D-Wave 2000Q System. D-Wave's technology utilizes quantum annealing, a specialized type of quantum computing well suited to solving combinatorial optimization problems, such as those facing autonomous fleets, utility grids, risk assessment, and supply chains.

Atos Quantum Simulator

The Atos Quantum Learning Machine (QLM) is a 30-qubit quantum simulator used by ***Oak Ridge National Laboratory*** and ***Argonne National Laboratory***. The QLM allows scientists to develop and experiment with quantum software. Powered by a powerful dedicated hardware infrastructure, the Atos QLM emulates execution as a quantum computer would.

Quantum Sensing and Communications

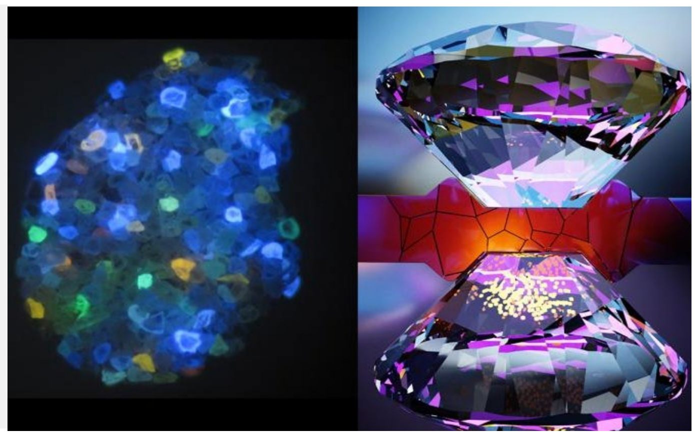
Quantum sensing and communications are highly researched fields within QIST today. Quantum sensing uses the extreme sensitivity of quantum phenomena to detect and measure target properties or signals. Applications range from detecting dark matter to earlier and more accurate prediction of earthquakes. The extraordinary accuracy of quantum sensing has the potential to improve precision in many disciplines.

Quantum communications resides at the intersection of quantum physics and information science, using the quantum properties of quantum objects, such as single and entangled photons, to transmit quantum information. Quantum communications networks can accelerate scientific discovery by linking next-generation quantum technology, such as quantum-based sensors and computers. Quantum Key Distribution, the secure generation of cryptographic keys using the principles of quantum physics, is likely the most well-known among the many applications made possible by quantum communications.

Quantum Sensing and Communications in the National Laboratories

Lawrence Berkeley National Laboratory is using quantum sensing to develop materials with improved strength and magnetism. Scientists used nitrogen-vacancy (NV) centers and atomic defects in the crystal structure of diamonds to explore phases of magnetic matter with submicron precision. Using NV centers imbedded into diamond anvil cells, researchers plan to use their device to explore the magnetic behavior of superconducting hybrid materials, which could transform how energy is stored and transferred.

To learn more visit photonics.com/Articles/Quantum_Sensors_in_Diamond_Anvils_Measure/a65424



SLAC National Accelerator Laboratory is using quantum sensors to increase the sensitivity of a dark matter radio, a highly sensitive radio used to search for axion signals. The dark matter radio detects axions in a manner analogous to how an AM radio detects broadcasted signals. With the use of quantum sensors, SLAC can test a larger sampling of frequencies that are likely to reveal the frequency of axions.

To learn more visit news.stanford.edu/2019/09/25/radio-

Argonne National Laboratory is developing superconducting detectors for particle detection and metrology, engineering defect centers for quantum sensing and communication, and designing and implementing quantum networks.

To learn more visit anl.gov/quantum

Los Alamos National Laboratory is developing methods to expand the range for secure quantum communications. Currently, quantum links are only effective for up to about 100 miles. LANL is connecting links over relay nodes to enable secure communications over longer distances. In addition, LANL is creating a network resilience and analysis tool that supports cost/benefit analyses to guide the placement of quantum links and nodes.

To learn more visit lanl.gov/science/centers/quantum/cryptography.shtml

Lawrence Livermore National Laboratory is investigating techniques that leverage quantum phenomena to achieve multi-photon quantum states that can support ultra-high-resolution sensing and imaging capabilities. These atomic-scale, optical and microwave sensing capabilities are expected to provide control and intrinsic self-calibration for real-time, high-impact applications. New quantum sensing capabilities, such as cold-atom gravity gradiometry and inertial motion sensors, will support LLNL's efforts to address mission-relevant challenges ranging from improved threat detection to GPS-free advanced navigation.

To learn more visit quantum.llnl.gov/

Testbeds at National Labs for Quantum Computing, Communication, and Sensing

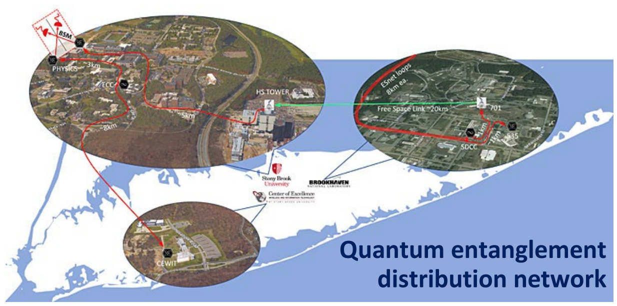
Quantum testbeds throughout national labs and a handful of universities are providing researchers and users with a means of testing various aspects of QIST. The map below shows the locations of current quantum testbeds in use at the national labs.

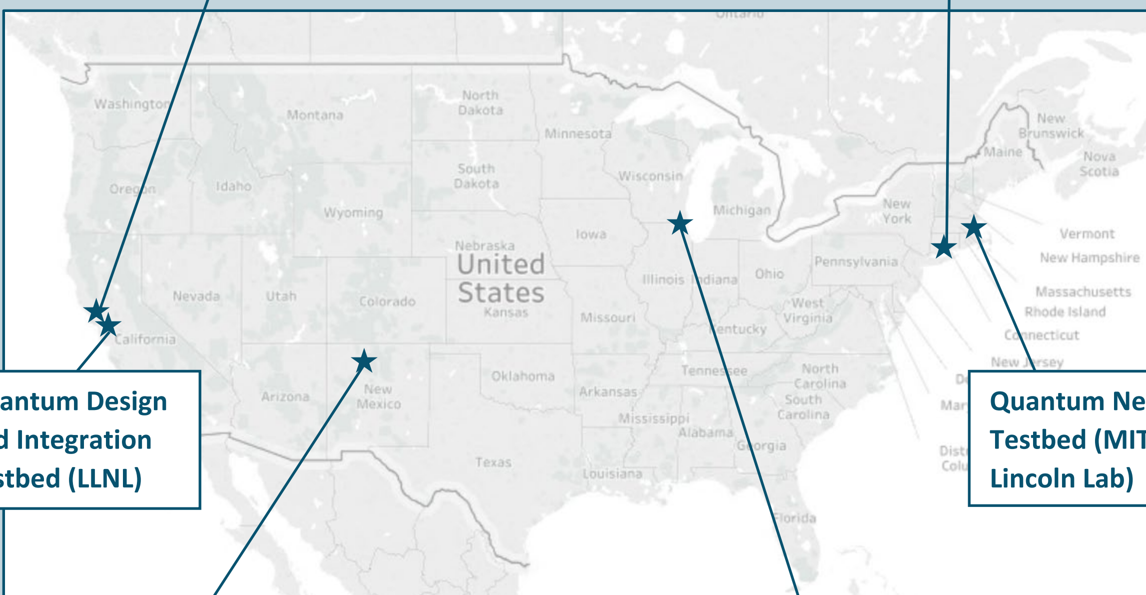
Advanced Quantum Test Bed (LBNL) (AQT)

The AQT was built at LBNL as an open resource for the research community. Researchers recently began testing superconducting architectures and will use the AQT to run simulation experiments in optimization, computation, machine learning, materials science, and high-energy physics.

To learn more visit: [aqt.lbl.gov/](aqt.lbl.gov/)

Quantum Network (BNL and Stony Brook University)





Quantum Design and Integration Testbed (LLNL)

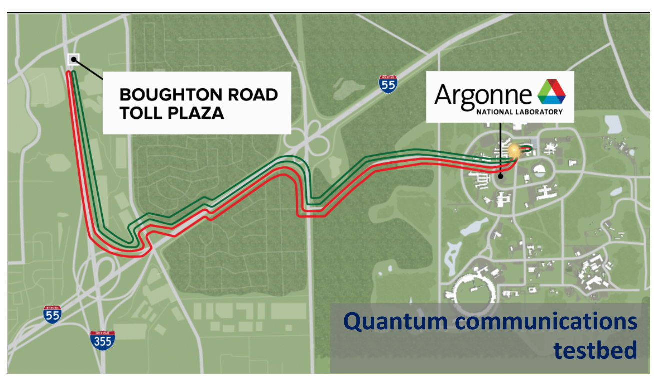
Quantum Network Testbed (MIT Lincoln Lab)

Quantum Scientific Computing Open User Testbed (SNL)

QSCOUT is based on trapped ions and serves the research community. QSCOUT will allow researchers to alter the quantum gates and pulse sequences to explore uses of quantum computing. The testbed will begin operation in steps, starting with a register of three qubits (QSCOUT 1.0). A round of proposals for use of the testbed took place in spring 2020.

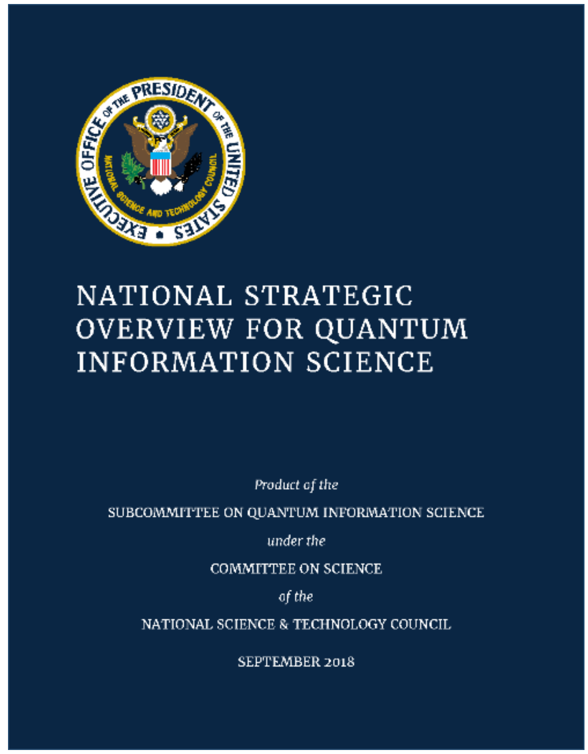
For more information visit: qscout.sandia.gov

Quantum Loop (ANL and University of Chicago)



Quantum Advancement is a National Priority

Research in Quantum Information Science (QIS) lays the foundations for technologies that will strengthen our national security, increase employment opportunities, expand the U.S. industrial base, and produce broad economic benefits. The bipartisan National Quantum Initiative (NQI) Act of 2018 (H.R. 6227) established into law a 10-year plan to support research and training in quantum information science and technology applications.[4]


NATIONAL STRATEGIC OVERVIEW FOR QUANTUM INFORMATION SCIENCE

Product of the
SUBCOMMITTEE ON QUANTUM INFORMATION SCIENCE
under the
COMMITTEE ON SCIENCE
of the
NATIONAL SCIENCE & TECHNOLOGY COUNCIL
SEPTEMBER 2018

The *National Strategic Overview for Quantum Information Science* focuses on six key policy opportunities: [5]

- **Choose a Science-First Approach.** Leading scientific agencies appointed to the Subcommittee on Quantum Information Science (SCQIS) will drive progress by articulating QIS Grand Challenges, formally coordinating federal efforts, fostering communications, and guiding diverse research approaches.
- **Create a Quantum-Smart Workforce.** Preparing a workforce to meet national QIS needs will require active participation by industry, academia, and government. Students will need engagement with QIS at all levels of education, including the potential to pursue Quantum Science and Engineering as its own discipline. Existing programs and novel outreach approaches could help attract additional candidates.
- **Deepen Engagement.** Formation of a U.S. Quantum Consortium will foster cross-sector consensus on R&D priorities, IP issues, and tech transfer mechanisms to increase awareness, funding, and joint partnerships.
- **Provide Critical Infrastructure.** Identifying infrastructure needs and pushing for infrastructure investment will aid QIS development. Developing user testbeds and adapting existing infrastructure (e.g., manufacturing facilities) can facilitate quantum technology advancement by all stakeholders.
- **Maintain National Security and Economic Growth.** Clarifying all implications of QIS developments is imperative to minimize risks to national security. Agencies can use mechanisms like the SCQIS to stay informed and effectively balance the risks and benefits of QIS.
- **Advance International Cooperation.** The NQI looks to attract and maintain top talent and expertise, strengthen relationships with trusted industry and government partners, maintain access to international technology, and identify both strengths and gaps of international actors to inform policy.

Strategic Vision for America's Quantum Networks

In February 2020, the White House's National Quantum Coordination Office released this guiding document. The goals of this effort focus on demonstrating foundational technology for quantum networks and working toward a quantum internet.

Document available at whitehouse.gov

[4] IOP Science. "The US National Quantum Initiative." February 22, 2019. iopscience.iop.org/article/10.1088/2058-9565/ab0441

[5] The White House. "National Strategic Overview for Quantum Information Science." September 2018. whitehouse.gov/wp-content/uploads/2018/09/National-Strategic-Overview-for-Quantum-Information-Science.pdf

DOE Funding Opportunities Align with National Interests

The Office of Science is responsible for maintaining DOE's QIST portfolio. Following the release of the *National Strategic Overview for Quantum Information Science,* the Office of Science has announced several funding opportunities to support and advance the needed R&D. Five of the six programs within the Office of Science (shown at right) now manage the resulting QIST projects, which have a total funding potential of $383.9 million. These projects address the following topics:

U.S. DEPARTMENT OF ENERGY | OFFICE OF SCIENCE

Office of Science Programs with QIST Funding Calls

Advanced Scientific Computing Research

Basic Energy Sciences

Fusion Energy Sciences

High Energy Physics

Nuclear Physics

- Materials and Chemistry for Quantum Information Science[6]
- Particle Physics and Fusion Energy Sciences[7]
- Quantum Computing and Networking[8]
- New Algorithms and Software for Quantum Computers[9]
- Interdisciplinary Research in Quantum Information Science and Nuclear Physics[10]
- Other QIS Projects[11]

Research Centers to Support the National Quantum Initiative

In support of the NQI, DOE announced it will invest up to $625 million to develop up to five National QIS Research Centers.[12] Each center will consist of a collaborative, multidisciplinary research team with engagement of academia, industry, and the government. The first competitive solicitation for centers closed on April 17, 2020. Two to five centers are likely to be selected through a peer review of the submitted proposals, with each center expected to operate for up to five years.[13]

[6] energy.gov/articles/department-energy-announces-37-million-materials-and-chemistry-research-quantum-information
[7] energy.gov/articles/department-energy-announces-214-million-quantum-information-science-research
[8] energy.gov/articles/department-energy-announces-607-million-advance-quantum-computing-and-networking
[9] energy.gov/articles/department-energy-provide-40-million-develop-quantum-computing-software
[10] energy.gov/science/articles/funding-department-energy-announces-68-million-research-quantum
[11] energy.gov/articles/department-energy-announces-218-million-quantum-information-science
[12] energy.gov/articles/department-energy-announces-625-million-new-quantum-centers
[13] science.osti.gov/-/media/grants/pdf/foas/2020/SC_FOA_0002253.pdf

DOE Partnerships Advancing QIST

QIST holds exceptional potential to solve long-standing and emerging problems across the U.S. economy. To expedite progress in QIST and achieve needed solutions, DOE has formed strategic partnerships among its program offices and with its laboratories, other federal agencies, industry, and academia.

These collaborative partnerships leverage resources to put quantum information power on a higher trajectory; create secure platforms for sharing very large, high-quality data sets; and pursue successful QIST applications in areas like national security, economics, medicine, and energy. Some partners may leverage DOE resources to create proprietary outcomes of commercial value, while others will advance basic research to sustain America's leadership in science and discovery. Examples of DOE's strategic partnerships are shown below.

NORTHWEST QUANTUM NEXUS

The **Northwest Quantum Nexus** is a coalition of research and industrial organizations in the Pacific Northwest working to advance scalable quantum computing for clean energy and develop the future quantum workforce needed to make the region a hub for quantum technology. Keystone partners are Microsoft, the Pacific Northwest National Laboratory, and the University of Washington.

Learn more at nwquantum.com/

CHICAGO QUANTUM EXCHANGE

The **Chicago Quantum Exchange** (CQE) facilitates information exchange, partnerships, and research on quantum technologies and applications by its members and partners. Led by the University of Chicago, Argonne National Laboratory, Fermi National Accelerator Laboratory, and the University of Illinois, CQE focuses on exploiting the laws of quantum mechanics to develop new devices, materials, and computing techniques.

Learn more at quantum.uchicago.edu/about/

THE quantum information EDGE

The **Quantum Information Edge**, led by LBNL and SNL, is a nationwide alliance of national labs, universities, and industry advancing the frontiers of quantum computing systems to address scientific challenges and maintain U.S. leadership in next-generation information technology. The alliance pursues solutions across a range of technology areas and integrates these efforts to build working quantum computing systems.

Learn more at thequantuminformationedge.org/

QED-C

The **Quantum Economic Development Consortium (QED-C)** was created to grow the quantum industry and supply chain in the U.S with support from NIST. QED-C brings together partners from industry, government, academia, and other areas to identify and address gaps in quantum technology and the quantum workforce.

Learn more at https://quantumconsortium.org/

DOE Leverages Unique Capabilities for QIST

DOE's National Laboratories are harnessing their massive scientific data sets, exceptional computing capacity, and specialized expertise to expedite QIST contributions across research domains. Additionally, the Labs use their advanced facilities, sensing capabilities, and modeling and computational techniques to increase capabilities in QIST and drive transformative breakthroughs.

The National Labs also use their skills in advanced data analytics, algorithm development, and modeling and simulation to help realize the potential of QIST in missions of national importance. These impressive capabilities attract high-value partners from various sectors. The resulting complementary partnerships can provide unparalleled insights and pave the way for game-changing innovations.

National Lab Capabilities in QIST

The National Laboratory System uses its world-class expertise and facilities to conduct basic discovery research, technology development, and demonstration.

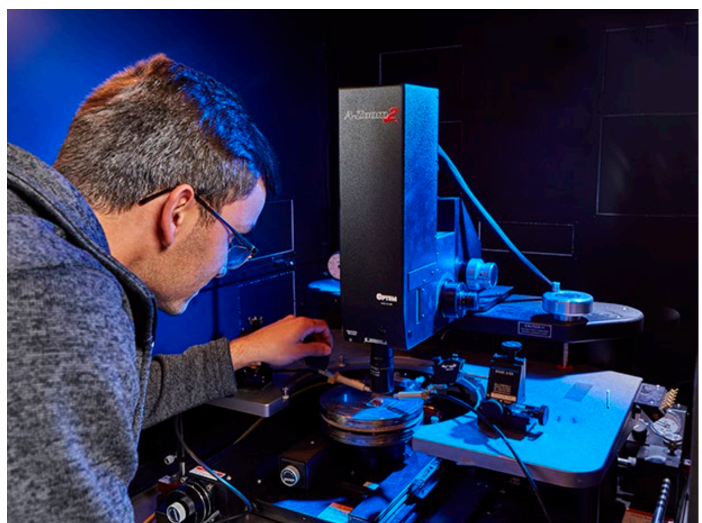
The following National Laboratories hold capabilities in QIST R&D:

- Argonne National Laboratory (ANL)
- Brookhaven National Laboratory (BNL)
- Fermi National Accelerator Laboratory (FNAL)
- Lawrence Berkeley National Laboratory (LBNL)
- Lawrence Livermore National Laboratory (LLNL)
- Los Alamos National Laboratory (LANL)
- National Energy Technology Laboratory (NETL)
- Oak Ridge National Laboratory (ORNL)
- Pacific Northwest National Laboratory (PNNL)
- Sandia National Laboratories (SNL)
- SLAC National Accelerator Laboratory (SLAC)

Examples of Quantum Capabilities at the DOE National Labs

The **Quantum Material Press** is in development at BNL's Center for Functional Nanomaterials. This system will be able to stack atomically thin ("two-dimensional") sheets into structures with unique quantum properties. It's a step towards realizing a vision by partners at MIT and Harvard for a fully automated robotic system that can catalog, store, and combine materials to create new quantum devices.

