2024

QUANTUM INFORMATION SCIENCE APPLICATIONS ROADMAP

For the:
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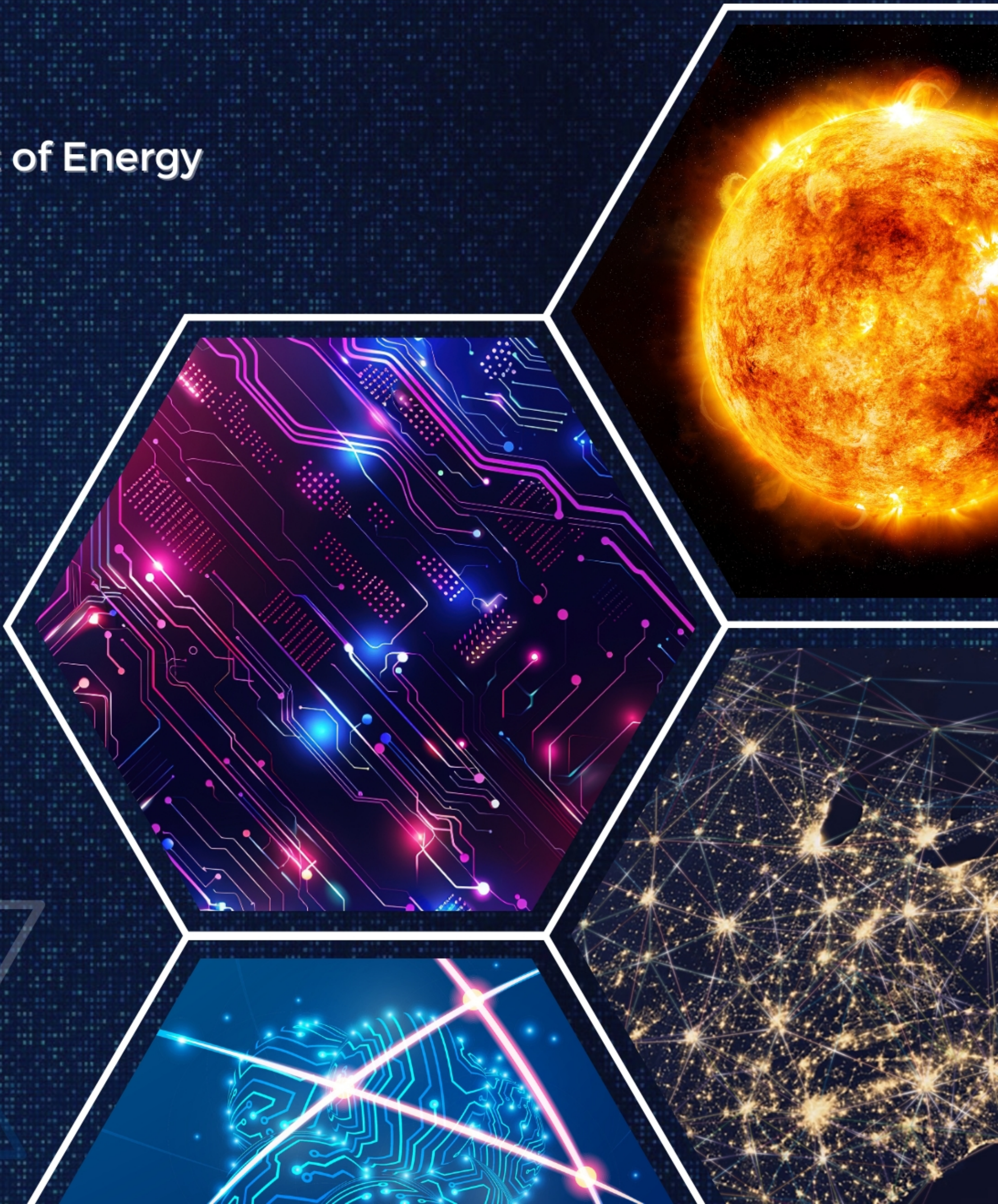

Department of Energy
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Washington, DC 20585

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Quantum information science (QIS) opens the door to revolutionize the way we process, store, and transmit information. The U.S. Department of Energy's (DOE) Office of Science plays a key role in QIS research & development (R&D). The Office of Science has provided sustained support for the development of QIS, leading to groundbreaking scientific discoveries and significant advances in our understanding of the natural world.

To inform QIS program activities, the Office of Science formed a committee of QIS experts spanning industry, academia, and DOE’s national laboratories to develop a roadmap for potential quantum applications relevant to DOE’s mission. I greatly appreciate the committee’s tireless efforts to deliver this report.

The following roadmap details technical challenges, guideposts, and milestones related to applications in **quantum computing, quantum sensing, and quantum networks**. The committee considered many factors and sources including scientific literature, detailed interviews with experts from a variety of related science and technology areas, and DOE’s current and past contributions to QIS and related fields.

This report provides us with several key takeaways. Notably, the precise nature and the full extent of quantum advantages, and the resources required to realize the impact of these technologies on DOE-related problems, remain an active area of research. While QIS has undergone significant fundamental advances over the last few decades, it is at a nascent stage of technology development. There are multiple fundamental and engineering challenges remaining. Overcoming each of these challenges will require substantial R&D, further scientific discovery, and innovation. For this reason, the timelines reported in the roadmap carry uncertainty. Advances need to be made, not only in QIS science and technology, but adjacent fields such as packaging, systems engineering, optical modulators, sources, detectors, integration, controls, new materials, etc. Additionally, advancements in one technology area will benefit others. For example, advancements in quantum computing will likely advance progress in quantum repeaters for networking.

This report details the scientific challenges underpinning technical milestones that need to be addressed for real world applications of QIS. DOE’s Office of Science is committed to supporting innovative research and working with stakeholders across the federal government and industry to realize the potential of QIS technologies for the nation.

Sincerely,

Harriet Kung
Deputy Director of Science Programs,
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2024 Quantum Information Science Applications Roadmap

for the U.S. Department of Energy

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Chapter 1

Executive Summary

The U.S. Department of Energy (DOE) is charged with "*ensur[ing] America's security and prosperity by addressing its energy, environmental and nuclear challenges through transformative science and technology solutions*" [1]. Historically, this broad mission has required significant agility from the DOE to adapt and respond to the challenges the nation has faced over many decades. The DOE's past and ongoing support for Quantum Information Science (QIS) perfectly illustrates this strategy. The field of QIS pursues the utilization of fundamental quantum phenomena in order to build more powerful computers, better sensors, and networks connecting these devices at the quantum level. The scientific and technological advances already underway and anticipated down the road include applications and capabilities of immediate interest to the DOE's mission.

In early 2024, the DOE tasked a committee of twenty experts from academia, national laboratories and industry to create roadmaps for applications within the quantum information science (QIS) field.[1] This document is the product of four months of intensive work by the committee, enriched by consultations with numerous additional experts and leaders in the field. The broadly shared consensus: QIS is a vibrant field with exciting recent progress on multiple fronts. QIS holds the promise of revolutionary breakthroughs that could rival the impact of the transistor's invention and the development of the microprocessor, which are foundational to much of today's technology.

Most quantum applications relevant to the DOE currently fall in one of three QIS application areas: quantum computing, quantum sensing, and quantum networking. The roadmaps in Chapters 2–4 discuss the state of the art and future outlook in these three areas. A summary of the central points follows.

Quantum Computing extends the frontiers of computation beyond the reach of traditional computers. Despite significant advances in classical computing, including artificial intelligence and machine learning, there are inherent limitations to the problems classical computers can solve. Quantum computers, operating on entirely different principles, have the potential to break through these barriers. Building on recent impressive progress in quantum computing, the realization of this long-term goal requires further investment into coordinated research at all levels as outlined in Chapter 2, from theory and algorithms to materials science and hardware development. With the appropriate support, it is very likely that breakthroughs will continue to occur over the next decades. With existing quantum computing platforms advancing on their trajectories towards maturation, the vision of large-scale, fault-tolerant quantum computers is becoming increasingly concrete. Exciting prospects exist for exploring the utility of different quantum processors of increasing sizes and capabilities for DOE-relevant QIS applications including, e.g., simulations for chemistry, materials, and calculating the strong forces in fundamental particle and nuclear physics.

Quantum Sensing uses new insights from quantum information science to provide fundamentally new methods of measurement. Using qubits as sensors allows for some of the most precise measurements achieved

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[1] Per DOE instructions, this document does *not* consider the topic of QIS workforce development.

by humanity, enabling technologies such as atomic clocks and their critical applications. The high spatial resolution achievable with several types of qubits also opens opportunities for sensitive, microscopic probes of materials, chemical samples, and biomedical diagnostics. The intrinsic stability, reproducibility, and robustness of certain qubit types render them excellent sensors that can be deployed in challenging and extreme environments, such as underground, in space, and near plasmas. Furthermore, there is a fundamental bound on the precision and sensitivity achievable with classical sensors, known as the "standard quantum limit." Quantum sensing provides a method to beat this bound by exploiting quantum correlations, thus expanding the observable universe. Chapter 3 outlines the fundamental research needed for developing and discovering new sensors, devising new sensing protocols and modalities, and improving these sensors through materials purification and device fabrication, as well as translational research to deploy and apply quantum sensors to a large range of applications for science and commercial purposes. Using quantum sensors for advancing science and wide-scale commercial deployment will require broad, ambitious investments in collaborative, interdisciplinary work that spans classical engineering and quantum science.

Quantum Networks seek to leverage the benefits gained by linking quantum resources. Such networks serve as glue to enable computing and sensing applications to scale and reach their full potential, as well as facilitate novel applications between computers and sensors that result in exponential advantages. Application examples discussed in Chapter 4 include connecting sensors via quantum channels to boost resolution and precision (improving telescopes to detect smaller and fainter objects, increasing timekeeping precision via networking atomic clocks), connecting sensors to quantum computers to increase sensitivity and reduce the number of measurements required for the desired precision (e.g., learning from quantum states with fewer measurements, detecting very faint signals in particle accelerators), and connecting quantum computers via quantum channels (improving computing power beyond what is possible on a single machine by linking machines, analogous to classical high-performance computing clusters used today). To realize these types of applications, investments are needed in hardware and theory to improve the production, routing, and repetition of quantum optical signals necessary for establishing entanglement between arbitrary nodes on the networks (the so-called network *core*), as well as the translation of signals from the network core to quantum systems at the nodes (the network *edge*).

Chapter 2

Quantum Computing to Extend the Frontiers of Computation

2.1 Introduction

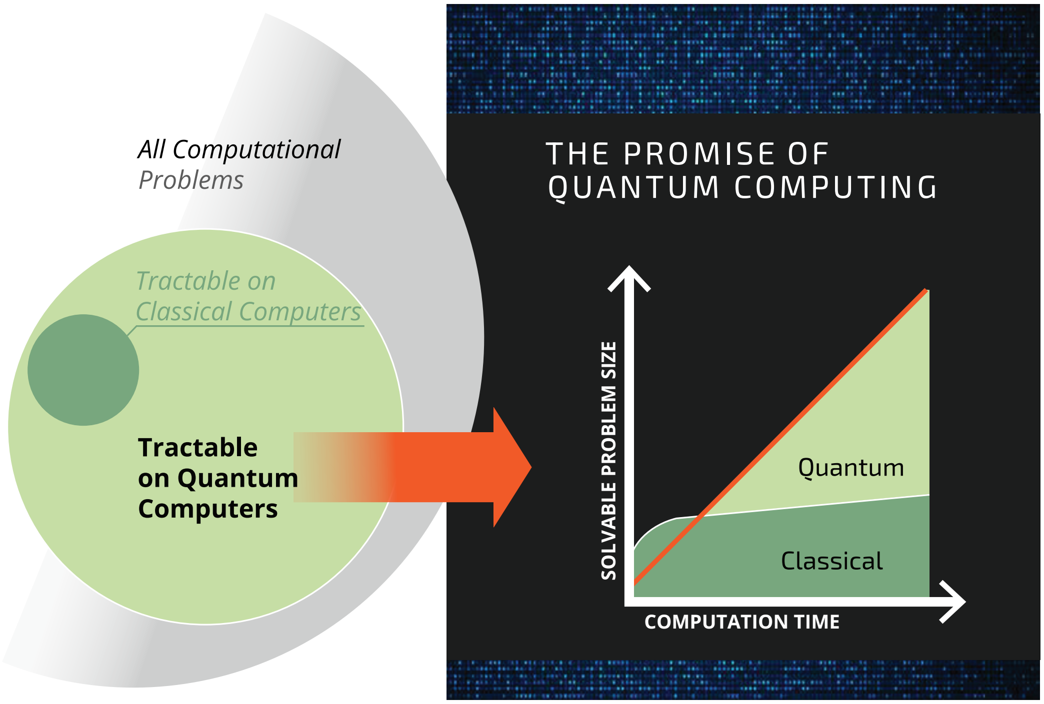

Fig. 2.1: Quantum computing extends the set of tractable computational problems. **Left**: From the set of all problems (light gray circle), ordinary computers only enable us to obtain solutions to a subset of tasks (dark green circle). Quantum computers will enlarge this set (light green circle) and thus facilitate the solution of problems otherwise intractable. **Right**: Certain tasks require impossibly long times on ordinary computers ("classical") for realistic problem sizes, but will be tractable on a future quantum computer ("quantum") due to the substantial improvements in computational efficiency.

Progress in science and technology is intimately linked to the fundamental question, "What can be computed and how difficult is it to obtain concrete solutions?". Despite the impressive power of modern supercomputers, certain computational tasks are still considered intractable. By leveraging the quantum-mechanical phenomena of superposition, interference, and entanglement, quantum computers are *fundamentally differ-*

ent [2] from all classical computing models (including conventional supercomputers, special-purpose accelerators like GPUs, artificial intelligence, etc.) and will enable us to address a broad range of scientific questions beyond our current reach (Fig. 2.1). Understanding which scientific areas will benefit the most from quantum computers, the precise nature of these quantum advantages, and the resources required to realize quantum computers capable of impacting DOE problems remains an active area of research [3–17]. Nevertheless, the research community has identified many scientific problems for which it is anticipated that quantum computers will have an impact [19–21].

Realizing quantum computing's full ambitious potential requires building large-scale quantum computing systems with excellent controllability. Various types of qubits currently under development include superconducting circuits [22, 23], trapped ions [24–26], neutral atoms [27, 28], quantum dots [29–31], and other emerging platforms [32–34]. In the last decade, science and industry have progressed from the first prototypes to quantum processors with hundreds of qubits. Much of this effort in the research community has been made possible through the activities of the DOE. In particular, the DOE has created five National QIS Research Centers (authorized by the National Quantum Initiative Act) [35–39], testbeds at Lawrence Berkeley National Laboratory [40] and Sandia National Laboratories [41], a user program (QCUP) at Oak Ridge National Laboratory [42], as well as provided funding for individual researchers and small research teams. In addition, individual labs in the DOE system have explored the applicability of quantum computing to lab-relevant problems [43, 44].

