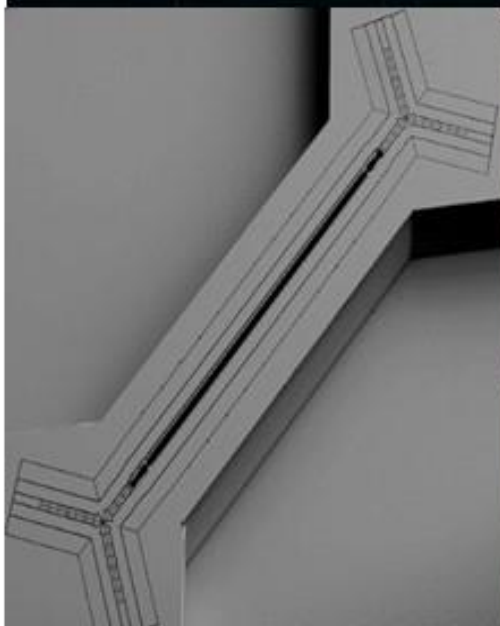
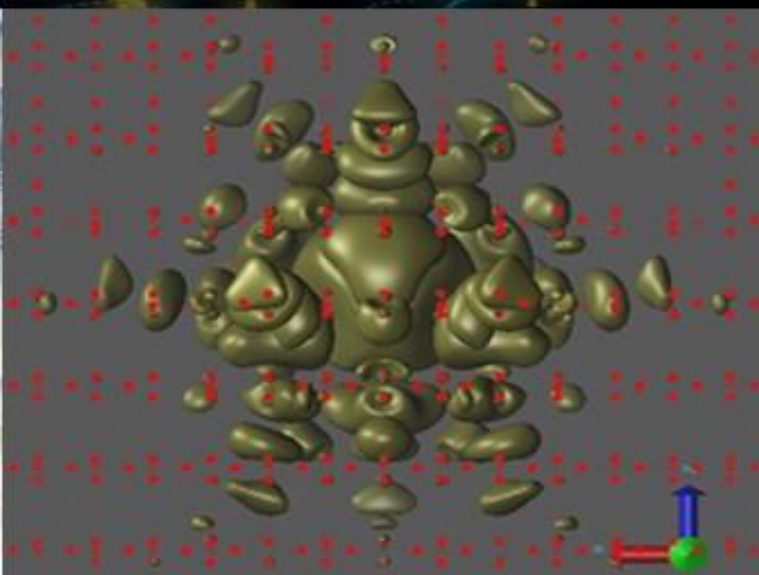
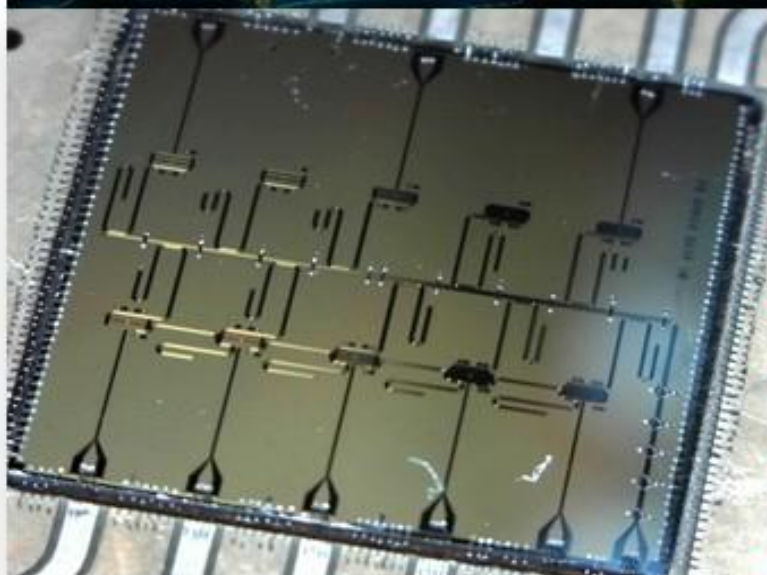
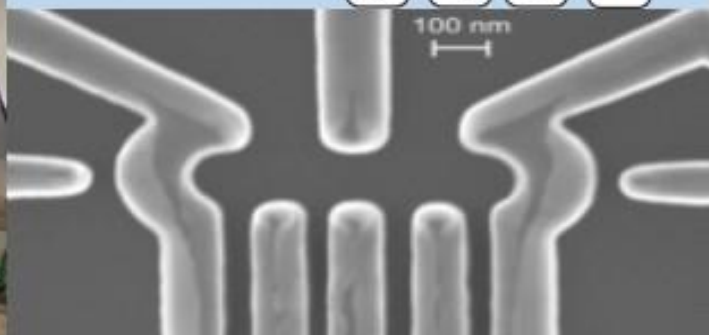
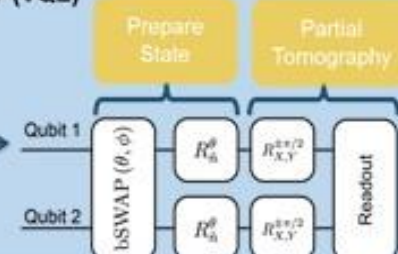


# ASCR Report on a Quantum Computing Testbed for Science



Quantum Chemistry (VQE)



# ASCR Report on a Quantum Computing Testbed for Science

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## Abstract

This report details the findings of the Quantum Testbed Stakeholder Workshop sponsored by the Department of Energy's Advanced Scientific Computing Research Program to identify opportunities and challenges in establishing a quantum testbed to advance quantum computing hardware and software systems that will enable science investigations. The workshop was held on February 14 – 16, 2017 in Washington DC and served as a forum for individual stakeholders from academia, industry, national laboratories, and government to provide their perspectives and ideas on the overarching goals and objectives of a quantum testbed, technical considerations, and how a quantum testbed program would be synergistic with other nascent quantum computing efforts in the US and worldwide. This report summarizes discussions on best practices for management of various types of collaborative research activities, including topics such as workforce training and building strong relationships with the research community. It also reviews specific technologies that have been identified by the ASCR Program as being important for the success of a quantum testbed whose overall goal is advancing quantum computing for scientific applications in the next five years.

