QUANTUM FRONTIERS
REPORT ON COMMUNITY INPUT TO THE NATION'S STRATEGY FOR QUANTUM INFORMATION SCIENCE

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INTRODUCTION

Under the Trump Administration, the United States has made American leadership in quantum information science (QIS) a critical priority for ensuring our Nation's long-term economic prosperity and national security. Harnessing the novel properties of quantum physics has the potential to yield transformative new technologies, such as quantum computers, quantum sensors, and quantum networks.

The United States has taken significant action to strengthen Federal investments in QIS research and development (R&D) and prepare a quantum-ready workforce. In 2018, the White House Office of Science and Technology Policy (OSTP) released the *National Strategic Overview for Quantum Information Science*, the U.S. national strategy for leadership in QIS. Following the strategy, President Trump signed the bipartisan National Quantum Initiative Act into law, which bolstered R&D spending and established the National Quantum Coordination Office (NQCO) to increase the coordination of quantum policy and investments across the Federal Government.

Building upon these efforts, the *Quantum Frontiers Report on Community Input to the Nation's Strategy for Quantum Information Science* outlines eight frontiers that contain core problems with fundamental questions confronting QIS today:

- Expanding Opportunities for Quantum Technologies to Benefit Society
- Building the Discipline of Quantum Engineering
- Targeting Materials Science for Quantum Technologies
- Exploring Quantum Mechanics through Quantum Simulations
- Harnessing Quantum Information Technology for Precision Measurements
- Generating and Distributing Quantum Entanglement for New Applications
- Characterizing and Mitigating Quantum Errors
- Understanding the Universe through Quantum Information

These frontier areas, identified by the QIS research community, are priorities for the government, private sector, and academia to explore in order to drive breakthrough R&D.

As background for this report, Federal agencies on the National Science and Technology Council Subcommittee on QIS have engaged with the QIS research community through public requests for information (RFI) [1] and through a series of QIS workshops, roundtables, and technical studies led by experts and stakeholders in the QIS R&D community. The NQCO analyzed the RFI responses and workshop readouts and found several recurring themes. This report summarizes and organizes the community input in order to focus the Nation's QIS research, academic, private sector, and Federal Government leaders on frontiers where key questions must be answered to enable the full potential of QIS. The Trump Administration remains committed to maintaining and strengthening America's QIS leadership and unleashing the promise of this emerging field to improve the prosperity, security, and well-being of the American people.

QUANTUM FRONTIERS IN BRIEF

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1. Expanding Opportunities for Quantum Technologies to Benefit Society

> ***"[W]hile the Strategic Overview takes a basic research-driven approach, applied research should not be neglected…it is important to accelerate the development of quantum technology toward usable results. This means balancing pure basic research with use-inspired research which is more likely to yield usable technology."*** *– RFI response*

The nature of information technology is governed by the rules of the universe itself, known as quantum mechanics. This realization helped establish the field of QIS. Presently, new technologies that harness unique quantum properties of coherence, entanglement, and measurement are emerging from fundamental advances in QIS. Developing practical, real-world applications for these technologies that benefit other scientists and end-users in a wide range of disciplines is now an important frontier for quantum information scientists and technologists. Two major areas of inquiry are key for making progress along this frontier: discovering what is fundamentally possible with quantum technology, including practical quantum advantages and a deeper understanding of the classical-quantum trade space; and engaging interdisciplinary QIS researchers with domain scientists and end-users early on, to work together and identify potential applications for QIS technologies and concepts in government, industry and other branches of science.

a. Elucidating Fundamental Capabilities of Quantum Technologies

Improving our fundamental understanding of how quantum technologies can provide meaningful advantages over conventional classical methods was a recurring theme in RFI responses. This includes: elucidating where improvements can be gained over existing technologies by utilizing quantum phenomena to accomplish specific tasks; characterizing entirely new capabilities enabled by quantum phenomena that have no classical counterparts; and understanding fundamental advantages for quantum metrology and quantum computing that can be derived from quantum networking.

For quantum computing, RFI respondents noted that advances in computational complexity theory could clarify the classes of problems for which quantum computational advantage is possible in principle, paving the way for building more useful quantum algorithms in the long term. In the near term, consideration of non-asymptotic regimes (corresponding to problem sizes that could be addressed by near-term digital quantum computers or simulators) and specific device parameters (e.g., actual time requirements for quantum gate operations and auxiliary tasks such as stabilization or error-correction protocols) will also be important for such analyses. The development of approaches for mathematically evaluating the potential for quantum advantage in analog quantum computation (quantum annealing, adiabatic quantum computation, and quantum emulation) is also an area for exploration.

> ***"Quantum complexity theory research should be encouraged to understand where quantum computing has the most value and why. Quantum algorithm research should focus on demonstrating incontrovertible quantum advantage on real quantum hardware for classically-intractable practical problems."*** *– RFI response*

RFI respondents also highlighted the potential value of heuristic approaches for finding applications of near-term quantum devices. Direct experimentation with quantum devices could establish what they are capable of in practice; applications for established quantum capabilities may then be sought.

> ***"The space to be explored in the next 10 years is vast and the first useful applications of these new technologies may come from actually just trying new ideas without requiring a long and slow period of developing the appropriate theoretical foundations."*** *– RFI response*

Members of the research community have also recognized the potential for demonstrating quantum advantage on noisy, intermediate-scale quantum (NISQ) devices. Near-term quantum computers and quantum emulators could be explored to realize transformative approaches with advantages for working on problems that can be mapped to a quantum algorithm or to a quantum system for computation or simulation. Developing new quantum algorithms suited to NISQ devices, and formal methods of resource estimation for evaluating their potential for quantum advantage, could facilitate near-term progress in this frontier.

> ***"Applications for NISQ computing are critical for the future of QIS because, in addition to the scientific insights they generate, they form the path to the longer term goal of fault tolerant quantum computation."*** *– RFI response*
>
> ***"What are the NISQ-era algorithms that offer quantum advantage for meaningful problems?"*** *– RFI response*

b. Engaging QIS Researchers with Domain Specialists and End-Users

The need to identify important real-world tasks for which quantum technologies may offer a promising solution was a common theme in the RFI responses. Prospective areas for exploration include biocompatible quantum sensors for in vivo characterization of biomolecules for diagnostic or research purposes; QIS-based metrology for environmental or industrial systems monitoring; quantum computing approaches to classically-hard problems such as modeling of chemical systems relevant to drug discovery or nitrogen fixation, and certain optimization and machine learning tasks; quantum networks to enable secure communications and blind quantum computation in support of data privacy and confidentiality; deployment of quantum networking for satellite communications; and further development and deployment of robust quantum-enabled navigation systems.