Learn more at bnl.gov/newsroom/news.php?a=214343



Lawrence Livermore National Laboratory (LLNL) is developing hardware, algorithms, and controls for QIS applications. LLNL scientists are also developing and optimizing materials for fabricating quantum devices and systems, while its Quantum Testbed Pathfinder Program tests new technologies for DOE's Office of Advanced Scientific Computer Research.

Learn more at quantum.llnl.gov/research

Examples of QIST Patents Available for Licensing

DOE funding of the National Laboratories leads to novel technologies that are often patented and later made available for commercial licensing. The following are examples of quantum technologies available for licensing:

Quantum Computing

Ultra-low noise materials and devices for cryogenic superconductors and quantum bits
Lawrence Livermore National Laboratory, US10318880

Semiconductor adiabatic qubits
Sandia National Laboratories, US9530873

Scalable quantum computer architecture with coupled donor-quantum dot qubits
Lawrence Berkeley National Laboratory, US8816325

Quantum coherent devices with reduced energy dissipation
Lawrence Livermore National Laboratory, US10586908

Quantum Communication

Multi-factor authentication using quantum communication
Los Alamos National Laboratory, US9887976

Polarization tracking system for free-space optical communication, including quantum communication
Los Alamos National Laboratory, US9866379

Quantum communications system with integrated photonic devices
Los Alamos National Laboratory, US9819418

Pilot-aided feedforward data recovery in optical coherent communications
Oak Ridge National Laboratory, US9768885

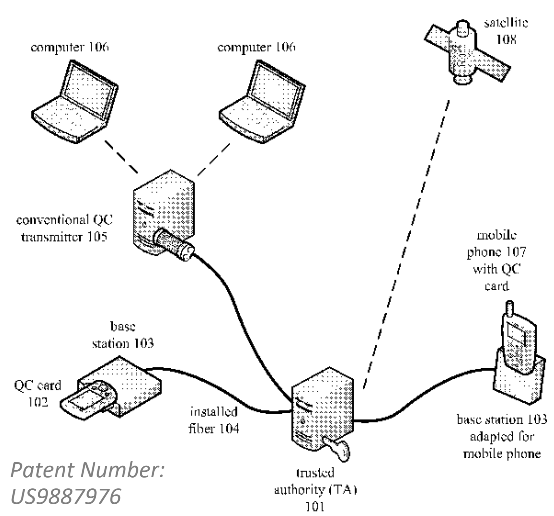
Quantum key distribution using card, base station and trusted authority
Los Alamos National Laboratory, US9680641

Great circle solution to polarization-based quantum communication (QC) in optical fiber
Los Alamos National Laboratory, US9287994

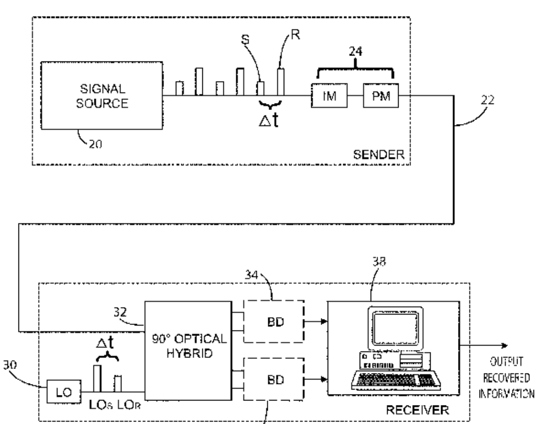
Laboratory Partnering Service (LPS)

LPS is an online platform managed by the Office of Technology Transitions (OTT) to provide public access to world-class DOE energy experts, facilities, and licensing opportunities at the National Laboratories.

For additional and up-to-date information on all available DOE technologies, please visit labpartnering.org/



Patent Number: US9887976



Patent Number: US9768885

Learn More

Organizations can select from among several mechanisms to partner on research with the DOE National Laboratories or to access specialized Lab facilities, capabilities, and expertise (Page 12).

OTT engages with stakeholders, collects partnership data, and raises awareness on the benefits of partnering with DOE. OTT works to expand the commercial impacts of the DOE R&D investment portfolio and highlight the successes achieved by DOE's public-private partnerships.

Contact OTT to learn how to access technical experts, acquire the latest reports, identify promising energy projects, and locate DOE-funded technologies.

Email: OfficeofTechnologyTransitions@hq.doe.gov

Website: energy.gov/technologytransitions/

InnovationXLab^{SM} Summits

DOE invests more than $10 billion each year in the 17 National Labs. The InnovationXLab^{SM} series of meetings is designed to expand the commercial benefits of this investment.

Each summit facilitates the exchange of ideas and information among industry, investors, National Lab researchers, and DOE program managers. The objectives of the summits are as follows:

1) **Catalyze** public-private partnerships and commercial hand-offs utilizing DOE's extensive Lab assets: technology, intellectual property, facilities, and world-leading scientists and researchers.
2) **Engage** the private sector to clarify industry's technical needs, risk appetite, and investment criteria—and thereby incorporate "market pull" into DOE's portfolio planning.
3) **Inform** DOE R&D planning to increase commercialization possibilities.

InnovationXLab^{SM} events are not technical workshops. They foster connections among decision makers and open commercialization opportunities.

Energy I-Corps Program

EIC is a training program designed to address the unique challenges in deploying federally funded technologies to advance the economic, energy, and national security interests of the nation. The National Renewable Energy Laboratory leads curriculum development and execution, recruits program instructors and industry mentors, and assembles teams from the following National Labs:

Project teams relevant to quantum computing have yet to be formed. For the latest info on Energy I-Corps project teams visit: energyicorps.energy.gov/

Technology Commercialization Fund

OTT administers the Technology Commercialization Fund (TCF) to help businesses move promising technologies from DOE's National Labs into the marketplace. TCF projects require non-federal funds to match or exceed the federal investment. One current project is relevant to quantum computing: **Development of Cost-Effective Quantum Key Distribution Systems for the U.S. Power Grid.**

For the latest on TCF projects, visit: energy.gov/technologytransitions/services/technology-commercialization-fund

Quantum Information Project Fact Sheets

U.S. Department of Energy

Project Fact Sheets

U.S. DEPARTMENT OF ENERGY

Office of Technology Transitions

The Office of Technology Transitions develops DOE's policy and vision for expanding the commercial impacts of its research investments and streamlines information and access to DOE's National Labs, sites, and facilities to foster partnerships that will move innovations from the labs into the marketplace.

A Molecular Approach to Scalable and Robust Qubits (NREL)

High spin states of triplet pairs in designed molecular systems have potential as qubits that have fast optical initialization and operate at room-temperature.

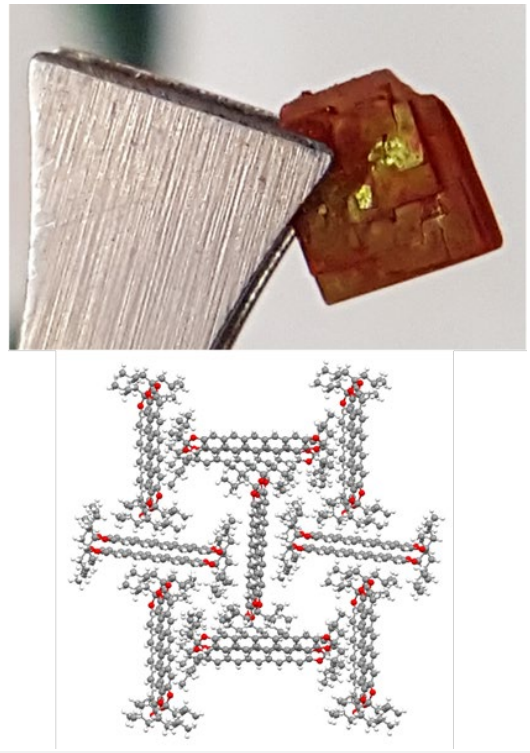
Critical Need

Entangled states lie at the heart of quantum computation, and shining light on certain types of molecules produces such states with high efficiency and unprecedented speed. These states, called "triplet pairs," have the potential for extremely long lifetimes and protection from spin decoherence that exists in other well-known qubit systems. For example, ultralow temperature or vacuum and ultraclean environments are not necessary for production or the potential operation of triplet pairs as qubits. The unknown fate of triplet pairs as the electrons naturally evolve after absorbing light has not been studied in detail but is crucial for directing the electronic states to the most ideal configuration. Molecular design and synthesis are powerful tools for creating the structure/function relationships required to meet the stringent parameters of practical quantum computation.

This project is funded by the U.S. Department of Energy, Basic Energy Sciences through a program supporting quantum information science (QIS) research. The team brings together theory, molecular design and synthesis, advanced spectroscopy, and device fabrication to fully test the original hypothesis of triplet pair qubits. Collaboration with other funded projects (e.g., NSF quantum institute at Colorado School of Mines) has been initiated for pooling of resources and expertise.

Project Innovation

The project utilizes specific triplet pair states called quintets that are amenable to detection and manipulation with magnetic and microwave fields. There are several innovations that advance this concept beyond prior fundamental work: (i) a full theoretical understanding of what drives the quintets into pure spin states with long lifetimes; (ii) synthetic control to produce the ideal intermolecular coupling geometries that are suggested by theory; (iii) advanced and customized instrumentation that enables optical and/or electrical detection of the spin state of the system. These advancements will allow us to further evaluate the potential of these molecular systems as qubits. Given promising results, our next challenge is to create scalable qubit arrays that include communication between triplet pairs that can be modulated so that logic operations can be performed. Much prior work in related fields toward molecular self-assembly and single molecule electronics/optics provides the basis for several intriguing approaches toward this important problem.



Photograph and crystal structure of candidate molecular system for entangled qubit generation through light absorption and singlet fission.

Project Partners

Lead: National Renewable Energy Laboratory

Program office: Office of Science/BES

Partners: University of Colorado-Boulder, Colorado School of Mines, University of Kentucky

Project Snapshot

Start Date & Duration: 10/1/18 – 09/30/21

Budget: $3.9M

QIST Keywords

Primary Keywords: Molecular qubits

Secondary Keywords: Scalable, room temperature, optically addressable

POC Name & Email: Justin Johnson, justin.johnson@nrel.gov

Potential Impact

Although much of the initial work represents the basic science of a unique photophysical phenomenon, we can envision impacts that stretch toward several fields. The primary application is qubit development and engineering, which currently is dominated by complicated and expensive equipment and techniques that leave much room for ease and energy efficiency of operation. We believe that access to molecular material systems with room temperature coherence properties and addressability with photons or electrons will lead to new applications in quantum information science. Besides their potential as qubits, these systems may serve as unique quantum sensors or detectors or may also play roles in other important areas of quantum technologies (e.g., sources of entangled photons). Quantum transduction is an important overall aspect of these systems, and the ability to partner molecules with other known spintronics materials will also be greatly advantageous. Underlying these technological advancements is the knowledge base that will be obtained through careful and thorough investigation of unique molecular systems, which may further broaden the application space beyond what is currently envisioned.

Project Milestones

- Develop theory for of quintet production and calculate parameters to predict spectroscopic splittings between spin states for synthesized and candidate dimers (completed)
- Develop synthesis of structurally defined pentacene dimers with extended bridges (completed)
- Measure spin dynamics via time-resolved electron paramagnetic resonance spectroscopy (completed)
- Further evaluate prospects of extending exciton spin coherence using molecular design (in progress)
- Understand full dynamical scheme of quintets using time-resolved optical spectroscopy (in progress)
- Measure high magnetic field luminescence in crystals to understand triplet pair interactions (in progress)
- Measure magnetoresistance effects in simple thin film device structures (in progress)
- Explore oligomer brush strategies for assembling aligned molecules on electrodes (scheduled)
- Attach triplet pair molecules to layered semiconductors for spin coherence transduction (scheduled)

Facility/Instrumentation Information

The spin resonance facility at the National Renewable Energy Laboratory is being utilized and upgraded for this project. Laser-induced and time-resolved electron paramagnetic resonance (EPR) spectroscopy is the primary tool for detecting the various spin states of the triplet pair. Pulsed microwave techniques are also being developed to measure the coherence time of certain spin states and to detection interactions with other magnetic species, such as nuclei. The ultrafast spectroscopy laboratory is also being used for understanding of the early time dynamics that leads to spin polarization in the target triplet pair states. High magnetic fields and low temperatures are accessed through a Quantum Designs Dynacool system customized with light input/output for detecting the change in fluorescence as resonance is achieved through level crossings of the triplet pairs. Additional functionality is being added through the design and fabrication of microwave resonators that enable tunable fields at a sample that is optically accessible.

Advanced Quantum Testbed at Lawrence Berkeley National Laboratory (LBNL)

Superconducting Quantum Processors at the Entanglement Frontier

Critical Need

The Advanced Quantum Testbed at LBNL (AQT) is part of an ASCR-funded program to deploy NISQ (Noisy Intermediate Scale Quantum) devices for quantum computations and simulations on its superconducting qubit platforms and precision superconducting electronics. The AQT collaborates with research partners to:

- Deploy superconducting qubit platforms and precision superconducting electronics.
- Share basic advancements in algorithms, materials, and measurement.

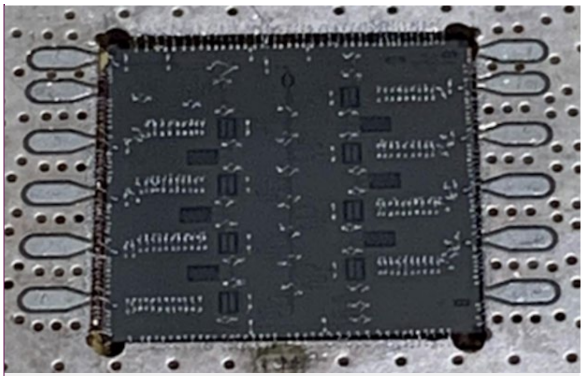
AQT has the following overall goals:

- Driving new ideas in algorithms and quantum hardware.
- Training the next generation of quantum scientists.
- Assembling and deploying quantum technologies for fundamental research.
- Sustaining innovation and development on a long-term horizon.
- Leveraging unique fabrication and packaging resources.
- Leveraging resources for metrology and validation.

Project Innovation

The AQT approach includes three main thrusts: quantum computation, quantum processor development, and the control stack. The three thrusts work synergistically to:

- Design, fabricate, and deploy superconducting qubit processors with varied topology and state-of-the-art gate/readout fidelities and coherence times.
- Enable continuous hardware improvements for both qubits and control circuitry.
- Provide access to users to push the boundaries of circuits to determine quantum capacity, including verification/validation, noise detection, suppression, mitigation, and fault tolerance.
- Extend the frontiers of quantum simulation experiments in optimization, computation, machine learning, materials science, and high-energy physics.



High coherence and high-fidelity eight qubit Quantum Processing Unit

"The AQT enables us to ask and evaluate the basic questions needed to guide the future development of quantum computers. It is an open resource for the community, including industry and academia, and allows researchers to evaluate superconducting architectures developed by testbed staff and collaborators for simulations in chemistry, materials, and other areas."

Irfan Siddiqi, Director of the Advanced Quantum Testbed.

Project Partners

MIT Lincoln Labs, UC Berkeley, Bleximo, Army Research Office (ARO)

Program Office: Office of Science/ASCR

Project Snapshot

Start Date & Duration: Sept 2018-Aug 2022

Budget: $31M

QIST Keywords

Primary Keywords: Quantum Computing, Quantum Processing unit, Quantum Simulation, Quantum Algorithms.

Secondary Keywords: Superconducting Electronics, Quantum Limited Amplifiers, Quantum Benchmarking, Coherence Science

POC Name & Email: Sarah Morgan SRMorgan@lbl.gov

Website: aqt.lbl.gov

Potential Impact

The Advanced Quantum Testbed at LBNL will allow scientists, with urgent problems that can be tackled with quantum computation and simulation, to explore what is possible with early prototype devices. Scientists will be able to:

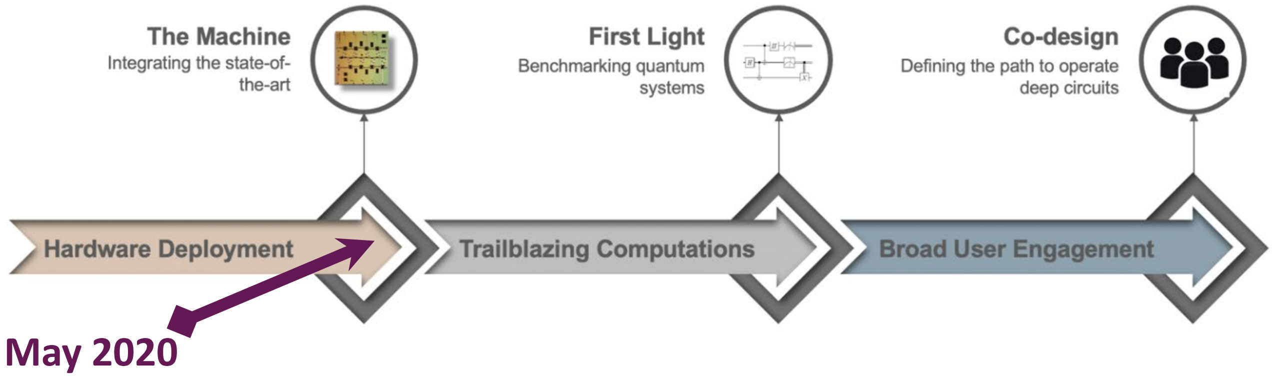
- Implement quantum algorithms of broad scientific interest.
- Execute experiments to verify and validate quantum hardware.
- Investigate noise mechanisms and fidelity loss.

We will partner with scientists in the community to:

- Explore the broad application space of quantum information science and technology.
- Realize computations and simulations that yield verifiable advantage over conventional computers.
- Define the next generation architectures and algorithms via co-design.

Project Milestones

- Co-design and co-fabricate chips at LBNL and MIT-LL: including 8 and 16 qubit, 3D flip-chip style Generation-I LBNL devices; and 5, 9 qubit MIT-LL chips.
- Co-fabricate Generation-III 32 qubit LBNL devices with varying degrees of connectivity.
- Demonstrate reduced error propagation in nearest-neighbor and high-connectivity devices using 3D integration.



Facility/Instrumentation Information

The AQT is collocated near unique nanoscale material characterization and optimization equipment and facilities at the Molecular Foundry. In particular, TEM, XPS, modeling, material treatment and passivation technology available at the Foundry is equal or beyond SOA anywhere in the world. These technologies enable high-coherence and high-fidelity operation quantum devices.

Advanced Software Framework Expedites Quantum-Classical Programming (ORNL)

XACC enables the programming of kernels of quantum code and orchestrates the compilation and execution of that code on currently available quantum processing units, a process that could drastically accelerate future scientific simulations.

Critical Need

To help researchers harness the potential power of quantum processing units (QPUs), which could enhance existing CPU-GPU computer architectures, a team from the Department of Energy's Oak Ridge National Laboratory developed an advanced software framework called XACC.

XACC offloads portions of quantum-classical computing workloads from the host CPU to an attached quantum accelerator, which calculates results and send them back to the original system. The framework uniquely enables the expression and compilation of quantum code in a number of quantum programming languages and dialects, providing an integration mechanism that spans across various research efforts.