## Executive Summary

Advances in computing are continuously enabling ever more powerful modeling and simulation tools that increase scientific understanding of complex phenomena relevant to the Department of Energy (DOE). Today, ASCR is developing platforms that will enable exascale class computing within 4-5 years. As the community moves toward exascale, a fascinating and challenging question emerges: what lies beyond exascale?

Quantum Computing (QC) represents the next frontier in world-changing computational capability. QC is a promising early-stage technology with the potential to provide scientific computing capabilities far beyond what is possible with even an exascale computer. The classes of problems that are uniquely suited to solution using QC are at the core of DOE's missions in materials science, high-energy physics, nuclear physics, and quantum chemistry. Research groups around the world are recognizing the game-changing capabilities of quantum computation and are investing in the long-term research needed to enable that promise.

Realizing quantum computers that will solve DOE-relevant problems beyond the scope of contemporary classically-based machines is a complex opportunity that presents formidable challenges. Interdisciplinary scientific research and technology development efforts involving physicists, applied mathematicians, computer scientists, materials scientists, and engineers will be required to harness the laws of quantum mechanics to build a quantum computer. Entirely new algorithms, architectures, and languages will be required. At present, commercial QC systems are not yet available, and the technical maturity of current QC hardware, software, algorithms, and systems integration is incomplete. Hence, there is a significant opportunity for DOE to provide the long-term leadership that defines the technology building blocks, and solves the system integration issues to enable this revolutionary tool.

The Quantum Testbed Stakeholder Workshop engaged the collective strengths of industry, academia, national laboratories, and government to discuss a path for quantum computing within DOE's Office of Science. This workshop builds upon the community engagement initiated in the 2015 ASCR workshop on Quantum Computing for Science. ASCR is committed to maintaining a high level of community engagement as the field and DOE's mission needs evolve.

At the outset of the workshop, the attendees recognized the value of a quantum computing testbed as a catalyzing force to bring the community together and focus it on the challenges of blending cutting-edge science with systems engineering to enable the application of QC to solve problems of interest to DOE. A testbed can also serve as a bridge between industry and academia to encourage transparency while these precompetitive technologies are being developed, lower the barriers for entry into the field by medium and small sized companies or academic research groups, and foster the establishment of metrics and standards to effectively compare the performance of engineering design tradeoffs.

One of the major barriers that was identified was the immaturity of not only the individual QC technology building blocks (including hardware and software), but also the system architectures and general infrastructure required to make effective design choices. The implication of this current state-of-the-art is that the principle of co-design arguably becomes even more important than it might be for design of conventional high performance computing (HPC) systems.

This workshop report provides a summary and assessment of the many elements that will need to be incorporated into a testbed to effectively weave together a diverse, high performing team to advance the state of the art in quantum computing and realize the long term economic and scientific promise of QC., and ASCR looks forward to continuing to engage the broader community to help define the future of QC.

# 1 Introduction and Motivation

## 1.1 Purpose of the Meeting and Agenda Overview

Quantum computing (QC) is a promising early-stage technology with the potential to provide scientific computing capabilities far beyond what is possible with even an exascale computer to solve specific problems of relevance to the Office of Science. Such capabilities include (but are not limited to) materials science, high-energy physics, nuclear physics, and quantum chemistry. Despite the rapid pace of progress in the underlying technologies of QC hardware, software, algorithms, and systems integration, commercial quantum computers capable of solving DOE-relevant computational challenges are not expected in the near term. Thus, there is a significant opportunity for DOE to define the necessary technology building blocks, and solve the system integration issues to enable a revolutionary tool optimized for DOE mission problems. Once realized, QC will have a world-changing impact on the scientific enterprise, economic competitiveness, and information processing in general.

Prior to this workshop, the DOE Office of Science's Advanced Scientific Computing Research (ASCR) program office hosted a workshop in 2015 to explore QC scientific applications. The goal of that workshop was to assess the viability of QC technologies in meeting the computational requirements needed to support DOE's science and energy mission, and to identify the potential impact of these technologies. That ASCR workshop report commented that research into QC technologies was progressing rapidly and that it was important for ASCR to understand the potential use of these new technologies for DOE-relevant applications as well as their impact on conventional computing systems. It also noted that scientific application development would make significant advances only when QC systems are available, even at the few-qubit level.

Subsequently, in February of 2017, ASCR sponsored a second workshop, the Quantum Testbed Stakeholder Workshop (QTSW), which brought together a diverse group of stakeholders from academia, industry, government, and DOE laboratories. The purpose of the QTSW was to identify opportunities and challenges in establishing a quantum computing testbed to advance QC hardware and software systems that could be used to enable scientific investigations. Prior to the workshop, whitepapers were solicited in a number of topic areas (the full list is in the Appendix). For example, stakeholders were asked to outline their individual capabilities and interests in QC hardware and software; comment on best practices for management of collaborative research facilities, including topics such as workforce training and building strong relationships with the research community; and review specific technologies that might be important for the success of a quantum testbed whose overall goal is advancing QC for scientific applications in the next five years.

The 2017 workshop was structured to serve as a forum for all stakeholders to provide their perspectives and ideas on the overarching goals and objectives of a quantum testbed platform and how that platform would be synergistic with other nascent QC efforts in the US and worldwide. The first day provided an introduction of the goals for the meeting, four plenary technical talks which provided a status update on key elements of the possible testbed design, and presentations by the DOE laboratories wherein they identified their individual capabilities and interests in QC and their use for science applications. The second day focused on programmatic issues, technical challenges, and the role of co-design in achieving an operational quantum computing testbed. Sessions on the third day explored the roles of industry and government in shaping a coordinated national QC vision, and the challenges in constructing functional QC by combining the work of many subfields.