The trajectory of quantum computing over the past decade is somewhat reminiscent of the early days of semiconductor devices and integrated circuits which ultimately led to the large-scale microprocessors that are ubiquitous today. Building large-scale and accurate quantum computers will have major impact on our understanding of science; the development thereof still requires significant research effort and broad investments into the full "stack" of technologies needed for quantum computing—covering materials aspects, devices and their integration, architecture considerations, algorithms, applications and theory, and so on.

Current quantum computers, with their limited ability to run complex circuits due to noise [45], are on the cusp of demonstrating "beyond-classical computations" (computations which are out of reach for classical approaches) [46–53]. Access to quantum computers, provided by testbeds at national labs [40, 41], cloud-based systems from industry [54–65], or on-premises installations from the same, have spurred diverse research into their utility [66–81], the development of tailored algorithms for them [66,82,83], and the creation and advancement of error mitigation techniques [84–88] to address the impact of noise. Leveraging all of these to make current and near-future quantum computers practically useful is a key area of research.

In parallel, concerted efforts are ongoing to implement the logical DiVincenzo criteria [19,89],[1] to demonstrate quantum error correction (QEC) and fault-tolerant quantum computing. The past several years have seen advances in QEC theory [90–94] as well as software and hardware tools for decoding and correcting errors [95–99], leading to demonstrations of key computational steps involved in QEC [100–112]. Continuing and enhancing these demonstrations is a critical step for bringing quantum computing to full fruition.

Thus, the current era now involves much activity both investigating the usefulness of available quantum computers as well as working to bridge towards fault-tolerant computers. For many applications of quantum computers, such as those described in Section 2.5, the feasibility of a positive impact by quantum computing has been validated. Realizing them generally includes algorithms, software, and hardware development, which builds on and is strengthened by DOE's prior investments. This effort will require contributions from industry, university researchers, and scientists at national laboratories in the US and around the world.

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[1] The logical DiVincenzo criteria outline the requirements necessary for error-corrected quantum computation.

2.2 Current hardware frontiers

Building a quantum system with sufficient capabilities to tackle the examples in this roadmap is a grand challenge. There have been several recent demonstrations of "logical qubits" on various platforms [108, 113–116]. Moving beyond these early demonstrations toward large, fault-tolerant quantum computers requires major efforts to improve every part of the hardware, as well as new, creative ideas at every layer of the stack, from materials, devices, and packaging, to systems engineering, hardware efficient architecture, and control, to software stacks, error correcting codes, and application-specific algorithms.

At the materials level, impurities and defects plague many qubit platforms and lead to time-varying behavior and instability that degrade the quantum computer's performance [117]. Improving device performance requires a better understanding of how to avoid, control, and eliminate these sources of noise. These efforts will require control over the materials properties to an exquisite degree, as well as device fabrication methods that do not degrade material properties or introduce new sources of noise. A collaborative co-design approach combining material resilience and high-precision fabrication with device and processor architectures that lessen the impact of noise will be important for advancing quantum hardware. Superconducting qubits can be sensitive to abrupt energy deposits caused by cosmic rays and ambient radioactivity [118–120]. Similar co-design efforts can be employed to understand and mitigate the impact of such radiation on large-scale quantum processing units based on superconducting qubits [121, 122].

At the devices level, new innovations in qubit design, couplers, and readout methods will help improve resilience to noise, long-term stability, gate fidelity, and connectivity. As another example, ion traps are generally compatible with CMOS processing, aiding fabrication at scale. However, issues remain to improve the reliability of such devices [123], and there are potential gains in seeking alternative materials and methods of trap fabrication [124]. Designing and modeling device geometries to match long-term architecture demands continues to be a very active area of research.

There are also many additional supporting classical technologies that require miniaturization, integration, and scaling to build a large-scale quantum machine. These devices are dependent on the specific quantum hardware platform, but include, among others, microwave attenuators, amplifiers, optical modulators [125, 126], switches, waveguides [127, 128], and detectors [129–131]. Integrating these components will also require new packaging techniques, new ways to handle the increased number of control signals sent to devices, and likely new materials.

Ultimately, similar to classical high-performance computing clusters, quantum computers will have modular designs with interconnects between processors [22, 26]. While there has been some work on interconnects of various qubit platforms, each qubit type has different requirements, and increasing the reliability and fidelity of such devices is still necessary (see Sec. 4.6.1).

Building quantum control hardware, the part of the system necessary for converting between classical instructions and quantum instructions, presents many new challenges as systems scale. The DOE has supported the development of several successful control hardware schemes that have begun to address these challenges [132–134], but continued research [135] is needed for simplifying calibration routines, improving timing and synchronicity, delivering low-latency classical processing of measurement results (critical for quantum error correction) of large systems, and reducing per-qubit costs.

Computer architecture became a stand-alone displine in the early days of classical microprocessors. Similarly, as quantum processors become more complex, building larger-scale systems will benefit from a broad program of quantum computer architecture that rethinks processor design and control, particularly from the point of view of hardware-efficient quantum error correction and modular quantum computing with quantum interconnects.

2.3 Past DOE successes

The Department of Energy plays a central role in the US quantum computing research ecosystem. This section highlights a subset of notable scientific advancements to illustrate the successes and payoffs from prior and ongoing DOE funding.

After the 2018 passage of the National Quantum Initiative Act, the DOE was granted authority to establish new and ambitious research centers, leading to five National Quantum Information Science Research Centers (NQISRCs): Co-design Center for Quantum Advantage (C2QA), led by Brookhaven National Laboratory [35]; Next Generation Quantum Science and Engineering (Q-NEXT), led by Argonne National Laboratory [36]; Quantum Systems Accelerator (QSA), led by Lawrence Berkeley National Laboratory [37]; Quantum Science Center (QSC), led by Oak Ridge National Laboratory [38]; and Superconducting Quantum Materials & Sciences Center, led by Fermi National Accelerator Laboratory [39]. These centers, alone with DOE-established testbeds, have galvanized the QIS community and led to breakthroughs across many dimensions of scientific research.

Firstly, new facilities and physical infrastructure have provided researchers with a foundation for novel science and engineering. The Quantum Garage at the SQMS Center, for example, is enabling QIS collaborations between the scientific community and industry [136]. The Q-NEXT Center established two new quantum foundries (at Argonne and SLAC) for advanced device fabrication [137, 138], and the DOE supported two new laboratories for characterizing quantum devices in low-background radiation environments: QSC's Quantum Underground Instrumentation Experimental Testbed (QUIET) [139] and a testbed at Pacific Northwest National Laboratory's Shallow Underground Laboratory [140]. Meanwhile, DOE quantum testbeds, the Advanced Quantum Testbed (AQT) at Lawrence Berkeley National Laboratory [40] and the Quantum Scientific Computing Open User Testbed (QSCOUT) at Sandia National Laboratories [41], provide researchers access to quantum processors with unrivaled transparency and robustness. Additionally, Oak Ridge National Laboratory [42] has been instrumental in connecting researchers to publicly available hardware.

Foundational materials innovations for improved qubit performance are a common theme across all efforts. To extend lifetimes of superconducting qubits and resonators, C2QA-enabled research developed a record-breaking tantalum-on-sapphire materials system [141, 142], while SQMS, inspired by decades of research in accelerator physics, has demonstrated new surface encapsulation techniques [143]. More broadly, C2QA has established a robust playbook for materials characterization and discovery utilizing user facilities such as NSLS-II and CFN at BNL. Q-NEXT researchers have boosted the coherence of optically-defined niobium trilayer junctions, which could allow for highly manufacturable superconducting qubits [144]. Meanwhile, a QSC effort to identify new materials platforms for topological qubits has characterized an exchange coupling in Bi_2Se_3/EuSe heterostructures, which could one day form the basis for Majorana modes [145].

Groundbreaking progress has also been achieved in building quantum computing devices. The QSA Center has created a quantum simulator based on 256 neutral atoms [146], designed and fabricated a trap for 200 ions [147], and built an advanced 4×4 flip-chip array of superconducting qubits featuring a crosstalk reduction by a factor of 50. SQMS's Quantum Garage is now hosting home-built 2D and 3D superconducting QPUs with advanced materials [136]. C2QA has built new superconducting devices implementing bosonic codes, pioneering a new dual-rail approach [148] and demonstrating a 2× suppression in logical error rates using tantalum qubits [115].

Improvements in control hardware and noise mitigation will be necessary to make advanced devices practical. A collaboration between QSC and SQMS led to the development of a highly successful open-source control hardware platform known as Quantum Instrumentation Control Kit (QICK) [132]. Researchers at QSA and the AQT also developed a next-generation control system known as QubiC [149], along with advanced packaging and flexible wiring. AQT and QSCOUT worked with an industry partner to produce noise-aware circuit compilation software, improving the performance of the testbed quantum processors [150].

Finally, algorithms research at DOE centers has led to multiple breakthroughs. QSA has created and demonstrated protocols for proof of quantumness [151]. SQMS researchers developed benchmarks for scaling up variational quantum eigensolver methods for the Kitaev model and implemented them on hardware systems [152]. QSC researchers developed a new framework for quantum machine learning of continuous-variable quantum systems capable of exponentially reducing input-output state training resources [153]. QSC also introduced a new quantum phase estimation simulator for modeling X-ray spectra for chemical systems [154]. Using a neutral-atom quantum simulator, a QSC group succeeded in performing advanced materials simulations in a kicked quasicrystal, showing anomalous localization and multifractality [155]. QSCOUT hardware was used to pioneer a new method of mapping quantum chemical dynamics and vibrational spectra of molecules onto a digital quantum computer with spectroscopic accuracy, even in the presence of real noise [215]. Meanwhile, a fundamentally new class of algorithms for simulating coupled harmonic oscillators was discovered at C2QA [156], along with approaches to simulating field theories that led to improvements over previously best-in-class algorithms [157].

This list represents just a fraction of the DOE-funded achievements in quantum computing over the past decade. The sum total of the DOE's support has been essential for bringing the field to the verge of the many future breakthroughs described in this roadmap.

2.4 Timeline and specific challenges

We present in Fig. 2.2 a timeline—including technology milestones, enabling research and infrastructure, and scientific results and applications—for four eras of quantum computing. While the exact timing of each era is uncertain, this framework does roughly correspond to published roadmaps from leading firms in the quantum computing industry [158–163].

The quantum processors developed in the past decade can be categorized as "noisy intermediate-scale quantum" (NISQ) devices [45]. However, recent limited demonstrations of quantum error correction (QEC) herald the start of a new era [100, 101, 107, 108, 113–115]. We expect the coexistence of these two types of devices, with an accelerating transition toward error-corrected devices, to continue for the next five years.

In the 5–10 year timeframe, the first small error-corrected quantum computers will become available. This will correspond with the first unambiguous demonstration of the logical DiVincenzo criteria, as well as scientific computing capabilities beyond the reach of classical computers, often referred to as "quantum advantage." Meanwhile, in preparation for larger and more sophisticated systems to come, the field will need to develop hardware for architectural building blocks such as quantum interconnects between quantum computers.

Continued scaling to large error-corrected quantum computers will take place in the 10–20 year timeframe. These systems will have distinct architectures from the preceding era: likely modular and possibly constructed of heterogeneous hardware modalities and qubit types. The scientific applications of such systems will be transformative. Examples (discussed in Sec. 2.5) include: simulations of non-perturbative quantum chromodynamics in three dimensions; simulations in chemistry that provide new insight into catalysis, energy storage, and drug discovery; speed-ups to many classical scientific computations; and more accurate solutions to real-world challenges.

The very large quantum computers built more than 20 years from now will be fault-tolerant, meaning their logical error rates will be low enough to be irrelevant even for lengthy computations. Although the full implications are unknown, the ability to solve computational problems unimaginable today will likely transform how scientific discovery is approached. Section 6.2 discusses in detail the road to such computers.

For this timeline to be realized, foundational research across the full computing stack will need to continue and expand, as discussed in Sec. 2.2. Meanwhile, more infrastructure for scientific collaboration and expansion of the community of quantum computing researchers—for example, research centers and user facilities–can catalyze further acceleration of technical progress. (See the "Enabling research and infrastructure" row in Fig. 2.2.) The DOE has traditionally played a central role in supporting both needs and has a unique opportunity to build upon its past successes in the decades to come.

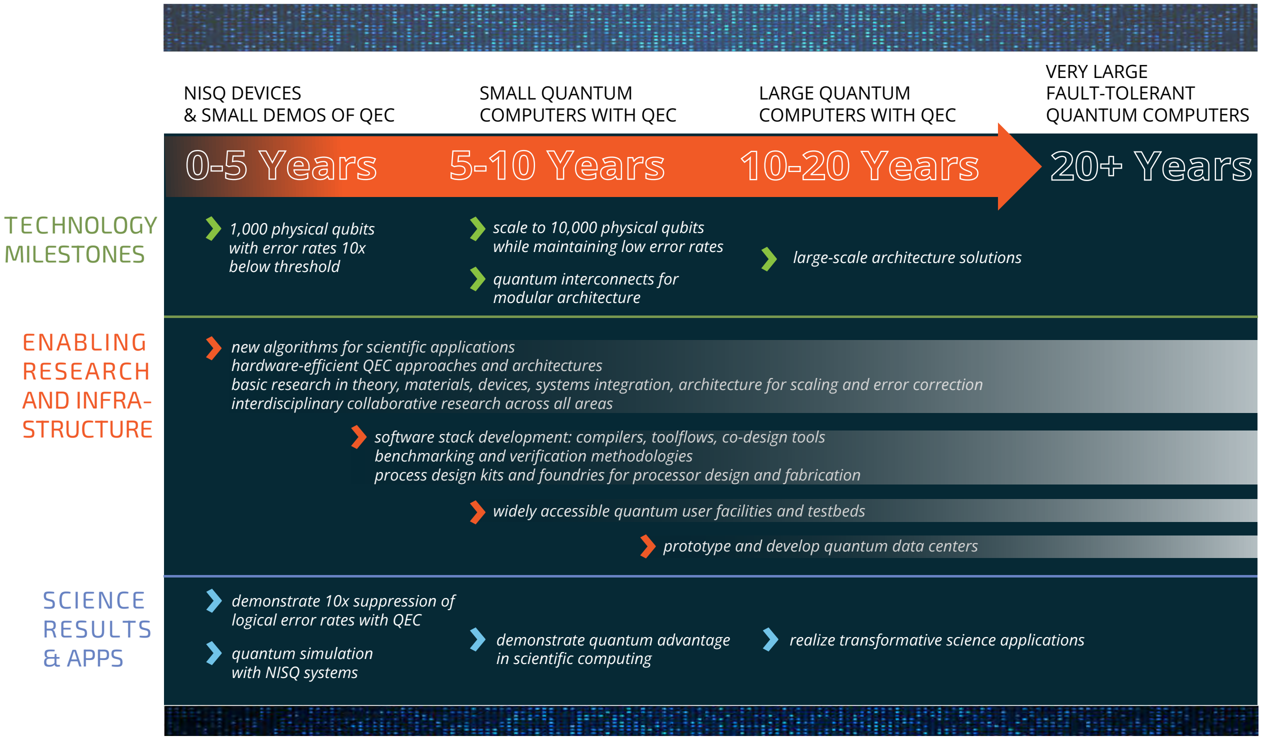

Fig. 2.2: Development of quantum computing capabilities relevant to the DOE mission. Over the next 20 years, the capabilities of quantum computing systems to tackle scientific problems relevant to the DOE will increase substantially. During this period, the role of quantum computers in accelerating scientific discovery will be fully established. Achieving the transitions between the eras noted requires innovations across the hardware, software, and systems stacks. Each era will unlock new scientific results, starting with modest beyond-classical computations, growing into problem-specific quantum advantages, and maturing into large-scale, scientifically relevant applications.