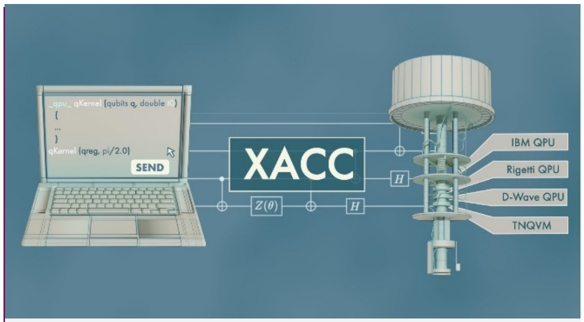
Additionally, this system-level quantum-classical software framework is compatible with any available quantum computer. XACC currently works with quantum computing platforms developed by IBM, Rigetti, D-Wave, and IonQ. The ORNL researchers were the first to build and demonstrate this type of hardware-agnostic software framework for today's quantum computers.

This work was funded by ORNL's Laboratory Directed Research and Development program and DOE's Office of Science.

Project Innovation

XACC promotes a service-oriented software architecture that enables developer extensibility in all aspects of the typical quantum-classical programming, compilation, and execution workflow. Such modularity and extensibility have directly enabled the integration of a diverse set of languages, compiler routines, and backend quantum hardware under a unified framework architecture.

The framework has defined a novel intermediate representation (IR) for compiled quantum programs compatible with a number of quantum computing paradigms, including digital gate, adiabatic, and low-level pulse programming. XACC uncovers routines for lowering quantum programming languages to this IR, as well as for lowering the IR to the native backend instruction set.



XACC integrates quantum computers from a number of vendors. Credit: Michelle Lehman/Oak Ridge National Laboratory, U.S. Dept. of Energy

"At its core, XACC is a way for users to program quantum-classical systems at a level familiar to those in the HPC community."

Alex McCaskey, computer scientist, Oak Ridge National Laboratory

Project Partners

Oak Ridge National Laboratory, Fermi National Accelerator Laboratory, Lawrence Berkeley National Laboratory, Argonne National Laboratory

Program Office: Office of Science

Project Snapshot

Start Date & Duration: Oct. 2016 - Preset

Budget: 2 FTE/year

QIST Keywords

Primary Keywords: Quantum Computing

Secondary Keywords: Quantum Software Development

POC Name & Email: Alex McCaskey mccaskeyaj@ornl.gov

Website: github.com/eclipse/xacc

XACC provides users with additional flexibility by supporting application programming interfaces in C++ and Python, and the team plans to extend this list to include Julia and other popular computer programming languages. These features allow the framework to integrate CPU-QPU processes into small-scale computing applications and large-scale high-performance computing (HPC) workflows.

Researchers have leveraged XACC in a variety of experimental settings in which the framework provided high-level quantum-classical application programming directly applicable to many quantum computers. In previous tests, the team used XACC to program and benchmark quantum chemistry applications by evaluating various molecules. ORNL scientists also used XACC to complete the first successful simulation of an atomic nucleus using a quantum computer.

Potential Impact

XACC represents the only system-level, HPC-friendly quantum programming, compilation, and execution framework. As such, it could potentially have an impact on future integration plans for CPU-GPU-QPU heterogeneous architectures. Its design and implementation are immediately amenable to integration with existing HPC applications, compilers, and parallel runtimes. Anyone can access XACC through the Eclipse Foundation, a major supplier of open-source software, to address scientific problems. Future CPU-GPU-QPU computing architectures could tackle complex workloads that would be unmanageable with current classical systems, potentially enabling new discoveries in fields such as quantum chemistry, nuclear physics, high energy physics, and machine learning.

Project Milestones

- Design of initial XACC quantum-classical workflow service interfaces (completed)
- Implementation of core service interfaces for quantum language parsing, compilation, transformation, and backend execution (completed)
- Demonstration of small-scale physical system simulation on nascent quantum hardware (completed)
- Implementation of core service interfaces for pulse-level, analog programming and execution (completed)
- Development of novel C++ compiler and quantum compiler subroutines leveraging XACC (in-progress)

Facility/Instrumentation Information

Oak Ridge National Laboratory's Computer and Data Environment for Science

Deterministic Synthesis of Quantum Metamaterials (ANL)

Vertically integrated modeling, characterization, and synthesis of quantum metamaterial systems.

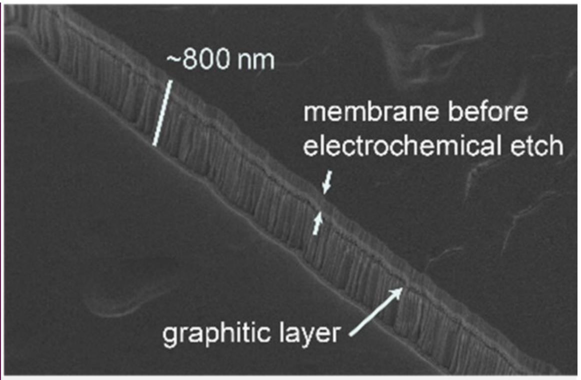
Critical Need

Technologies based on the manipulation of individual charges, spins, photons, and phonons in superconducting and solid-state platforms are key for revolutionary quantum technologies with applications in computation, nanoscale sensing, and communication. While manipulation and detection schemes have been achieved using ever-evolving optical microscopy techniques, complex superconducting circuits, and photonic/photonic sophistry, the inherent fragile nature of these solid-state quantum states provides stringent restrictions on the ability to interface with them. As these systems are fundamentally material-based, these challenges demand relentless progress of fundamental characterization capabilities, material understanding, and synthesis control.

As part of the quantum metamaterials effort, our team combines expertise in creation and control of single electron and nuclear spin states in wide bandgap semiconductors, superconducting quantum circuits, and microwave frequency mechanical systems – all operating and manipulated in the quantum regime. Cutting across these areas will be a focus on optimization and materials synthesis, discovery and integration, and fundamental understanding of materials-based quantum systems.

Project Innovation

This project combines materials growth, defect creation, new materials, and hybrid system integration to form a holistic and deterministic methodology to quantum metamaterials synthesis. Specifically, we combine theory (MICCoM), on-site synthesis of host materials and defects (diamond CVD, nitride PVD and ALD, oxide MBE, etc.), and unique characterization capabilities (Advanced Photon Source, confocal microscopy, X-ray photoelectron spectroscopy, etc.) to provide a vertically integrated approach to quantum information science relevant material systems. This approach aims to optimize the integration of disparate quantum systems, identify new opportunities in QIS applications, and continues to advance the state-of-the-art capabilities and expertise in each of their individual disciples with the ultimate goal of achieving a unified, hybrid quantum coherent system. Such hybrid quantum architectures stand to play a key role in the development of the quantum technologies underpinning the advancement of quantum computing, communication, and sensing.



Diamond membranes (~200 nm thick) for hosting quantum point-defects - made using smart-cut technique and CVD overgrowth.

Project Partners

Argonne National Laboratory and the University of Chicago

Program Office: Office of Science/BES

Project Snapshot

Start Date & Duration: 2017 – Present

Budget: $3.9M

QIST Keywords

Primary Keywords: Quantum Metamaterials, Addressable Quantum States

Secondary Keywords: Material Characterization, Material Synthesis, Material Modeling, Hybrid Systems, Quantum Transduction

POC Name & Email: David Awschalom (awsch@anl.gov); F. Joseph Heremans (heremans@anl.gov)

Website: anl.gov/msd/quantum-information-science

Potential Impact

These homogeneous or hybrid quantum architectures stand to play a key role in the development of the quantum technologies underpinning the advancement of quantum computing, communication, and sensing. These fields stand to benefit from a fundamental understanding of the interplay between qubits and their materials systems. This approach could revolutionize classically restricted technological systems with enhanced or outright revolutionary fundamentally quantum behaviors and properties.

Program Milestones

- Engineered defect spins in isotopically purified environments
- Hybrid quantum systems exploring mechanical control of defect spins in SiC
- Exploration of new transition metal defects in SiC for tailored quantum applications

Facility/Instrumentation Information

Theoretical modeling and computing resources are available through MICCoM. General growth capabilities and nanofabrication of various photonic devices and components is performed at Argonne's Center for Nanoscale Materials (CNM) and UChicago's Pritzker Nanofabrication Facility (PNF). This is in compliment to specialized quantum material growth facilities. CVD reactor(s) at Argonne National Laboratory (ANL) are used for isotopically controlled diamond crystal growth with in-situ doping capabilities. A sputtering tool at ANL is dedicated and optimized for the synthesis of piezoelectric AlN growth. Molecular beam epitaxy facilities at ANL are used for complex, rare-earth doped, quantum relevant oxide growth with atomic layer control. Quantum metamaterials relevant characterization uses a combination of established and emerging facilities. Multiple advanced XRD characterization techniques are performed at and in collaboration with various sectors and beam scientists of the Advanced Photon Source. Broadband Vis-IR confocal microscopy and general material characterization is made possible with collaborative facilities at both Argonne National Laboratory and the Pritzker School of Molecular Engineering (UChicago).

Enabling Chemical Sciences Simulations on Quantum Computers (LBNL)

Quantum algorithms team delivers algorithmic, computational and mathematical advances to enable scientific discovery in chemical sciences on quantum computers.

Critical Need

Chemistry simulations are an early exemplar of quantum computing, demonstrating the potential of various types of quantum devices to aid in scientific discovery in the chemical sciences. Quantum chemistry is ripe for exploring various new types of algorithms that have a potentially broad applicability. The Quantum Algorithms Team (QAT4Chem), led out of Lawrence Berkeley National Laboratory and funded by the Department of Energy Office of Advanced Scientific Computing Research through the Quantum Algorithms Team Program, is an integrated team of quantum algorithm developers, mathematicians, and computer scientists that has been designing and delivering novel algorithms, compiling techniques, scheduling tools, and linear algebra approaches for chemical sciences that has broken new ground in modeling physical processes in chemistry and advanced machine learning on near-term quantum computing platforms.

Project Innovation

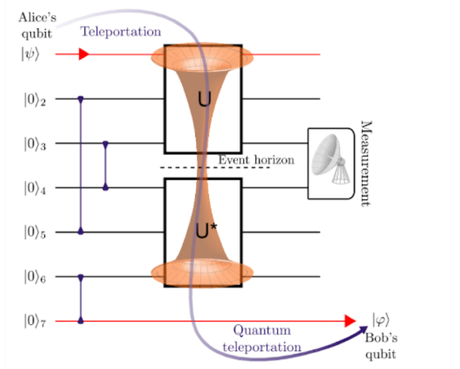
New sparse techniques for algorithms and approaches used in simulating chemical systems were developed that deliver a lower circuit depth [1]. In partnership with NASA, low depth circuits for k-local gates in quantum approximate optimization algorithm (QAOA) and chemistry algorithms were demonstrated.

The efficient generation of thermal states is important for modeling chemical systems. A scheme for engineered thermalization of quantum many-body systems in an analogue quantum system was developed in collaboration with researchers from Sandia National Laboratories.

A simple algorithm was developed to solve the quantum linear system problem (QLSP) with near-optimal complexity [2]. The algorithm does not rely on phase estimation, variable-time amplitude amplification, or in fact any amplitude amplification procedure.

An artificial quantum spiking neuron, inspired by classical neuromorphic computing, was built that relies on encoding the function of the neuron in the time evolution of a small spin-Hamiltonian. An initial demonstration shows the neuron can discriminate between Bell states.

One of quantum computing's largest challenge is handling the errors due to noisy near-term intermediate scale quantum (NISQ) computer hardware. For the first time we show experimentally that error detection codes can enable scientific discovery on NISQ quantum computers, improving the accuracy of an end-to-end chemical simulation of the hydrogen molecule on a quantum computer [3].



First demonstration of verified quantum information scrambling in a quantum system using the protocol developed by Yao and Yoshida in the trapped-ion experiment from the University of Maryland [3].

"Quantum information science will become an increasingly important element of our research enterprise across many disciplines."

Horst Simon,
Berkeley Lab's Deputy for Research,
Lawrence Berkeley National Laboratory

Project Partners

Lawrence Berkeley National Laboratory, Argonne National Laboratory, University of California, Berkeley, University of Toronto

Program Office: Office of Science/ASCR

Project Snapshot

Start Date & Duration: October 1, 2017; 3 years

Budget: $4.5M

QIST Keywords

Primary Keywords: Quantum Computing, Chemistry Algorithms

Secondary Keywords: Machine Learning, Optimizers, Error Mitigation

POC Name & Email: Wibe Albert de Jong
wadejong@lbl.gov

Website: qat4chem.lbl.gov

A partnership between Google and the University of California, Berkeley developed an efficient and noise resilient approach to perform measurements for quantum chemistry simulations on near-term quantum computers. A protocol was developed that can discriminate between decoherence errors and information scrambling, providing a way to verify quantum circuits. This protocol was subsequently validated experimentally on a trapped-ion quantum computer from the University of Maryland [4].

Compilers are used to translate algorithms describing scientific problems of interest to an optimal set of operations to be performed on a classical computer. Computer scientists and applied mathematicians collaborating with quantum information scientists have been delivering key advances in compiling and optimizing quantum computer simulations. A novel scalable circuit synthesis approach using numerical optimization and gradient descent has been developed that is capable of delivering computational quantum circuits that are in some cases are near-optimal and in other cases can drastically reduce the number of operations as compared to other numerical decomposition techniques.

Stochastic classical optimizers that are robust to noise are needed for variational quantum eigensolvers and computational quantum circuit optimization. A large suite of optimizers was tested for robustness and have been packaged and made available as an open-source package for integration in quantum computing software stacks [5]. Multistart optimization approaches were developed that improve the QAOA's ability to solve important graph clustering problems on NISQ computers.

Potential Impact

Our proposed research has the potential for a broad impact across quantum computing and scientific communities. The dynamics and machine learning algorithms developed by the team will immediately enable researchers in chemical sciences and other engineering domains to exploit quantum architectures. These new algorithms will also provide a solid foundation for algorithmic development and exploitation of quantum computers in other research and engineering domains. The successful development of new quantum linear algebra and stochastic optimization approaches by the project will impact quantum and classical computing alike. Finally, our advances in compiler and quantum circuit optimization will be integrated in open-source software frameworks and will benefit all developers of quantum algorithms.

Project Milestones

- Demonstration of developed protocol that verifies quantum information scrambling in a quantum system
- Developed an artificial quantum spiking neuron for machine learning on quantum computers
- Released and validated a large suite of stochastic classical optimizers on github.com/scikit-quant
- Developed and demonstrated new error mitigation approaches on near-term intermediate scale quantum computers
- Design of novel scalable circuit synthesis to find the optimal circuit of an algorithm
- Developed an algorithm that solves the quantum linear system problem with near-optimal complexity

Facility/Instrumentation Information

The development of the algorithms and software tools required the high-performance computing resources of the National Energy Research Scientific Computer Center (NERSC), a DOE User Facility, and collaborating with the Advanced Quantum Testbed. Both facilities are located at Lawrence Berkeley National Laboratory.

[1] J. Lee, W.J. Huggins, M. Head-Gordon, K.B. Whaley. Generalized Unitary Coupled Cluster Wave functions for Quantum Computation, J. Chem. Theory Comput. 15, 311 (2018)

[2] L. Lin, Y. Tong. Optimal quantum eigenstate filtering with application to solving quantum linear systems. arXiv:1910.14596 [quant-ph]

[3] M. Urbanek, B. Nachman, W.A. de Jong. Quantum error detection improves accuracy of chemical calculations on a quantum computer. arXiv:1910.00129 [quant-ph]

[4] K.A. Landsman, C. Figgatt, T. Schuster, N.M. Linke, B. Yoshida, N.Y. Yao, C. Monroe. Verified quantum information scrambling. Nature 567, 61 (2019)

[5] scikit-quant (2020): pypi.org/project/scikit-quant/

Environmental Radiation Could Interfere with Quantum Computers (PNNL)

Experiments show radiation present in the environment limits the performance of current superconducting quantum computers and requires mitigation strategies.

Critical Need

Quantum computers perform calculations by communication among a series of connected qubits, the basic unit of quantum computing. The performance of qubits relies on achieving and maintaining quantum coherence over relatively long periods. Hardware developers must improve quantum coherence times to make quantum computing realistic. Loss of coherence, or decoherence, occurs when qubits change their state unexpectedly. Current causes of quantum decoherence are not well understood, but recent research between Pacific Northwest National Laboratory (PNNL) and the Massachusetts Institute of Technology (MIT), has pointed toward an ultimate performance goal.

Project Innovation

A series of experiments tested the effect of ionizing radiation on the performance of superconductor-based qubits. The research team, including scientists from PNNL and MIT, showed that radiation equivalent to that found naturally in the environment reduces quantum coherence times.1 In the first carefully controlled experiment of its type, the research team used radioactive copper produced at the MIT research reactor to slightly elevate radiation levels a superconducting aluminum transmon qubit. The experiment showed increased quantum decoherence while a complementary experiment showed increased coherence times when similar qubits were shielded from naturally occurring radiation.

The discovery may have long-term impact on the design and construction of quantum computers. It showed that naturally occurring radiation, primarily cosmic rays and trace radioactivity in common building materials, will limit coherence times to a maximum of a few milliseconds. And that maximum might be reached only if the current 100 microsecond limit from still-unknown causes could be removed. Reducing and mitigating the impact of ionizing radiation will be critical for realizing fault-tolerant superconducting quantum computers. In the longer term, quantum computers may need to be located underground, where cosmic radiation is reduced. In addition, radiopure materials with reduced levels of natural radiation-emitting isotopes may eventually be required.

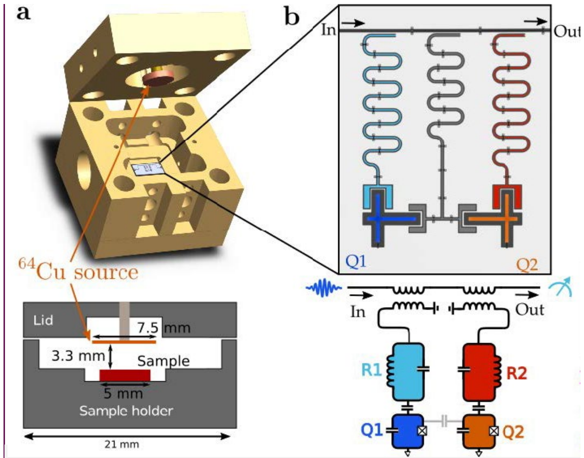


Illustration of the sample holder and the 64Cu radiation source. The copper radiation source is mounted 3.3 mm above the silicon chip containing the superconducting aluminum transmon qubits. b) False-color micrograph and circuit schematic of the qubit sample.

"Reducing and mitigating the impact of ionizing radiation will be critical for realizing fault-tolerant superconducting quantum computers."

Brent VanDevender, Physicist, Pacific Northwest National Laboratory

Project Partners

Pacific Northwest National Laboratory,

Program Office: Office of Nuclear Physics

Project Snapshot

Start Date & Duration: Oct 1, 2018; 1 year

Budget: $110,000

QIST Keywords

Primary Keywords: Physics

Secondary Keywords: Qubit Hardware

POC Name & Email: Brent VanDevender brent.vandevender@pnnl.gov

Website: pnnl.gov

Potential Impact

Reducing or otherwise mitigating the impact of ionizing radiation will be critical for realizing fault-tolerant superconducting quantum computers. The work suggests a potential future in which quantum supercomputing 'farms' are placed in underground facilities to escape from high-energy ionizing cosmic rays. The instruments themselves, cooled to near absolute zero, would reside in specially designed shielding 'tombs' to block the ever present naturally occurring radioactivity in construction materials, such as concrete. These precautions are routinely employed in existing, modern-day deep underground experiments studying the fundamental particles of the universe.

Given existing knowledge and experience in building shielded, low-radiation environments for deep underground science experiments, it would be possible to test relatively quickly the questions raised by these recent research results. Research partnerships among academic institutions, national laboratories, and the private sector would provide the tools, expertise and engineering capabilities to bring a shielded, low-background underground facility for quantum device testing to fruition. An opportunity exists now to pursue a range of facilities from research test beds containing a shielded dilution refrigerator within an existing deep underground science laboratory to the creation of new, dedicated private sector facilities.