## 1.2 Plenary Talks

This session consisted of four presentations covering representative technologies, applications, and verification and validation techniques. The first two plenary speakers discussed two quantum computing technologies in detail: trapped-ion QC, and superconducting-qubit QC. These leading quantum computing technologies achieve gate and readout fidelities at the 99.9% level or better, but have different advantages and disadvantages. For example, ions have demonstrated a higher single-qubit gate fidelity, but superconducting qubits have a faster clock speed. While the gate fidelity numbers are impressive, they are significantly less reliable than conventional CMOS and other transistor-based technologies. This leads to the third plenary talk, which surveyed possible applications of imperfect near-term technologies for QC, and the need for verification and validation techniques for QC devices, the topic of the fourth plenary talk.

*Ion Trap Quantum Computing*, Dr. Christopher Monroe, *University of Maryland*

Trapped ions are one of the leading candidate technologies for implementing quantum information processing. In this technology, atomic ions are confined in free space with electromagnetic fields supplied by nearby electrodes. Qubits stored in trapped atomic ions are represented by two stable electronic levels within each ion. Using laser cooling, these effective spin states can be initialized and detected with near-perfect accuracy using well-established optical techniques.

A particular advantage of ion trapped qubits is that, whereas most physical platforms have nearest-neighbor interactions only, a multi-qubit trapped-ion system features an intrinsic long-range interaction that is optically gated and connects any pair of qubits, resulting in a highly-connected graph. These gates are decomposed into laser pulses that are pre-calculated to implement the desired qubit operation through the Coulomb-coupled motion along with an appropriate deconvolution at the end. Linear chains of order 10 qubits have been successfully used in proof-of-principle demonstrations of canonical quantum algorithms and quantum simulations.

Practical applications of QC require quantum control of large networks of qubits to realize gains and speed increases over conventional devices. Current laboratory implementations of ion trap qubits require many optical elements and complex lasers. The field is currently attempting to miniaturize such setups with robust components that can be connected via a modular approach. Entanglement within a module can be achieved with deterministic near-field interactions through phonons, while remote entanglement between modules can be achieved with a probabilistic interaction through photons. Such an architecture paves a path towards a flexible, large-scale QC platform that promises less spectral crowding and thus potentially less decoherence as the number of qubits increases. Demonstrations indicate that generating such modular entanglement can be faster than the observed remotely entangled qubit-decoherence rate, thus motivating the feasibility of this approach.

*Superconducting Circuit Quantum Computing*, Dr. William Oliver, *Massachusetts Institute of Technology & MIT Lincoln Laboratory*

Superconducting qubits are another leading candidate for a quantum testbed. Superconducting qubits are anharmonic oscillators that feature transition frequencies around 5 GHz. Their main features are lithographic scalability, nanosecond-scale gate speeds, and the need for cryogenic temperatures.

To date, the most advanced superconducting qubit demonstrations feature linear chains of 9 qubits. Prototype error detection protocols have been demonstrated by UCSB/Google, IBM, and Delft.

These demonstrations store quantum information in the superconducting qubits. An alternative approach used by the Schoelkopf group at Yale stores the quantum information in a microwave cavity that is made slightly anharmonic by a qubit. This “resonator cat-state memory” has demonstrated a prototype error correction scheme as well.

Looking forward, it would be highly beneficial to develop testbeds of 10-100 qubits in order to test new algorithms, identify roadblocks to scalability, and address those issues. Testbeds of this size will almost certainly require 3D integration. Ideally one would like the flexibility to control each and every qubit, and wiring laterally from the edges is challenging. Additionally, such testbeds need to be controlled with microwave electronics, and for larger numbers of qubits, the form factor of the electronics becomes an issue.

#### Near-term Practical Applications of Quantum Devices, Dr. Jarrod McClean, *Lawrence Berkeley National Laboratory*

To set near-term expectations, first-generation quantum testbeds, comprising 5-15 qubits, will not solve useful algorithmic problems. The ideal behavior of such a testbed can be simulated with relative ease on classical computers. So what is first generation quantum testbed good for? This is often a question in rapidly evolving and promising scientific and technical fields, and the realm of quantum computing is no different.

In QC, one of the first key milestones is “quantum supremacy” - defined as the completion of a well-defined computational task that all the classical resources on earth today could not complete within a reasonable window of time, by using elements that could be used to comprise a universal quantum computer. While some of the earliest milestones generate excitement both in the science and technology community and in the public eye, such milestones might not correspond to tasks that are practically useful in an application sense. There will likely be a gap between the first demonstration of quantum supremacy and the first use of a quantum computer for a practical application that exceeds the capabilities of conventional HPC. This gap, sometimes called the post-supremacy gap, could be surmounted through the development of near-term applications. A focus on applications can help maintain momentum and government focus between the pending demonstrations of quantum supremacy and the development of the *error-corrected* QC systems that will be required to solve relevant DOE problems.

Promising candidates for quantum speedups on near-term devices have been identified in the areas of optimization, quantum simulation, and representations in machine learning. A particular focus of interest is the topic of quantum simulation for quantum chemistry. One example of an application for such a device is the study of the nitrogenase enzyme that is responsible for nitrogen fixation in nature. Recent developments include coherence-time friendly methods that have the potential to get us to this valuable milestone without full quantum error correction. A key aspect of these algorithms is the careful use of quantum-classical couplings and co-design. Such an achievement has the potential to cement quantum computers into the landscape of applied technology.