2.5 Example applications of quantum computing

This section presents examples showing the breadth of opportunities for quantum computing to impact DOE science problems (Fig. 2.3). We stress that other examples exist and are of no less importance [19–21]. Some of these opportunities have previously been highlighted in Office of Science reports, many of which precede the significant growth in DOE investment in quantum computing [18, 164–174]. In the intervening years and thanks in part to these investments, a sharper understanding of the requirements for realizing meaningful quantum computing impacts across the Office of Science has been gained. (This similarly applies to quantum sensing and quantum networking applications discussed in Chapters 3 and 4.) This roadmap reflects the importance of preparing for the eventual use of fault-tolerant quantum computers to achieve revolutionary impacts on DOE problems, while finding creative ways to use increasingly mature quantum computers in the meantime. In each example, we consider the motivation, state of the art for classical and quantum computing, and a discussion outlining how we expect research to progress as quantum computing technologies mature according to the timeline in Fig. 2.2. Fully realizing scientific impacts in these areas requires engaging a broad range of subject matter experts, as well as new developments in quantum algorithms, software, and hardware, both from industry and the DOE research community.

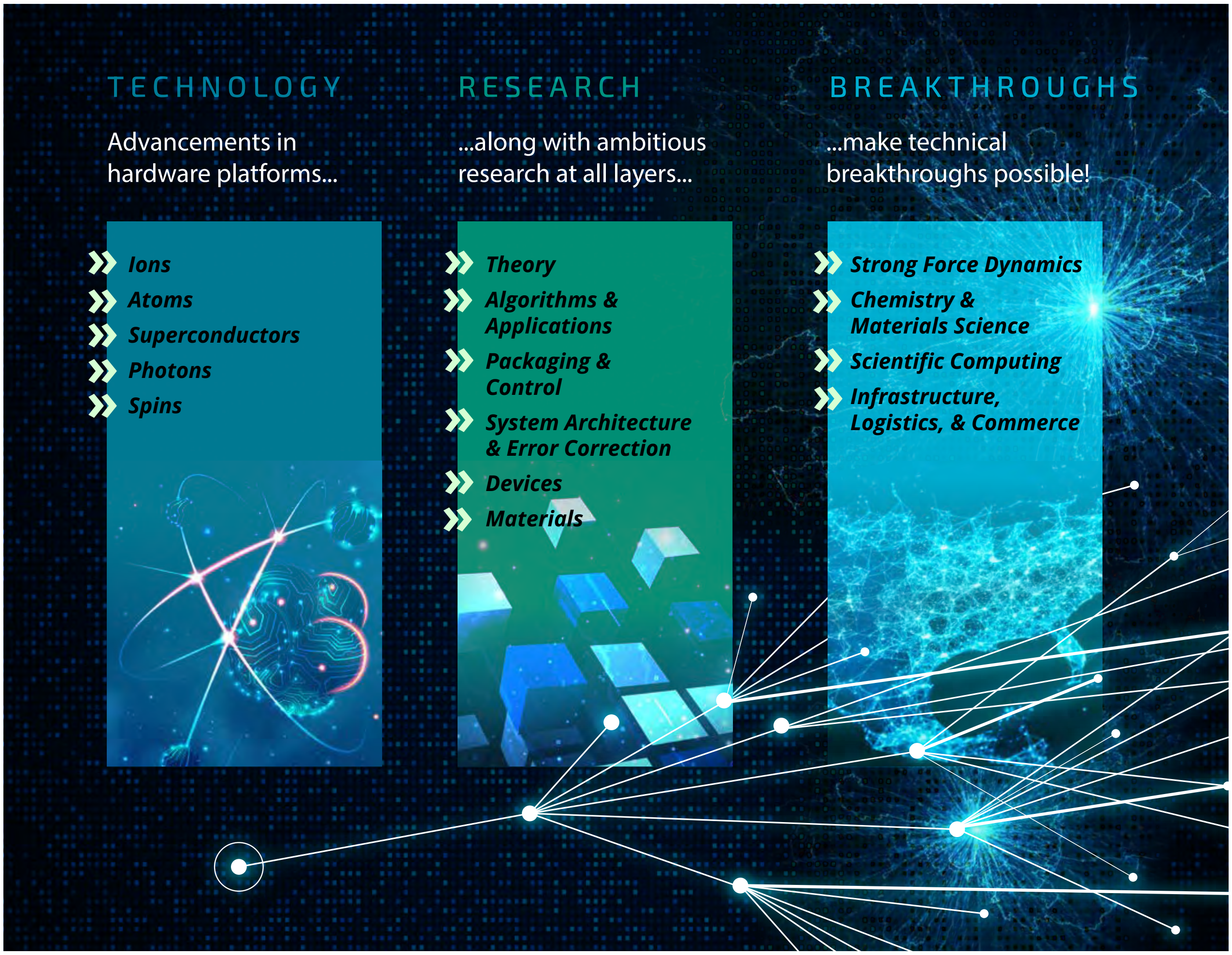

Fig. 2.3: Realizing scientific breakthroughs by accelerating the development, deployment, and use of quantum computing systems. Industry, national labs, and universities are developing a variety of hardware platforms for quantum computing. Research in theory, algorithms and applications, packaging and control, system architecture and error correction, devices, and materials — especially collaborative research cutting across these domains — will speed up the arrival of useful quantum computations at the forefront of science. Four examples of such possible breakthroughs are discussed in this report. The DOE is well-positioned to lead the way in making quantum computers impactful and practical for scientific applications.

2.5.1 Simulating the dynamics of the strong force

Motivation

The strong interaction binds quarks and gluons into hadrons (e.g., protons and neutrons) and holds protons and neutrons together in atomic nuclei. Interactions between quarks and gluons are described by a theory called quantum chromodynamics (QCD) that has been known for over 50 years [175]. QCD has the property that the coupling between particles grows with distance [176, 177]. This fact makes the binding between quarks and gluons so strong that they can never be observed in everyday life, and it also makes analytical calculations of the properties of hadrons impossible. While hadrons are responsible for almost all of the mass of the matter that we observe today, the details of how such hadrons form are still a mystery. This lack of knowledge impacts our understanding of the evolution of the universe shortly after the Big Bang and affects how well we can use facilities like the Large Hadron Collider or the Electron Ion Collider to search for new fundamental interactions or particles such as the elusive dark matter. Using quantum computers to predict hadronization dynamics has the potential to transform our ability to probe the deepest secrets of the universe [178].

State of the art

Classical computers: On classical computers, numerical simulations of the strong interaction [179] are limited to time-independent properties of hadrons, such as their mass. Understanding how hadrons form from quarks and gluons requires simulating the dynamics of this process and calculating correlation functions. While a theoretical formulation for dynamical simulations exists [180], the number of possible states is unimaginably large, and first-principles calculations are impossible on classical computers, instead requiring models with uncontrolled uncertainties.

Quantum computers: Because quantum computers can simulate quantum processes more directly than classical computers, they require dramatically fewer resources than their classical counterparts [181]. However, existing quantum computers are not yet powerful enough to perform the necessary simulations. In addition, a more detailed theoretical understanding of quantum simulation still needs to be fully formed. Quantum simulations to date have been performed in lower-dimensional systems (i.e., 1 or 2 spatial dimensions) and have been guided by theories with simpler interactions than the complete QCD picture [182].

Path to reliable quantum calculations at the forefront of science

The ultimate goal of simulating the dynamics of the strong force will require advances on many fronts. Broader quantum computing research towards the realization of large general-purpose fault-tolerant quantum computers will be essential to achieving this goal. More directed theoretical research specific to better simulating the strong force using a quantum computer is also crucial. The important scientific questions that need to be addressed are broad and will require strong multi-disciplinary collaboration.

Many details of the quantum simulation algorithms that will be used in these calculations remain topics of ongoing research. This includes the most efficient approaches for time evolution, state preparation and measurement, and the most interesting observables to estimate. It will also be critical to further develop Hamiltonian lattice gauge theories to make predictions with controlled uncertainties. Various algorithmic approaches can be pursued, and these might differ in their performance across quantum hardware platforms. Having a variety of approaches to calculating the same quantities available will also be crucial for verification. Application-specific hardware might also realize large performance gains, bolstering the importance of DOE remaining invested in hardware research. Accordingly, co-development efforts (as instantiated in existing DOE NQIRCs) involving scientific experts in all these areas are required.

As mentioned, studies of dynamics in one spatial dimension are ongoing, and over the next five years, simulations of QCD in two spatial dimensions should become possible. Such simulations require most of the theoretical techniques that will be needed for the full 3-dimensional simulations. While these will require many fewer computational resources, they will provide great insight into the dynamics of hadronization. It will also allow the study of hardware requirements for efficient QCD simulations. The ultimate goal of simulations in 3 spatial dimensions will require fault-tolerant hardware, but provide answers to many questions that are outside our current scientific understanding.

2.5.2 Chemical and materials simulations with unprecedented accuracy

Motivation

Quantum simulations of chemical and materials systems are among the most widely studied applications of quantum computers [183–186], with prospective commercial and scientific utility in an enormous variety of problems ranging from catalysis [187, 188], to energy storage [189–191], to drug discovery [192, 193], to better understanding quantum materials [194, 195]. Simulating these problems on classical computers forces chemists and materials scientists to choose between accuracy and efficiency in their calculations [196]. Either the calculation is efficient but ultimately an approximation, or it is inefficient but capable of achieving arbitrarily high accuracy. Quantum simulation algorithms offer the prospect of circumventing this dilemma, enabling accurate and efficient calculations on sufficiently powerful quantum computers.

There are countless open problems throughout chemistry and materials science thanks to the combinatorial explosion of possibilities combining elements from the periodic table. Among these many instances are prospective examples with significant scientific and societal impacts. For example, there is some hope that a sufficiently powerful quantum computer could help us develop alternatives to the Haber-Bosch process, responsible for 2% of global energy consumption [187,188,197,198]. Quantum simulations of electronic dynamics and light-matter interaction are expected to be another important application for quantum computers. These problems are intrinsically more difficult to simulate classically and often require less accuracy. Effective or model Hamiltonians present another opportunity for scientifically interesting quantum computation with reduced resource requirements.

State of the art

Classical computers: Classical computational chemistry and materials science are highly mature scientific disciplines with dozens of open-source and commercial software packages implementing a wide variety of methods [199–204]. These software packages are capable of running on platforms ranging from laptops to DOE's largest high-performance computing systems. They enable the calculation of a wide variety of properties, ranging from total energies to reaction rates, to optical and magnetic properties and ultrafast dynamics, and will continue to advance. However, they are ultimately limited in their accuracy.

Quantum computers: Quantum computational chemistry is rapidly maturing, and near-term demonstrations cover an enormous breadth of techniques, from variational hybrid algorithms [205–209], to non-variational algorithms [210], to enhancements of quantum Monte Carlo methods [211,212], to other algorithmic primitives [213–216]. Quantum advantage has yet to be achieved in chemical/materials simulation, though increasingly sophisticated chemistry and materials simulations have been executed on ever more capable systems [66,217].

Path to reliable quantum calculations at the forefront of science

It is widely believed [218–222] that fault-tolerant quantum computers are required for simulations that are on the margin of classical tractability [188, 198]. Even so, reductions of multiple orders of magnitude in the estimated resources have been realized [187, 188, 198] and future research in algorithms, quantum error correction, and architectures will continue to improve these estimates as hardware matures.

Within the next 5 years, calculations on very specific molecules or materials that are on the boundary of classical tractability might cross that boundary, and some of these demonstrations might benefit from augmentation by HPC resources [66, 185]. At the same time, the field will begin to implement and verify algorithmic primitives for those machines. With future fault-tolerant quantum computers, classically intractable calculations become possible, putting us on a path to revolutionary advances in chemistry and materials science. The higher accuracy that can be expected from quantum simulations could eliminate uncontrolled approximations that afflict classical methods and enable new scientific discoveries in the process.

2.5.3 Enhancing scientific computing applications

Motivation

There are numerous physics simulation applications (e.g., plasma physics, fluid dynamics, structural mechanics, and astrophysics) that are likely to be enhanced by sufficiently capable quantum computers. A quantum algorithm and resource estimates for one such class of calculations in plasma physics have recently been identified [223]. Such simulations—and the broader field of scientific computing—stand to be impacted by quantum algorithms for solving ordinary and partial differential equations (ODEs and PDEs) [224–228], linear algebra [229–234], and machine learning [235–238]. Even challenging nonlinear ODEs/PDEs might benefit from sufficiently powerful quantum computers [239], and recent evidence for an exponential quantum advantage in simulating highly structured classical systems [156] suggests that other classical physics applications might be discovered. The Harrow-Hassidim-Lloyd (HHL) algorithm presented the first exponential quantum advantage for linear systems solvers [229], laying the foundations for the broader field of quantum linear algebra. In recent years, powerful new concepts have greatly facilitated more generic quantum algorithm development [240, 241]. Other linear-algebra-relevant algorithms include those for matrix decomposition [240, 242], matrix diagonalization [243], and other basic linear algebra subroutines [244, 245]. For machine learning, quantum algorithms have been proposed to accelerate tasks such as clustering [246–250], classification [251–253], and several others [254–259].

State of the art

Classical computers: Classical algorithms for ODEs and PDEs are very mature, with a wide spectrum of methods for rendering their solutions as structured linear algebra problems. Numerical linear algebra is essential to these applications and proportionally mature. While the DOE has broad expertise in this area, ranging from the performance-limiting instabilities in fusion plasmas to understanding the synthesis of elements in supernovas, improving these simulations remains an active topic of research.