> ***"[Identify] key problems that need QIS as a tool for solutions, from modeling and understanding complex physical phenomena to optimization problems to cryptography and security; characterizing problems and their quantum requirements."*** – RFI response

RFI responses also noted that efforts to find meaningful applications for quantum technologies would be accelerated by connecting QIS scientists and engineers with experts from other domains to explore potential use cases. This could expedite the timeline for finding new solutions to critical societal challenges and enable informed technology design strategies from an early stage. Reciprocally, as an added benefit, this work would provide a new lens through which to advance fundamental QIS by motivating new experiments, stimulating new hypotheses, and inspiring theoretical advances. Collaboration and continued discussion across QIS, computing, mathematics, engineering, and other application domains will be needed to reveal what can—and cannot—be accomplished uniquely with quantum technologies, and to achieve this potential in actual devices.

> ***"In a co-design approach, the problems can help drive the design and the engineering and scientific research while at the same time the scientific and engineering advances can drive designs to motivate new approaches to solving problems."***
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> *– RFI response*

An overarching goal for R&D in this frontier is to demonstrate quantum technologies that offer advantages for practical tasks. How might quantum technologies bring better, cheaper, or never-before-possible solutions to other scientists and end-users, and to society at large? Discoveries in this area would help to further establish the value proposition of QIS, beyond its role in expanding the boundaries of human knowledge.

2. Building the Discipline of Quantum Engineering

> ***"Quantum engineering should be established as a new discipline or a sub-discipline in engineering schools which requires developing curricula and textbooks both at undergraduate and graduate levels."*** *– RFI response*
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> ***"As new quantum information science-based technology ('quantum technology' for short) develops, the U.S. will need a new type of profession that has not previously existed: the quantum engineer. Quantum engineers will not be—and will not need to be—specialists in the detailed physics of QIS but will instead be expert in the use and extended application of the new systems, tools and possibilities enabled by QIS."*** *– RFI response*
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> ***"One element to U.S. Government engagement with academia on workforce development should be promoting the development of the field of quantum engineering, not as classical engineering to support quantum technologies (i.e. classical control electronics or thermal control systems), but as its own discipline where there are models of abstraction permitting useful engineering of quantum systems…quantum-engineering-focused research efforts will be required for developing the engineering models that appropriately abstract away the details of the complex underlying effects, while still allowing academic courses that teach these models to provide engineers with the appropriate intuition and depth of understanding."*** *– RFI response*

Advances in QIS and technology have led to compelling proof-of-principle experiments with gate-based and analog quantum computing, and demonstrations of quantum sensing with unprecedented capabilities and precision. However, many technical and systems-level challenges still remain to be overcome before today's quantum control capabilities are considered as standard ingredients for planning and constructing complex devices. This is especially true for products defined by a broad range of specifications and practical constraints for real-world applications. The emerging discipline of quantum engineering may bridge this gap by creating new perspectives on topics ranging from designing and integrating components, to optimizing and verifying functionality, and providing useful abstractions and heuristics. As illustrated by some RFI responses, these are among the variety of concepts currently referred to as quantum engineering. Pathways for progress in this frontier include: understanding what makes designs scalable and useful; integrating the development of quantum hardware, software, and support technologies; developing and using system-level architectures; and creating the new discipline of quantum engineering.

a. Integrating Quantum Hardware, Software, and Support Technology

Physical elements that were identified in several RFI responses and workshop reports as needing to be characterized, integrated, and optimized by quantum engineers include qubit arrays, refrigeration devices, electronics, optics such as silicon nitride waveguides and delay lines, single-photon detectors, vacuum systems, wiring and feedthroughs, lasers and stabilization components, radiofrequency and microwave technologies, and device packaging. Other hardware research areas that RFI responses suggested may be improved and integrated with an engineering approach are: the development of quantum memory technologies; efficient methods of quantum state preparation—especially for loading classical data into quantum information storage, processing, or communication devices; and the transduction of quantum states between heterogeneous components of quantum systems.

On the software and systems side, important research areas identified in RFI responses include development of modular software designs, methods for mapping computational problems to the specific hardware configurations of early devices, and exploration of programming languages built upon hardware-informed semantic models. Major research opportunities include further development of system architectures and abstractions and community-acceptable metrics and standards (once technologies have reached the appropriate level of maturity) for use in system validation, verification, and performance benchmarking and to inform technology selection and system optimization for specific use cases.

> ***“Whether it be in quantum computing, quantum software, or other QIS disciplines, a hybrid approach that integrates various quantum systems will be important to make breakthroughs. This means facilitating the combination of the best of various quantum systems to build new devices, capabilities, and platforms based on multiple different physical realizations.”*** *– RFI response*
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> ***“Longer term, the use of abstractions to enhance productivity will be needed, once quantum resources are more plentiful….We must establish the sorts of modularity and layering commonly needed for scalable systems.”***
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> *– Next Steps in Quantum Computing: Computer Science’s Role (Computing Community Consortium 2018)*

b. Exploring System-level Architectures, Abstractions, and Testing

Establishing essential principles of quantum engineering that enable researchers to build and use quantum systems at various levels of abstraction without having to start from first principles is considered groundbreaking for QIS R&D. Research community members also suggested that quantum engineers should work closely with domain experts to pioneer new applications that drive the design and experimental testing of tools, techniques, and architectures, and which could lead to near-term use cases for quantum technologies, as noted for frontier A.

> ***“[W]e have found the most fruitful work results from programs that enable close collaborations between quantum engineers and application domain experts.”***
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> *– RFI response*

c. Enabling Modular Systems

At the hardware level, systems of tens of entangled qubits have been demonstrated experimentally for several different qubit types, including superconducting, trapped ion, and photonic as examples provided in the RFI responses. These experiments illustrate that it is possible to access unique regimes for quantum information processing. However, as they grow in number, qubit systems generally become increasingly difficult to prepare, couple, and control, and their inherent complexity makes them concomitantly more difficult to understand, model, and validate—posing significant challenges for realizing systems of a larger scale. RFI responses highlighted the need to develop techniques, protocols, models, and validation approaches to enable heterogeneous, modular, and scalable designs, fabrication methods, characterization techniques, and packaging of qubit technologies.