#### Characterization and Control of Quantum testbed Devices, Dr. Robin Blume-Kohout, *Sandia National Laboratories*

A critical capability that testbeds would provide is the ability to probe and characterize the noise, errors, and other imperfections that occur in the real-world gates that will make up the testbed. Since mitigating those errors (via quantum error correction) is expected to occupy the

overwhelming majority of future quantum processors' time, characterization of real-world noise is one of the most important applications for the testbed. To achieve this goal, testbeds must be equipped with fast, flexible control systems that can implement arbitrary quantum circuits, and are not hamstrung by memory limitations.

A variety of techniques have been used to characterize qubits and the operations (gates) performed on them. Currently, the two dominant techniques are *randomized benchmarking* (RB), and *gate set tomography* (GST). In these methods, data is gathered by performing and repeating a variety of *quantum circuits* on the testbed device; it is then collated and analyzed by a classical algorithm to estimate how the qubits are misbehaving. Both RB and GST admit multiple variations, but as of yet do not address gatesets that involve more than two qubits. This is an area of active research, as is expanding these protocols to probe specific noise/error properties. Future protocols that directly probe the effect of changing how we implement gates will be critical for improving our devices and stabilizing them against drift.

In recent years, characterization protocols have rapidly grown more complex. There is a trend towards both larger, more powerful noise models, and larger, more structured sets of circuits. For example, current 2-qubit GST experiments use  $\sim 27,000$  different circuits to estimate  $\sim 1,200$  distinct noise parameters. We expect these numbers to grow. This trend supports increasingly powerful debugging and QEC design, but it also demands certain features of the testbed's control system. Moreover, future characterization tools must also scale in a resource-friendly manner. A testbed's control systems should be designed with these, and other, future needs in mind.

### 1.3 DOE Laboratory Capabilities for Quantum Computing

The goal of this discussion was to provide a forum for the DOE laboratories to share their capabilities and interests in quantum computing and testbed operations. Participating labs were Argonne National Laboratory (ANL), Fermi National Accelerator Laboratory (FNAL), Los Alamos National Laboratory (LANL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Oak Ridge National Laboratory (ORNL), Pacific Northwestern National Laboratory (PNNL), Stanford Linear Accelerator National Laboratory (SLAC), and Sandia National Laboratories (SNL).

The number and maturity of the technologies that the individual laboratories have to contribute to achieving the goals of the quantum computing testbed varies. Several of the laboratories have made significant and sustained investments that are directly relevant using their internal LDRD funding, coupled with institutional facility resources. However, the breadth of technologies and skills that will be required to achieve the goals of the quantum testbed, and its later spinoff systems may require robust teaming to engage the best from many of the laboratories represented at the workshop. A few notable areas are below.

Materials characterization. Many of the DOE laboratories have complementary and unique materials characterization capabilities that can be used to understand the fundamental performance of qubits and the materials in which they are constructed. This capability ranges from designing and optimizing nanoscale materials parameters specifically for qubits to modeling of quantum devices. In some cases, the labs have also invested in unique facilities that could guide qubit construction and help provide insight into failure modes.

Device development and manufacturing infrastructure. DOE has major investments in cleanrooms, fabrication facilities, and engineering support for nanodevices, integrated circuits, and superconducting sensors and detectors that can currently produce ion-trap, SC circuit, and silicon-

based dot qubits. Many of these capabilities are one of a kind. For example, Sandia's microelectronics fabrication facility is a flexible production facility capable of processing silicon and III-V materials to produce finished materials. The DOE lab complex also has a number of prototyping facilities to make one-off devices for answering basic science questions about device characteristics and to support a fast cycle for testing and improving novel devices.

Applications and algorithm users. The DOE laboratories have physical science applications that will benefit from quantum simulation, with the primary candidates being in quantum chemistry, nuclear physics, high-energy physics, and material science. Circuit-based QC algorithm development has focused on basic operations, such as factoring or linear algebra, but most of these gate-based computing efforts show great promise in supporting DOE missions in the future. The DOE labs also have a long history of fielding, testing, and benchmarking emerging technologies on real mission applications, whether they are new accelerators, new computers, or new sensors.

User facilities and operations experience. Many of the DOE laboratories have long, successful track records in building, operating, and upgrading large-scale facilities and open user programs for computing, light sources, neutron sources, and other capabilities. These world-class facilities have experience fielding equipment that requires massive power and cooling, and supporting thousands of users with complex workflows. Smaller facilities, such as the nanoscale science research centers offer a somewhat different user model with closer interaction between users and facility staff and a suite of unique fabrication and characterization capabilities that could prove valuable for developing novel QC devices. In contrast to many of these facilities, the cycle-time of a QC testbed is expected to be in the range of every 3-6 months, owing to rapid technology refreshes, and in order to support these shorter timeframes a QC testbed may need to adopt a modular, easily-upgradable design, with in-house expertise and on-call user support for rapidly debugging user experiments in real time.

The combination of the nanoscale science research centers and other resources across the DOE lab complex, such as large clean rooms, production-class fabs, and high performance computing centers, has the potential to accelerate progress in QC for science.

## **2 Building the Future Quantum Computer with a Testbed**

### **2.1 Best practices for management of and access to a quantum computing testbed**

Now and throughout their history, DOE and the Office of Science have sponsored a wide range of scientific facilities, each with its own unique culture and governance model that fosters scientific advances through positive user experiences. As such, numerous examples of organizational structure and culture exist that will provide a first-class user experience. By the same token, there are examples in which actions of the management team resulted in lessons learned. This section explores some of these examples, and highlights the expert input in these areas offered by the workshop attendees at this breakout session.