Quantum computers: Much of the progress in quantum scientific computing applications has been due to the quantum algorithm development referenced above. Absent any further improvements, algorithms are likely to require fault-tolerant quantum computers to implement [260], but algorithms amenable to pre-fault-tolerant systems are being developed [261–267]. While a few demonstrations of algorithms for scientific computing on current hardware exist [268–270], the study of quantum algorithms for scientific computing is still maturing.

Path to reliable quantum calculations at the forefront of science

The continued development of quantum algorithms for scientific computing applications will remain an important research area for the next 5–10 years. In parallel, advancing quantum algorithms for ODEs/PDEs, linear algebra, and machine learning is essential. Algorithms for quantum linear systems provide a motivating example. Since the HHL algorithm was proposed 15 years ago, substantial improvements over the past 5 years have led to theoretically optimal quantum linear systems solvers [230–234]. Achieving similar improvements in the other algorithms would expand and accelerate the realization of the impacts of quantum computers in scientific computing. Finally, exploring novel quantum advantages (e.g., in space [271]) might lead to unexpected opportunities for impacts on broader classes of problems.

2.5.4 Enabling more efficient management of infrastructure, logistics, and commerce

Motivation

Optimization is a ubiquitous computational challenge that impacts scientific discovery and everyday tasks alike. Finding optimal solutions to problems with many variables is critical to applications including the management of supply chain uncertainties, determining better shipping routes, and smart allocation of resources in power grids,[2] or improving manufacturing processes. The difficulty of these tasks can be substantial due to the rapid growth in the number of possible solutions as the number of variables increases. In many cases,

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[2] The strategy of harnessing QIS in the modernization of the power grid was previously highlighted in the DOE Grid Modernization Initiative's strategy document, as updated in 2020 [272].

even small improvements in optimization performance or solution accuracy can lead to significant real-world impacts.

State of the art

Classical computers: *Combinatorial optimization* seeks an optimal solution among a large set of candidates, which is vital in contexts ranging from traffic routing to deploying energy resources in a power grid. Mature classical software packages exist for exactly and approximately solving combinatorial optimization problems, with heuristics handling being capable of handling millions of variables. However, the runtime of exact classical algorithms grows exponentially with the size of the problem, rendering full optimization impractical. Managing market risk in energy trading or optimizing an investment portfolio are common problems amenable to *optimization with Monte Carlo methods*. Classical Monte Carlo methods are also quite mature but can face accuracy obstacles related to sampling rare events.

Quantum computers: Quantum algorithms may fall short of achieving the most impressive (exponential) speedup for optimization tasks [273–279]. However, Grover's algorithm and the closely related amplitude estimation algorithm belong to a larger set of well-understood quantum algorithms achieving a quadratic improvement over the best classical algorithms. Whether this speedup yields a practical quantum advantage when accounting for fault-tolerance overheads [280, 281] remains to be seen. The possible improvements achievable by quantum search heuristics like Quantum Approximate Optimization Algorithm (QAOA) and Quantum Adiabatic Optimization (QAO) are less well understood. Small-scale combinatorial optimization problems have been implemented on available quantum hardware [74, 78, 79, 282–285]. Research into using amplitude estimation for Monte Carlo-based optimization in trading portfolio management is underway [286–290], with small examples validated on hardware [291, 292].

Path to reliable quantum calculations at the forefront of science

Some modest optimization problems may already be solvable with current hardware [77–80]. The feasibility of scaling to practical problem sizes on such hardware, while maintaining sufficient solution accuracy, remains an open challenge. More work is needed to identify specific problem classes and regimes where quantum computers are most relevant, especially given the maturity of classical solvers [293–295]. Theoretical research is needed to establish speedup guarantees for different types of optimization problems, develop new quantum algorithms, and tabulate resource estimates. Future studies could assess whether quantum speedups are diminished or erased in end-to-end analyses [20] taking into account aspects such as the encoding of large classical data on the quantum side [296]. Combining classical optimization and quantum computing expertise will likely facilitate attaining meaningful and impactful quantum calculations, where possible.

Chapter 3

Quantum Sensing to Enable Unprecedented Precision and New Discoveries

3.1 Introduction

Quantum information science gives us new insight into how the physical world can be measured. As the quantum behavior of a system is preserved for longer periods of time, it becomes more sensitive to small signals in the environment. While this sensitivity poses a challenge to the long-term goal of quantum computing, it provides new opportunities for sensing and metrology. For example, fundamental limits to sensitivity can be improved by using quantum information concepts such as entanglement and quantum nondemolition measurement [297], which enable ultrahigh precision timekeeping [298], improved navigation [299], testing fundamental physical theories [300–302], probing materials at nanometer and single-atom length scales [303, 304], robust sensing in extreme environments [305, 306], sensing biological systems down to the single-molecule level [307, 308], and biomedical applications [308, 309].

There are two major areas of research and technology development in quantum sensing: (1) using qubits as sensors and (2) using quantum correlations to improve sensor performance. Both areas build on a rich history of building sensors with techniques from atomic physics and metrology, and expand the capabilities, functionality, and precision of sensors by leveraging QIS and quantum engineering toolkits.

Qubits such as single atoms or solid-state defects have several properties that make them attractive as sensors. First, they can be prepared in a superposition of internal energy levels that is highly sensitive to the quantity to be probed. Second, the calibration of the sensor is connected to fundamental constants and is therefore known *a priori* and exactly reproducible between laboratories and over time. Finally, atoms are very small, enabling spatial resolution at the nanometer scale in principle.

These properties have been exploited for decades to make atomic clocks, which can currently measure the passage of time with an error of less than half a second over the age of the universe and observe the gravitational redshift over laboratory scales [310, 311]. Furthermore, measurements of cold atoms and molecules have provided the most stringent tests of the standard model, allowing for searches of new physics over a wide parameter space [312, 313].

More recently, the high spatial resolution of solid-state atomic defects has been deployed to probe microscopic properties of materials and to detect very small concentrations of molecules, down to the single molecule and even the single atom level. Combining this extreme spatial resolution and high sensitivity with quantum control methods gives access to fundamentally new information, such as how microscopic properties of materials fluctuate in time over very small scales. Such sensors will open a new frontier for understanding

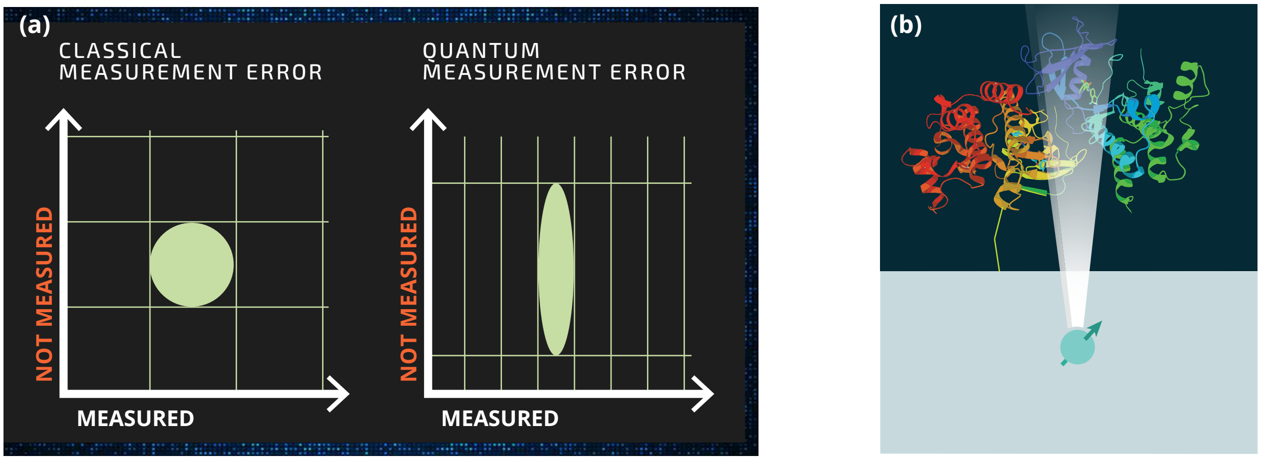

Fig. 3.1: Quantum resources for sensing. (a) Measurements are subject to a fundamental precision limit imposed by quantum mechanics called the "standard quantum limit." This corresponds to the minimum measurement uncertainty, depicted as the grid size of classical measurement error (left). In quantum measurements, uncertainty can be reallocated into an irrelevant measured parameter, thus squeezing the grid and allowing for more precision in the quantity to be measured (right). (b) A solid-state spin qubit (ball pierced by arrow) can be used as a sensor with extremely high spatial resolution, similar to MRI measurements but at the atomic scale. The cartoon shows a nitrogen vacancy center in diamond used as a qubit to take a high-resolution cross-sectional "image" of a protein attached to the surface of the diamond.

materials, devices, chemical systems, and biomedical diagnostics.

Once a sensor has been designed and engineered to avoid parasitic environmental noise, it eventually hits a limit dictated by quantum mechanics – the standard quantum limit – that arises from fundamental principles of measurement and uncertainty [314]. Fortunately, quantum mechanics also provides a method to surpass this precision limit by using entanglement. Thus, quantum sensing allows for the measurement of very weak signals that are otherwise unmeasurable, enabling new technologies and scientific discoveries.

A paradigmatic example of the power of quantum sensing is the Laser Interferometer Gravitational-Wave Observatory (LIGO), which has spawned a new era of gravitational astronomy [315]. Through careful engineering of the stability and low-noise measurement of the interferometer, LIGO achieved a performance limited only by quantum noise and succeeded in detecting the first gravitational wave. Following this milestone, the next frontier in sensitivity improvement was to use a so-called "squeezed vacuum," in which the quantum noise is squeezed into another part of the measurement (see Fig. 3.1a), allowing the parameter related to gravitational wave observation to exhibit less noise [316]. This step, a prime example of quantum tricks in action, allowed LIGO to increase the volume of the universe it can observe by a factor of eight. The same principle can be applied to a wide range of sensing and metrology tasks: once classical engineering brings a sensor to the quantum-noise limit, quantum tricks can be deployed to boost the sensitivity even further.

Developing quantum sensors to their full potential will require significant classical engineering in mitigating noise. This noise includes environmental noise such as vibration and temperature fluctuations, magnetic and charge noise arising from constituent materials and impurities, fluctuations in the sensor readout (optical, microwave, or electrical), pulse errors in the qubit driving protocol, and aliasing due to the necessary periodic interrogation required for quantum protocols. The coming years will require fundamental research in developing and discovering new sensors, devising new sensing protocols and modalities, and improving these sensors through materials purification and device fabrication, as well as translational research to deploy and apply quantum sensors to a large range of applications for science and commercial purposes. Here, we outline some of the common themes of this research frontier along with four example applications of quantum sensors: precision measurement for new physics, sensitive and high-resolution probes to understand materials, robust and deployed sensors, and biological, chemical, and biomedical sensing.

Fig. 3.2: Overview of quantum sensing platforms, resources, challenges, and applications. Multiple types of quantum sensing platforms are under development, offering different advantages for particular applications. They each feature a suite of quantum resources that can be exploited for specific sensing tasks. Taking advantage of these quantum resources and deploying quantum sensors for useful applications will also require a significant effort in classical engineering for each sensing platform. Applications range from fundamental physics and materials research to deployed sensors in extreme environments and chemical and biomedical diagnostics.

3.2 The current frontiers of quantum sensing

3.2.1 Physical platforms

There are numerous physical platforms that are actively explored as quantum sensors (see Fig. 3.2). Atoms, ions, and molecules in specialized environments such as vacuum chambers or vapor cells can have exceptionally long quantum coherence times, and are by their nature identical, allowing for highly accurate and reproducible measurements. These systems have been deployed for a number of fundamental science and precision technology use cases, including atomic clocks [317, 318], magnetometers [319], gravimeters [320], and probes of fundamental constants such as the magnetic or electric dipole moments of fundamental particles [312, 313].

Solid-state defects such as nitrogen vacancy centers in diamond [303–305, 307, 308] and other emerging atomic-scale impurities in semiconductor and insulating host materials [30, 321] can mostly realize the functionality of atomic sensors, but with the additional benefit of stable operation in ambient conditions. The solid-state form factor also allows placing sensors extremely close to the target of interest, which can increase sensitivity and spatial resolution for localized signals. These qubits are already commercially deployed as material probes [303, 304], and are actively developed for bulk and nanoscale magnetic field sensing [305], as well as nanoscale nuclear magnetic resonance (NMR) [322] and thermometry [323].

Other solid-state qubit technology has found application in sensing. For example, superconducting qubits are used as single photon detectors for dark-matter searches [324], and there is a long synergy between superconducting qubits and superconducting detectors. Additionally, quantum control techniques such as laser cooling have been used to improve the performance of micro- and nano-mechanical sensors, which can be used as inertial sensors or as probes of fundamental physics.

3.2.2 Common themes

Quantum sensing and metrology is a highly active area of research, with many lab-scale demonstrations of key concepts. However, applying such techniques and platforms for useful quantum advantage will require ambitious, interdisciplinary science and engineering efforts. This research can be accelerated with broad, large-scale investments to develop quantum resources and push classical engineering in myriad quantum sensing platforms to expand the bounds of what can fundamentally be sensed. Across the different physical platforms and applications of quantum sensors, there are several common themes of research and development.

A common theme is the classical engineering required to eliminate classical noise and achieve quantum-limited noise performance. The fragility of quantum states makes them sensitive to many perturbations beyond the particular quantity of interest; thus a high degree of sensor stability, materials engineering and purification, and device engineering is required to reach the standard quantum limit.

Furthermore, quantum sensors will need to be engineered for robust applications in the field. With proper design, quantum sensors can remain robust under various conditions, such as environmental noise, fluctuations in operational parameters, and hardware imperfections. As one example, using weak enough signals to see a quantum advantage and dealing with harsh and varied environments are currently limiting advances in techniques such as quantum radar and quantum LiDAR [325]. Achieving this robustness will necessarily involve employing a combination of environmental isolation, advanced materials, and adaptive algorithms, ensuring quantum sensors are practical and reliable for real-world applications.

Moreover, ongoing theoretical investigations in quantum sensing are crucial in this endeavor and encompass a wide range of areas. These include a better understanding of material properties and finding new uses for quantum sensors.

In the near future, widely deployed sensors can also take advantage of multiplexing and multimodal sensing to achieve new functionality, such as measuring correlations across sensors. Such large-scale measurements will also require new methods for handling large datasets in real-time. Just as multimodal astronomy has enabled fundamentally new ways to learn about the universe, multimodal sensors will allow for many independent measurements simultaneously, expanding the scope of our observations.

One major task is generating and manipulating quantum resource states in different platforms, including devising strategies for harnessing and distributing entanglement, producing states with a high degree of squeezing, and using quantum non-demolition measurements of entangled sensors or particles. A key outstanding goal in the community is to exploit the information encoded in a many-body state, in which many particles are highly entangled, in order to achieve better sensitivity or access to new types of information about the system under test.