"Developing common terminology and metrics will allow researchers in different groups to communicate more clearly and encourage better exchange of ideas and enable faster progress." *– RFI response*

"Several QIS areas remain in an early phase of research, where the engineering of a core technology is relatively immature." *– RFI response*

Members of the R&D community identified a range of technical challenges that would benefit from the application of engineering principles, including: optimizing quantum materials, fabrication, and manufacturing methods to meet hardware requirements; establishing specifications, parameters, and a common terminology for quantum system design that can be shared across qubit technologies and disciplines; developing new models of system behavior and efficient emulation techniques for comparison with actual performance; inter-qubit communication and connectivity; and methods for debugging systems that do not perform as intended. These methods could enable design and development of stable, self-contained collections of physical quantum hardware and control systems that would serve as the basis for a modular approach to system design.

"Focus on how to build quantum computers with a modular architecture. This will require bringing together [experts] from engineering, as well as system architects and computer scientists, to think about how to make interfaces and how to scale those interfaces." *– RFI response*

A vision of progress in this frontier is to build a broadly applicable set of quantum engineering principles, tools, and specifications for designing quantum systems that are stable, sophisticated, compact, and cost-effective enough to be useful and usable in a range of different environments and contexts. They would also lay the groundwork for designing and deploying large-scale, quantum computing and communication technologies and infrastructures.

3. Targeting Materials Science for Quantum Technologies

"In applications of quantum computing, qubit quality is inextricably tied to materials quality, particularly in solid-state platforms. The longer coherence times and lower error rates needed to advance the aims of error-corrected quantum computing will come fastest through a full predictive capacity for materials performance, one that is able to guide fabrication well enough to deliver desired QIS characteristics with consistency and without trial-and-error processes. An improved understanding of materials might also uncover new or better ways to fabricate error-protected qubits, which if found and made reliably could represent a transformative leap toward logical-qubit creation." *– RFI response*

Quantum information can be coded into different physical systems: ions, atoms molecules, or solid-state materials and superconducting circuits, and photons or phonons—each with its own advantages and challenges. Coherence in each system generally depends on how the qubits and interconnections are fabricated and controlled. Fundamental knowledge of the quantum properties of matter can inform the design of high-fidelity qubit systems to minimize the potential for noise and error. Developing and applying new and precise methods for characterizing and fabricating these physical components according to engineering specifications will accelerate advances in system development. Key areas ripe for progress include: using materials science to improve device performance, and pursuing new approaches to materials design, fabrication, and characterization.

"Research opportunities encompass (1) development of new in situ and in operando characterization and feedback techniques to discover materials with improved properties and functionalities; (2) characterization and control of quantum material properties on all length and time scales relevant to function, including tools to reveal the often subtle forms of emergent and topological order; and (3) prediction of the fundamental properties of quantum materials, including emergent order, behavior far from equilibrium, and functionality in the presence of disorder."

– Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology (DOE 2016)

a. Using Materials Science to Improve Device Performance

RFI respondents identified key opportunities for communication and collaboration between QIS researchers and those in fields such as materials science, chemistry, and condensed matter physics to leverage current knowledge and tools for improving the quality and resilience of the materials currently in demand for building quantum devices. Established theory and experimental techniques from these fields will aid in the design, characterization, fabrication, and evaluation of improved near-term devices. Building a robust approach for mapping materials characterization knowledge to estimated quantum bit and quantum device performance will advance this frontier.

"[D]evelop and optimize new advanced materials, including solid-state hosts for atom-like qubits (e.g., diamond and other semiconductors), materials with emergent properties (analogous to graphene and topological insulators), and materials developed by learning lessons from evolved (natural) biological and chemical materials."

– Quantum Sensors at the Intersection of Fundamental Science, Quantum Information Science, & Computing

b. Pursuing New Approaches to Materials Design, Fabrication, and Characterization

Members of the research community noted the opportunity to build on existing knowledge to advance the theories, tools, and techniques that will enable researchers to explore the fundamental quantum nature of materials, predict material properties, devise new synthesis and integration processes, and target new kinds of materials to outperform those currently in use. Key research pathways include exploration of artificial intelligence-driven materials science; improved chemical simulation techniques; 3-D atomic-scale imaging; scanning probe techniques for quantum materials characterization and quantum device readout; higher-sensitivity magnetic resonance tools; and other new measurement and modeling capabilities suited to extreme conditions.

"Quantum device coherence times, gate fidelity, and other metrics must be improved using new materials, processes, designs, and approaches. Goals for device improvement should be tied to actual system performance needs based on the best system estimates possible." *– RFI response*

Researchers noted that progress in realizing topological materials could yield entirely new, inherently error-protected qubits that are expected to be much more resilient to noise than approaches currently deployed. This area of exploration will involve substantial challenges in realizing quantum information primitives in such systems, beyond the initial difficulties of showcasing topological behavior in such materials in the first place. Demonstration of topological protection of quantum information in materials remains a wide-open question, with many potential pathways for success.

Opportunities were also highlighted for coupling a deeper understanding of materials properties with higher-resolution, more precise, and more easily scalable fabrication and manufacturing processes to enhance the ease with which materials can be customized, including fabrication techniques to enable the bottom-up construction of qubits from the atomic or molecular components. Collaboration between quantum engineers and those studying materials science would enable the development of models for optimizing materials selection for desired function and performance based upon controllable properties, such as density of states, tunneling energies, and resonance frequencies, and the qubit-relevant characterization of materials-related decoherence mechanisms.

> ***"How can we develop a fast, iterative synthesis technology that integrates in situ fabrication and characterization and is informed and/or directed by first principles theory and machine learning, thereby enabling rapid convergence toward a desired quantum-coherent property[?]"***
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> *– Opportunities for Basic Research for Next-Generation Quantum Systems (Basic Energy Sciences Roundtable, DOE 2017)*

Progress in this frontier has the potential to enhance researchers' abilities to fabricate high-quality qubits and other specialized materials for quantum device components reliably and according to desired specifications, by design. It could also spur progress towards next-generation quantum materials with increased resilience to noise, supporting efforts to build stable, compact, and low-cost quantum devices with the potential for practical deployment.