Project Milestones

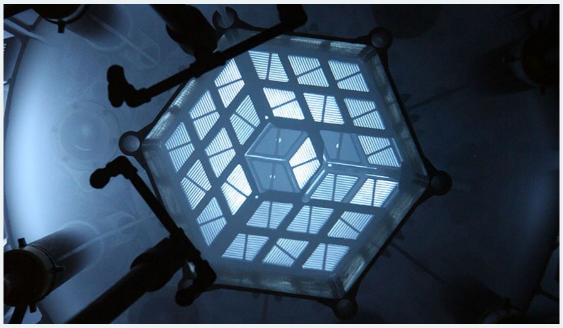
- Demonstration of reduced coherence time correlated with in correlation with elevated radiation levels. (Completed)
- Demonstration of increased coherence time with radiation shielding. (Completed)

The research team performed work at the MIT Reactor. This work was supported in part by the U.S. Department of Energy Office of Nuclear Physics under an initiative in Quantum Information Science research (Contract award # DE496 SC0019295, DUNS: 001425594); by the U.S. Army Research Office (ARO) Grant W911NF-14-1-0682; by the ARO Multi-University Research Initiative W911NF-18-1-0218; by the National Science Foundation Grant PHY-1720311; and by the Assistant Secretary of Defense for Research and Engineering via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002.

Facility/Instrumentation Information

Pacific Northwest National Laboratory possesses unique and world-leading capabilities in low-radioactive-background detection techniques that were critical components to the experiments.

The research reactor and superconducting qubit fabrication facilities at MIT and its Lincoln Lab were equally important.



MIT Research Reactor

[1] Impact of ionizing radiation on superconducting qubit coherence. arxiv.org/pdf/2001.09190.pdf

Experimental Observation of Exceptional Surfaces (ANL)

This work provides a new pathway to engineer non-Hermitian systems and opens up new application opportunities such as robust mode conversion and high-sensitivity sensing.

Critical Need

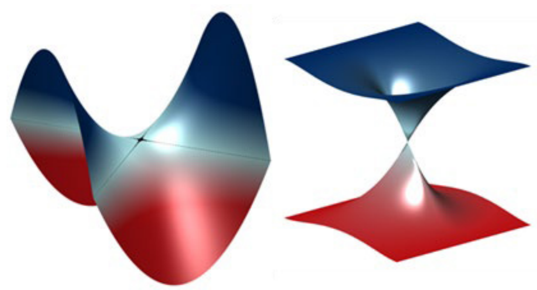
Observation of energy level singularities enters a higher dimension in this work by Zhang et al.[1]. Exceptional points (EPs) are singularities of eigen-energies in a non-Hermitian system that is open to the environment. Intriguing phenomena have been previously observed around EPs, including exceptional sensitivity, unidirectional signal propagation, etc. However, these demonstrations of EPs are limited to zero-dimensional points and one-dimensional lines.

In this work by Zhang et al., an exceptional surface (ES) – a continuous three-dimensional surface of EPs – is experimentally observed for the first time. This is achieved by constructing a four-dimensional synthetic space, taking advantages of the multiple independent tuning knobs of a cavity magnon polariton system. Magnon polaritons are hybrid excitations of electromagnetic waves and spin waves, which have recently emerged as a promising candidate for coherent information processing. The observed ES in the magnon polariton system can further coalesce into an exceptional saddle point in the four-dimensional space, which exhibits novel complex anisotropic behaviors.

This work was performed, in part, at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

Project Innovation

Non-Hermitian physics such as exceptional points have been recently heavily studied in integrated photonics. In this project, the authors demonstrated the great potential of hybrid magnonic systems as a versatile platform for studying non-Hermitian processes. Although hybrid magnonics have been recently widely studied for coherent/quantum information processing, its potential for non-Hermitian physics has been long ignored. In fact, such systems possess large flexibility and tunability, making it convenient to explore non-Hermitian processes especially in high dimensions. This project utilizes the rich tuning mechanisms in hybrid magnonics and constructed a previously unachievable high-dimensional parameter space, leading to the observation of high-dimensional exceptional points and the novel exceptional saddle point.



Left graph plots exceptional point conditions in a three-dimensional parameter space (x, y and z) which forms an exceptional surface, as calculated from experimental measurements at Argonne. Exceptional saddle point marked by X. Right graph plots energy dissipations of the two modes which show anisotropic behavior at the exceptional saddle point (near the intersection of blue and red surfaces.)

"Our work opens up exciting new possibilities for quantum information processing with highly desired functionalities"

Xufeng Zhang, Assistant Scientist, Center for Nanoscale Materials, Argonne National Laboratory

Project Partners

Argonne National Laboratory, Imperial College London, UK

Program Office: Office of Science/BES

Project Snapshot

QIST Keywords

Primary Keywords: Non-Hermitian Quantum Mechanics, Magnon Polaritons

Secondary Keywords: Quantum Sensing, Quantum Transduction

POC Name & Email: Xufeng Zhang, xufeng.zhang@anl.gov

Potential Impact

The demonstration in this project provides a new approach for studying non-Hermitian physics, which will enable a class of novel studies on that topic. In particular, this study bridges hybrid magnonics with non-Hermitian physics, not only pointing out a new direction for studying hybrid magnonics but also providing a new physical platform for non-Hermitian physics. The combination of these two research topics, which both are attracting intensive attention recently, will enable new capabilities such as novel magnon-based signal conversion, magnon exceptional-point sensing, etc.

Project Milestones

- Novel microwave cavity development (completed)
- Non-Hermitian physics study on the novel cavity magnonic platform (completed)

Facility/Instrumentation Information

This project utilized the Magneto-Electro-Optical Spectrometer at the Center for Nanoscale Materials, Argonne National Laboratory, for device characterization.

[i] X. Zhang, K. Ding, X. Zhou, J. Xu, and D. Jin, “Experimental Observation of an Exceptional Surface, in Synthetic Dimensions with Magnon Polaritons.” Physical Review Letters 123, 23702 (2019).

Foundations of the National Quantum Internet (BNL)

Building and scaling quantum communication networks is among the most important technological frontier of the 21st century. Quantum networking, if fully realized, will have large societal impact with a range of applications in national security and science - unconditionally secure communication, distributed quantum computing, ultra-precise measurements, and novel scientific instruments.

"A quantum Internet-of-Things will open up whole new areas of scientific research."

Paul Dabbar,
Undersecretary of Energy for Science

Project Partners

National Labs: BNL, ESnet (LBNL), ORNL, LANL

Program Office: Office of Science and NNSA

Academia: Stony Brook University, New Jersey Institute of Technology

Industry: Qunnect, Inc.

Project Snapshot

QIST Keywords

Primary Keywords: Quantum Internet

Secondary Keywords: Quantum Communication

POC names and E-mails:

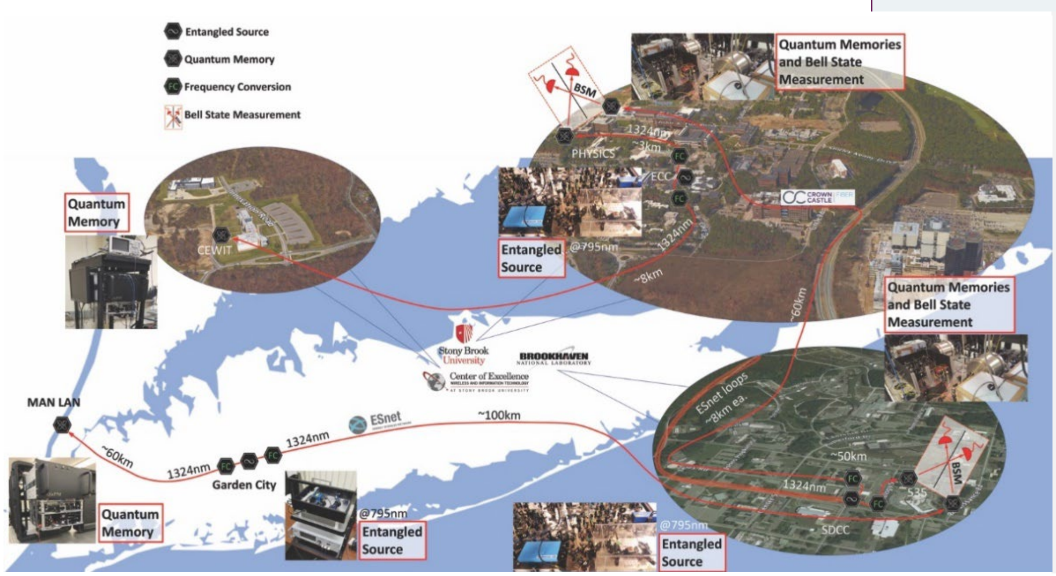
Eden Figueroa - efbarragan@bnl.gov

Gabriella Carini - carini@bnl.gov

Critical Need

By networking a myriad of sensors and processors, the Internet has revolutionized the use and processing of information across the globe. We are now at the cusp of a new revolution: networks that can transfer and process quantum information (qubits), in addition to classical information (bits).

As a consequence, the February 2020 White House document, A Strategic Vision for America's Quantum Networks, notes it is of "paramount national relevance to elevate current U.S. research in this area to the level of worldwide leadership." Brookhaven National Laboratory and Stony Brook University are working collaboratively toward this international leadership by demonstrating groundbreaking quantum networking experiments.



Using room-temperature quantum memories to distribute entanglement over long distances without detrimental losses is one goal of the Long Island Quantum Information Distribution Network, known as LIQuIDNet. This joint effort between Brookhaven Lab, Stony Brook University, and ESnet will help set the stage for a nationwide quantum Internet.

Project Innovation

The quantum internet is composed of many sub-systems: quantum communication hardware, timing systems to synchronize quantum information transmission, and large classical communication components to control long distance quantum nodes.

The team has built and developed several key building blocks for the quantum internet, such as room temperature quantum memories, scalable entanglement sources, and the classical optical control infrastructure [1-3]. These quantum networking technologies have been used to create an integrated, working quantum network testbed on Long Island, N.Y., that produced the longest distance entanglement distribution experiment in the United States in 2019. Recently our collaboration achieved the first intercampus communication of polarization states tuned for quantum memory operation, using a 68 km fiber infrastructure connecting BNL and SBU campuses.

The team has now focused its research efforts on the critical components needed for large-scale long distance quantum communication, such as quantum repeaters. Using room-temperature quantum memories to distribute entanglement over long distances without detrimental losses is one goal of the Long Island Quantum Information Distribution Network, known as LIQuIDNet. This joint effort between Brookhaven Lab, Stony Brook University, and ESnet will help set the stage for a nationwide quantum Internet.

Potential Impact

A nationwide quantum Internet would have transformational impact on science and national security, including:

- Unconditionally secure communications and agreement protocols.
- Ultra-precise sensors, clocks, and long-baseline quantum-enabled telescopes
- Privacy-preserving ("blind quantum") computing to process and transmit critical information.
- Distributed quantum computing built on many small systems connected using quantum network to implement large scale quantum algorithms.

Project Milestones

- Demonstrate long-distance quantum entanglement distribution using in-campus network infrastructure – Completed 2019, 18 km/11 mi. (longest in United States at the time).
- Connect Brookhaven Lab quantum local area network (LAN) with Stony Brook University quantum LAN with single-photon qubit transmission and quantum cryptography capability – lab-to-lab fiber connection is completed (70 km/42 mi.). Creation of entanglement between two quantum memories over 120 km / 80 mi. is in progress.
- Extend entanglement distribution across Long Island to New York City to develop a large quantum communication network infrastructure based upon entanglement swapping that outperforms counterparts found in China and the European Union – vision, groundwork in progress.

Facility/Instrumentation Information

The Quantum Information Technology (QIT) laboratory at Stony Brook has developed room-temperature quantum network prototypes, connecting several quantum memories and qubit sources. Additionally, the Quantum Information Science and Technology (QIST) laboratory at Brookhaven National Laboratory has focused on the development of portable entangled sources and quantum transduction devices [4].

Together, the two labs will allow for the design and implementation of a quantum network prototype that exceeds 100 km in optical fiber [5]. Using quantum memories to enhance entanglement swapping will enable entanglement distribution over long distances without detrimental losses. ESnet and Crown Castle fiber infrastructure already has been used to demonstrate sending custom IR pulses between Brookhaven and Stony Brook campuses. In the near future, this quantum network prototype can be extended to the Manhattan Landing (MANLAN) in New York City, setting the stage for a nationwide quantum-protected information exchange network.

[1] M.Namazi, G. Vallone, B.Jordaan, C. Goham, R.Shahrokhshahi, P. Villoresi and E.Figueroa. Free space quantum communication with quantum memory. Physical Review Applied 8, 064013 (2017).

[2] M.Namazi, C. Kupchak, B.Jordaan, R.Shahrokhshahi, and E.Figueroa. Unconditional polarization qubit quantum memory at room temperature. Physical Review Applied 8, 034023 (2017).

[3] bnl.gov/newsroom/news.php?a=214491

[4] nature.com/articles/s41598-020-62020-z

[5] arxiv.org/abs/1808.07015

Integrated Development Environments for Quantum Computing (LBNL)

Developing and delivering an open-source computing, programming, and simulation environment that supports the large diversity of quantum computing research at DOE

Critical Need

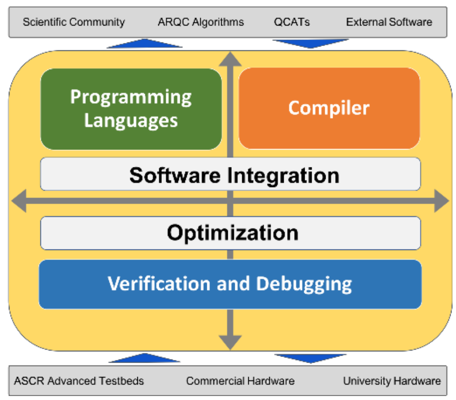
Recent advances in quantum computing have clarified the potential of the technology to accelerate many key science and engineering applications ranging from quantum chemistry and high-energy physics to machine learning. While these demonstrations remain proof-of-principle, there is a growing need to expand the programmability and testability of these devices. This will require more sophisticated research and development software environments to support the integration of critical concepts with the rapidly changing diverse hardware landscape.

The newly funded multi-institutional effort, "Advancing Integrated Development Environments for Quantum Computing through Fundamental Research (AIDE-QC) led out of Lawrence Berkeley National Laboratory (LBNL), will develop and deliver an open-source computing, programming, and simulation environments that support the large diversity of quantum computing research at DOE.

AIDE-QC is funded by the Department of Energy (DOE) Advanced Scientific Computing Research (ASCR) through the Accelerated Research in Quantum Computing program.

Project Innovation

AIDE-QC will address critical aspects of computer science research that accelerate the integration of near-term intermediate-scale quantum (NISQ) devices for scientific exploration. Advances that will be pursued include the development of new and better high-level programming languages accessible by domain scientists, leading-edge platform agnostic compilers supported by fast classical numerical simulators and robust tools for validation, and verification and debugging of simulations run on NISQ quantum hardware. All the software components developed by the different research thrusts of AIDE-QC will be integrated in an open-source and easy-to-use quantum software development environment. Novel error-mitigation techniques for near and mid-term hardware devices will be developed, and next-generation optimization algorithms in service of quantum computing will be integrated across the software stack.



Five thrusts drive our research to program emerging QC platforms and support the broader DOE quantum community.

"Sophisticated software development environments are essential for broad accessibility to quantum computing."

Bert de Jong, Senior Scientist, Lawrence Berkeley National Laboratory

Project Partners

Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory, Sandia National Laboratories, Argonne National Laboratory, Los Alamos National Laboratory, University of California, Berkeley, The University of Chicago

Program Office: Office of Science/ASCR

Project Snapshot

Start Date & Duration: October 1, 2019; 5 years

Budget: $17.5M

QIST Keywords

Primary Keywords: Quantum Software Development Environment

Secondary Keywords: Programming Models, Compilers, Optimizers, Debugging

POC Name & Email: Wibe Albert de Jong
wadejong@lbl.gov

Website: aid-qc.org

Some of the early advances include the extension of the XACC quantum-classical software framework that enables pulse-level programming for superconducting, gate-model quantum computers [1], the release of the first version of QFast, a quantum synthesis tool designed to produce short circuits and to scale well [2], and a novel circuit partition approach to produce optimal circuits on modular quantum computing architectures.

Potential Impact

The open-source software development environment developed by AIDE-QC will be a critical link between the domain scientists and the quantum hardware ecosystem. It will provide a research and simulation environment that will allow scientists from across the DOE complex and beyond to effectively use the immense power of quantum computers in their quest for scientific discovery.

Project Milestones

- Language abstractions enabling expression of algorithms across scientific domains
- Cross-platform compiler with circuit synthesis, resource optimization and analysis tools
- Scalable techniques for verification of results from NISQ platforms
- Development of debugging tools to analyze circuit execution errors
- Next-generation optimization algorithms in service of quantum computing
- Extensible programming, compilation, and hardware-agnostic execution workflow for scientific quantum computing

Facility/Instrumentation Information

We will leverage ASCR's high-performance computing facilities to establish versatile, scalable and accurate numerical simulators in order to provide a state-of-the-art platforms for debugging and testing algorithms and software developed by the research community. During the development of the integrated software development environment, the high-performance computing resources of the National Energy Research Scientific Computer Center (NERSC), a DOE User Facility located at Lawrence Berkeley National Laboratory (LBNL) is utilized. Development of validation and verification will require collaborations with the Advanced Quantum Testbeds at both LBNL and Sandia National Laboratories. In addition, the IBM Q Hub at Oak Ridge National Laboratory will be used for testing, capability demonstration, and benchmarking.

[1] T. Nguyen, A. McCaskey. Enabling Pulse-level Programming, Compilation, and Execution in XACC, arXiv:2003.11971 [quant-ph]

[2] E. Younis, K. Sen, K. Yelick, C. Iancu. QFAST: Quantum Synthesis Using a Hierarchical Continuous Circuit Space. arXiv:2003.04462 [quant-ph]

[3] J.M. Baker, C. Duckering, A. Hoover, F.T. Chong. Time-sliced quantum circuit partitioning for modular architectures. CF '20: Proceedings of the 17th ACM International Conference on Computing Frontiers, 98 (2020)

National Security Applications Drive Quantum Sensor Advances (LLNL)

Lawrence Livermore National Laboratory (LLNL) is working with the private sector to develop and field-test advances in quantum sensing that offer the speed and sensitivity needed for national security and defense applications.

Critical Need

Quantum sensing applications are among the earliest applications of quantum technologies, and LLNL is partnering with U.S. companies to advance development of quantum sensors for national security applications.

Novel quantum technologies are needed to enable fast, highly accurate, real-time analysis applications. Indeed, quantum sensors inherently possess the advantages of high precision, environmental control and isolation, and intrinsic self-calibration.

The precise, high-resolution measurements needed for security can only be achieved using quantum technologies.

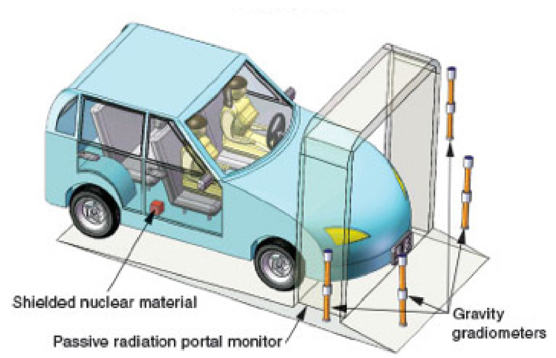
Project Innovation

Building on the well-established capabilities of gravity gradiometry, which has long been used in geology, LLNL collaborated with AOSense to develop a quantum version of this technology, known as cold-atom gravity gradiometry. Cold-atom gradiometers can easily 'see' Earth's tides, recording variations in the local gravity field of Earth as it is strained by the sun and moon.

The cold-atom interferometry sensor developed through this collaboration measures subtle changes in gravity, making it possible to rapidly acquire accurate, local-gravity measurements that are free of the calibration limitations of conventional sensors, and therefore provide an accurate mass-map of interrogated objects, at the sensitivity needed to detect threats.