3.2.3 Past DOE successes

Many past DOE investments have led to major advances in quantum sensing. Recent results using spin squeezing and quantum scrambling have demonstrated improvement in the precision of atomic clocks (QSA). New protocols that measure correlations among quantum sensors allow for fundamentally new types of information to be learned, such as measuring the gravitational redshift at small scales with atomic clocks (QSA) and gaining access to dynamics in materials with NV centers in diamond (QNEXT, BES programs). Achieving the deepest sensitivity to dark sector particles and axion-like particles through experiments utilizing superconducting cavities and qubits, including robust B-field sensors (SQMS, HEP programs) [326–328].

Within the DOE's HEP program, the Axion Dark Matter eXperiment (ADMX) has been designed to measure the extremely weak conversion of axion dark matter to photons with measurements beyond the standard quantum limit [329]. These experiments are crafted in the context of theoretical calculations to guide the most likely parameter space for finding new physics, for example through the QuantISED program.

The DOE has also been instrumental in supporting work to develop new qubit sensors, particularly in materials growth, characterization, and fabrication at DOE user facilities. The lowest loss superconducting resonators achieved thus far are based on tantalum (C2QA), and the lowest loss bulk cavities have been demonstrated at Fermilab (SQMS), opening the door to new quantum detectors and sensors. There are also several DOE facilities for quantum diamond growth and fabrication, including at Argonne National Lab and the Princeton Plasma Physics Laboratory (QNEXT, FES programs, BES programs), as well as novel qubit synthesis efforts led by LBNL (FES programs, BES programs).

A major role of the DOE has been the deployment of large facilities with high throughput capabilities, which also serve as educational platforms and democratize access to quantum technology for research and education. Some of the new flagship facilities created by the National Quantum Initiative Science Research Centers include the SQMS Quantum Garage at Fermilab, the QSC QUIET and LOUD twin underground and above-ground facilities at Fermilab, the Q-NEXT Argonne Quantum Foundry at ANL, the SLAC Detector Microfabrication (DMF) Facility supported by Q-NEXT, the QSA-developed magnetoARPES facility at the ALS, LBNL, and the C2QA multi-probe scanning microscopy facility at BNL.

3.3 Example applications of quantum sensing

For each of the four applications outlined below, there are many different activities on various quantum sensing platforms. We summarize some of the activities and the current state of the art in the following. Since a comprehensive account is beyond the scope of this report, we instead provide illustrative examples. Each example application concludes with a summary of key areas and themes that would benefit from large-scale investment.

3.3.1 Precision measurement for new physics

The progress of scientific discovery is often propelled by the development of new measurement techniques. In the 19th century, breakthroughs were fueled by the study of light, electric currents, and magnetic fields. The emergence of quantum mechanics and insights into the atom's microscopic structure stemmed from the challenges presented by particle interactions with each other and with light. The 20th century saw significant advances with the creation of large-scale particle accelerators and colliders to probe atomic structure, powerful telescopes for cosmic observations, and precise lab experiments to test our fundamental theories. Quantum sensing promises to extend the reach of these endeavors by improving the sensitivity, precision, and range of measurable physical quantities. By pushing the measurement frontier and significantly cutting the time needed to achieve sensitivity goals, quantum sensors could unlock answers to some of physics' most profound mysteries, including the nature of dark matter and dark energy, the formulation of a quantum gravity theory, and the reasons behind matter's dominance over antimatter in the universe [312, 330, 331].

Atomic clocks have already had a transformative impact on society and commerce through their use in global navigation satellite systems, unit definitions, and network synchronization, amongst many other applications. Thanks to their remarkable precision, comparisons between atomic clocks and across clock networks have set stringent limits on fundamental constants [332–334] and modifications to relativity [335], and have also been used to search for certain ultralight dark matter candidates [336]. The ultimate precision of an individual atomic clock is limited by the electromagnetic frequency of a specific atomic transition probed by the clock. Microwave atomic clocks, as used in global navigation satellite systems and setting the definition of the second, have been surpassed by optical atomic clocks, which are currently our most precise time-keeping devices. New clocks based on shorter wavelength nuclear transitions have the potential to improve precision even further [337]. Other methods for improving clock accuracy include frequency comparisons between atomic clocks and entanglement of the clocks themselves, as discussed in Sec. 4.3.2.

Atom interferometers utilize spatial superpositions of quantum states and subsequent interference of ultracold clouds of atoms to measure minute accelerations, rotations, and gravitational forces. They are also increasingly finding applications in probing fundamental physics, including tests of the weak equivalence principle, precision measurements of the fine-structure constant, searches for ultralight dark matter, and even searches for exotic dark energy candidates. Networks of entangled atom interferometers can enhance the sensitivity of these experiments significantly, expanding their discovery potential and offering new tests of exotic modifications to quantum mechanics such as gravity-induced wave-function collapse [338].

Quantum sensors have also formed the basis of new detectors in many experiments searching for new physics. For example, microwave and mm-wave frequency detectors capable of detecting single photons can measure such signals below the standard quantum limit, which allows for much faster searches for low-mass dark matter (e.g., axions). Furthermore, superconducting resonators are actively used to search for dark matter over an extensive frequency range, from 100 Hz to tens of GHz (8 orders of magnitude in energy) [324], and they have long been explored as microwave detectors for astronomy [339]. Solid-state quantum sensors (e.g., using NVs in diamond) show promise for directional detection of rare massive particles with very low cross-sections, potentially allowing the discrimination of (hypothesized) weakly interacting massive particle (WIMP) dark matter from the background of neutrinos [340]. There is also an excellent opportunity for the development of networks of quantum sensors optimized to search, e.g., for different types of dark matter, violations of Lorentz and CPT symmetry, temporal variations or oscillations of fundamental physical constants, anomalous spatial variations or oscillations of physical constants, and long-distance breakdowns in standard quantum mechanics interpretations of entanglement.

Path to discovering new physics with quantum sensors

Pushing the frontier of quantum sensing is not a solitary endeavor. It requires the collective efforts of the community to undertake major research in improving all sensing platforms outlined here: cold-atom, trapped ion, superconducting, and molecular-based quantum sensors, including novel kinds of optical atomic, molecular, nuclear clocks and clock networks, cold-atom and molecule-precision spectroscopy experiments, atom-like systems in the solid state, and atom interferometers. Community efforts will be essential to realize quantum sensor performance beyond the standard quantum limit and to enhance the accuracy and sensitivity to new physics by employing non-classical entangled and spatially delocalized states. Multi-resonator entanglement techniques combined with squeezing would enable measurements below the standard quantum limit with applications ranging from dark matter searches to gravitational wave sensing [341–345]. New emerging tools offer enhanced control that will unlock the full potential of entanglement and other quantum resources in these systems, such as optical tweezers, differential comparisons, multi-ensemble sensors, and networks of sensors.

3.3.2 Sensitive and high-resolution probes to understand materials

Our capacity to create, enhance, and produce technologies shaping the modern world is fundamentally linked to our understanding and manipulation of materials. Quantum sensors, with their exceptional sensitivity and spatial resolution, enable measurements beyond the reach of conventional materials characterization methods. Individual qubits can measure minuscule electric and magnetic fields, as well as local temperature, strain, and noise from fluctuations and dynamics. The capability of qubits to assess local dynamics heralds a new era in the use of multiple sensors or sensor arrays, and ultimately, quantum entangled sensors, offering a groundbreaking tool for material science.

Nitrogen vacancy (NV) centers in diamond provide unique opportunities in studying condensed matter systems: they are quantitative, noninvasive, physically robust, offer nanoscale resolution, and may be used in ambient conditions and across a wide range of temperatures [303, 304] and pressures [346, 347]. In recent years, NV centers have been used to achieve nanoscale resolution measurements of magnetism [348, 349] and current flow [350, 351] in condensed matter systems. Furthermore, NV centers have the unique advantage that they can probe quantities that go beyond average magnetic fields – leveraging techniques from magnetic resonance, they can be used to perform high-precision noise sensing, allowing for probes of dynamics and nonequilibrium physics [352–354].

There is also active research in alternative qubits for materials sensing, including in layered, two-dimensional materials such as hexagonal boron-nitride (hBN) [355–357], in which exotic material properties can serve as powerful tuning knobs for the qubit [358–360]. The two-dimensional host material allows for integration into devices and materials of interest [361–363].

In addition to engineering single qubits as sensors, there is great promise for the use of many entangled sensors in a solid-state spin ensemble to achieve sensitivities beyond the limit imposed by classical correlations. Although there are many proposals and small-scale demonstrations of such concepts, the realization of such a sensor remains an important frontier [364, 365].

Superconducting circuits, resonators, and cavities can also be used as quantum sensors. A well-established example is the superconducting quantum interference device (SQUID), which has been a standard tool for measurements of magnetism in materials for many decades. SQUIDs have been used to study a wide range of quantum materials including high-temperature superconductors [366], candidate topological superconductors [367], 2D materials [368], topological electronic materials [369, 370], and quantum spin liquids [371]. Although SQUIDs are among the most sensitive magnetometers, their performance degrades as they shrink, leading to a trade-off between spatial resolution and sensitivity. A grand challenge in this area is to realize higher-resolution probes by reducing flux noise which plagues not only quantum sensors based on superconducting circuits but also superconducting qubits in quantum processors.

Path to new materials science with quantum sensors

The past decade has been focused on developing quantum sensors and exploring and demonstrating their potential for particular applications. Development focused on exploiting and measuring correlations, devising new protocols to expand the scope of materials phenomena that can be sensed, and building tools for massively multiplexed sensing will open up new frontiers in the understanding and applications of condensed matter systems. Harnessing large-scale entanglement for sensing would enable fundamentally new tools. Turning a quantum information lens onto materials science and condensed matter physics will lead to new understanding of complex materials. Achieving these goals will require collaborative, interdisciplinary efforts in theory, experiment, and materials science.

Developing these platforms over the next 5–10 years will require improving diamond surfaces and removing defects in the bulk down to sub-parts per billion levels to create a quiet environment. Material quality must be preserved during microfabrication and device integration, and new qubit protocols and experimental methods need to be devised for increasing the speed, throughput, and sensitivity of materials measurements.

In parallel, the community should now turn to using such sensors to learn materials science and discover new condensed matter phenomena. This activity will require an interdisciplinary, concerted effort that bridges basic science and translational research in a manner reminiscent of other tools that are now routinely used to understand materials, such as synchrotron radiation sources, X-ray diffraction, electron microscopes, and scanning probes. Transitioning quantum sensors out of quantum research labs and into widely used tools for materials science and condensed matter physics will require advances in materials, devices, and fabrication in concert with fundamental research in new sensing protocols and modalities. Some steps have already been taken along these lines, with commercially available scanning probe platforms based on NV centers [372]. These interdisciplinary goals will benefit from deep, long-term investments in diamond materials growth and microfabrication [373] that mimic the ecosystem we currently have in place for understanding and controlling silicon.

3.3.3 Robust and deployed sensors

Quantum sensors can be intrinsically robust, making them well-suited for extreme environments and myriad applications in the field. Examples include harsh environments, such as high temperatures and radiation environments, as well as demanding operational requirements, such as the small size and low power constraints when sensing within the human body or the confines of small autonomous vehicles.

For example, certain quantum sensors, such as highly-excited Rydberg atoms, are identical and intrinsically calibrated to fundamental constants, which can make them more stable in demanding applications and eliminate the need for complicated or expensive calibration routines [374]. These properties make them well suited for sensing in extreme settings like plasmas and ion-beam sources [375]. As another example, quantum optical pumped magnetometers (OPMs) can tie magnetic field measurements to fundamental constants, and technological improvements over the last ten years have made them suitable for space applications [376].

Furthermore, quantum sensors can be very small, down to the scale of single atoms, making them less sensitive to radiation damage because they have a small area to absorb radiation. For example, sensors in fusion plants will be exposed to extreme neutron radiation (up to 1022 neutrons/m^2), high temperatures (up to 200°C) and rapidly fluctuating high magnetic field environments (8 T/s). Any sensor to be used in such a machine will need to not only survive under these conditions, but maintain performance for long enough to provide stable, high-sensitivity measurements. NV centers in diamond can operate at high temperatures, and irradiation will generally not change the sensor properties, making diamond quantum sensors particularly well suited for studying fusion and other extreme radiation environments.

Gravitational measurements are some of the most interesting tools available to image through the earth's surface. Applications range from identifying underground mineral deposits to monitoring glaciers, ocean levels, and underground aquifers. Existing gravity sensor technologies suffer from drifts that limit their use in long-term measurements, and the instruments that do minimize these drifts are large, expensive, and typically immobile. Quantum gravity sensors (gravimeters) and gravity gradient sensors (gradiometers) based on atom interferometry leverage the inherent stability of individual atoms to provide low-noise, low-drift measurements of the shape of the earth and local gravitational variations. Current atom interferometry technology aims to compete in sensitivity with large gravity space missions such as GRACE and GRACE Follow-on [377], while improving long-term stability and only requiring a single satellite.

Path to deploying quantum sensors in diverse and extreme environments

Deploying quantum sensors in extreme environments is a complex task that necessitates a broad, interdisciplinary effort. This effort should bring together quantum sensor design, materials synthesis, device fabrication, and quantum sensing protocols research with systems engineering, device packaging, application-specific integrated circuits, and translational efforts. Such collaboration is crucial for ensuring the robust performance of quantum sensors in extreme environments. For example, in the case of NV center sensors for plasma science and fusion, materials engineering to create robust sensor substrates and mitigate radiation damage will be key. Programs to link such efforts to end-users in the scientific community and industry will be crucial for driving progress.

Next-generation quantum instruments will maintain high sensitivities in dynamic, terrestrial environments by taking their cue from the most advanced optical atomic clocks, measuring gravity while confined to only a few millimeters within a three-dimensional lattice of atoms [298]. Advances in photonic integrated circuit

(PIC) laser technologies will also dramatically lower the size and cost of these devices, which in turn will open up an array of new applications and use cases [378].

A particularly interesting frontier is the design of sensors for measuring differences among quantum sensors to achieve higher precision by avoiding shared noise. For example, quantum gradiometers have the unique potential to minimize common-mode noise from vibrations by measuring two atomic populations simultaneously resulting in improved deployed resolutions [379]. This, coupled with the intrinsic long-term stability of atom interferometers, will pave the way for sensors especially well-suited for observations of changes to our Earth, with the potential to measure millimeters of change to global ocean and glacier levels year over year [380].

3.3.4 Biological, chemical, and biomedical sensing

Many advances in our understanding of biology, disease, and human health depend on technology to detect very small signals and minute concentrations of molecules, sometimes from deep within a living organism such as a human body. The sensitivity, resolution, and functionality of quantum sensors enable new probes for chemical, biological, and biomedical applications. However, advancing quantum sensing technologies requires an interdisciplinary approach that integrates quantum sensor design, materials science, and system engineering for specific biological and medical use cases. Near-term life science applications will likely be centered around existing quantum sensor technologies, such as nitrogen-vacancy (NV) centers in diamond or optically pumped atomic magnetometers (OPMs).