4. Exploring Quantum Mechanics through Quantum Simulations

"The intellectual roots of [quantum computing] go back decades to pioneers such as Richard Feynman who considered the fundamental difficulty of simulating quantum systems and 'turned the problem around' by proposing to use quantum mechanics itself as a basis for implementing a new kind of computer capable of solving such problems. Although the basic theoretical underpinning of [quantum computing] has been around for some time, it took until the past 5 years to bring the field to an inflection point: now small and intermediate-scale machines are being built in various labs, in academia and industry."

– Next Steps in Quantum Computing: Computer Science's Role (Computing Community Consortium 2018)

Engineered quantum technologies can be used to efficiently simulate and emulate intrinsically quantum systems to elucidate their properties. Such efforts have already improved our understanding of previously mysterious phenomena and have the potential to lead to stunning progress in foundational and applied science. Quantum information technologies, such as NISQ computers and analog quantum simulators available over the next 5 years, will offer the chance to improve our understanding of quantum systems through computation, simulation, experimentation, and other studies. Key areas for progress include: leveraging quantum devices to improve approaches for the classical, quantum, and hybrid simulation of quantum behavior from many-body physics to chemistry to materials science; demonstrating quantum advantages based on quantum simulation; and developing new algorithms for NISQ-era devices, and exploring their performance in the presence of noise.

"A quantum, rather than classical, simulation is naturally better equipped to explore the state space spanned by quantum systems."

– Quantum Computing: Progress and Prospects (National Academies of Sciences, Engineering, and Medicine 2019)

a. Developing Quantum Simulation Applications

Many researchers noted the potential for quantum devices to improve our understanding of the science and engineering of a range of quantum systems. Key areas of opportunity include: chemical electronic structure calculations; nuclear vibration and rotation calculations for molecular spectroscopy; many-body chemical dynamics and chemical reactions; equilibrium properties, phase diagrams, and other materials properties; and other many-body dynamics and complex physical phenomena such as protein folding, high-temperature superconductivity, or nuclear fission. Simulation of these systems could be conducted via analog or gate-based quantum computers, quantum emulation, or simulations run on classical computers.

"[T]he answer to the question whether quantum mechanical resources of a quantum computer are required for accurate computation of molecular electronic properties is then also highly relevant. If the answer is affirmative, then this makes a perfect practical case for quantum computing. Otherwise, if we can show that quantum chemistry may be described classically in spite of its quantum nature, this can open the door to efficient exact solutions of these problems on a classical computer….Regardless of which way the question is resolved, the chemistry community stands to benefit, gaining a tool for simulating the electronic structure of molecules." *– Quantum Information and Computation for Chemistry (NSF 2016)*

b. Implementing Algorithms on Available Devices and Exploring Their Performance

This frontier also reflects the opportunities to advance and implement quantum algorithms and protocols for studying these and other quantum systems. Examples of quantum algorithms highlighted by the research community include quantum phase estimation, adiabatic state preparation, quantum imaginary time evolution, Hamiltonian simulation, real space simulation, and fermionic simulation. Hybrid quantum-classical approaches, which leverage quantum hardware for specific computational steps within a larger algorithm, include the variational quantum eigensolver (VQE) for ground-state energy optimization and the quantum approximate optimization algorithm (QAOA). A key element of this work will be establishing performance benchmarks for comparing different algorithms—both theoretically and empirically—and for comparing quantum algorithm outputs to the best-known classical results. Insights gleaned from this work could also inform new or improved classical computational approaches, helping to establish their capabilities and limitations.

"It is clear that one will rely on hybrid quantum-classical algorithms for many years to come, and there remain many open questions. One is how to best adapt quantum algorithms within existing quantum-classical frameworks."

– Enabling the Quantum Leap: Quantum Algorithms for Chemistry and Materials (NSF 2019)

This specific use case of NISQ devices provides a promising context to study how noise affects algorithm implementation, varies with different hardware configurations, and scales with system size. Research would benefit from empirically validated resource estimation strategies and the development of noise models in support of system validation—perhaps enabled by quantum and approximate circuit simulators. Quantum and classical simulation methods could also be used to model and optimize other quantum technology components, such as elements of quantum networks.

"Estimating resources for quantum algorithms using realistic quantum computing architectures is an important near-term challenge. Here, the focus is generally on reducing the gate count and quantum circuit depth to avoid errors from qubit decoherence or slow drifts in the qubit control system. Different types of quantum hardware support different gate sets and connectivity, and native operations are often more flexible than fault-tolerant gate sets for certain algorithms. This optimizing of specific algorithms to specific hardware is the highest and most important level of quantum computer co-design."

– Quantum Computer Systems for Scientific Discovery (NSF 2019)

A vision for this frontier is to demonstrate transformative quantum advantage for solving many-body quantum physics, quantum chemistry, or materials science problems, while improving researchers' abilities to engineer quantum hardware and software. It could also lead to models for how best to leverage quantum and classical computing resources complementarily for different kinds of problems. At a fundamental level, it will help to illuminate practical efficiency, accuracy, and precision limits of various methods for the computational study of quantum systems.

5. Harnessing Quantum Information Technology for Precision Measurements

> ***"State-of-the-art detectors and sensing are developed and employed to perform precision measurements that probe the laws of nature, to discover new particles and states of matter, and to develop capabilities for national security needs."***
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> *– Nuclear Physics and Quantum Information (Nuclear Science Advisory Committee, DOE, NSF 2019)*

Several cutting-edge metrology techniques already demonstrate key benefits from quantum control and QIS-related approaches, including atomic clocks, atom interferometers, magnetometers, and nuclear magnetic resonance (NMR) imaging systems. In this frontier, there are opportunities to improve precision and accuracy, develop new measurement modalities, improve methods for deploying these technologies in the field, and pioneer new applications for precision measurements. Key areas for exploration include: improving understanding of quantum-related limits to accuracy and precision for systems that can be deployed in the field to enhance navigation capabilities and for realization of standards; new modalities and applications for quantum sensing in situ and in vivo; and using entanglement and small-scale quantum computers to improve measurement technologies.