Five panelists with experience managing, operating, and using various scientific facilities funded by both DOE and the National Science Foundation (NSF) were asked to provide their individual input to seed a group discussion. Panel members were from the NSF, DOE's Basic Energy Sciences (BES) Program, the Center for Integrated Nanotechnologies, the Argonne Leadership Computing Facility, and the Combustion Research Facility (CRF). Collectively, the panel discussion yielded the following key points:

1. The process of defining metrics and program goals must include the needs of the user community. While this may seem obvious, there were multiple examples from the panel discussion in which this point was not observed, to the detriment of the facility.
2. Input from a group representing the entire user community is important to guide investments and directions. This seemed especially important to the panel given the relative immaturity of QC technology.
3. Past experiences strongly suggest that an agile and flexible management team that develops a roadmap and works closely with all relevant stakeholders is better positioned for long term success.
4. It takes time to build a user community for a facility or testbed. The existence of a physical location where people can visit in person and interact in multiple ways has been shown to facilitate co-design by accelerating the development of a vibrant community. If only virtual access to a testbed were available, then the time required to build the user community would likely be increased.
5. Moreover, the management/access model must be flexible and change as the technology and testbed matures. With the accelerated cycles of learning expected in the early development of a testbed, QC system modifications would be expected on a 6-month cycle, not a multiyear cycle. As noted above, flexibility and agility in designing and implementing facilities-related improvements in significantly reduced cycles would also be needed to enable flexibility in the management/access model.

In addition to the summary points above, the whitepapers and group discussion included the following key points:

Lessons learned from experiences at other user facilities. The NSF representative shared an example of a prior NSF center focused on development of microwave interferometer technology that he believed presented challenges analogous to those facing a quantum testbed program. Both programs involve relatively immature technology pushing the boundaries of what is possible with an unclear system integration path for ultimately blending that technology into a functional system. The NSF program was successful for a number of reasons: the community identified the most challenging engineering issues and took ownership of the final objective; the goals and metrics evolved as the technology matured; the program was led by agile program leaders who were also practitioners in the field; and importantly, the ambition and goals were matched by the available budget. Another facility manager offered a negative counter-example regarding a facility that developed a new capability only to have very few users. In retrospect, it is believed this occurred because the user base was not surveyed to uncover and document the community needs prior to facility planning.

The role of a testbed in bridging the gap between the academic and industry communities. In general, discussion participants felt that the national laboratories can be an effective bridge between these communities because they offer professional staff that can be tasked with transitioning academic advances into initial practice. Because the path to maturing qubit assemblies and the interface layers between hardware and software is ill-defined, there is a need for an environment where accelerated cycles of learning, or “failing fast,” is rewarded without possible repercussions on careers. The national laboratories provide just such a working environment and therein provide value at the early stages of technology maturation. Another

observation about the testbed is that it can lower the barriers for academia and industry to enter the field by providing a way to prove (or not) their technology building block by injecting it into an operational system. New users would not require a fully functioning system of their own to test their building block concept. Others noted that an issue exists in testbed concept between hardware development time, when the QC will not be operational, and the actual time that the testbed is being used for scientific simulations. While both are important, many participants considered making qubit systems available to users a high priority for a testbed, and that new technology could be incorporated into the testbed when available and appropriate. There is much to be learned about how ensembles of qubits work that can help inform the next generation of hardware. Finally, it was noted in this session and others, that the testbed could enable training for students who might then launch careers in industry.

The impact and importance of interface standards. There was a diversity of thought about the importance of, and priority for, setting interface standards. Standards can help broaden the user base by clarifying how new technology building blocks can be integrated into an operating QC system, thereby leading to a more engaged user community and driving innovation in all the stakeholder communities. However, standards can also impede progress by unduly constraining the solution space, especially if not broadly agreed to by the user community. Thus, helping to recognize when a standard may be required, and then helping to foster a community-based standards development process could be one of the roles for a quantum testbed advisory panel. In both cases, standards should be flexible enough to evolve rapidly as the hardware/software stack matures. A secondary benefit of the identification of standards could be the development of a language to describe QC performance. Currently, there is no standard or even rough agreement on what constitutes a QC, how to compare one QC to another, or how to describe the performance of individual elements with the QC system. As the hardware and interface software layers (stack) become available, the communities' lexicon will also evolve to allow performance of system elements to be compared so the QC can be optimized for the problem at hand.

Metrics for success. The panel members described what their centers used for metrics of success. In many cases, metrics were the number of publications and number of users served. These are reasonable metrics for an established facility mostly stocked with mature tools but may not be the best metrics for a quantum testbed where the technology is rapidly evolving, especially if accelerating system-integration innovations is a testbed goal. Pulling from the NSF example mentioned above, technical performance metrics may be the most appropriate in the first few years. It was noted that there is an inherent tension between maintaining the testbed strictly for user access and the continual churning of hardware and software that is at the heart of co-design. One suggestion for the early stages of the testbed was to run in a campaign mode, alternating between cycles of operation and engineering improvement. This suggestion was supported by the success of an NSF center that operated in technology operation/improvement cycles until a reasonably stable prototype was available to serve as a secondary testbed.

Possible role of an Advisory Panel (AP). Both the panel and discussion participants expressed support for an advisory panel to counsel the testbed management on success metrics, oversee progress, and serve a significant role in growing the user base through academic interactions and their own potential involvement in the testbed program. One of the examples from the NSF center highlighted the value added by advisory panel members who are leading experts in the field in helping to set and achieve near-term and long-term objectives for the testbed. These functions are critical to maintaining user engagement, utilizing the best contributors from across the DOE

complex, and maintaining the support of the broader community. The AP can also help evaluate and prioritize proposals for user access in the context of the overall roadmap when the requests for access begin to exceed the ability of the testbed to accommodate them. A frequently repeated suggestion was to not get bogged down in process. Finally, the early stages of a quantum testbed are likely to be capital-intensive; prioritizing available capital resources and leveraging other programs such as hardware/software programs in the academic, industry and national labs will be critical.