For example, nuclear magnetic resonance (NMR) is a workhorse technique for detecting molecules and determining molecular structure, but requires large samples and bulky superconducting magnets. Quantum sensors based on NV centers can perform high-resolution NMR spectroscopy on dilute concentrations of molecules in very small quantities of liquid, down to picoliter volumes [308, 322] and even single molecules [381]. Potential applications include ultra-sensitive and high-throughput chemical analysis relevant to drug discovery and natural products research, as well as the monitoring of chemical reactions in individual biological cells. Combined with existing microfluidic assays, these ultra-sensitive detection assays will eventually enable monitoring and screening for infectious diseases. These ultra-sensitive assays could be implemented into high-throughput screening devices that enable the detection of proteins related to diseases, such as cardiovascular diseases or diabetes, at an early stage and, therefore, significantly improve treatment options.

Quantum sensors also allow for more precise and practical localization of magnetic signals from the human body, e.g., from the brain (MEG) and heart (MCG). In particular, optically pumped atomic magnetometers (OPMs) enable sensitive human MEG and MCG using more compact, versatile, and adaptable apparatus than previous technologies [308]. OPMs do not require low temperatures (like older SQUID technology), thus simplifying the sensor architecture and allowing smaller sensor-to-sample distances. Another benefit of OPMs is their ability to detect vector magnetic fields, which helps differentiate signal and background fields. Recent progress in developing miniaturized OPMs integrated into sensor arrays in helmets and other configurations have opened new frontiers for monitoring human electromagnetic activity; and are beginning to be used by researchers and clinicians to study, among other things, human brain activity under different functional and developmental states, the effects of injuries, and disorders such as epilepsy.

Quantum light sources such as squeezed light or entangled photons can provide new ways to perform measurements in the life sciences, including improvements to the sensitivity of spectroscopy and microscopy, and measurements with much weaker excitation light intensity. Lower light intensity is critical to prevent photo-induced damage of light-sensitive organisms. Entangled photons and squeezed light have been shown to excite two-photon fluorescence with much lower light levels than with standard two-photon absorption performed with femtosecond pulsed lasers [382]. This entangled two-photon absorption combines the benefits of localized excitation and deep sample penetration from two-photon absorption with low light levels, making it a promising technique for bioimaging. Additional applications of entangled photons include quantum ghost imaging [383] and interferometric imaging [384], which can provide additional observables for imaging and benefits for depth of field and resolution.

Path to quantum sensing for chemistry, biology, and medicine

Developing broadly useful quantum sensors for biological, chemical, and biomedical applications will require interdisciplinary collaboration between quantum physicists, engineers, biologists, chemists, and clinical researchers to tailor these technologies to specific applications. A key aspect is the creation of an ecosystem that supports the translation of quantum sensing innovations from proof of concept to applications in fundamental biology and medicine. This includes creating funding mechanisms for translational research and establishing partnerships with industry and clinical stakeholders. Eventually, clinical trials will be necessary to benchmark these technologies in real-world scenarios.

For nanoscale NMR, several key technical developments are needed for wide-ranging impact in the chemical and life sciences: integration with microfluidics for high-throughput screening of single cells and small chemical samples, higher sensitivities, deterministic single-molecule placement, and increased spectral resolution. Furthermore, advances in optical systems for wide-field NV-based imaging and spectroscopy could be applied to highly parallel single-cell studies and chemical analysis of candidate pharmaceuticals at the picoliter-scale. The ultimate goal is to make these techniques widely available beyond the physics community, e.g., leading to easy-to-use and scalable chip-scale NV-NMR spectrometers for analysis of very small chemical and biological samples.

Further improvements in OPMs for MEG and MCG are required before this quantum sensor technology can achieve widespread use in hospitals. For example, scaling up OPM sensor arrays, to provide superior sensitivity and spatial resolution to SQUID-based MEG, will require the suppression of crosstalk between individual OPMs. The main advantages of OPM-MCG for clinical applications are its potential for portability, low cost, and electrode-free application. Improved robustness and efficient packaging (i.e., miniaturization) of OPMs are needed to realize this potential, requiring further research to improve sensitivity, field amplitude dynamic range, and isolation from environmental perturbations, to enable engineering trades for practical operation in real-world settings.

The application of imaging with entangled photons to biological or biomedical research requires improvements in sources, detectors, and strategies for their use. Benefits of quantum imaging include the potential for increased resolution, contrast, and lower noise for the same excitation. Strategies for increasing the intensity of dim entangled photon sources and squeezed light sources will boost the applicability of quantum imaging techniques. Ghost imaging with entangled photons promises to reduce sample photodamage and extend long observation windows [385]. Additionally, quantum imaging approaches often perform measurements photon-by-photon and would benefit from improvements in arrays of single-photon counting detectors. Increased timing resolution, pixel count, data throughput, detection efficiency, and wavelength range directly improve the use of quantum imaging in practical applications, making them increasingly competitive with standard imaging techniques.

3.4 Timeline and specific challenges

For each of the sensing applications outlined in this roadmap, there is an active community working on near-term improvement and development of numerous sensing platforms and modalities. Taking full advantage of these quantum resources will require significant investment in theory, hardware development, materials research, experimental physics implementation, translational research, and classical engineering. We outline some key research areas and milestones over the next decade and beyond for quantum sensing, summarizing activities of broad importance and essential for the four applications above.

	1-5 Years	5-10 Years	10+ Years
PRECISION MEASUREMENT FOR NEW PHYSICS	*Quantum control techniques to extend searches for new physics with quantum sensors* *Develop new precision measurement platforms for next-gen searches for new physics*	*Next-gen quantum sensing searches for new physics, targeting parameter space with highest potential for new discoveries* *Entanglement enhanced searches for new physics with beyond-classical capabilities*	*Quantum sensors and sensor networks for axion and ultralight dark matter search over large parameter space.* *Use quantum sensors to explore interface between relativity and quantum mechanics.* *Integrate quantum sensors with particle accelerators and detectors to enhance their performance.*
SENSITIVE HIGH-RESOLUTION PROBES FOR MATERIALS ANALYSIS AND DESIGN	*Ultrahigh sensitivity magnetometers near the quantum noise limit,* *Discovery of new qubits for sensing* *Nanometer resolution magnetic imaging of currents, magnetic phases* *Noise sensing for dynamics*	*Integrated probes and instruments for high-throughput materials science* *Measure correlation functions in materials* *Exploit many-body physics, squeezing, entanglement for better sensitivity*	*User facilities with quantum sensors* *Commercial deployment of materials analysis tools* *Nanoscale sensors with quantum advantage*
ROBUST AND DEPLOYED SENSING RESULTS	*Improvements in size, weight & power, component integration, robustness to bring state-of-the-art quantum sensors into the field* *Materials development for radiation, thermal, and chemical resilience*	*Demonstrate prototypes in the field* *Demonstrate sensors in fusion environments*	*Mid-scale and large-scale manufacturing and deployment for scientific applications* *Technology translation to commercial partners*
BIOLOGICAL, CHEMICAL, AND BIOMEDICAL SENSING	*Sensor integration with relevant geometry for biological and chemical sensing and imaging, materials development and surface functionalization* *New protocols for measuring dynamics and small signals*	*Translation to bioenergy, capture of* CO_2*, biomedical and clinical applications* *Quantum sensing and imaging in physiologically relevant conditions* *Demonstrate high-throughput, high-sensitivity chemical sensing*	*Technology transfer to clinical settings, bioenergy and a bioeconomy* *Wide-scale deployment of biological and chemical assays*

Fig. 3.3: Key activities and milestones for quantum sensors in each of the four application areas over 1–5 years, 5–10 years, and for the 10+ year time frame, assuming significant investments over this time period.

Chapter 4

Quantum Networks to Harness the Power of Linked Quantum Resources

4.1 Introduction

One of the most remarkable features of quantum entanglement is nonlocality: measurements of one quantum particle can influence the state of an entangled partner, even when the two are separated by arbitrarily large distances [386]. Such effects eschew our everyday experience of the world, yet have been confirmed with ever-increasing precision in Bell inequality tests for over 40 years [387–393] — an achievement recognized by the 2022 Nobel Prize in Physics [394]. The nonlocality inherent in quantum entanglement implies that the very phenomena underpinning QIS applications in computing and sensing can be realized across spatially separated devices when linked by quantum entanglement. While classical networks operate by transmitting information back and forth between nodes, quantum networking unlocks entirely new paradigms in which nodes sharing *entangled* resources can support applications impossible with classical physics, such as quantum teleportation [395–397]. (Even quantum networks lacking entanglement can still offer value in cryptographic applications like quantum key distribution [398–400].) However, *establishing* long-distance entanglement becomes increasingly challenging as distances grow, since transmission loss can severely suppress successful entanglement distribution. Entanglement swapping can be utilized to mitigate this problem.

A future quantum internet [401, 402] could support numerous applications. Fig. 4.1 offers a simplified conceptual vision, where quantum computers and sensors connect to a networking infrastructure combining fiber-optic and free-space channels. The network core combines sources of entangled photons with quantum switches or routers, linking devices within or between networks. Quantum repeaters effectively "catch and release" photons before they are lost to extend the distances supported [403–405]. At the network edge, quantum transducers convert quantum information from the transmitted photons to the matter qubits at the nodes. Like the conventional internet, the quantum internet ideally will be application-independent, providing an essential service (e.g., entanglement between any two points) that users can exploit for *any* application of interest. Nevertheless, several projected applications are particularly relevant to the mission of the DOE Office of Science. Figure 4.1 highlights a few examples, which can be classified according to the type of interactions supported: sensor to sensor (Sec. 4.3), sensor to computer (Sec. 4.4), and computer to computer (Sec. 4.5).

4.2 Previous DOE contributions and successes

The potential of quantum networking for scientific discovery and its significance to the DOE are well-established [18, 406–408]. Through base programmatic funding from Advanced Scientific Computing Research (ASCR) — as highlighted by Early Career Awards and four quantum network programs [409] —

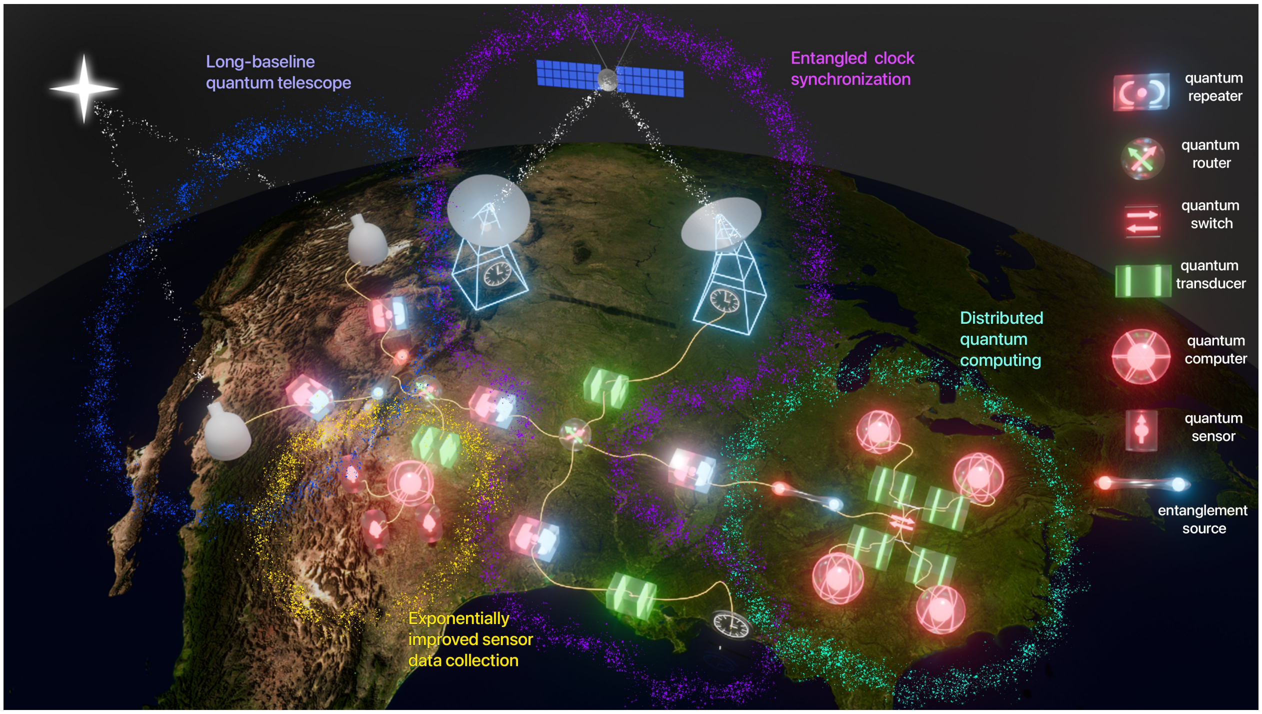

Fig. 4.1: Sketch of a continental-scale quantum network. Basic quantum network components (sources, switches, routers, and repeaters) connect quantum nodes that perform a variety of applications, some linking sensors to sensors (long-baseline telescopes, clock synchronization) sensors to computers (exponentially improved data collection), and computers to computers (distributed quantum computing). Each application is based on distributed entanglement over some spatial scale.

and the National QIS Research Centers, the DOE Office of Science has invested heavily in quantum networking research over the last half-decade. DOE's leadership in advanced classical networking, exemplified through infrastructure such as ESnet [410], uniquely positions it to bridge the gap between conventional network engineers and physicists who have historically dominated quantum networking research. Collaboration and cross-pollination between the two communities will be critical for scaling up towards a quantum internet, an often-overlooked synergy ideally suited to DOE strengths. Among the many scientific accomplishments supported by the DOE so far, perhaps the most salient contributions center on the development of quantum network testbeds anchored by national labs (in alphabetical order): Argonne National Lab and Fermilab [411–415], Brookhaven National Lab [416], Lawrence Berkeley National Lab [417], and Oak Ridge National Lab [418–424]. Furthermore, significant advances have been made towards the development of quantum repeaters in the telecom band. These advances involve devising new material systems for quantum memories and integrating them with silicon nanophotonics to realize indistinguishable photon emission and spin-photon entanglement (C2QA [425,426] and Q-NEXT [427]). Additionally, the use of exotic single photons has shown promise in improving transduction between flying qubits and memory qubits (QSC [428]). Moreover, theoretical work has been conducted using entangled sensors for the detection of dark matter (SQMS [341]).

4.3 Linking sensors for increased resolution

Sensors harnessing the properties of quantum mechanics (see Chapter 3), have already shown large impacts in multiple fields. By linking quantum sensors together via networks that enable entanglement, their measurement resolution and sensitivity can be boosted even further.