> ***"Attaining strong quantum enhancements in detection (e.g., quantum illumination) and in sub-Rayleigh quantum imaging represent significant challenges. Equally important is the construction of compact and robust quantum sensors, detectors, and imagers that are suitable for deployment in extreme environments."***
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> *– Future Directions of Quantum Information Processing. A Workshop on the Emerging Science and Technology of Quantum Computation, Communication, and Measurement (Virginia Tech Applied Research Consortium, DOD 2016)*

a. Deploying Quantum Technology for Improved Accuracy and Precision

Precision position, navigation and timing (PNT) applications already use quantum technology, but typically have practical constraints on size, weight, power and cost (SWAP-C). Bandwidth and reliability also matter. Members of the R&D community highlighted the exploration of attaining superior performance while satisfying overall package requirements as a critical direction that combines measurement science with quantum engineering. Positioning with millimeter accuracy and time-transfer with sub-nanosecond accuracy are available in the laboratory. However, their transition to practical quantum technologies, including designing and manufacturing rugged components for practical deployment, remains a challenge.

The entire set of System International (SI) units is now tied to constants that can be realized using quantum phenomena. This was a key reason for the redefinition of the kilogram in 2019. Connecting measurements in the field and on the factory floor directly to fundamental constants, by using QIS technology is a capability that will affect many fields of science and technology. New procedures can replace some time-consuming and elaborate calibration chains that were required for conventional approaches to metrology. This frontier will also leverage QIS to enable better precision and accuracy.

> ***"There are many laboratory demonstrations of quantum sensors with performance eclipsing fielded instruments, presenting opportunities for significant return on investment for engineering/development….Clocks, accelerometers, and magnetometers may be the best opportunities."***
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> *– Applications of Quantum Technologies (Defense Science Board, DOD 2019)*

b. Creating New Modalities and Applications for Quantum Sensing In Situ and In Vivo

While quantum advantages for sensing can be profound, part of this frontier entails identifying compelling use-cases that justify such quantum control as opposed to simply increasing flux or system size in standard approaches. Community-identified opportunities for exploration of precision measurements include high energy physics detectors; spectroscopy in chemistry labs; NMR techniques that combine cutting-edge spatial resolution with spectroscopic chemical shift sensitivities; geodesy and mapping; hydrology and mineral exploration; astronomy with quantum-enhanced telescopes; and a variety of bio-science applications ranging from electroencephalography (EEG) and magnetoencephalography (MEG) to studies of vision, photosynthesis, cellular dynamics, and magnetotaxis.

> ***"[H]ighly entangled systems of trapped ions can be used not only for quantum simulation…squeezing can perform extraordinarily precise measurements of force, with implications for searches of ultralight dark matter. Measurement of forces and fields is a basic operation of precision measurement and tests of fundamental symmetries, and some of the most exciting developments today take advantage of QIS techniques."***
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> *– Opportunities for Nuclear Physics and Quantum Information Science (DOE 2019)*

Researchers also recognized that new measurement modalities with quantum states of light, next generation atomic clocks, ultracold molecules, matterwave interferometers, color centers in crystals, and other systems, offer new capabilities and in some cases unprecedented precision and accuracy based on quantum coherence and superposition. However, to push this frontier even further, demonstrating the clear advantages for metrology using *entanglement* and many-body quantum states with non-classical correlations is seen as an important next step. Using squeezed vacuum states for Advanced LIGO is a major achievement in this direction. Exploring this frontier will enable improved performance with increasing degrees of entanglement, for useful applications in other scientific fields.

> ***"[S]cientists have created new opportunities for understanding and constructing quantum matter where many-body physics is no longer feared as a hurdle for precision measurement, but rather a new frontier to advance precision and accuracy."***

– Manipulating Quantum Systems: An Assessment of Atomic, Molecular, and Optical Physics in the United States (National Academies of Sciences, Engineering, and Medicine 2020)

c. Using Entanglement and Quantum Computers to Improve Measurements

Extending this concept to sensor arrays and other networked quantum systems (e.g., a network of entangled clocks) was identified by the research community as a cutting-edge opportunity for quantum metrology. In principle, optimal entanglement and measurement using quantum pre- and post-processing enable new domains of metrology. One suggested direction to explore is to use many-body quantum states, prepared with quantum circuits or small-scale quantum processors, to enable metrology. This would utilize cutting-edge QIS technologies to expand the precision measurement frontier.

"[Q]uantum technology is already having an impact in metrology and fundamental discovery (gravitational waves; LIGO). Five years is a very realistic timeframe for demonstrating the usefulness of quantum sensing technology in particular."

– RFI response

Progress in this frontier could lead to deployment of quantum sensors in new contexts and scientific domains. These devices are expected to push the limits of accuracy and precision, and to be realized via new underlying sensing mechanisms. In PNT, quantum technologies are likely to enable new levels of accuracy and time transfer capabilities in field campaigns. In metrology, quantum effects can be used to disseminate standards tied to defined SI units. Deployment of novel quantum sensing technologies is a major goal, as is identification of key use cases where entanglement and small quantum computers can improve metrological outcomes in applied settings.

6. Generating and Distributing Quantum Entanglement for New Applications

> ***"[O]nly a small number of scientific techniques and technological applications take advantage of the unique phenomena of quantum superposition and entanglement."***
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> *– Opportunities for Basic Research for Next-Generation Quantum Systems (Basic Energy Sciences Roundtable, DOE 2017)*

Progress in distributing entanglement has stimulated great interest in quantum networks as an enabling platform for quantum technologies. Interconnecting quantum devices by entangling qubits in separate modules may be a key pathway for scaling up quantum computers. Furthermore, distributing quantum information across spatially separated nodes is expanding the intellectual domain of quantum communication into the larger field of *quantum networking*. Inventing the physical layer components to distribute entanglement, developing algorithms, applications, protocols, and use cases for various quantum network systems, and understanding the integration of components and protocols into systems-level architectures are areas to explore in this frontier.

> ***"Quantum communication systems require repeaters and quantum memory…early technology demonstrations exist but repeaters and memory are far from levels of performance to be useful."*** *– RFI response*

a. Developing Foundational Components for Quantum Networks

RFI respondents and workshop reports named several foundational technologies that need further development before long-distance quantum networks can be realized. These range from quantum repeaters to memories and interconnects. An outstanding challenge is the development of quantum repeaters that are efficient and scalable, possess sufficient bandwidth, and are deployable. Likewise, plug and play modules for quantum memory remain an open R&D track, despite early progress on protocols.