The balance between onsite and virtual access to the testbed. Transparency of the system design and full access to the controls of the QC were believed to be critical to achieving rapid progress. These principles were balanced by the recognition that full access carries risk to the operation of the hardware. These two views can be mitigated by a graded approach to access that will evolve with time. While the first testbeds are being assembled, access could be via onsite visits or email discussions with the professional team that is in daily contact with the hardware/software stack. As the systems mature or as more testbeds are developed, significant advantages could be realized by opening up access to one of the testbeds via a virtual access portal. The IBM experience offers several lessons—the virtual access portal generated a large number of users, an engaged public response, and valuable metadata on how the system was actually used. However, the QC experts expected to be the testbed’s early users will likely desire to operate with greater transparency and with the ability to control more qubit parameters. The IBM web interface was also achieved at a significant overhead cost that may not be the best use of resources in the short term. One of the roles of the testbed management team and advisory panel would be to monitor the demand signals for offsite access and adjust resources to meet that user desire. Finally, given the world-wide interest in QC technologies the QC testbed should both expect and actively encourage engagement with the international community, with due regard for export control restrictions.

## **2.2 Staffing and Workforce Development**

It is anticipated that staffing an experimental quantum computing testbed will require a cross-disciplinary approach with an engaged workforce from varied backgrounds. This section summarizes staffing and workforce development considerations raised in a group discussion and in the whitepapers.

Composition of testbed staff. The different skill sets needed to develop and realize a successful testbed include domain scientists in the areas of computing hardware, cryogenics, vacuum design, atomic and molecular physics, lasers and optics, electronics, physics and engineering. One also needs quantum algorithm developers and implementers. National Laboratories possess a broad set of personnel who can be tasked with working on several projects simultaneously. While a dedicated full-time staff may be optimal for an unconstrained budgetary environment, staffing of the testbed could initially be drawn from existing talent at the Laboratories.

Appropriate staffing depends on the phase of testbed development. Workshop participants identified phases of testbed development with different staffing requirements: 0) planning for the hardware; 1) building the physical testbed; 2) transitioning the testbed to operations; 3) a longer period of standard testbed operations; 4) upgrade of the testbed (which repeats the cycle). Note that this testbed cycle mimics the typical developments found in many of the ASCR computing centers. Scientists and engineers would work together to provide requirements and planning during phase 0. Likely, significant PhD level engagement across several disciplines will be required during phases 1 and 2, including electronics, vacuum, cryogenics, atomic and molecular physicists,

HPC experts, and fabrications experts. Some participants suggested that it could require several QC hardware experts to get a testbed up and running. During phase 3, the testbed would be operational and require the engagement of hardware technicians, research scientists, and software engineers to effectively utilize the hardware. It is possible that phase 3 might require involvement of fewer individuals than the other phases; however a significant effort to engage the broader research community will also likely be required during this phase. Effective community engagement will likely involve staff at several levels, ranging from instrument scientists to science domain experts and interface developers. Planning for future upgrades (phase 4) is similar to phase 0.

Software development can proceed in parallel. As plans develop for successive generations of the testbed, it would be logical to pursue a parallel strategy for testbed software development. This effort could involve slightly different skill sets. Users of the testbed will need to be informed about plans for software development for the quantum computing system. It may be possible to utilize other successful open-source software approaches from the Office of Science, such as the one utilized by the NWChem code development community.

Finally, participants noted that QC is not yet sufficiently well-developed to predict staffing needs and that any model for a testbed should build in flexibility to adapt this rapidly changing field.

### **2.3 User Community Development and Interactions**

A panel of experts from across various industries participated in a discussion outlining user communities across these industries in order to provide useful examples for a quantum testbed. Panel members were from Los Alamos National Laboratory, the University of Washington's Institute for Nuclear Theory, the Association of Universities for Research in Astronomy (AURA), and IBM. Panelists made the following key points:

1. A lesson from the astronomy community is that user facilities, especially those based on new or cutting-edge technology, are best-served by a world-class staff who are both professionally invested in the facility and at the same time transparent and accountable to the users.
2. Longer-term face-to-face interactions focused on solving research problems have proven more effective than short, presentation-heavy workshops in accelerating progress in areas that cross disciplinary boundaries. The INT representative presented an example of a visitor program that has been effective in bringing new ideas into nuclear physics as well as sharing concepts in nuclear physics that have enriched other disciplines.
3. Exploring applications of quantum computing is often a high-risk endeavor for scientists not already working in the field. Lowering the stakes by providing opportunities for researchers to do small projects has been an effective means of engaging new users.
4. Well-developed interfaces are critical for non-expert users. As discussed below, testbed staff may provide an adequate interface for a first-generation testbed while a more sophisticated remote access capability is being developed.

The subsequent discussion highlighted how development of a user community and fostering a vibrant, community-wide interaction are critical to the success of a testbed.

The importance of the user / operator interaction. The panel shared key insights on the important elements of a functional user interface, noting the role of testbed staff. In particular, it was emphasized that the QC systems operators who interact with users are one of the testbed's most

important resources. It will be important for users to have a set of experts who operate the testbed devices to serve as intermediaries between the users and the testbed. In the same vein, most users will likely not interact with the testbed directly or be physically present in the same room as the qubit devices. This mediated-access model will ensure the deepest reach to the most potential users, especially beginners, and will ensure that the users cannot physically damage the testbed. Before a fully automated, remote interaction model is developed, it may be useful to have staff guide the users, in a way similar to how the nanoscience centers such as CNMS, or certain telescope facilities managed by AURA, work. At CNMS, users may tell a staff scientist that they want to make nanostructure X. Users may rely on staff to execute much of the lithography to carry out that process. In a similar way, early users may tell the quantum testbed staff to set up the quantum processor to run simulation Y. The staff can take a leading role in actually making sure the machine is ready to go in the proper configuration to run Y, if such tasks have not yet been automated. Nonetheless, many of the users will also be expected to have expertise in quantum information science, and in the particular qubit technology used. These advanced users may wish to propose experimental upgrades to the testbed and contribute to future software and hardware development. A model for testbed operation that allows advanced users greater flexibility could significantly enhance test scientific productivity. Further, since one important function testbed could serve is to discover the failure modes of early-stage devices, it is conceivable that more knowledge could be gained from early device failure than success. Advanced users may be allowed to physically interact with the testbed devices and in doing so, might be provided access to an enhanced set of controls versus those which a lay-user might experience through the remote interface. While none of the existing user models discussed by the panel appear to be a perfect fit for a quantum testbed, discussion participants felt that a combination of the IBM Quantum Experience's remote access model and AURA's flexibility in supporting a broad spectrum of users - from mediated-access users to power users who interact directly with the hardware - could be effective.