4.3.1 Linking telescopes for high-precision astronomical imaging

Motivation

Telescopes and optics have been used to study our universe for hundreds of years, serving as the forefront to advancements in basic and applied science, such as cosmology, astronomy, and navigation. Improving telescope resolution and sensitivity in the visible spectrum allows us to study more of the universe, with examples including "starspots" on stars other than the sun (shedding light on how a star's magnetic field affects temperature), topographical features on exoplanets (elucidating planetary properties and formation), the innermost regions of protoplanetary disks (revealing information on star and planet formation), very faint stars (such as variable stars and binary systems, important for benchmarking galactic distances), and the environments surrounding massive stars (deepening our understanding of mass loss and mass transfer in rotating systems) [429].

Fig. 4.2 illustrates possible resolution improvements when observing the dwarf planet Pluto from Earth. [1] Each pane, from left to right, displays enhanced resolution achieved by either spacing telescopes further apart or utilizing shorter wavelength light, transitioning from Pluto as 1-2 pixels to revealing surface details. Incorporating quantum memories at each telescope boosts sensitivity, allowing for the detection of fainter features.

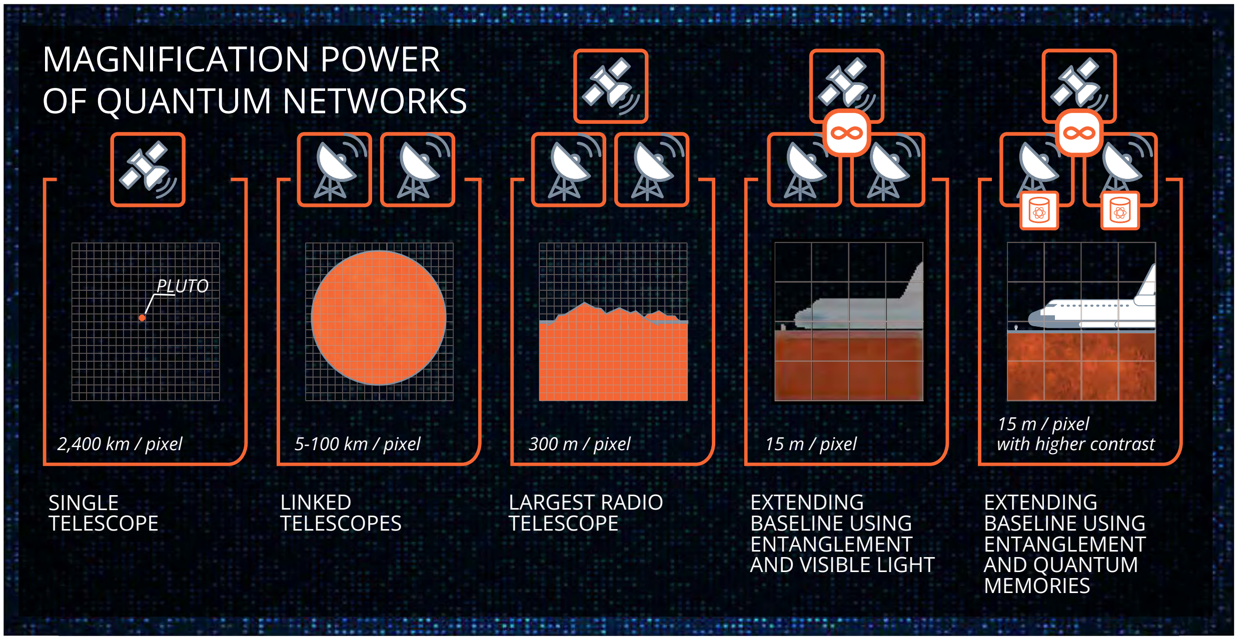

Fig. 4.2: Example views of the dwarf planet Pluto from Earth using telescopes of increasingly extended baselines. First panel: resolution using a single telescope like Hubble or James Webb [430]. Second panel: linking telescopes using standard radio techniques or visible interferometry [431, 432]. Third panel: resolution from the largest radio telescope combining data from locations spanning the globe [433]. Fourth panel: improved resolution combining the baseline of the largest radio telescope with entanglement in the visible regime, making it possible to see $\sim$15 m-scale features, depicted by a space shuttle for scale. Fifth panel: if quantum memories are also available at the satellite locations, the ability to see very dim objects improves, depicted here by an increase in contrast.

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[1] Pluto is merely an example; the telescope could be directed toward any object of interest with similar resolution and sensitivity improvements.

State of the art

The performance of a telescope is determined by its sensitivity and resolution. The resolution of a single telescope, for example the Hubble or James Webb Space Telescope, is limited by the diameter of its objective and the wavelength of light collected. This resolution can be significantly improved through a telescope array, now standard in radio astronomy [434, 435], which creates an effective objective much larger than a single telescope and interferes collected photons from one telescope with another. Interfering visible-wavelength photons further increases resolution, but presents many challenges since current schemes require that photons be physically combined [436]. Therefore, the maximum achievable baselines with visible light are currently limited by photon loss and optical-phase control in the channels connecting the telescopes.

Envisioned future

Quantum networks could extend short-wavelength telescope array baselines significantly by harnessing quantum entanglement. In one method [437], entanglement is generated continuously between telescopes using "cheap" terrestrial photons, which will then be available to interfere with astronomical photons, producing the necessary entanglement between telescopes. The distance between telescopes can be extended if quantum repeaters are used, thus eliminating the problem of photon loss between sites.

Instead of continuously generating entanglement, one can place quantum memories at each telescope. These quantum memories store the entanglement between sites until there is an incoming photon, which can also be stored in a quantum memory before joint detection [438, 439]. This scheme reduces requirements on the entanglement generation rates, but likely demands transduction between photons and longer-lived physical or logical qubits and reliable gate operations for nonlocal parity checks on the quantum memories to extract photon information.

Additionally, beyond reducing loss between telescope sites, a large network of telescopes with small quantum memories at the telescope locations can lead to additional, more fundamental sensitivity improvements (similar to Sec. 4.4). Since coherence can be preserved across the entire array, a quantum Fourier transform can be performed instead of the typical classical Fourier transform, improving sensitivity by roughly $\sqrt{N}$ where N is the number of telescope sites [439].

4.3.2 Global clock synchronization for testing fundamental physics

Motivation

Optical atomic clocks are currently the best timekeeping devices available [317,318,335,440]. Developments in such clocks have already unlocked new precision records in a variety of fundamental science applications, including testing the validity of Einstein's theory of general relativity [335] and adding limits to temporal variations of the fine structure constant [334]. Linking distant optical atomic clocks stands to further improve our ability to measure small time variations. Networks of atomic clocks are particularly suited to search for dark matter, mysterious and as yet unobserved matter that comprises the vast majority of the universe's total mass. In one theory, as a large dark matter object passes through a network, initially synchronized clocks will become out of sync, and the signature of time discrepancies then encodes the dark matter object's structure [441]. As a terrestrial application, measurement of small vertical clock motions relative to Earth's gravitational field can indicate underground volcanic processes (such as an inflating or deflating magma chamber) [442].

State of the art

Perhaps the most famous success of clock comparisons is the Global Positioning System (GPS) which, under the right conditions, can measure vertical displacements of the Earth to within 1 cm for short integration times and 1 mm after long integration times [442]. GPS satellites each carry multiple microwave atomic clocks and are regularly synchronized to an ensemble frequency standard at the Naval Observatory in Washington D.C. Additionally, frequency comparisons between optical clocks via terrestrial optical fiber links have already been used to improve the precision of the clock system beyond that of an individual clock [443].

Envisioned future

To improve our ability to use clocks to detect very small time shifts, increasing the number of clocks in a frequency-comparison network and expanding the distance between them are essential steps. Since frequency comparisons do not require quantum state preservation, the infrastructure to do so is somewhat relaxed and can be done via fiber optics (land and undersea) or through precise space links with satellites in orbit.

However, instead of simple frequency comparisons, if the clocks are entangled, the precision can increase beyond the standard quantum limit to the ultimate allowed precision, the Heisenberg limit [444, 445]. This precision enables the detection of smaller time shifts, thereby allowing researchers to identify subtler interactions with dark matter and impose tighter constraints on variations of fundamental constants. To entangle clocks that are separated by long distances, a similar scheme is needed as for entangling light collected by telescopes — entanglement can be distributed through the use of entangled sources and the distances between detectors can be increased through the use of quantum repeaters.

4.4 Linking sensors to quantum processors for finding rare or small signals

Typically, quantum sensors undergo minimal quantum manipulation after they are exposed to a signal of interest, and are measured quickly to reduce their state to classical information that can be easily stored, processed, and analyzed. If instead the states of the linked sensors or quantum devices are allowed to remain in a quantum memory and be manipulated by quantum operations before reduction to classical data by measurement, a number of new enhancements and applications become available, including exponential enhancements in learning from physical systems, detecting small signals amid noise, and identifying particle trajectories in a single shot.

4.4.1 Networks for faster learning from quantum states

Sometimes it is necessary to discover properties or answer questions about the state of a physical system by using repeated measurements of that system. It was recently shown that if a small quantum processor can manipulate the states beforehand, learning the properties of that state can occur with exponentially fewer measurements than techniques without state manipulation [446, 447]. This advantage in the number of measurements is distinct from purely computational advantages in that it cannot be overcome by even an infinite amount of classical computation. This result was validated with 40 qubits that, even in the presence of real experimental noise, retained many orders of magnitude speedup over all possible single-copy measurement schemes [3]. Remarkably, while the advantages depend on the multi-qubit nature of the state or sensor, many do not require the underlying sensor state to be entangled or pure.

4.4.2 Finding rare or small signals in particle accelerator outputs

The initial research on exponential learning advantages in quantum states primarily concentrated on ensembles of qubits. However, subsequent advancements expanded this theory to encompass systems resembling sensor arrays, cavities, and general photonic channels. As a result, its applicability has been broadened to include dark matter or other exotic particle detection applications [448, 449]. One advantage of these methods is the ability to extract a small signal in a very noisy background from exponentially fewer measurements.

More recent work has shown that the use of entangled arrays of qubits may be used to identify trajectories of individual particles weakly interacting with the sensors with a single shot, a capability that is provably impossible with unentangled or classical sensors [450].

As an application of these powerful new results, one can imagine the detection and identification of novel or rare particles such as axions, dark matter, and unique particle accelerator products [300]. Such aggressive goals require further development of the theory and close collaboration with experimental teams developing novel sensors and transduction technology. Despite the above challenges, preliminary results suggest that this unique combination of sensing and computation can reveal otherwise invisible facets of our universe and drive the discovery of new physical phenomena.

4.5 Linking quantum computers to increase processing power

The advantages of modular and networked computing systems over their monolithic counterparts are well-established for classical computing. For example, networked computing systems (i.e., almost all HPC systems) enable high-speed multi-party computation and communication over vast geographic distances. Meanwhile, performance at the single-core level has generally plateaued in classical computing, so that optical networking has become critical in advancing today's supercomputers [451] and datacenters [452]. Even for computation by a single party, modular designs improve robustness, scalability, and price while remaining flexible to future design improvements. These advantages are expected to translate to networked *quantum* computing systems, yet with the ability to take advantage of new quantum effects — most notably, entanglement — to enable applications not possible in a purely classical world.

At a basic level, a quantum link is required between two quantum computers in order to effectively create a larger quantum computer without incurring an exponential overhead in some resource [453, 454]. Techniques like state [395] and gate [455] teleportation can be used to combine separate quantum computers composed of either the same or separate physical hardware platforms. In the latter case of computers composed of multiple hardware platforms, one can exploit the natural advantages of different systems, e.g., speed in computing or lifetimes in storage, rather than accept the tradeoffs inherent to a homogeneous architecture. In all cases, modular design of quantum computing systems allows one to separate and maintain control systems in a way that is more easily scaled up and replaced if a component is damaged. Moreover, connections enabled by networked architectures may be more flexible than those natively available in the qubit systems themselves.

In addition to simply scaling computing systems, quantum communication between quantum computers offers novel opportunities. This includes an exponential reduction in communication overhead [456]. In today's big data ecosystem, one of the most significant expenses is the storage and transmission of large quantities of training data. Thus the reduction in communication overhead for quantum devices means some machine learning problems are solvable using exponentially fewer bits than classical devices [457, 458]. To be concrete, the same information that would require exabytes of classical information ($>10^{18}$ bits) would only need tens of qubits. Unlike some quantum advantages, these advantages are unconditional in the sense that no amount of classical computation can close the communication gap.

Some applications of quantum networks lack a natural classical analog and represent fundamental resources of the quantum world we can leverage. For example, quantum information is fundamentally fragile in a way that enables fundamentally new capabilities in privacy and security, such as proven deletion of user data [459], currency that can't be copied [460], or computations one can run on the cloud while revealing nothing to the server [461]. While some of these applications focus on security, it has been noted that this perspective provides novel tools we may use to interrogate our universe [447, 462], like quantum position verification [463]. Such applications require quantum communication or networking to enable, but they are especially exciting due to their impossibility without quantum technology.

4.6 Timeline and challenges

4.6.1 Science and technology challenges and metrics

Network core

Realization of the overall vision highlighted in Fig. 4.1 and articulated through specific applications in Secs. 4.3–4.5 will require sustained research addressing challenges on multiple fronts. Ultimately, the network *core* will be responsible for producing, routing, and repeating the quantum optical signals necessary for establishing entanglement between arbitrary nodes on the network. Analogous to the classical internet, the quantum network core can thus be viewed as providing a generic service — entanglement distribution — to those connected to it. Accordingly, a natural measure of network quality is the number of entangled bits per second (ebits/s), i.e., the number of ideal entangled qubits (known as Bell pairs) supplied over a given link in a unit time [464], or more generally the rate of Bell pairs which could be obtained after performing measurements on a larger number of noisier resource states (so-called "entanglement distillation") [465–467].

In the quest to maximize performance, quantum networks face a variety of technical challenges. It is useful to classify challenges in terms of those based on channel and architecture. The former encompasses issues related to the transmission medium itself, such as signal loss and noise. Quantum repeaters [403–405] are designed to address signal loss. Although a variety of important experiments entangling matter qubits over deployed fiber have been demonstrated [391, 468–473], no repeater surpassing the throughput of the equivalent "repeater-less" lightpath in terms of end-to-end efficiency has been demonstrated at the time of writing. Accordingly, an important early milestone on the path toward a quantum internet will be a repeater attaining better performance than the passive medium itself.

Noise is likewise a major challenge for quantum network channels, whether from background light in free space or crosstalk from co-propagating classical signals in optical fibers. Quantum-classical coexistence appears particularly urgent for quantum communications to leverage the vast lightwave infrastructure available today. Although a growing number of experiments have demonstrated both coarse [414, 474–477] and dense [421, 478, 479] wavelength-division multiplexing coexistence, dark fiber — i.e., strands devoid of any shared classical traffic — remain by far the medium of choice in quantum communication experiments. Ongoing research in quantum-classical coexistence is needed, with the critical turning point arising when performance is so reliable that quantum network architects will no longer need to consider whether quantum light shares the fiber with classical signals or not in their buildouts.