> ***"Quantum interconnects (QuICs) present special challenges, as they must allow the transfer of fragile quantum states between different physical parts or degrees of freedom of the system. The diversity of QIT [quantum information technology] platforms (superconducting, atomic, solid-state color center, optical, etc.) that will form a 'quantum internet' poses additional challenges. As quantum systems scale to larger size, the quantum interconnect bottleneck is imminent, and is emerging as a grand challenge for QIT."***
>
> *– Development of Quantum InterConnects for Next-Generation Information Technologies (NSF 2019)*

b. Enabling Quantum State Transduction

Quantum interconnects are needed for coupling the often heterogeneous elements of quantum systems. Researcher-identified avenues for exploration include: coherent transduction of quantum states in atomic, optical, microwave, electronic, and solid state systems; quantum frequency conversion; quantum control of spin states, charge states, polarization, spatial modes, orbital angular momentum, and other degrees of freedom such as spectral-temporal encoding; higher dimensional qubits; and manifestations of entanglement with continuous variables. Furthermore, practical methods to generate and distribute entanglement must mitigate loss, noise, and errors to meet specifications (e.g., data processing rates and compounded efficiency or throughput) needed for applications such as those discussed below.

> ***"[L]arge-scale networks of superconducting quantum computers—quantum networks—are impossible without new ways to distribute entanglement over long distances, necessitating the development of efficient quantum state transduction."*** *– RFI response*

c. Integrating Quantum Networking Systems

Researchers have identified a need for infrastructure and engineering to facilitate entanglement distribution over a range of distance scales. Entanglement distribution over short ranges, from cryostat to cryostat, across integrated photonics devices, or between qubits in a single system are key challenges. Aerial and satellite platforms equipped for free-space communication of quantum states and for interconnecting local networks (e.g., terrestrial fiber-optics based quantum intranets) are also pursued in this frontier. Infrastructure and protocols for entanglement distribution and research testbeds or facilities (e.g., with switching, purification, interconnections, and hybrid classical-plus-quantum methods) require substantial exploration.

> ***"[O]ptical telescopes connected across the globe in a quantum network could allow determination of apparent positions of stars with unprecedented precision. Evolution of the above ideas will depend very much on theoretical efforts to develop concepts of experiments and to evaluate their sensitivity."***
>
> *– Quantum Networks for Open Science Workshop (DOE/ASCR 2019)*

d. Exploring Quantum Networking Algorithms, Applications, Protocols, and Approaches

Members of the R&D community also pointed beyond the physical layer, towards opportunities to explore applications of quantum networks such as distributed quantum computing, blind quantum computing, end-to-end quantum encryption, secure software distribution, and entangled sensor arrays. In addition to entirely new algorithms and applications, networking protocols may need refinement or large-scale revision to work on nascent quantum network testbeds. A variety of network architectures may be envisioned, or encountered in the real world, and algorithms for distributed quantum computing will need to account for network topologies. Applications of sensor networks, including long baseline telescopes, Heisenberg-limited interferometry, and improved clock synchronization align both here and with frontiers 1, 2, and 5.

> ***"Quantum networking resources such as entanglement and teleportation are still not well understood among domain scientists who could exploit them to solve new classes of scientific problems."***
>
> *– Quantum Networks for Open Science Workshop (DOE/ASCR 2019)*

A key opportunity on this frontier is for researchers to develop and validate a sufficiently complete set of foundational quantum networking components that work together so long-distance quantum networks can then be designed, established and operated to distribute entanglement to multiple nodes on (and around) Earth. During the same period, novel algorithms could enable exploration of new applications for quantum networks. Several concepts such as blind quantum computing and quantum-enhanced telescopes could be tested and improved with empirical studies using quantum network testbeds or prototypes. Feasibility studies for space-based missions to distribute entanglement will combine concepts from quantum engineering (and technology readiness levels) with fundamental studies of entanglement generation, distribution, and utilization. Furthermore, new concepts for sensor arrays and distributed quantum computers are likely to be discovered as proofs-of-principle unfold.

7. Characterizing and Mitigating Quantum Errors

"The grand challenge…for the Nation is understanding and experimentally realizing quantum error correction and, ultimately, fault tolerance at large scales."

– RFI response

Quantum systems are inherently sensitive to their environment, which inevitably leads to errors. This is a fundamental issue because controlled interactions make qubits useful, yet untamed interactions cause decoherence. The frontier of preserving coherent superpositions and entangled states long enough to perform valid quantum computations therefore relies on understanding how to diagnose, avoid, and mitigate quantum errors. Fighting such decoherence is essential for quantum metrology and networking, too. In addition to materials science and topological protection discussed in Section 3, improved control will be needed with explorations ranging from quantum error correction to decoherence-free subspaces and new approaches for fault-tolerant quantum computing. Key themes include: optimal characterization and control for multi-qubit systems, including use of measurement, feedback, and novel encodings; development and exploration of novel universal computing approaches in the fault-tolerant domain; and use of current devices to expand the limits of performance for qubits.

"A variety of techniques have been used to characterize qubits and the operations (gates) performed on them. Currently, the two dominant techniques are randomized benchmarking (RB), and gate set tomography (GST)….Future protocols that directly probe the effect of changing how we implement gates will be critical for improving our devices and stabilizing them against drift."

– ASCR Report on a Quantum Computing Testbed for Science (DOE 2017)

a. Characterizing and Controlling Multi-qubit Systems

Exploring how, and to what extent, characterizations of 2-qubit gates enable predictions of system performance may be key for designing and controlling quantum computers at scale. New techniques may be needed to fully predict how errors propagate in complex quantum processors and networks. Characterization and modeling can guide the development of optimal gate operations, help mitigate coherent errors and crosstalk, and stabilize devices against drift. Quantum error mitigation opportunities named by members of the R&D community include improved materials (Section 3), multi-qubit measurements and feedback, improved control techniques and platform designs, and extensions to the fundamental theory of quantum error correction with novel encodings and protocols that may improve the threshold for fault-tolerance, and reduce overhead costs in terms of resources (qubits, gates, and times) for implementing logical qubits.