The role of early adopters in driving innovation. A first-generation testbed is likely to have two distinct user groups: the first being expert quantum information researchers, and the second being early adopters seeking to learn about QC in order to develop applications better suited to later-generation testbeds. Avid users of the early testbed may be those who build or are capable of building an operating testbed itself, with a focus on verification, validation, fault tolerance, and other aspects of making a functional system. These "power users" can also be particularly valuable members of a user group that aims to provide grassroots troubleshooting and community-based support for new users. At the same time, forward-thinking domain scientists from nuclear physics, chemistry, quantum field theory, and other disciplines are also likely to be among the early adopters. These fields represent those in which quantum algorithms could provide substantial advances if a scalable testbed capable of running large scale algorithms were available. The early testbed would likely see a large proportion of physicists and quantum algorithm developers testing new algorithm snippets and demonstrating fault-tolerant schemes (including encoding and quantum error correction). As the testbed grows, primarily in number of qubits available, and becomes capable of running more complex algorithms, the user community is expected to evolve and take on a larger number of domain scientists. The users at this stage should not need to be experts in quantum information science in order to take advantage of such a testbed.

Enabling the user community. The panel provided ample successful strategies for engaging new users and developing a community of scientists from outside the quantum information science field. Several user models currently in use, including one from Los Alamos National Laboratory,

provide hands-on courses to train users in this new technology. At IBM, extensive online tutorials are provided, including videos with robust documentation. The astronomy community user model has benefitted greatly from having expert users work in tandem with new and inexperienced users in order to streamline access to complicated instruments while simultaneously propagating knowledge across the broader user community. In quantum computing, each domain science might have its own approach to user community development. The challenge of training QC users is even observed in the current few-qubit systems that exist in laboratories. For example, there is a significant learning curve to implement modest gate set tomography algorithms for new users of the systems. A model that draws from each of these strategies and provides a broad spectrum of outreach and community development will have the highest probability of ensuring the testbed mission's success.

Fully engaging a user community. Multiple examples were discussed that describe how user communities become invested and participate in the smooth operation and productivity of a testbed. A model espoused by the astronomy community, in which users are active developers of the testbed in terms of both future software and hardware, potentially has many parallels with a quantum computing testbed. This model ensures that users help develop a testbed into something that maximizes usefulness, and it ensures that the testbed operators and management remain cognizant of new qubit technologies that could be integrated into the system. On the other hand, while such a model is well-suited for a narrower domain science where most users are astronomers, it may not be fully compatible with the broad base of different domain sciences expected to comprise the quantum computing testbed user community because different domain sciences may have different ideas of the direction that testbed development could take. A hardware upgrade may be suitable for one domain, but not another. In contrast, current quantum computing testbeds at IBM and LANL have more abstract levels of interaction, in which users do not have access to low level hardware and do not participate in testbed development. This model is advantageous in that the chances of breaking a device are minimized and a broader developer community could likely be nurtured without requiring users to understand all aspects of hardware operation. At the same time, it would be important to ensure that new improved technologies could be incorporated and the testbed were not frozen into suboptimal solutions. Helping strike a balance between these modes of operation could be a role for an advisory panel.

### **3 Principles for Quantum Computing Co-design**

In the classical digital computing world, co-design [1] is typically thought of as a design cycle in which application performance is improved with respect to some metric (for example performance, power consumption, etc.), by using application software design to inform hardware design and vice versa. The hardware design space might include register set size, cache size and associativity, the number and connectivity of cores on a node, and the connectivity between nodes. Typically, there are many designs possible within the same cost, power and target peak performance. The application software design space can be explored by rethinking the fundamental mathematical models and algorithms employed, by re-engineering parallel decomposition and scheduling, and by tuning for vectorization, cache blocking, and multi-threading. At a scale much larger than a single scientific application, the entire ecosystem of hardware and software for a broad community of users can be optimized by using the co-design process resulting in a path for combined application software and system architecture evolution.

ASCR, in partnership the national laboratories and computer vendors, has used co-design as a critical methodology in the Exascale Computing Initiative with impacts in diverse application

areas from combustion to materials modeling. Currently, a new set of Co-design Centers focused on computational technologies like adapted mesh refinement (AMR) are funded as part of the Exascale Computing Project. Co-design of a quantum computer is as important, or even arguably more important, than in a classical computer. Because of the relative immaturity of QC hardware, architectures, and software, QC system development will both learn from classical co-design process and promote even newer development methods.

Speakers from LANL and the University of Maryland initiated a group discussion by presenting lessons learned from classical co-design and thoughts on how quantum co-design might proceed. Key points presented include:

1. Establishing a common vocabulary and building a community across diverse disciplines are both challenging and absolute necessities, especially with non-traditional partners.
2. An expanded multi-scale co-design approach spanning all the way from materials science to programming could be very effective for early-stage post-Moore's Law technologies such as QC. A testbed strategy could make this large endeavor more tractable by breaking the problem into manageable chunks.
3. Exploring QC architectures, multi-qubit gate implementations, and qubit connectivities through co-design will accelerate the development of useful devices. Specific hardware implementations may not be universal, but lessons learned could apply to other applications.