The second major category of challenges, architecture, includes resource allocation, quantum switching and routing, and timing (synchronization and latency). All of these considerations are shared by classical networking, where lightwave technology, electronic packet switching, and the TCP/IP stack [480] jointly provide a reliable and scalable architecture. Unfortunately, the unavailability of standard optical-to-electrical conversion — and thus digital logic — for processing quantum signals (measurements collapse the quantum state) severely constrains the tools available for quantum networks. Additionally, with the timing and latency requirements for coordinating and maintaining entanglement across spatially separated nodes, quantum network architectures must address a slew of challenges beyond those faced in typical internet communications.

Progress toward scalable quantum optical backbones has advanced steadily, with recent accomplishments including flex-grid bandwidth management [481, 482], proposals for quantum network stacks [419, 483, 484], forays into packet switching [485, 486], centralized control based on software-defined networking (SDN) [411, 487, 488], and a variety of timing approaches to synchronize and correlate distant quantum measurements [412, 416, 488–490]. Yet, so far no solution even remotely approaching the reliability and universality of TCP/IP has emerged. Ultimately, the mark of success for a quantum network architecture will be its transparency to the end user, who should be able to successfully *use* a quantum network without knowing how it works. At that point, quantum networks will truly provide a service that could reasonably be likened to the conventional internet.

Network edge

While the network core is focused on providing *resources* — e.g., entanglement — it is the network edge where such resources will be leveraged for *applications* like those in Secs. 4.3–4.5. These edge nodes will need to perform various functions using components such as quantum processing units, entanglement generators, memories, and measurement detectors.

Photons, due to their weak interaction with the environment and ability to carry quantum information over long distances with minimal loss, are preeminent as quantum information carriers or *flying qubits*, with the low-loss telecom bands (1310–1625 nm) particularly advantageous [491]. For this reason, we anticipate that the network core will likely evolve into a relatively homogeneous and standardized architecture. But this standardization will certainly not prove to be the case for the network edge, which is expected to develop heterogeneously given the diversity of *stationary qubits* currently under development including but not limited to ions, atoms, and superconductors. Not only can different applications place widely varying requirements on the quality of network service;[2] each edge node will need to be able to interface efficiently with network photons through transduction and, depending on the application, store quantum information for periods of time comparable to network latencies.

Different transducers, such as photon-photon, phonon-phonon, photon-spin, and ion-superconducting, will therefore be necessary to perform multiple tasks in a full-stack quantum network, including storage, repeaters, and interfaces with other technologies [494, 495]. As one example, the challenges of quantum transduction are perhaps most pronounced for superconducting qubits, where high-efficiency microwave-optical transducers are needed to convert information between the optical regime of telecom flying qubits and the microwave regime of stationary superconducting qubits, which can differ in energy by five orders of magnitude. High-efficiency conversion at low photon counts is challenging and currently out of reach with existing devices, although important recent results, novel designs, and demonstrations on different platforms suggest promising future directions [342, 496–501].

4.6.2 Timeline

A possible timeline for developing the specific examples presented in this Applications Roadmap is shown in Fig. 4.3. The technological developments are categorized into "network core" and "network edge" and can be pursued in parallel. The technological advances in each section, however, are generally sequential with different milestones building upon each other.

Arguably, the most critical building block for interconnected quantum networks is the quantum repeater, which will allow campus- and metropolitan-scale networks to increase arbitrarily in size. Another possible disruptive technology would be the development of optical fibers capable of transmitting visible light long distances with very low loss, which could obviate — or at least reduce — the urgency of quantum repeaters. Advances in other QIS pillars (computing and sensing) could likewise disrupt this timeline. For example, many requirements for quantum computers are shared with quantum repeaters, making advances in quantum computing readily transferable to quantum networking. Similarly, because some quantum sensor modalities rely on the conversion of quantum states between two systems, they share important commonalities with transduction, producing strong synergies between sensing and networking research as well.

Overall, allocating resources toward the essential elements of a quantum network, such as repeaters, routers, switches, transducers, entanglement sources, quantum computers, and low-loss optical fibers, as well as establishing connections between these components, will yield significant benefits. These investments will result in heightened sensitivity, enhanced precision, and increased capabilities of the interconnected devices.

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[2] E.g., quantum key distribution can accept much higher physical error rates [492] than fault-tolerant quantum computing [493].

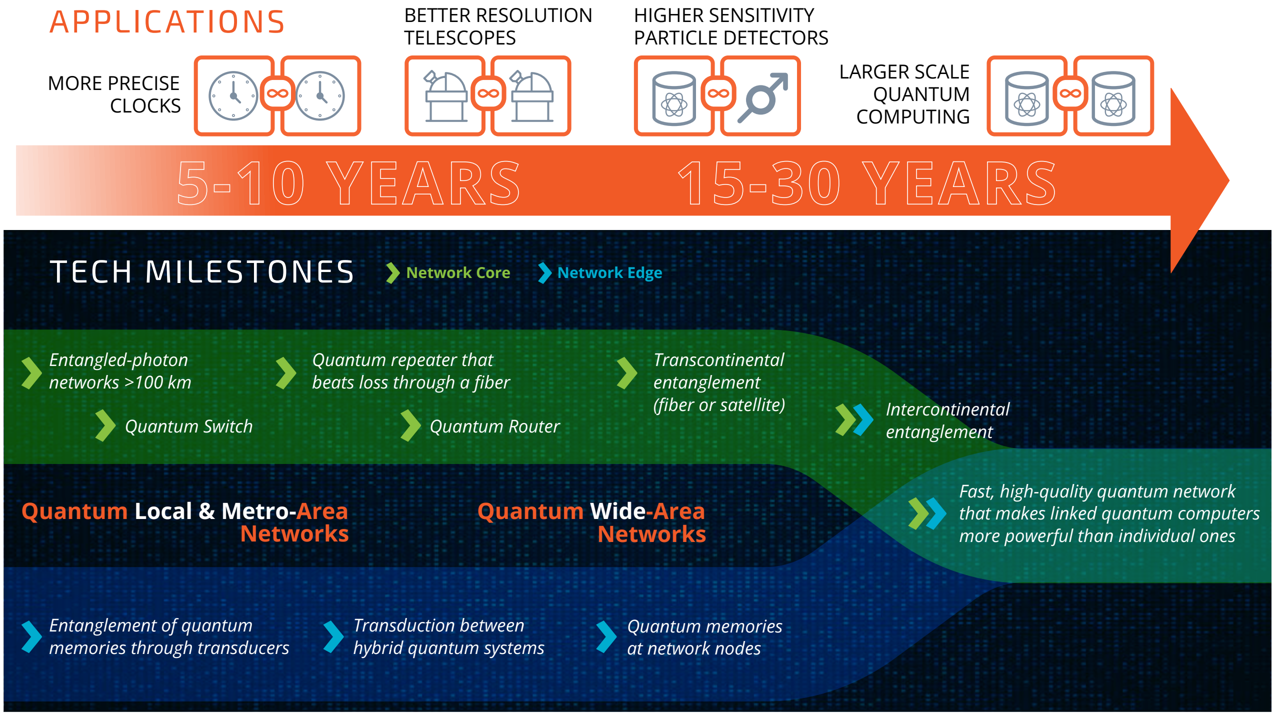

Fig. 4.3: Timeline for developing quantum network applications. Applications appear at the top of the timeline with corresponding technological developments shown below, categorized into “network core” and “network edge.”

Chapter 5

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Chapter 6

Supplementary Material

6.1 Basic quantum concepts explained

Qubit A qubit, short for quantum bit, is the quantum analog of the bit and the smallest building block of a quantum processor. A qubit refers to a two-state quantum system, but qudits, which are multi-state (>2) quantum systems are also investigated.

Interference Interference is a wave phenomenon that occurs when two (or more) waves travel through the same spatial region. Each wave has wave crests and troughs. If crests of wave 1 coincide with troughs of wave 2, then the two waves can eliminate each other (destructive interference). If crests and crests coincide, the two waves add up to form a larger wave (constructive interference).

Entanglement Consider two objects A and B. For concreteness, we may think of two bits or qubits. Ordinarily, we expect that we can specify the configuration or state of these two objects by recording their individual states: bit A is in state 0, and bit B is in state 1. Quantum physics allows so-called entangled states in which, e.g., two qubits inhabit a joint state that cannot be expressed in terms of two individual qubit states. The Bell state $(|00\rangle + |11\rangle)/\sqrt{2}$ illustrates this case. Neither qubit is in a definite state of its own in this case; rather, the qubits share one joint state. Entanglement leads to new correlations not found in classical physics and is known to be a necessary resource required for certain types of quantum speedup.

Entanglement swapping In the standard instantiation of entanglement swapping [502, 503], Alice and Bob begin with separate pairs of entangled qubits and send one qubit from each pair to a central station (Charlie), who performs a joint measurement on each; this will then entangle the two unmeasured qubits that never interacted. Since no single qubit needs to travel the entire separation between Alice and Bob, but only to Charlie (who can be placed right in the middle), the distance of entanglement can be doubled; piecing many of these operations in parallel provides one path toward quantum repeaters: devices that increase the reach of entanglement by segmenting long, high-loss channels into smaller elementary links where entanglement can be established with higher probability [403–405].

Quantum error correction Physical errors in classical computing are usually rare and simple, with bit flips (randomly changing a 0 to a 1 or vice versa) constituting the typical error type. Quantum computing is different in that several different types of qubit errors will occur at significant rates. Without interventive strategies, these errors severely limit the utility of quantum processors. Quantum error correction protocols introduce redundancy (e.g., by encoding the quantum information of a single logical qubit in several physical qubits), combined with clever schemes for detecting and correcting the physical errors.

Fault tolerance Quantum fault tolerance implies that large quantum computations can be performed accurately even in the presence of physical errors. One path to fault tolerance uses the full implementation of quantum error correction, combined with the use of schemes that carry out each logical gate operation through a sequence of basic operations on the groups of physical qubits that redundantly encode the quantum information. Such fault tolerance comes at the price of an increase in the required number of physical qubits and physical gates to implement the logical computation.

Standard quantum limit The fundamental precision limit determined by quantum uncertainty.

Squeezing The reallocation of noise from one parameter to another to achieve higher precision in the measurement of interest, beyond the standard quantum limit. By making the measurement noisier in one variable (such as the position), the measurement can be less noisy in another (such as the momentum).

Superposition A classical bit can take on two values: 0 or 1. At any given time, the bit is either in state 0 or in state 1. For a qubit, the quantum analog of the bit, the possibilities are far richer: a qubit can be in so-called superposition states to which both the 0 and the 1 state contribute with varying proportions.

Quantum nondemolition measurement A measurement constructed such that the uncertainty in the measured quantity does not increase because of the measurement.

Quantum transduction The process of coherent quantum state transfer between different types of qubits, such as between a stationary qubit (e.g. spins, charges, currents) and a flying qubit (e.g. photons, phonons).

6.2 The path to fault tolerance

Expanding upon Sec. 2.4, we discuss the timeline and challenges in the development of quantum error correction in the four eras identified: E1, NISQ devices and small demos of QEC (0–5 years); E2, small quantum computers with QEC (5–10 years); E3, large quantum computers with QEC (10–20 years); and E4, very large fault-tolerant quantum computers (20+ years). Numerous challenges abound, both in realizing the described hardware systems as well as successfully capitalizing on them. Hence, the field needs a "dual-path" approach to development: advance to E4 as soon as possible, and find increasingly useful computations for the hardware systems available in each era. New innovations and ideas for quantum algorithms will be especially important [66, 83, 185, 216, 252, 504–507].

E1 (NISQ devices and small demos of QEC) describes the current era of quantum computing, characterized by noisy systems which are rapidly approaching the most advanced classical capabilities, the need for error suppression and mitigation techniques to achieve maximum system performance, and increasingly-sophisticated demonstrations of the computational primitives required for QEC (albeit without simultaneously fulfilling the complete set of criteria for error correction). The novel use of these systems may be useful for realizing certain, limited applications [66]. The main challenges for E1 include: (a) advances in QEC and demonstrations thereof, (b) developing new scientific applications and algorithms by engaging with the broader DOE researcher community, (c) initiating engagement with experts in advanced classical computing for building powerful, high-throughput, low-latency control hardware for future QEC systems, (d) benchmarking, verifying, and quantifying quantum advantage(e) ensuring sufficient access to quantum computing platforms to enable novel research.

E2 (small quantum computers with QEC) describes an era wherein systems unambiguously demonstrate all criteria of error correction, but with underlying physical error rates close to the thresholds of the error correction codes used [508–510]. Such systems may be capable of accurately running circuits acting on hundreds of qubits with hundreds of millions of operations, which would likely be truly beyond classical capabilities. The field will need to adapt to their distinct capabilities [511], as well as their drawbacks such as the significant overhead of fault-tolerant operation. Progress will continue on previously devised paradigms for quantum algorithms and applications that do not require QEC. The main challenges for E2 include: (a) establishing and operating a user facility allowing the general DOE scientific community access to quantum computing systems,[1] (b) successfully integrating advanced classical computing and control capabilities with quantum computers in support of larger-scale quantum error correction, and (c) identifying and de-risking challenges to scaling towards E3 and E4, including supporting foundational research in quantum transduction techniques.

E3 (large quantum computers with QEC) refers to the availability of systems operating well below threshold error rates, capable of reliably running circuits acting on thousands of qubits with billions to trillions of operations. Now quantum computing will start to deliver transformational results to the scientific community, making predictions well beyond the reach of classical computers, as discussed in Section 2.5. The main challenges for E3 include: (a) ensuring that a well-established user facility exists, (b) helping the general DOE scientific community to begin capitalizing these systems to transform how research is done, and (c) updating and porting classical software codes to encompass new programming and architecture models of quantum computers.

E4 (very large fault-tolerant quantum computers) encompasses the availability of systems operating well below threshold, and capable of running circuits acting on tens of thousands of qubits with more than 10^{12} operations. These systems' transformative potential for scientific discovery is previously discussed in Sec. 2.4. For example, the ability to simulate many processes will change what type of measurements provide scientific information into foundational questions and how new technology will be developed.

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[1] This could be in the form of access to general-purpose quantum processors or more specialized hardware for different scientific domains. The DOE has already established the Quantum Computing User Program (QCUP) [42] and two testbeds based on different technologies (superconducting qubits at AQT and trapped ions at QSCOUT) [40, 41]; a future user facility could build on or compliment these. One could also imagine additional testbeds based on different hardware platforms to explore the tradeoffs of various qubit technologies.

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