Additionally, LLNL's industry collaborations related to quantum sensing also include novel solutions aimed at enabling high-precision navigation in areas where GPS navigation is not viable. The solutions use inertial motion sensors to provide navigation that does not rely on GPS.

In collaboration with AOSense, LLNL's quantum sensing experts are investigating the use of atom-interferometer gyrosocopes for inertial navigation. These devices enable "dead reckoning" navigation, which works by advancing the sensor position from the previously known position using the sensor's gyroscopic and acceleration data. AOSense instruments were successfully field tested and validated using LLNL navigation codes on instrumented vehicles providing comparison high precision navigation solutions.



One of LLNL's advances in quantum sensing technology enables deployment of passive radiation detectors that increase the chance of discovering nuclear material hidden inside a vehicle.

"Gravity gradiometry measures the local variations in acceleration due to gravity. Oil and mineral prospectors use this technique, for instance, to measure changes in subsurface density. That information allows them to pinpoint subsurface anomalies and more accurately target oil, gas, and mineral deposits. Our application instead focuses on mapping the density distribution of a passing vehicle."

Brent Young, President, AOSense, Inc.

Project Partners

Lawrence Livermore National Laboratory, AOSense, Inc., Vector Atomic, Inc.

Program Office: U.S. Department of Homeland Security, Domestic Nuclear Detection Office

Project Snapshot

Start Date & Duration: 2010-ongoing

QIST Keywords

Primary Keywords: Quantum Sensing

Secondary Keywords: Gravity Gradiometry, Cold-atom Interferometry, Inertial Navigation

POC Name & Email: Stephen Libby
libby1@llnl.gov

Website: quantum.llnl.gov

LLNL is also working with Vector Atomic, a California-based startup company, which is pursuing another path toward deploying mobile quantum sensors for inertial navigation and timing that also do not rely on GPS. The devices will determine the position and orientation of a vehicle by precisely measuring its linear and rotational acceleration through the quantum interference of atomic wave functions.

To achieve the small size and low-power usage needed for these mobile quantum sensors, Vector Atomic is using the capabilities of LLNL's Advanced Manufacturing Laboratory (AML) facilities and staff to incorporate Livermore-developed micromirror array technology, which controls and directs light using microscale structures to manipulate arrays of tiny mirrors.

The cooperative research and development agreement (CRADA) partnership as described by LLNL engineer Robert Panas, "will allow us to merge these two technologies. Our micromirror technology can modulate and tune the laser power for the atomic sensors more accurately than any other available technology. The result will be a device that can operate in demanding environments with substantial jostling and shaking. We expect the combined product to represent an improvement of more than an order of magnitude over current inertial navigation systems."

Potential Impact

Quantum cold atom gravity sensors being demonstrated through a collaboration between LLNL and AOSense will enable the rapid detection of hidden or shielded threats. Similarly, such gravity sensors could be used to detect tunnels and underground facilities. For defense applications, quantum sensing could also provide the ability to navigate in areas where GPS navigation may not be possible, such as in submarines and tunnels or areas where GPS is disabled. Additionally, the technology developed to address national security challenges will undoubtedly expand to other industries, such as oil and gas pipeline mapping, mineral extraction and exploration, and archaeological surveying.

Facility/Instrumentation Information

LLNL is partnering with AOSense to develop cold-atom gravity gradiometers that can provide an accurate mass-map of interrogated objects. They are also investigating the use of atom-interferometer gyroscopes for internal navigation.

Additionally, LLNL is working with Vector Atomic to develop mobile quantum sensors for inertial navigation that incorporate LLNL-developed micromirror array technology. In this partnership, Vector Atomic is using the capabilities of LLNL's Advanced Manufacturing Laboratory to adapt the laser-based technology for use in a demanding mobile environment.

Open Source Quantum Chemistry Software (PNNL)

Computational scientists at Pacific Northwest National Laboratory collaborated with Microsoft to develop an open source quantum chemistry tool kit.

Critical Need

Quantum chemistry lies at the heart of many of many energy-intensive problems that will need to be solved to achieve a renewable energy future. Realizing this promise requires scalable quantum chemistry tools that allow users to translate descriptions of electronic structure problems to optimized quantum gate sequences executed on physical hardware.

Many of these problems require interdisciplinary knowledge and subject matter expertise. There is a need to leverage the tools of quantum computing without requiring specialized quantum computing knowledge. To this end, quantum chemistry experts at Pacific Northwest National Laboratory (PNNL) teamed with Microsoft to develop a quantum chemistry library, under the open-source MIT license, that implements and enables straightforward use of state-of-art quantum simulation algorithms.

The project received support from the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences. It was supported in part through the Quantum Algorithms, Software, and Architectures (QUASAR) Initiative, conducted under the Laboratory Directed Research and Development Program at PNNL. The NWChem software package was supported by the Environmental Molecular Sciences Laboratory (EMSL), a DOE user facility located on the campus of PNNL and supported by the DOE Office of Biological and Environmental Research.

Project Innovation

The library is available in Q#, a programming language designed by Microsoft software specialists to express quantum algorithms at scale1. It interfaces with NWChem, a leading electronic structure software package developed at PNNL. The innovation lies at the interface, Broombridge, which describes second-quantized Hamiltonians, along with metadata required for effective quantum simulation. Further research in this area continues, with software development efforts to extend its capabilities.

NWCHEM performs a quantum chemistry calculation

"Researchers everywhere will be able to tackle chemistry challenges with an accuracy and at a scale we haven't experienced before."

Nathan Baker, Data Scientist, Pacific Northwest National Laboratory

Project Partners

Pacific Northwest National Laboratory, Microsoft Research, Quantum Architectures and Computation Group

Program Office: Office of Science/BES

Project Snapshot

Start Date & Duration: FY2018, ongoing

Budget:

QIST Keywords

Primary Keywords: Computing

Secondary Keywords: Software Development

POC Name & Email: Nathan Baker, nathan.baker@pnnl.gov

Website: pnnl.gov

Potential Impact

This software development project exemplifies the necessary collaboration that will need to occur for chemists, physicists, and computer scientists to access state-of-the-art quantum computing tools necessary to solve pressing societal concerns. This toolkit has already been used to enable progress in energy storage and energy conversion technologies, two essential advances needed to move toward a sustainable energy future. This toolkit makes the power of quantum computing available to for instance, chemists studying the enzymatic conversion of nitrogen into ammonia, an essential ingredient in fertilizers that feed our major crop plants such as corn and wheat. The ability to harness this enzymatic conversion at scale would greatly reduce the need for fossil fuel inputs in agricultural production, enabling a growing population to feed itself more sustainably, while protecting the environment.

Further, this innovative, open-source software package can serve as a building block for the development of new software libraries, platforms, and even programming languages to facilitate the entry point of a new generation of researchers into the interdisciplinary field of quantum computing. Attracting the best and brightest talent to tackle quantum computing challenges will be essential to accelerate progress.

Project Milestones

The Microsoft Quantum Development Kit chemistry library was developed and released. The chemistry library utilizes PNNL's NWChem, an open-source, high-performance computational chemistry tool developed by the U.S. Department of Energy's Office of Science to enable quantum solutions to solve computationally complex chemistry problems. November, 2018.

Facility/Instrumentation Information

NWCHEM was developed through support from the Environmental Molecular Sciences Laboratory (EMSL), a DOE user facility located on the campus of PNNL.

[1] docs.microsoft.com/en-us/quantum/libraries/chemistry/?view=qsharp-preview

ORNL Researchers Advance Performance Benchmark for Quantum Computers (ORNL)

ORNL researchers have developed a quantum chemistry simulation benchmark to evaluate the performance of quantum devices and guide the development of applications for future quantum computers.

Critical Need

While still in their early stages, quantum computers have the potential to be exponentially more powerful than today's leading classical computing systems and promise to revolutionize research in materials, chemistry, high-energy physics, and across the scientific spectrum.

But because these systems are in their relative infancy, understanding what applications are well suited to their unique architectures is considered an important field of research.

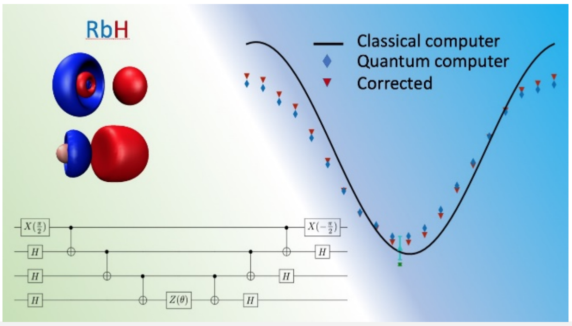
The Quantum Computing Testbed Pathfinder program addresses this need by developing benchmarks which connect application-inspired computation with low-level metrics and controls characterization. The project delivered a suite of high-level chemistry computations which help satisfy this need.

ORNL partnered with IBM under the Quantum Computing Testbed Pathfinder program to obtain access to quantum processors, while additional access to the IBM and Rigetti processors was provided by the Quantum Computing User Program at the Oak Ridge Leadership Computing Facility, which provides early access quantum computing systems as well as educational outreach and internship programs. Support for the research came from DOE's Office of Science Advanced Scientific Computing Research program.

Project Innovation

The team calculated the bound state energy of alkali hydride molecules on 20-qubit IBM Tokyo and 16-qubit Rigetti Aspen processors. These molecules are well understood, allowing researchers to effectively test the performance of the quantum computer. Using new error analysis techniques, the team showed that quantum computers can reach chemical accuracy in multiple problem instances with the execution of quantum circuits over the cloud.

Of equal importance is the fact that the quantum calculations also included systematic error mitigation, illuminating the shortcomings in current quantum hardware.



The benchmark will help the community evaluate and develop new quantum processors. (Below left: schematic of one of quantum circuits used to test the RbH molecule. Top left: molecular orbitals used. Top right: actual results obtained using the bottom left circuit for RbH).

"This work is a critical step toward a universal benchmark to measure the performance of quantum computers, much like the LINPACK metric is used to judge the fastest classical computers in the world."

Raphael Pooser, principal investigator of the Quantum Testbed Pathfinder project, ORNL

Project Partners

Oak Ridge National Laboratory, Virginia Tech, Duke University, IBM Q, IonQ

Program Office: Office of Science/ASCR

Project Snapshot

Start Date & Duration: September 2017, 5 yrs

Budget: $1.55M/yr

QIST Keywords

Primary Keywords: Quantum Computing, Quantum Benchmarks

Secondary Keywords: Software Development

POC Name & Email: Raphael Pooser; pooserrc@ornl.gov

Website: testbed.ornl.gov

Potential Impact

Quantum chemistry, along with nuclear physics and quantum field theory, is considered a quantum "killer app," i.e., it is believed that as they evolve quantum computers will be able to more accurately and more efficiently perform a wide swathe of chemistry-related calculations better than any classical computer currently in operation, including Summit, the world's fastest computer located at ORNL.

Project Milestones

- Implementing a suit of application-inspired benchmarks in chemistry and other domains on today's quantum computers ✓
- Benchmarking error characterization at the quantum control and single-qubit level ✓
- Predicting the application benchmark performance based on low level characterization – in process (2021 planned)
- Providing a frontier to aid in the discovery of quantum advantage – in process (2022 planned)

Facility/Instrumentation Information

- Oak Ridge Leadership Computing Facility
- IBM Q Hub
- Rigetti Quantum Cloud Services

Quantum Communications for Critical Infrastructure Protection (LANL)

Keeping electric grid communications safe with quantum physics

Critical Need

Nationwide deployment of quantum technologies will require interoperable systems from multiple vendors. An operator must be able to "plug-and-play" a quantum device without regard for the underlying physics. It is essential to deploy quantum technologies without the undue burden on operators that would result from disparate technologies. Existing quantum links are limited in range to ~100 miles, in practice much less. We will demonstrate that a succession of such links, joined by relay nodes located in physically secure locations, can overcome this limitation. Extending this distance by linking systems through trusted nodes is contingent on physical security of the node. These devices, while possible, have not been demonstrated in a laboratory setting and are decades away from deployable at scale.

Finally, we are developing a network resiliency analysis tool which will allow us to quantitatively assess the added security these systems provide, and thereby to make informed cost/benefit decisions about scale and location of their deployment.

This effort is supported by the DOE Office of Cybersecurity, Energy Security, and Emergency Response (CESER).

Project Innovation

By developing and implementing a systems-level approach to interoperable trusted relay nodes, we will bring the security assurances of quantum communication systems to long-haul distances and evaluate the improvement of overall system resilience from the installation of quantum secured communication lines and trustworthy nodes.

The Alternating Current Optimal Power Flow (ACOPF) problem plays a central role in power systems optimization. The optimal placement of trustworthy nodes and secure channels requires solving a large amount of ACOPF problems where a subset of components is compromised due to a cyber-attack. Being able to provide global optimality guarantees for the ACOPF problem is critical for providing protection guarantees against such cyberattacks.

Our optimization engine, Gravity, is able to model the grid's reaction to damage (e.g. line failure, loss of generation, etc.). It can model hundreds of thousands of cases in a reasonable amount of time.

The project strategy is to simulate very many attack scenarios, both with and without quantum-secured links, and measure the impact of the attack. We will then be able to quantify the relative benefit of the quantum links as a function of their placement in the network, in order to make informed choices about installing these systems.

Quantum communication terminals installed in EPB's Chattanooga substation.

"The sustained and growing threat of cyberattacks to our energy infrastructure requires us to think differently, to act proactively"

Rick Perry, former Secretary of Energy, June 2018

Project Partners

Los Alamos National Laboratory

Oak Ridge National Laboratory

Virginia Tech, Qubitekk, Inc., EPB, Inc.

Program Office: Office of Cybersecurity, Energy Security, and Emergency Response (CESER)

Project Snapshot

Start Date & Duration: start FY17, end FY20

Budget: 2.5 M

QIST Keywords

Primary Keywords: Cyberphysical Security

Secondary Keywords: Cybersecurity, Secure Communications, Quantum Mechanics

POC Name & Email: Raymond Newell, PhD
raymond@lanl.gov

Potential Impact

- Secure SCADA and ICS networking over long-haul distances
- Extend security benefits of quantum communications to nodes as well as links
- Remove (or greatly reduce) requirements for physical security at quantum secured communication end points and nodes.
- Demonstrate interoperability of different Quantum Communication systems
- Bring security benefits of quantum communications to longer-range links
- Show that quantum communication systems can exchange cryptographic key material over different physical-layer implementations
- Optimal placement of trust-worthy nodes and secure quantum links in order to minimize the impact of cyber-physical attacks on the power grid.
- Accurately measure the impact of cyber-physical attacks using mathematical modeling of the physical laws underlying power networks

Project Milestones

- Upcoming Joint Field demonstration with Oak Ridge National Laboratory, Qubitekk, and EPB at EPB's power distribution network in Chattanooga, Tennessee: February 2019

Facility/Instrumentation Information

LANL's optimization engine, Gravity, is used to model the grid's reaction to damage.

[1] ornl.gov/news/ornl-teams-los-alamos-epb-demonstrate-next-generation-grid-security-tech
[2] eurekalert.org/pub_releases/2019-02/drnl-otw021219.php
[3] phys.org/news/2019-02-ornl-teams-los-alamos-epb.html
[4] dailyenergyinsider.com/news/17730-oak-ridge-los-alamos-labs-join-utility-epb-to-demonstrate-next-gen-grid-security/
[5] "ORNL & LANL team with EPB on next-generation grid security tech," Federal Technology Watch, Volume 17 Issue 7 page 3, February 18, 2019.

Quantum Computing Algorithms for Clean Energy Systems Research (NREL)

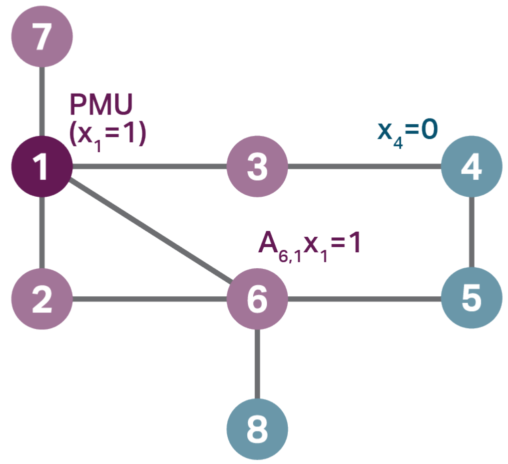
Near-term quantum computing algorithms implemented on noisy intermediate-scale quantum computers may hold the key to solving hard computational problems in optimization, artificial intelligence, and quantum simulation of matters relevant to the development of advanced clean energy systems.

Critical Need

Difficult computational problems in optimization, artificial intelligence, and simulation of quantum mechanical systems lie at the heart of efforts to develop clean, renewable, and sustainable power and transportation systems. Alongside classical simulation and machine learning on advanced computing systems, quantum computing is a novel computational paradigm primed to help solve such problems. Quantum computing recently passed the so-called "quantum supremacy" threshold with Google's 53-qubit Sycamore processor that was able to sample the output probability distribution from a random quantum circuit in 200 seconds, a task practically infeasible for even the world's largest supercomputer.[1] However, useful applications for such noisy-intermediate scale quantum (NISQ) computers have yet to be discovered. A team of researchers at the National Renewable Energy Laboratory (NREL), in collaboration with the Colorado School of Mines and funded by NREL's Laboratory Directed Research and Development (LDRD) program, is investigating use cases for NISQ devices with applicability to the development of clean energy systems.

Project Innovation

Two unique properties of quantum computers—entanglement and superposition—allow for their increased computational power. For instance, in combinatorial optimization superposition allows a NISQ device to represent an exponential number of solutions in superposition on a linear number of computational resources. Then, by using quantum optimization heuristics such as quantum annealing or the quantum approximate optimization algorithm, the various solution amplitudes are interfered such that when the terminal state of the computer is measured repeatedly, the optimal solution is ideally found with high probability. The team at NREL has demonstrated reformulation for and solution of the optimal phasor measurement unit placement and Markov decision problems on the D-Wave 2000Q processor and is looking towards additional use cases in mixed-integer programming and reinforcement learning.[2,3]



Minimum domain set formulation of quadratic unconstrained binary optimization (QUBO). Red is a placed PMU, red and pink are observed nodes as a result, and blue nodes are unobserved.

Project Partners

National Renewable Energy Laboratory

Colorado School of Mines

Project Snapshot

Start Date & Duration: 10/01/2019 – 09/30/2022

Budget: $600,000

QIST Keywords

Primary Keywords: Computing

Secondary Keywords: Software/Applications Development

POC Name & Email: Peter Graf, Peter.Graf@nrel.gov

The property of entanglement is what allows for efficient simulation of quantum mechanical systems on NISQ devices since entanglement is typically the feature that frustrates classical methods. Application of NREL's variational quantum state preparation research will be relevant to understanding the properties of strongly correlated topological materials, which have potential applications to low power consumption electronics and novel quantum computing architectures.

Potential Impact

Quantum computing algorithms for optimization, artificial intelligence, and simulation of quantum mechanical systems may eventually play a role in addressing the difficult computational problems involved in developing cleaner, more renewable, and more sustainable power and transportation systems.

Project Milestones

- Combinatorial optimization on quantum hardware
- Machine learning applications
- Synthesis of quantum computing and HPC capability

Facility/Instrumentation Information

This project utilizes classical high-performance computing resources at NREL (Eagle supercomputer), the D-Wave 2000Q processor hosted at Los Alamos National Laboratory, named Ising, and various other gate-model quantum processors.

[1] F. Arute et al., "Quantum supremacy using a programmable superconducting processor", nature.com/articles/s41586-019-1666-5

[2] E. B. Jones et al., "On the Computational Viability of Quantum Optimization for PMU Placement", arxiv.org/abs/2001.04489

[3] E. B. Jones et al., "K-spin Hamiltonian for Quantum-Compatible Markov Decision Processes", Manuscript in Preparation

Quantum Information Science and Engineering Network (QISE-NET): Bridging National Laboratories, Academia, and Industry to Build Tomorrow's Quantum Engineers (ANL)

QISE-NET is a one of-a-kind national training program for graduate students pursuing careers in quantum science and engineering.