> ***"Uncovering new types of error correction and mitigation suitable for near-term simulators is an open problem. Furthermore, there is a natural trade-off between the coherence of a system and the degree of programmability and tunability. Understanding and exploring this trade-off is important in developing quantum simulators. There is also an opportunity in the development of algorithms with this trade-off in mind, leading naturally to the concept of co-design, i.e., developing applications for specific hardware and architectures. Such efforts will benefit from the convergence of various areas of expertise, including experimental physics, quantum control theory, computer science and software, and engineering."***
>
> *–Quantum Simulators: Architectures and Opportunities 2019*

b. Approaching the Fault-tolerant Domain

Quantum error mitigation will enable explorations of universal computing with systems approaching the fault-tolerant regime. Experiments in this direction can stimulate co-design efforts, for example with error-aware implementations of algorithms supported in ways that minimize use of particular gates, operations, or states that are prone to decoherence (as mentioned in Sections 2 and 4). Several R&D community inputs pointed out that developing a full stack—from physical to logical qubits and compilers with software to implement higher-level quantum circuits—opens a series of new directions for research. Explorations include new performance benchmarks (e.g., quantum volume or test-piece calculations) where results depend on error mitigation. Verification and validation will take on new urgency as fault-tolerant modules and co-processors become available. Error-correcting quantum repeaters and fault-tolerant approaches for adiabatic quantum computing and analog quantum simulation are related research challenges.

> ***"Research on quantum error correction can benefit enormously from using the current and near-term quantum computer hardware (often referred to as Noisy Intermediate Scale Quantum [NISQ] computers), which will allow error correction codes and protocols to be developed from in situ studies on real hardware rather than using idealized theoretical models."*** *– RFI response*

c. Using Current Devices to Expand the Limits of Qubit Performance

At the same time, even as error-corrected systems are in development, several voices have been clear that there is much to be learned from exploring newly available, albeit imperfect, technologies. Problems can be mapped to device-specific architectures to seek value in the near-term (as mentioned in Section 4). Explorations identified in this direction include examining what amount of error mitigation is required to realize useful computations, development of useful low-depth algorithms (e.g., approximate optimization), and finding practical strategies for tailoring quantum error mitigation techniques to specific hardware for specific applications.

"Quantum states are fragile; a great challenge is developing devices and techniques to reduce noise in quantum devices. All avenues should be explored, including topological materials and/or device designs that promise to reduce quantum state fragility, new error mitigation techniques, and quantum error correction codes."

– RFI response

In pursuit of fault-tolerance, both evolutionary and revolutionary pathways are being explored. Experiments with state-of-the-art qubits can push the envelope of performance, even with incremental developments. Improvements in support technologies such as lasers, microwave electronics, cryogenics, and foundries can provide valuable steps in this direction. Work at testbeds can hone quantum control methods (e.g., dynamical decoupling, pulse sequencing, and error correction), by facilitating learning through experimentation to develop and apply device-specific models of noise, control, and errors. Some of the more revolutionary approaches that were named include topological qubits (touched upon in Section 3), use of cluster states and symmetry-protected states as a resources for measurement-assisted quantum computing, studies of higher dimensional qubits such as oscillator encodings, and other novel qubit architectures.

"Quantum computers are intrinsically far more vulnerable to error than classical computers. Thus our hopes that large-scale quantum computers will be built and operated someday are founded on the theory of quantum fault tolerance, which establishes that reliable quantum computation is possible when the noise afflicting the computer has suitable properties. Recent insights are broadening the class of noise models for which fault-tolerant quantum computing is provably effective, and clarifying the overhead cost of overcoming noise."

– Report of the Workshop on Quantum Information Science (NSF 2009)

The vision for this frontier is to develop reliable logical qubits and other techniques for achieving fault tolerance. Development of more sophisticated error-corrected systems will benefit from improved methods for characterizing system performance and error propagation. Error corrected networks and processors would serve as a next generation of hardware to support testing and stimulate development of new algorithms and protocols for verification and validation. While both incremental and revolutionary approaches to enable large-scale fault-tolerant systems will continue to be explored, near-term applications for smaller-scale fault tolerant machines could be tested with a variety of architectures and contexts. Aside from its practical importance for quantum technologies, theoretical work on quantum error correction may stimulate further discoveries about fundamental mathematical and physical foundations of the universe, as discussed more in Section 8.

8. Understanding the Universe through Quantum Information

"This 'entanglement frontier' is exciting because, knowing that highly entangled systems of many particles are hard to simulate with digital computers, we may anticipate that surprising, illuminating, and useful new phenomena will occur in sufficiently complex quantum systems."

– Grand Challenges at the Interface of Quantum Information Science, Particle Physics, and Computing (DOE Study Group Report 2014)

QIS is a marvelous source of new perspectives on the mathematical and physical foundations of the universe. It has begun to transform the way we think about computation by exploring the limits of what can be computed with physical systems, and could provide new opportunities for testing quantum mechanics and other fundamental scientific theories in new regimes. Quantum technologies also provide new ways to search for physics beyond the standard model of particles and fields, often via precision measurements. In this frontier, foundational QIS research opens new scientific vistas. Three major themes underlie this frontier: exploring the mathematical foundations of computation and information through the lens of quantum computing and quantum information theory; using concepts from QIS and new applications of quantum simulation to explore the limits of physical theory, from dark matter to quantum gravity; and leveraging precision measurement and many-body quantum systems to test the expectations of the standard model of particle physics, and search for phenomena beyond the current model.

"Some important areas of research in entanglement theory aim to: deepen understanding of fundamental physical and mathematical aspect of quantum vs classical correlations (notably, 'monogamy' of entanglement, also in relation to the 'quantum marginal problem,' or relevant to temporal as opposed to spatial correlations); further push aspects of the characterization and quantification of entanglement within a resource-theory framework (with possible ramifications ranging from quantum thermodynamics to high-energy physics); ultimately, explore generalizations of the very notion of entanglement, that may incorporate 'locality constraints' more general than currently envisioned and may allow [researchers] to unveil the nature and role of entanglement in topological quantum matter or in the emergence of space-time geometry."

– Executive Summary of 2015 NSF Conference on Mathematical Sciences Challenges in Quantum Information (NSF 2015)

a. Exploring Mathematical Foundations of Computation and Information

Fundamental questions about computation (e.g., *Can quantum computers efficiently simulate any process that occurs in nature?* And, *for what computations might exponential speedup be achieved over classical approaches?*) raised in QIS workshops touch on quantum complexity theory, quantum resource theory, and quantum computing. Fundamental research on the cybersecurity implications of quantum technologies, and mitigation strategies, is a common area of interest for mathematics, computer science, and QIS experts. Open questions on the theoretical limits of error correction and topological quantum computing, and the universality of adiabatic quantum computation are also discussed in the RFI responses and workshop reports.