Critical Need

QISE-NET is devoted to advancing academic and industrial efforts in the science and engineering of quantum information. It addresses the vital need to develop a national workforce of quantum scientists and engineers for the US to lead in quantum science and technology.

Each cohort in the network includes sets of triplets, with each triplet comprising the graduate student, mentor from industry or a national laboratory, and the university PI. Through these triplets, the network seeks to prepare students with knowledge, understanding and expertise in multiple convergent fields that will serve the second quantum revolution.

The network also increases interactions between academia, national laboratories and industry to advance quantum science and technology by cross-sector sharing and leveraging of facilities, expertise, and scientific and technical challenges. QISE-NET, which was the first of its kind, is now the model for similar programs starting up across the country. It enables students to build connections and develop pathways to careers with industry.

QISE-NET is co-led by the University of Chicago and Harvard University and managed by the Chicago Quantum Exchange, a leading national hub for the science and engineering of quantum information and for training tomorrow's quantum workforce. Funding is provided by the National Science Foundation.

Project Partners

Mentoring institutions include several national laboratories and companies: Argonne National Laboratory, Sandia National Laboratories, Oak Ridge National Laboratory, Brookhaven National Laboratory, and Los Alamos National Laboratory, and IBM, Raytheon BBM, and Adamas Nanotechnologies.

The program is managed by the Chicago Quantum Exchange, which includes founding members Argonne National Laboratory and Fermilab, University of Chicago, and University of Illinois at Urbana Champaign, as well as member institutions University of Wisconsin-Madison and Northwestern University.

Ami Greene, a graduate student at MIT and member of the first QISE-NET cohort, engages with other attendees during the inaugural Chicago Quantum Summit at the University of Chicago in 2018. Credit: John Zich

"QISE-NET provides an innovative model for training that workforce by embedding students in companies and national laboratories to drive collaborations that advance the frontiers of quantum science and engineering,"

David Awschalom, Liew Family Professor of Molecular Engineering at UChicago; Senior Scientist at Argonne National Laboratory; Director of the Chicago Quantum Exchange; and the QISE-NET Director.

Project Snapshot

Start Date & Duration: 2018 – Present

Budget: $2.5M

QIST Keywords

Primary Keywords: Workforce Development

POC Name & Email: David Awschalom
awsch@anl.gov

Website: qisenet.uchicago.edu/

Project Innovation

This network of triplets provides a unique, critically needed student experience in quantum science. Students work within a focused academic-industry and academia-national laboratory collaboration, which includes thesis development, specific research goals, extended visits at the industrial partner's site, and network-level mentoring opportunities. Together, the student and their mentors take on a pressing research question that they pursue during their course of study.

This novel approach to integrating research, education and technology transfer is highly convergent and cross-cutting in nature. These triplets originate from a variety of fields, including materials science, chemistry, device engineering, physics, computer science, and industrial research.

Program Outputs

The QISE-NET program's first cohort of students has published more than 23 papers and have given more than 20 presentations on their work since the program began in 2018. A selection of paper citations is included below.

"Handling leakage with subsystem codes." Natalie Brown, Michael Newman, and Kenneth Brown, New Journal of Physics. 21. (2019) iopscience.iop.org/article/10.1088/1367-2630/ab3372

"Quantum algorithms and lower bounds for convex optimization." Shouvanik Chakrabarti, Andrew M. Childs, Tongyang Li, and Xiaodi Wu, Quantum 4, 221 (2020). dx.doi.org/10.22331/q-2020-01-13-221

"Sublinear quantum algorithms for training linear and kernel-based classifiers." Tongyang Li, Shouvanik Chakrabarti, and Xiaodi Wu, Proceedings of the 36th International Conference on Machine Learning (ICML 2019), PMLR 97:3815-3824, 2019. arxiv.org/abs/1904.02276v1

"Superfast encodings for fermionic quantum simulations." Kanav Setia, Sergey Bravyi, Antonio Mezzacapo, and James D. Whitfield**.** Phys. Rev. Research **1**, 033033 (2019) doi.org/10.1103/PhysRevResearch.1.033033

"Fundamental Principles for Calculating Charged Defect Ionization Energies in Ultrathin Two-Dimensional Materials." Tyler J. Smart, Feng Wu, Marco Govoni and Yuan Ping, Physical Review Materials, 2, 124002 (2018). doi.org/10.1103/PhysRevMaterials.2.124002

"Measurement of a superconducting qubit with a microwave photon counter." A. Opremcak, I. V. Pechenezhskiy, C. Howington, B. G. Christensen, M. A. Beck, E. Leonard Jr., J. Suttle, C. Wilen, K. N. Nesterov, G. J. Ribeill, T. Thorbeck, F. Schlenker, M. G. Vavilov, B. L. T. Plourde, R. Mcdermott. *Science* 21 Sep 2018: doi.org/10.1126/science.aat4625

Project Milestones

- 2018 – accepted 20 students as part of the network's first cohort
- Spring 2020 – accepted 18 students into the network's second cohort
- Fall 2020 — students accepted into the network's third cohort

Facility/Instrumentation Information

Students accepted into the QISE-NET program who work with mentors at national laboratories have access to the cutting-edge facilities at those laboratories. National laboratory mentors include Argonne National Laboratory, Sandia National Laboratories, Oak Ridge National Laboratory, Brookhaven National Laboratory, and Los Alamos National Laboratory.

Quantum Loop: A Metropolitan Scale Quantum Communications Testbed (ANL)

Researchers have leveraged existing metropolitan optical fiber networks to perform quantum optical measurements over tens of kilometers under real-world conditions.

Critical Need

The prospect of communication protected by the laws of quantum physics is promising for next-generation ultra-secure networks and represents a natural means for connecting quantum technologies. The most promising way of realizing quantum communication networks is using optical photons, which can send quantum states across long distances. While the challenging experiment of communicating these states via light has been performed at the lab scale, considerable development is needed to scale these systems for viable long-distance communication. Among these developments is the search for bright and coherent, single photon sources that emit in the telecom band and couple to quantum memories. Furthermore, as the distances between nodes continue to increase, optical losses in the fiber will start to dominate requiring the development of quantum repeater technology.

As part of the Quantum Link project, researchers are utilizing existing underground commercial optical fiber connections to perform quantum optical communication experiments on the scale of dozens of kilometers. The fiber network will be used as a testbed for new single photon emitters, quantum memories, and communication protocols, with new nodes coming online across the Chicago metro area. This testbed will demonstrate the feasibility of linking disparate quantum systems and is an important step for the development of long-range quantum communication.

"An exciting part of this experiment is that it takes place outside of the lab and moves into the real world where there are temperature changes and vibrations and noise. This will give valuable insight in possibly creating a national quantum internet."

Paul Kearns, Director, Argonne National Laboratory

Project Partners

Argonne National Laboratory, The University of Chicago, Qubitekk, Inc.

Program Office: Office of Science/BES

Project Snapshot

Start Date & Duration: 2018 - present

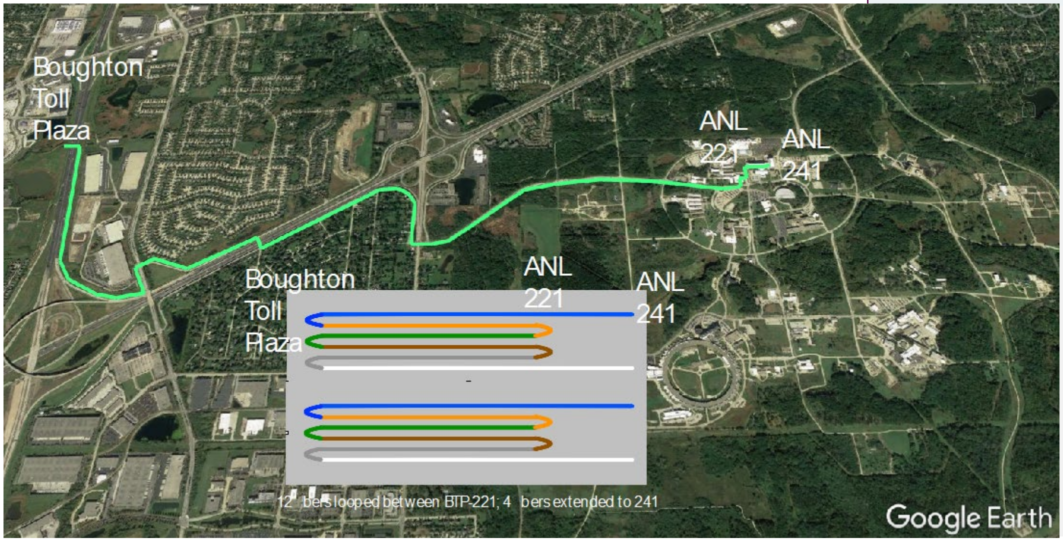
QIST Keywords

Primary Keywords: Quantum Communication, Quantum Internet, Solid-State Quantum Systems

Secondary Keywords: Entanglement

POC Name & Email: POC Name & Email: David Awschalom (awsch@anl.gov)

Website: anl.gov/msd/quantum-information-science



Satellite image schematically showing the fiber connections of the quantum loop experiment. Courtesy of Linda Winkler, Argonne National Laboratory.

Project Innovation

Optical fiber networks have been the infrastructure of choice for long-distance, high bandwidth telecommunication. In these networks, signal loss is compensated for by the use of repeater nodes, which simply read in the weak signal and then rebroadcast it using a telecom laser. Such an approach is incompatible, however, with quantum communication protocols where measuring the quantum state of a photon will fundamentally alter it. As a result, researchers seek quantum memories that can temporarily store a quantum state and then emit a photon that is entangled with that state. To reduce the transmission loss through optical fibers, these photons should ideally be in the near infrared telecom band.

Starting from Argonne National Laboratory, pairs of entangled photons were sent through two loops of optical fiber extending to a nearby highway toll plaza and back again several times for a total loop length of 40 km. Time coincidence measurements were performed in the lab using a superconducting nanowire single photon detector to confirm the spectral entanglement between photons sent through each of the two loops. Using a commercial fiber switch, the researchers were able to direct photons through either the loop or through an in-lab fiber network on command. Through this experiment, the researchers demonstrated the utility of this network and commercially available systems as a testbed for new quantum communication technologies. Testing under real-world conditions requires consideration for factors such as temperature swings in the fiber and vehicle traffic, which may add noise to the system.

Unique to this project, is the use of solid-state single-photon emitters with a natural coupling to quantum memories via nearby nuclear spins. One target technology for fiber-based quantum memories centers on ions of the element erbium (Er) inside a host oxide crystal. Er has an optical transmission that emits single photons in the telecom band. Argonne and University of Chicago scientists have grown crystals doped with Er ions and have fabricated nanophotonic devices at the Center for Nanoscale Materials, a DOE Office of Science user facility at Argonne, to enhance the brightness of these quantum defects. These devices are being tested both in the lab and in the Quantum Link testbed as potential quantum memories. Soon, the fiber link will extend a distance of 50 km, adding an additional node at Fermi National Accelerator Laboratory (FNAL), developing a two-way quantum link network on metropolitan scale for quantum communications.

Potential Impact

Materials that can effectively store and transmit quantum states by the production of telecom-wavelength photons have great potential in fiber optic-based quantum communication. It is one thing to test these systems in a lab; it is another to test them in real-world fiber network conditions. This project gives us the unique opportunity to test these new materials and develop new protocols for feasible fiber-based quantum communication.

Project Milestones

- Testing of the “quantum loop,” two 40 km-long loops of dedicated fiber. (completed)
- Construction of node at Fermi National Accelerator Laboratory. (in progress)
- Growth/fabrication of materials/devices for telecom single photon sources and quantum memories. (in progress)

Facility/Instrumentation Information

Quantum optics measurements were performed in the laboratory using the dedicated underground fiber network in the vicinity of Argonne National Laboratory. The entangled photon source was provided by Qubitekk, Inc. a partner of the Chicago Quantum Exchange (CQE). Erbium-doped crystals are grown at Argonne National Laboratory and photonic devices are fabricated at Argonne’s Center for Nanoscale Materials (CNM).

Quantum Performance Laboratory (QPL) (SNL)

The Quantum Performance Laboratory is an R&D group at Sandia National Laboratories that develops and deploys cutting-edge techniques for assessing the performance of quantum computing hardware to serve the U.S. government, industry, and academia.

Critical Need

Quantum computing is undergoing a revolution, with the rapid emergence of testbed-class quantum computers that can run unique quantum programs, and promise someday to enable quantum algorithms that solve key problems. The leading edge of this hardware – until recently, limited to individual qubits in research labs – is now full-stack multiqubit "NISQ" (noisy intermediate-scale quantum) processors accessed over cloud interfaces.

The critical questions about every such device are "What can it do?" and "How well does it perform?" But claims about performance are often based on opaque metrics with no clear relation to applications, which go unverified and unchallenged. Sandia National Labs has been developing testing, benchmarking, and characterization protocols to answer these urgent questions since 2013, and in early 2019 stood up the Quantum Performance Laboratory (QPL) to serve the U.S. and global quantum computing community. The QPL's primary mission is R&D around the performance of quantum computers – how to measure it, what limits it, and how to guide development toward useful quantum advantage.

The QPL's Innovative R&D Mission

The QPL combines research into the capabilities and behavior of quantum processors, development of new techniques and protocols for measuring and assessing that performance, and active engagement and outreach with the entire U.S. quantum computing community. We study the failure mechanisms of real-world qubits and processors. We create meaningful metrics of low- and high-level performance, predictive models of multi-qubit quantum processors, and concrete, tested protocols for evaluating as-built experimental processors. And we enable scientists and engineers around the world to use cutting-edge diagnostics and benchmarks by maintaining and supporting the open source pyGSTi software package, which provides an extensive suite of tools and algorithms for evaluating individual qubits and many-qubit processors. The QPL collaborates with industry and academia to develop new performance assessment tools and apply them to newly developed quantum computing platforms, publishes results in scientific journals including Nature Communications, Physical Review X, and Physical Review Letters, and sponsors high-impact international workshops to nucleate and nurture the quantum performance research community. In addition to its R&D capabilities, the QPL also provides quantum hardware assessment capabilities directly to DOE and the U.S. Government.

www.pygsti.info

QPL created pyGSTi, an open-source software for modeling and characterizing noisy quantum information processors

"Understanding the capabilities, faults, and performance of specific quantum computing processors is essential to make good use of the processors available today, and to guide development of the next generation."

Robin Blume-Kohout
Lead, Quantum Performance Lab

Sponsors and Partners

Sandia National Laboratories' QPL is supported by DOE's Advanced Scientific Computing Research (ASCR) program, and other US Government sponsors. The QPL has partnered and collaborated with other national labs (including LBNL and ORNL), as well as academic and industrial partners across the nation.

QPL Snapshot

Start Date & Duration: Officially inaugurated in 2019, QPL's R&D history dates to 2013.

Budget: Approximately $2.5M (FY19)

QIST Keywords

Primary Keywords: Computing

Secondary Keywords: Hardware Performance Assessment

POC Name & Email: Robin Blume-Kohout rjblume@sandia.gov

Website: qpl.sandia.gov/

The QPL's Impact on Quantum Computing

Since 2013, quantum computing has exploded into prominence, thanks to dramatic leaps in experimental capability, engineering accomplishments, and repeated surges of funding from government and private industry. Today, in situ quantum computers have outpaced theorists' ability to characterize their behavior and performance. Sandia National Laboratories and the QPL have been at the forefront of the ongoing effort to understand, characterize, and measure the performance of these new and potentially revolutionary devices. QPL innovations that changed the landscape of performance assessment include:

- Introduction and popularization of gate set tomography (GST) as the first method for comprehensively characterizing every aspect of quantum logic gates to arbitrarily high accuracy, and eliminating systematic "calibration" errors.
- Creation and release of the open source pyGSTi (pygsti.info) software package for quantum characterization, verification, and validation (QCVV), which provides easy-to-use GST and a host of other techniques.
- Direct randomized benchmarking (DRB), a streamlined and scalable extension of the popular "randomized benchmarking" protocol for assessing the performance of 1-3 qubits, which enables benchmarking up to 10 qubits.
- A framework for volumetric benchmarking of large quantum processors that unifies almost all extant benchmarking approaches within a common framework and enables simple yet detailed visualization of devices' capability.
- New protocols to characterize drift, context dependent and non-Markovian errors, and crosstalk in quantum devices.
- The first international workshop on Assessing the Performance of Quantum Computers, which brought together 80 scientists, experts, and stakeholders from government and industry in September 2019 to discuss, innovate, learn, and chart the future of benchmarking and characterizing quantum computers in the NISQ era.

QPL Goals and Mission

The QPL's ongoing goal is to make it possible for experts, stakeholders, and sponsors of quantum computing R&D to understand and assess the capabilities of as-built quantum computers. To this end, we develop:

- Models, metrics, and characterization protocols for probing the detailed low-level behavior of quantum computing components – e.g., qubits, logic gates, measurements, and other elementary operations – and enabling experts to build reliable predictive models that can be used by customers and sponsors to predict program outcomes.
- Benchmarks and performance assessment techniques to measure high-level holistic performance of integrated quantum computing systems, compare them fairly against each other, and validate low-level models.
- Clear, easily understood, and powerful hardware models that describe what a given quantum computing system or component can – and can't – do reliably, and allow customers and users to predict what they'll be able to do with it.
- Powerful, easily used open source software tools that enable a wide range of users to measure, visualize, and analyze the performance of as-built qubits, processors, and quantum computing components.

Our mission, quite simply, is to solve and eliminate the mysteries from quantum computer performance, making it easy for everyone involved to understand what's feasible, what's not, and why hardware behaves as it does.

Unique Capabilities and Resources

The QPL's unique role as a trusted and reliable resource for both the DOE and the rest of the US Government and for industrial and academic research labs is made possible by Sandia's unique positioning as an FFRDC that does not compete with (or pick sides within) private enterprise, and by the unique depth and breadth of quantum computing expertise at Sandia. The QSCOUT trapped-ion quantum computing testbed, part of DOE/ASCR's Quantum Testbeds for Science program, is especially critical for the QPL's ongoing ability to test and evaluate benchmarks and characterization protocols on real hardware before releasing them for use on external testbeds in academia and industry.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2020-3577 O

Quantum Scientific Computing Open User Testbed (QSCOUT) (SNL)

A quantum computing testbed based on trapped ions that is available to the research community as an open platform for a range of quantum computing applications.

Critical Need

Quantum information processing has reached an inflection point transitioning from proof of principle scientific experiments to small noisy quantum processors. To accelerate this process, it is necessary to provide the scientific community with access to testbed systems that provide full specifications, enable low-level access to native gate implementations, make vertical integration approaches possible, and provide ways to fully specify scheduling of gates.

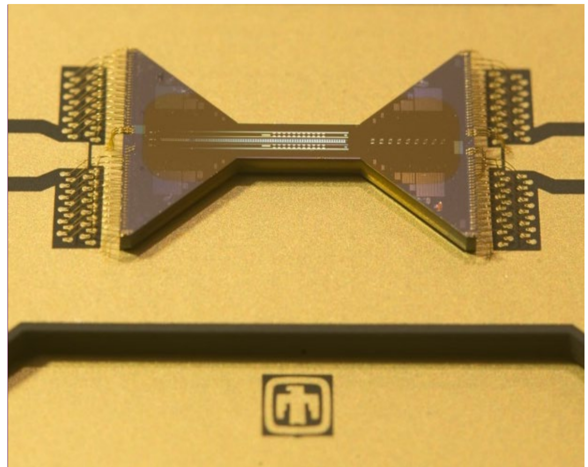
Access to noisy intermediate-scale quantum (NISQ) systems is needed to understand and optimize the noise properties, learn how to characterize and validate quantum operation, and to incubate the development and optimization of quantum algorithms for scientific applications.

Project Innovation

The Quantum Scientific Computing Open User Testbed (QSCOUT) is a 5-year DOE program funded by the Office of Science's Advanced Scientific Computing Research (ASCR) program to build a quantum testbed based on trapped ions that is available to the research community. As an open platform, it will not only provide full specifications and control for the realization of all high-level quantum and classical processes, it will also enable researchers to investigate, alter, and optimize the internals of the testbed and test more advanced implementations of quantum operations. QSCOUT will be made operational in stages, with each stage adding more ion qubits, greater classical control, and improved fidelities.

We will leverage the specific strengths of trapped ion systems: the identical qubits with long qubit coherence times, the high-fidelity single and multi-qubit operations possible in these systems, the low cross-talk addressing of individual qubits in the register, and the all-to-all connectivity available in trapped ion quantum registers.

In the first stage, we will make a quantum register of 3 qubits available. Parallel single qubit gates and sequential two-qubit Mølmer-Sørensen gates between any pair of qubits will be available. Target fidelities for single qubit operations are 99.5%, target fidelities for two-qubit gates are 98%. At the beginning of a computation, each quantum bit is prepared in the $|0\rangle$ state of the z-basis. At the end of a computation the entire quantum register is measured in the z-basis. For each measurement of the quantum register, the state of each qubit will be available to users.



Peregrine microfabricated ion trap which is used to store a chain of ytterbium ions to implement a quantum register.

"QSCOUT is a trapped ion quantum processor developed by scientists and made available to scientists to explore the power of quantum computation to solve scientific problems"

Peter Maunz, Principal Investigator, Sandia National Labs

Project Partners

Sandia National Laboratories, IARPA, Duke University, Tufts University

Program Office: Office of Science

Project Snapshot

Start Date & Duration: 10/2018 – 9/2023

Budget: $25 million

QIST Keywords

Primary Keywords: Quantum Computing

Secondary Keywords: Testbed, Trapped Ions, Scientific Computing

POC Name & Email: Peter Maunz
plmaunz@sandia.gov

Website: qscout.sandia.gov/

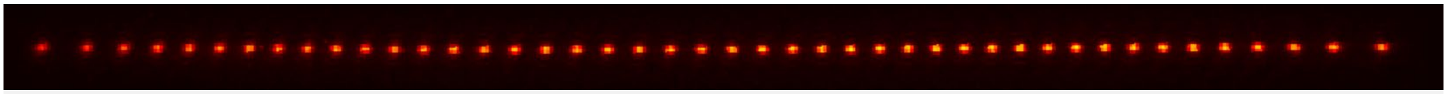
Potential Impact

The QSCOUT system will enable the understanding of noise properties of current quantum processors, it will teach us how to calibrate, characterize, and validate quantum processors. It will also help us to understand the limitations of current testbed systems and develop the next generation of larger more capable quantum processors featuring more quantum bits and higher fidelities. Furthermore, the availability of a real testbed system will nurture the development and optimization of quantum algorithms to solve scientific problems on quantum processors available in the future.

QSCOUT will also serve the greater quantum information sciences community by providing the possibility to develop the next generation of quantum computer scientists in academia, industry, and government.

Project Milestones

Milestone	Completion	Status
Testbed 1.0: Critical design review	4/15/2019	Complete
Testbed 1.0: Subsystem completion	8/7/2019	Complete
Testbed 1.0 completion	6/15/2020	In progress
Call for user proposal	3/20/2020	Complete
Proposal submission deadline	5/2/2020	In progress
First run for users	7/15/2020	



A chain of ytterbium ions stored in a Sandia microfabricated surface ion trap.

Facility/Instrumentation Information

The QSCOUT hardware will be realized as a trapped ion system. A chain of ytterbium ions will be stored in a Sandia surface ion trap, which offers excellent optical access for state preparation, detection and qubit manipulations. Qubits are encoded in the hyperfine clock states of each ytterbium-171 ion and a chain of ions serves as the qubit register. Single- and multi-qubit operations are implemented with optical Raman transitions using a 355nm pulsed laser. Imaging of an acousto-optical modulator (AOM) array onto the ion chain is used to realize individual addressing of qubits in the register. At the end of a computation, the quantum state of each qubit in the register will be read out and reported for each qubit and each detection event. This is achieved with standard fluorescence detection by imaging the chain of ions on an array of multi-mode fibers connected to an array of individual photomultiplier tubes.

The QSCOUT system is programmed using Just Another Quantum Assembly Language (Jaqal). Jaqal was developed to enable the QSCOUT objectives of providing full implementation specifications of the underlying native trapped-ion quantum gates, enabling users to optimize existing and introduce new native gates and vertical integration approaches. Furthermore, Jaqal provides users with full control of sequential and parallel execution of quantum gates. Jaqal specifications are available at qscout.sandia.gov/jaqal.html.

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Quantum Spin Probes for Biological Electronic Circuitry (NREL)

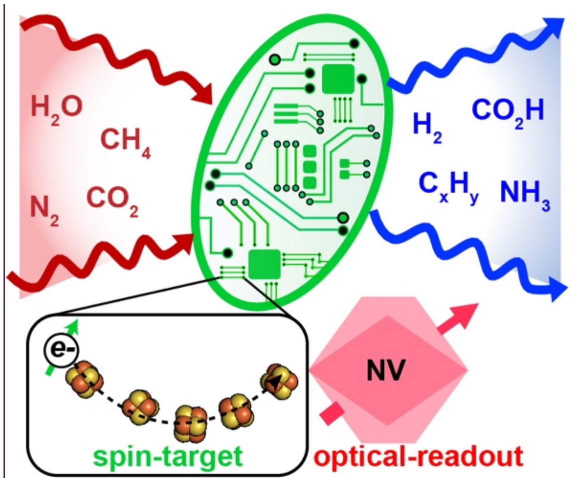
Developing optical magnetic resonance tools to investigate the quantum sensing capabilities of nitrogen-vacancy in diamonds for measuring electron-transfer reactions and chemical processes in biological systems.

Critical Need

Ranging from photosynthesis to cellular respiration, the complexity of electron-transfer mechanisms in biology calls for novel methods that can capture the underlying kinetics and dynamics of electron carries, donors, and acceptors which comprise the basic 'circuitry' of the cell for energy conversion. A fundamental understanding for how electron-flux is controlled through pathways is critical toward directing energy to reduced products and fuels with precise selectivity and control in engineered systems. Nitrogen-vacancy (NV) centers have emerged as promising probes for real-time quantum sensing applications and are being investigated here for sensing electron-flow through the detection of spin-dependent reactions. This is a two-year seed project funded by the NREL Lab Directed R&D program.

Project Innovation

Where physics meets biology: NV centers offer unique optical and magnetic properties that merge quantum sensing capability with biological compatibility. An interdisciplinary team at NREL comprised of biologists, spectroscopists, and physicists are joining efforts to leverage the extraordinary centers to provide simple optical readouts for electron-flow of desired targets in biological pathways for energy conversion. The NV center, an atomic defect in diamond formed by a vacancy adjacent to a nitrogen atom, is photostable with long spin coherence times and is sensitive to external magnetic and electric fields. Placement of the NV center near model biomolecules containing redox active metal sites can lead to a shortening of the relaxation time due to short-range magnetic dipole interactions. Scientists are using this concept to develop optically detected magnetic resonance (ODMR) tools for monitoring the oxidation-reduction of metal sites common to electron-transfer pathways that form electrical 'circuits' and 'wires' in the cell. In these schemes, tuning the magnetic field to match the Zeeman energy of desired targets makes it possible to relate experimental observables of the NV center to the proximity and oxidation state of the metal site. Following this notion, incorporation of NV centers near targeted biomolecules will make it possible to extract dynamic information for relating the electron flux through specific biochemical pathways and reactions.



Nitrogen-vacancy (NV) centers provide optical readouts for electron flux through complex 'circuits' in the cell formed from electron-transfer centers such as Fe-S clusters that couple oxidation-reduction reactions to energy transformation.

"An innovative approach for tracing quantum phenomena of electron-transfer processes in biological pathways with applications in harnessing electrons for energy rich products"

Paul King
Principal Scientist/Group Manager NREL

Project Partners

David Mulder, CO-PI, Justin Johnson, CO-PI

Yilin Shi, Post-doctoral Researcher

Project Snapshot

Start Date & Duration: October 2019, 2 years

Budget: $500,000

QIST Keywords

Primary Keywords: Quantum Sensing

Secondary Keywords: Electron-transfer, Magnetic Resonance, NV Centers

POC Name & Email: David Mulder, david.mulder@nrel.gov

Website: nrel.gov/bioenergy/

Potential Impact

From observation to control, capturing the quantum phenomena behind the electron-transfer reactions that link biochemical processes to energy conversion is expected to reveal guiding principles for directing electron-flux in catalytic systems. The ODMR tools will enable new methodology for real-time monitoring of the electric-potential of ‘wires’ that span large distances in the cell by selective incorporation of NV centers at targeted locations and reaction interfaces. This may allow for the visualization of selective photobiological processes such as the energy transduction and quantum coherence of photosynthesis. Successful development of the quantum sensing techniques can also be combined with other microscopy and fluorescence imaging to map complex ‘circuits’ and higher ordered interactions in the cell, with the possibility to engineer reactions cascades for driving electrons to desired products under certain conditions. The new capabilities will also enable precise time and space measurements in other molecular and material systems, broadly relevant to nanoscale technology for novel electronics, correlated electron systems, and nanoscale semiconductors.

Project Milestones

- Design, validate, and optimize ODMR detection schemes with existing spectroscopic equipment (in-progress)
- Develop model biomolecular system for incorporation of NV centers near redox active metal sites (in-progress)
- Carry out relaxation time measurements of NV centers in the model system (scheduled)
- Test advanced ODMR chip-based designs for ultra-fast measurements (scheduled)
- Partner with other teams for extending quantum sensors to biological, chemical, and material systems (scheduled)

Facility/Instrumentation Information

ODMR techniques are being developed across the NREL Spin Resonance Facility and optical laboratories for integrating magnetic resonance capabilities with versatile optical detection schemes. The Spin Resonance Facility houses multiple electron paramagnetic resonance (EPR) spectrometers and supports multi-disciplinary research for examining electronic and molecular structures that span chemical, biological, and material systems. NREL personnel, such as post-doctoral researcher Yilin Shi with unique expertise in magnetic resonance and software programming, are creating robust platforms for simultaneously probing optical and magnetic driven signals. Coupling chip-based microwave resonators to unique time-resolved fluorescence and transient absorption spectrometers at NREL will further unite ODMR approaches with ultra-fast capabilities.

Quantum Supremacy Milestone Harnesses Summit Supercomputer (ORNL)

A partnership between Oak Ridge National Laboratory, Google, and NASA Ames Research Center has demonstrated the first example of a quantum computer surpassing a supercomputer.

Critical Need

Tracking the rapidly growing performance of quantum computers is essential for identifying when these systems are ready to deliver practical solutions to the most challenging computational problems. Verification and validation using the world's most powerful computing systems, like the Summit supercomputer at the Oak Ridge Leadership Computing Facility, is an essential part of evaluating when quantum computers reach this supremum of computation.

A recent partnership between ORNL, Google, and NASA demonstrated a historic milestone when the Google Sycamore processor consisting of 53 qubits outperformed a task known as random circuit sampling (RCS). The RCS task was designed specifically to measure the performance of quantum devices, and the results provide a proof of concept for quantum supremacy by establishing a baseline for the comparison of time-to-solution and energy consumption. The research was supported by DOE's Office of Science and used resources at the Oak Ridge Leadership Computing Facility, a DOE Office of Science User Facility.

Project Innovation

The simulation of a random quantum circuits on 53 qubits took 200 seconds on the Sycamore quantum computer. After verifying numerical simulations of similar circuits on the Summit supercomputer, the team extrapolated that the conventional calculations would have taken more than 10,000 years to complete with current state-of-the-art algorithms. These numbers provide the first experimental evidence of quantum supremacy and critical information for the design of future quantum computers. The researchers also estimated the performance of individual components to accurately predict the performance of the entire Sycamore device, demonstrating that quantum information behaves consistently as it is scaled up—a necessary property for the design of large-scale quantum computers.

A library developed by the OLCF for performing tensor algebra operations on multicore CPUs and GPUs allowed the team to take advantage of all of Summit which, along with the IBM system's 512 gigabytes of memory per node, increased the speed of the simulation 46-fold per node (using 4,550 of Summit's nodes) as compared to the previous implementation that ran solely on CPUs.

Oak Ridge National Laboratory's Summit Supercomputer

"This experiment establishes that today's quantum computers can outperform the best conventional computing for a synthetic benchmark. There have been other efforts to try this, but our team is the first to demonstrate this result on a real system."

Travis Humble, ORNL researcher and Director of the laboratory's Quantum Computing Institute

Project Partners

Oak Ridge National Laboratory, Google, NASA Ames Research Center

Program Office: Office of Science

Project Snapshot

Start Date & Duration: 2019

QIST Keywords

Primary Keywords: Quantum Computing

Secondary Keywords: Simulation

POC Name & Email: Travis Humble, humblets@ornl.gov

Potential Impact

Once realized, quantum computers have the potential to be much more powerful than today's leading classical computers, and exponentially more energy efficient. For example, Google's Sycamore quantum processor was found to be approximately 10 million times more energy efficient than Summit in the performance of this task.

Facility/Instrumentation Information

This research used the IBM Summit supercomputer at Oak Ridge National Laboratory, currently ranked as the world's fastest system.

[1] *F. Arute et al., "Quantum supremacy using a programmable superconducting processor," Nature 574, 505 (2019)*

Quantum Transducers for Applications in Quantum Computing, Communications, Sensing, and Networks (SLAC National Accelerator Laboratory)

Utilizing the millimeter-wave regime to develop transducers for energy-efficient exchange of quantum information.

Critical Need

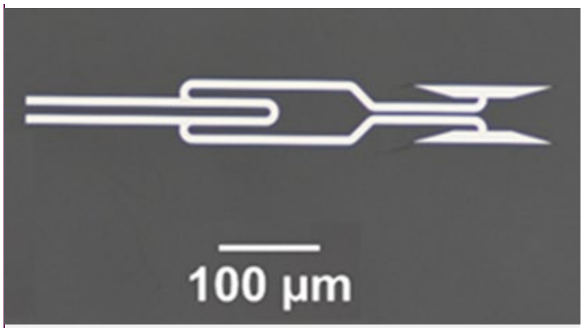
Quantum transducers are utilized to exchange information between disparate quantum devices or systems. The ability to coherently transfer quantum information across different platforms, from one frequency to another and across a broad temperature range, is critical to a number of quantum applications ranging from computing to communications to sensing. For quantum sensing, transducers have the potential to broaden the energy range of dark matter searches beyond what is presently possible by separating the receiving and measuring functions of a sensor. Transducers are also the foundation for quantum network nodes, which serve as gateways between a diverse array of rapidly evolving quantum subsystems and optical networks that move photons with different temporal and spectral properties over long distances. Such networks would enable both quantum communication and distributed quantum computing. Quantum transducers are a critical component of future quantum information systems and technologies.

QIS research at SLAC is funded by two awards from the Department of Energy Office of Science program offices in High Energy Physics and Advanced Scientific Computing Research. The awards are for projects focusing on connecting various quantum devices so that quantum information can be transferred efficiently and with high fidelity.

Project Innovation

The direct transfer of quantum information between two extreme wavelengths is highly inefficient, limiting the performance of micro-wave circuits that operate at millikelvin temperatures. This project aims to use a "quantum bus" that uses the mm-wave range as an intermediate stage. Then, a two-step transduction can be performed, starting with the microwave to mm-wave transduction before moving to higher temperatures and frequencies. This two-step transduction has decreased thermal losses compared to the direct transfer from mm-wave to higher temperatures, leading to a higher overall efficiency.

Beyond the mm-wave regime, this project seeks to develop systems for ultra-low loss, efficient and tailorable quantum frequency conversion, and to build from these components the capability to interface with quantum bits and memories. These subsystems will form the basis for nodes of a future quantum network, whereby ultra-low-loss and high-bandwidth connections are made between quantum systems, which can interface with telecom photonic networks and emitters.



A prototype micro-antenna that exhibits dual resonances at 50 and 105 GHz. Such a device forms the basis of a millimeter-wave transducer to link quantum devices.

"Energy-efficient quantum transduction with high fidelity is critical to a broad array of QIS technologies"

Paul Welander, Staff Scientist, SLAC National Accelerator Laboratory

Project Partners

SLAC National Accelerator Laboratory

Stanford University

Program Office: Office of Science/HEP and ASCR

Project Snapshot

Start Date & Duration: FY20, 4 years

Budget: $2.3 Million

QIST Keywords

Primary Keywords: Transduction, Nodes, Photonic Networks, Millimeter-Wave

Secondary Keywords: Computing, Sensing, Communications

POC Name & Email: Emilio Nanni, nanni@slac.stanford.edu

Website: qis.slac.stanford.edu/, qfarm.stanford.edu/

Potential Impact

One potential impact of an efficient quantum transducer is in the search for dark matter. A significant portion of the candidate dark matter spectrum spanning the μeV-eV range lacks techniques for processing or transducing quantum states, thereby greatly limiting the possible reach of quantum sensors. Indeed, transduction from the mm-wave regime would also greatly benefit dark matter searches. The frequency range for axions above ~10 GHz (~40 μeV) is beyond the reach of current experiments. Development of resonant structures that may couple to the axion field at mm-wave frequencies is actively being pursued by a number of groups. Transduction from mm-wave to either microwave or optical frequencies will permit quantum-limited photon counting with well-developed devices.

In a broader sense, the improvements in transduction between quantum states plays a vital role in linking the classical world to the quantum world, playing a role in the advancement of various applications. In particular, networks that transport quantum information will play a key role interfacing quantum computers, devices and sensors. When linked together via an energy-efficient, high-fidelity and high-bandwidth quantum network, the combined potential of quantum devices and technologies has incredible potential to drive scientific discovery forward, leading to new capabilities and scientific tools to transform our understanding of nature and advance U.S. energy, economic, and national security interests. Quantum transduction plays a vital role in applications in computing, sensing, networks, and communications, all a vital role in the future of QIST.

Project Milestones

Demonstrate a quantum transducer, whereby quantum information is coherently exchanged between a superconducting qubit at microwave frequencies and a resonant high-Q device at mm-wave frequencies. We aim to study the behavior of such devices, understand their limitations, and explore routes to optimize for efficiency and fidelity.

Demonstrate quantum photonic network nodes relying on transduction and quantum frequency conversion, linking quantum bits and memories. Interface such nodes with telecom photonic networks and emitters, while remaining sufficiently versatile and extensible to operate with a multitude of encodings and frequencies essential to QIST.

Facility/Instrumentation Information

This project utilizes facilities at both SLAC National Accelerator Laboratory and Stanford University. Facilities include micro- and nanofabrication cleanrooms (including Nano-X at SLAC and SNF at Stanford), cryogenic testbeds for low-noise device measurements, the Geballe Laboratory for Advance Materials, and an array of laser laboratories including the Nonlinear Optics Lab. This project is a collaborative effort between institutions, and part of Quantum Fundamentals, Architectures, and Machines (Q-FARM), a joint initiative between SLAC and Stanford.

Synchrotron X-rays Catch Sound Waves that Drive Quantum Spins (ANL)

Unique nanoscale X-ray microscopy instrumentation allowed researchers to directly watch atoms move in a quantum material as sound waves passed through them

Critical Need

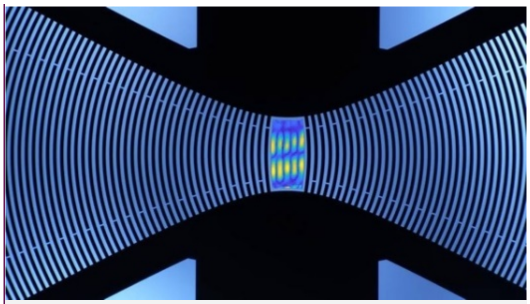
Communicating quantum information is a challenging task. It is difficult to move information stored in electron spin within a device. However, since different quantum systems represent quantum information in different ways, combining more than one type into a hybrid system could take advantage of the strengths of each one. For instance, optical photons can send quantum states across long distances. An electron's spin state can store information, which allows scientists to expand the binary information storage system used in traditional computing. In this study, researchers created a hybrid quantum system that acoustically drives transitions in electron spins. Unique X-ray microscopy instrumentation allowed researchers to directly watch atoms move in a quantum material as these sound waves passed through them. For part of the work, they used the Center for Nanoscale Materials (CNM) and the Advanced Photon Source (APS), both U.S. Department of Energy (DOE) Office of Science user facilities. The study provides a step towards bringing quantum technology closer to reality.