"Although several theoretical models of quantum computation exist and are well-studied, such as quantum circuits, topological quantum computation, dissipative quantum computing, quantum walks, and the adiabatic quantum computing model, each model has its pros and cons in the context of an actual hardware implementation. The space of possible quantum computational models is far from fully charted, and developing models in a co-design approach with quantum hardware development may benefit both."

– 2015 DOE ASCR Workshop

Investigating how complex quantum states can be prepared or efficiently approximated could inform the development of performance benchmarks, and also elucidate the origins of thermodynamics and non-equilibrium dynamics (e.g., via studies of time crystals, chaos, pre-thermalization, and quantum information scrambling). At the same time, advances in QIS are spurring improvements in classical computation—for example, with simulated quantum annealing or new approaches to Boson sampling that raise expectations for demonstrable quantum advantages. One workshop report suggested QIS can help answer the question, "Are there other fundamentally different models of computing that have not yet been developed?"

b. Expanding the Limits of Physical Theory

"[T]he field should think carefully about which key, longstanding questions in physics could be solved using quantum technology." *– RFI response*

Research in QIS has begun to shed light on other interwoven areas of physics and other scientific fields. For example, research on entanglement can address fundamental questions about the emergence of spacetime, entropy of black holes, correspondence with wormholes, and the foundations of thermodynamics. Research areas described in workshop reports and RFI responses include: how quantum computational analysis of quantum walks can extend scattering theory; how quantum error correction codes and multipartite entanglement can inform searches for new phases of matter and topological states; and how the anti-de Sitter/conformal field theory (AdS/CFT) correspondence and associated dictionary for translating results can be used to inform quantum gravity theory, and explore properties of gauge theories at strong coupling where perturbative analysis is not possible. Furthermore, quantum networks and computers can test quantum mechanics in new regimes by exploring fundamental limits for coherence and entanglement. QIS can help explore the question, "What credible deviations from conventional quantum theory are experimentally testable?" (e.g., gravitationally induced decoherence, spontaneous wavefunction collapse models, or nonlinear corrections to the Schroedinger equation).

"Focus on simulating quantum systems that cannot be studied in a lab, such as black holes." *– RFI response*

c. Testing the Standard Model of Particle Physics

For fundamental physics, in addition to improvements in gravitational wave detection and precision measurements of fundamental constants, QIS can provide new approaches to testing expectations from the standard model of particle physics, and conjectured extensions to that field. Examples include: searches for dark matter and dark energy; tests of fundamental symmetries such as charge, parity, time (CPT) and Lorentz invariance; and searches for variation of fundamental constants in time or space. QIS methods such as coherent spectroscopy, atom interferometry, or advanced magnetometry enable searches for permanent electric dipole moments of fundamental particles (tests of CP-violating physics), measurements of the fine structure constant (useful for tests of quantum electrodynamics), searches for axion-like particles (dark matter candidates), and fifth-force searches. This frontier will improve our understanding of the foundations of the physical universe.

"Ultra-precise measurements of quantum phenomena can be used as extremely powerful probes of new physics at very high energy scales, e.g., by testing fundamental physical symmetries and laws, and by searching for new phenomena such as that associated with the 'dark sector.' For example, one of the most exciting opportunities at the Quantum Frontier is searches for an electric dipole moment (EDM) of the electron, as well as related quantities in atomic nuclei, which arise at a measurable level only from charge-parity (CP) violation beyond that in the Standard Model." *– DOE Quantum Sensors Report*

This frontier recognizes the value of QIS R&D for deepening foundational knowledge, with the potential to yield unexpected discoveries, new scientific concepts and tools that translate to other disciplines, and yet unknown applications and technologies downstream. QIS research provides opportunities to test, refine and extend fundamental mathematical and physical theories that we use to describe the nature of the universe; develop a more complete understanding of what can and cannot be efficiently computed; and elucidate the value of quantum resources for computing, engineering and science itself.

SUMMARY AND OUTLOOK

Within these frontiers, what are the most pressing grand challenges facing QIS? The answer to that depends on one's objectives. The breadth of responses and details of R&D pursuits encouraged in the RFI responses and QIS workshop reports provide a broad range of opportunities for research agencies to consider and pursue according to their missions. This community input, received in multiple venues from U.S. and worldwide technical experts, has been organized into eight technical areas identified here as quantum frontiers. The frontiers are broad areas at the forefront of QIS that contain numerous quantum questions that should be explored early on, and hard technical challenges that must be overcome before applications can be developed.

Ensuring sustained American leadership in QIS hinges on coordinating core research programs across the pillars of QIS U.S. Government funding: the civilian, intelligence, and defense agencies. For each mission, the grand challenges and priorities may be different, but there are common hurdles where coordinated efforts can accelerate progress. The synopsis of R&D community perspectives presented here is intended to gently guide this coordination by pointing towards quantum frontiers to explore.

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The National Quantum Initiative (NQI) provides an overarching framework to strengthen and coordinate QIS R&D activities across U.S. Departments and Agencies, private sector industry, and the academic community. The NQI entails a whole of government effort to accelerate quantum research and development, as legislated by the NQI Act of 2018. The NQI Act authorizes the National Science Foundation (NSF), the Department of Energy (DOE), and the National Institute of Standards and Technology (NIST) to strengthen QIS Programs, fund Centers, and support Consortia. The NQI Act also calls for a coordinated approach to QIS R&D efforts across the Federal Government, including the civilian, defense, and intelligence sectors. NQI activities are coordinated through the NSTC Subcommittee on Quantum Information Science (SCQIS), with support from the National Quantum Coordination Office (NQCO).

ABOUT THE NATIONAL QUANTUM COORDINATION OFFICE

The National Quantum Coordination Office (NQCO) coordinates QIS activities across the U.S. federal government, industry, and academia. Legislated by the NQI Act of 2018 and established within the White House Office of Science and Technology Policy, the NQCO oversees interagency coordination of the NQI Program and QIS activities; serves as the point of contact on Federal civilian QIS activities; ensures coordination among the consortia and various quantum centers; conducts public outreach, including the dissemination of findings and recommendations of the NSTC Subcommittee on Quantum Information Science and the NQI Advisory Committee; promotes access to and early application of the technologies, innovations, and expertise derived from U.S. QIS activities, as well as access to quantum systems developed by industry, universities, and Federal laboratories to the general user community.

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