Project Innovation

When exposed to stress and strain, materials can display a wide range of different properties. By using sound waves, scientists have begun to explore fundamental stress behaviors in a crystalline material that could form the basis for quantum information technologies.

In a study by researchers at the DOE's Argonne National Laboratory and the Pritzker School of Molecular Engineering at the University of Chicago, scientists used X-rays to observe spatial changes in a silicon carbide crystal when using sound waves to strain buried defects inside it[1]. The work followed on an earlier recent study in which the researchers explored controlling the ground state spin state of the defect's electrons when the material was similarly strained[2].

Because these defects are well isolated within the crystal, they can act as a single molecular state and as carriers of quantum information. When the electrons trapped near the defects change between spin states, they emit energy in the form of photons. Depending on which state the electrons are in, they emit either more or fewer photons in a technique known as spin-dependent readout.



An x-ray image of sound waves (courtesy Kevin Satzinger and Samuel Whiteley)

"We're interested in how to manipulate the original spin state with acoustic waves, and how you can spatially map out how the mechanics of the strain with X-rays,"

F. Joseph Heremans,
Materials Science Division,
Center for Molecular Engineering,
Argonne National Laboratory

Project Partners

Argonne National Laboratory

The University of Chicago

Program Office: Office of Science Facilities (Center for Nanoscale Materials and Advanced Photon Source)

Project Snapshot

QIST Keywords

Primary Keywords: Spin Defects

Secondary Keywords: X-ray Microscopy

POC Name & Email: Martin Holt
mvholt@anl.gov

In the experiment, the researchers sought to assess the relationship between the sound energy used to produce the strain on the defects in the crystal lattice and the spin transitions indicated by the emitted photons. While the defects in the crystal naturally fluoresce, the additional strain causes the ground spin of the electron to change state, resulting in a coherent manipulation of the spin state than can be measured optically.

To characterize the lattice and defects, Argonne researchers used the CNM's Hard X-ray Nanoprobe on the shared CNM/APS beamline. Through a newly developed technique called stroboscopic Bragg diffraction microscopy, Argonne scientist Martin Holt and his colleagues were able to image the lattice around the defects at many different points throughout the strain cycle.

Potential Impact

Materials harnessing quantum behavior could revolutionize applications in communication, sensing, and computation – but the exact relationship between materials properties and quantum behavior is sometimes not well understood – time resolved synchrotron microscopy gives us new tools to correlate dynamic strain with optical response.

Project Milestones

- Demonstrate correlation of dynamic strain with enhanced photoluminescence of quantum defects (completed)
- Image secondary acoustic waves re-emitted by scattering from engineered structures (in-progress)
- Create a 3D time-resolved movie of an acoustic wave interacting with a defect using Bragg ptychography (in-progress)

Facility/Instrumentation Information

Stroboscopic scanning X-ray diffraction microscopy measurements were performed at the Hard X-ray Nanoprobe Beamline, operated by the Center for Nanoscale Materials at the Advanced Photon Source, Argonne National Laboratory (contract no. DE-AC02-06CH11357). This work also made use of the University of Chicago MRSEC (NSF DMR-1420709) and Pritzker Nanofabrication Facility, which receives support from the SHyNE, a node of the NSF's National Nanotechnology Coordinated Infrastructure (NSF ECCS-1542205).

[1] Whiteley, S. J., F. J. Heremans, G. Wolfowicz, D. D. Awschalom, and M. V. Holt. "Correlating dynamic strain and photoluminescence of solid-state defects with stroboscopic x-ray diffraction microscopy." Nature communications 10, no. 1 (2019): 1-6.

[2] Whiteley, Samuel J., Gary Wolfowicz, Christopher P. Anderson, Alexandre Bourassa, He Ma, Meng Ye, Gerwin Koolstra et al. "Spin–phonon interactions in silicon carbide addressed by Gaussian acoustics." Nature Physics 15, no. 5 (2019): 490-495.

The Fundamental Algorithmic Research for Quantum Computing (FAR-QC) (SNL)

A multi-party collaboration led by Sandia National Laboratories which aims to develop novel resource-efficient quantum algorithms to advance capabilities in quantum simulation, optimization, and machine learning.

Critical Need

Researchers in the FAR-QC project are developing novel algorithms to advance fundamental capabilities in quantum simulation, optimization, and machine learning, leveraging an interdisciplinary team of physicists, computer scientists, and mathematicians. Through rigorous asymptotic scaling analysis of these algorithms, the FAR-QC team is pinpointing problems and domains in which quantum resources may offer significant advantages over classical counterparts. Understanding the benefits and limitations of quantum computing are vital in remaining on the leading edge of science and technology and impacting the DOE mission.

FAR-QC is sponsored by the DOE, Office of Science, Office of Advanced Scientific Computing Research (ASCR) Accelerated Research in Quantum Computing program. FAR-QC builds upon work initiated in the QOALAS project, sponsored by the DOE/ASCR Quantum Algorithms Teams program.

"Quantum algorithms to harness the potential of emerging and future quantum processors are essential in fulfilling the promise of quantum computing."

Ojas Parekh, Principle Investigator,
Sandia National Labs

Project Partners

Sandia National Laboratories (Lead), Oak Ridge National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, Berkeley Lab, University of Maryland, Caltech, Dartmouth, University of Southern California, QuSoft, Centrum Wiskende & Informatica, University of Amsterdam, Paderborn University, and Microsoft .

Program Office: Office of Science/ASCR

Project Snapshot

Start Date & Duration: FY20-FY24

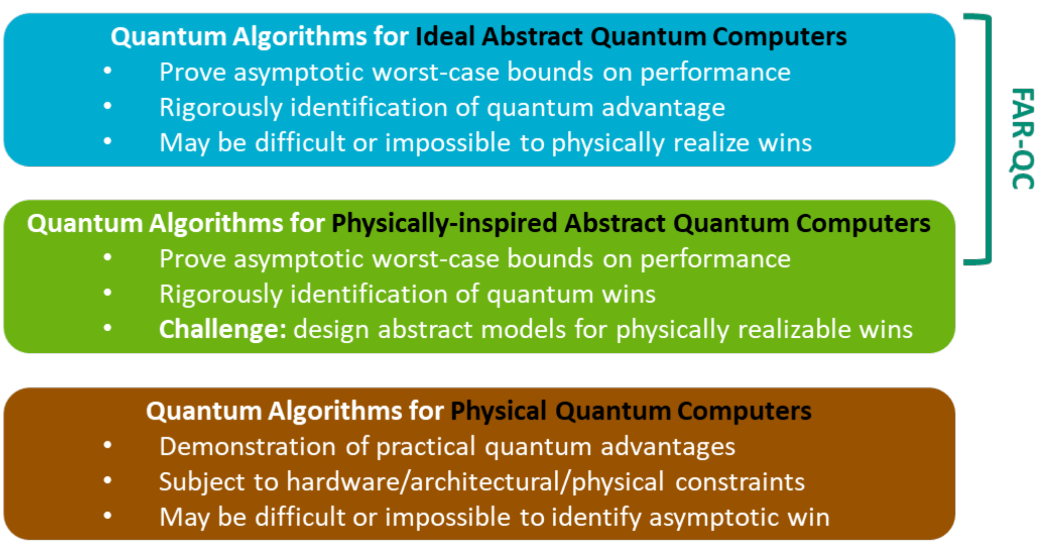
Budget: $18.5 million

QIST Keywords

Primary Keywords: Quantum Computing, Quantum Algorithms

Secondary Keywords: Resource-efficient Quantum Algorithms, Simulation, Optimization, Machine Learning

POC Name & Email: Ojas Parekh odparek@sandia.gov



FAR-QC: Continues to develop quantum algorithms for fundamental applications in optimization, simulation, and machine learning, with an additional emphasis on a "grassy" layer to allow theoretical quantum advantages (blue "sky" layer) to inform potential practically realizable quantum wins (brown "earthy" layer)

Project Innovation

FAR-QC is at the forefront of designing quantum algorithms enabling scientific applications, through four interrelated thrusts. FAR-QC's simulation thrust is advancing the quantum frontier for both dynamical and non-dynamical simulation, as well with cross-cutting techniques. FAR-QC's optimization thrust aims to deliver new quantum-accelerated approaches for fundamental optimization problems as well as classical and quantum techniques for approximating physically relevant properties of quantum Hamiltonians. FAR-QC's machine learning thrust focuses on theory of quantum learnability, learning quantum states and dynamics, and learning representations of high-dimensional domains. An overarching theory and practice thrust strives to bridge the gap between abstract theoretical algorithms and more practical resource-efficient implementations.

Potential Impact

Developing algorithms through the quantum perspective has brought insights into unique advantages of quantum resources for shaping future quantum systems and applications, as well as new classical algorithms. Additionally, the produced algorithms help fill a need for quantum applications and algorithms to complement, validate, and leverage near-term quantum systems developed within the DOE complex and beyond. It is intended that some of the algorithms produced will serve as a template for implementations on emerging and future quantum architectures.

Project Outputs

An approximation algorithm for the MAX-2-Local Hamiltonian problem
(Sean Hallgren, Eunou Lee, Ojas Parekh)

Quantum Algorithms for Simulating the Lattice Schwinger Model
(Alexander F. Shaw, Pavel Lougovski, Jesse R. Stryker, Nathan Wiebe)
(arxiv.org/abs/2002.11146)

High-Precision quantum algorithms for partial differential equations
(Andrew M. Childs, Jin-Peng Liu, Aaron Ostrander)
(arxiv.org/abs/2002.07868)

Quantum Coupon Collector
(Arinivasan Arunachalam, Alksandrs Belovs, Andrew M. Childs, Robin Kothari, Ansis Rosmanis, Ronald de Wolf.)
(arxiv.org/abs/2001.10520)

Can graph properties have exponential quantum speedup?
(Andrew M. Childs, Daochen Wang)
(arxiv.org/abs/2001.10520)

A Theory of Trotter Error
(Andrew M. Childs, Yuan Su, Minh C. Tran, Nathan Wiebe, Shuchen Zhu)
(arxiv.org/abs/1912.08854)

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User-focused Development Environment at the Quantum Design and Integration Testbed (LLNL)

LLNL's co-design approach to developing quantum systems addresses user-identified performance requirements, while offering a unique environment that fosters the knowledge needed by our nation's future quantum science innovators.

Critical Need

Quantum science holds the potential to deliver exponential gains in computational capabilities and enable simulation of physical phenomena that are beyond the reach of today's largest supercomputers, such as the dynamics of chemical and nuclear reactions. However, in today's quantum ecosystem, it is often challenging to bring together quantum system developers with the scientists who will benefit from innovative quantum applications.

In this rapidly evolving field, a "co-design" approach is needed—a collaborative development environment where the users' needs are integral to the system design process.

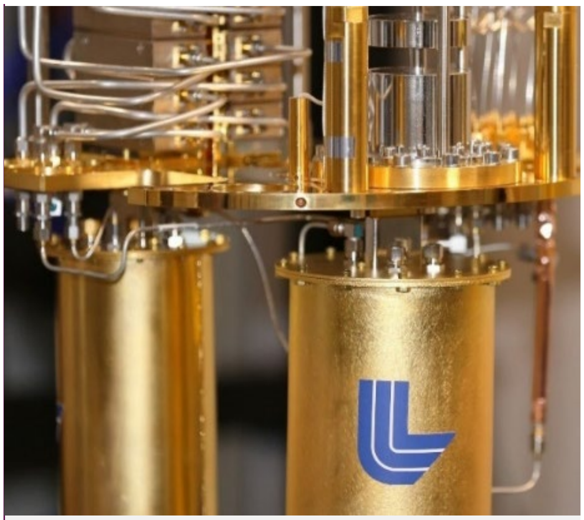
This approach will foster innovation for quantum application users who come from a broad range of disciplines, including physics, optics, engineering, materials science, and computer science. It's also key to creating simulation tools that can solve complex challenges in national security, energy security, and our nation's technology leadership.

Project Innovation

LLNL's Quantum Design and Integration Testbed (QuDIT) fosters a unique research environment that focuses on collaborative co-design involving quantum system developers and quantum application scientists. The current research focus on quantum simulation brings together scientists from a variety of fields, who are working to develop novel algorithms for each application area.

QuDIT developers are exploring control solutions for the quantum simulation environment that can significantly accelerate computing times on near-term quantum hardware, while minimizing decoherence. By working closely with users, developers strive to add functionality that meets user-identified needs.

Likewise, user teams develop a deeper understanding of the physics of the underlying quantum hardware, gaining the knowledge they need to design their own quantum software programs and execute them on the QuDIT platform. Providing this physics-level system access can allow quantum algorithms to perform 10-100 times better than they could on a black-box quantum computing system.



The hardware platform for LLNL's Quantum Design and Integration Testbed

"My team works hand-in-hand with testbed developers as we investigate quantum simulation of nuclear dynamics. This interaction accelerates our ability to generate new ideas regarding how to enhance testbed performance, as well as how to chart the most successful path to leveraging the capabilities of quantum technology to simulate nuclear properties across nuclides."

Sofia Quaglioni, Deputy Group Leader, Nuclear Data and Theory, LLNL

Project Partners

Lawrence Livermore National Laboratory, UC Berkeley, UC Merced

Program Office: Office of Science/ASCR and FES, NNSA (ASC)

Project Snapshot

Start Date & Duration: 2016 - ongoing

QIST Keywords

Primary Keywords: Quantum Simulation

Secondary Keywords: Quantum Computing; Quantum Testbed; Quantum Algorithms

POC Name & Email: Jonathan DuBois dubois9@llnl.gov

Website: quantum.llnl.gov

Potential Impact

Quantum simulation will allow advances in science areas currently limited by high performance computing capabilities. Applications range from chemistry and nuclear physics simulations to fusion reactor design and grand-unified physics theories. However, near-term quantum computing systems require expertise in the computers themselves, as well as the targeted science applications.

LLNL's quantum testbed is preparing the next generation of quantum simulation physicists by pairing them with system developers in a co-design process that benefits both groups. These co-design teams explore how the quantum system hardware and software stacks can be developed simultaneously in order to meet the needs of each science application. In addition, the testbed platform supports this co-design approach, enabling users to reconfigure system software and tailor the system to solve specific science problems.

For example, teams have already developed algorithms for nuclear spin interactions and 3-photon mixing. Moreover, through our close ties with industry and academia, we are cultivating the infrastructure for quantum computing with the goal of improving coherence times, modularity, and scalability.

Project Milestones

- 2017 – First quantum testbed installed at LLNL
- 2018 – Second quantum testbed at LLNL came online
- 2019 – Testbed used to demonstrate ~20x improvement in effective circuit depth for first realistic simulation of spin dynamics in nucleon interactions
- 2020 – Testbed used to demonstrate 30x improvement in effective circuit depth to enable unprecedented exploration of 3-wave mixing problem for fusion energy sciences

Facility/Instrumentation Information

LLNL's Quantum Design and Integration Testbed (QuDIT) contains several dilution refrigerators that can operate at the temperatures required to maintain coherent superconducting quantum states. Radiofrequency electronics are available for producing a variety of signals required for arbitrary quantum gates on the simulator. Simulator designs consist of 3D resonator cavities with transmons inside, which are used as multi-state devices.

Unlike conventional universal quantum computers, QuDIT utilizes multiple quantum states in each quantum mode. Rather than confine each device to a two-state qubit, these multiple modes allow a multiplicative increase in the computational power of each element. The states also offer all-to-all connectivity, rather than relying on a 2D lattice to transfer state entanglement from one end of the chip to the other, which reduces the probability of decoherence for large quantum states.

A focus on high fidelity characterization, fast feedback broadband control, and computation tools enabled by high performance classical computing allows real-time software reconfigurability of the underlying quantum logic operations available to users.

[1] Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-BR-806479

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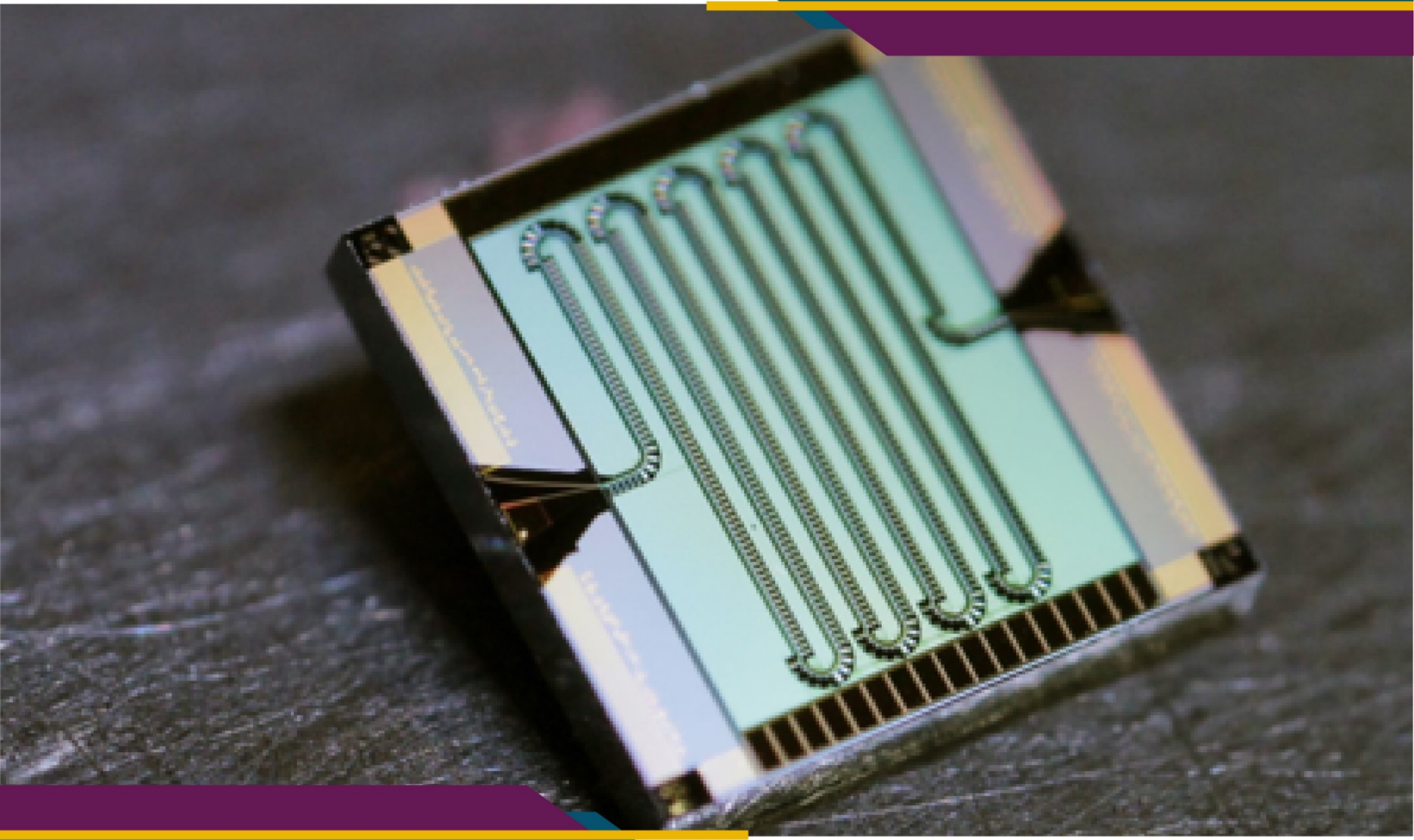

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