The subsequent group discussion identified key elements for testbed operation that will enable rapid and effective iteration of the co-design loop and therefore improvements in capabilities:

1. Development of a broad range of benchmark problems based on DOE mission needs.
2. Agile and effective planning for deployment of improved qubit architectures, accounting for any asymmetries in relative progress in hardware and software and allowing for intercomparison of hardware instantiations.
3. Local instantiations of hardware, permitting much lower-level interactions, parameter adjustments, and optimizations than would be available through pre-defined APIs.
4. A flexible software architecture enabling multiple hardware instances, a variety of programming languages, adapted to different developer communities (for example, domain specific languages), and transformation between various intermediate representations to be supported.
5. Performance modeling, emulation, and simulation tools that can use classical compute resources to the extent possible to develop algorithms and test the software stack and aid in hardware design.

Principles of quantum computing co-design are evolving. In contrast to the classical computing co-design space, the current co-design space for quantum computing is in many ways much less mature. The number of algorithms for a given application (even the number of algorithms for any application) is far fewer, and the understanding of their utility to important use-cases, as well as resource consumption is not as well-known as in the classical case. In addition, though considerable research, development, and engineering efforts have been made in the fabrication of physical qubits, such investment has targeted mostly improving the number and quality of qubits rather than exploring tradeoffs in system design and ties to application needs. Moreover, differentiation in the type of error correction that can be implemented for the leading qubit systems would be a significant addition to the co-design space. Altogether, each class of qubit hardware is

very different from the others, much more so than different CMOS-based chip designs. A testbed could enable a library of well-defined results including data about chip, gate, and qubit characterization data that will fuel future research, and spur design of benchmarks enabling QC system comparison

QC systems will combine classical and QC elements. Co-design for quantum computing is likely to be a more challenging endeavor than in the classical digital space for the reasons mentioned above, and also because an early testbed will likely involve both classical and quantum components where the classical computer controls and interprets the results of the quantum submodule. The optimization that will be required to join both technologies is largely unexplored. Compared to the standards and engineering capital available in the classical computing world (fabrication processes, circuit design libraries, instruction set architectures, compiler theory, programming models, etc.) much more needs to be developed for classical/quantum hybrid systems.

Co-design as a tool to bridge communities. The communities that must be brought together for successful quantum co-design are more diverse than that required for classical computing co-design. In addition to the application domain scientists, applied mathematicians, computer scientists, and classical software and hardware engineers, the community needs to be augmented with scientists, typically physicists, and engineers (microwave, optical) who can design and build quantum hardware, implement error-correction, and validation and verification protocols. The skill sets of the domain scientists, applied mathematicians, and computer scientists involved must start to evolve to span the models, algorithms, and programming paradigms appropriate for quantum computing. An early testbed device will likely involve the co-design of both quantum and classical hardware, so the classical and quantum skill sets should not be siloed. Creating a focal point around which a quantum co-design community can form, collaborate, and begin to share their experiences and goals will maximize return on investment and accelerate progress,

The importance of control algorithms and the software stack. Until very recently, the software control systems that drive current QC experiments have been restricted to labs where the devices are fabricated, were not often shared, and had minimal formal structure. For co-design to be successful, a common software stack must be expanded upwards from the hardware layers to enable easier composition of simulations by domain scientists—for example, allowing remote web-based access, and expanding downward to enable robust and efficient connections to the hardware itself. In addition to a complete software stack, quantum hardware must start to evolve towards common interface standards not just for input/output, but also for calibration data and hardware metadata. In addition, the testbed community must also educate itself broadly on the key challenges and tradeoffs at each level of the design process; doing this will require the testbed community to develop a common shared vocabulary that bridges disciplines that have thus far been unfamiliar with each other.

#### **4 Technical Considerations for a Quantum testbed**

The availability of a testbed can nurture the development of hardware, architectures, quantum algorithms, and simulations for scientific applications. Technical considerations and informed trade-offs are crucial for the implementation of a quantum testbed, as these will determine the feasibility of realizing the testbed, the computational power of the testbed, and the usability of the testbed system. These issues were discussed by the workshop attendees in multiple technical-focused breakout sessions, which are summarized in this chapter.

The technical breakout sessions focused on the following topics:

- 4.1 Design and emulation tools - Output of these tools can characterize the impact of computing model, size, performance, and qubit connectivity on testbed performance.
- 4.2 Hardware characterization, verification and validation - A summary of available verification and validation tools, and a discussion of their ability to predict the performance of quantum algorithms on a testbed system.
- 4.3 Analog simulation - Using one quantum many-body system to simulate the properties of another.
- 4.4 Tools for making a quantum testbed useful - Properties of a user interface and operating system to facilitate the efficient implementation of quantum algorithms, adaptations of compiler and optimizer to the strengths of disparate qubit implementations, as well as the quantum control capabilities needed for calibration, verification and validation and to implement algorithms.
- 4.5 Superconducting qubits - Properties, status, and challenges with this qubit technology.
- 4.6 Trapped ion qubits - Properties, status, and challenges with this qubit technology.
- 4.7 Emerging qubit technologies - Survey of promising qubit technologies in addition to superconducting or trapped-ion qubits.
- 4.8 Interconnects - Long range interconnects between qubits and their impact on the ability to scale the number of qubits in a testbed system.

#### **4.1 Design and Emulation Tools**

In this session, participants discussed the status and efficacy of software tools used for the design and performance evaluation of QC devices. The discussion was initiated by speakers from the Georgia Tech Research Institute (GTRI), Lawrence Berkeley National Laboratory (LBNL), and Pacific Northwest National Laboratory (PNNL). Take-away points from the discussion included:

New modes of quantum computing emulation needed. Performing a “brute-force” Hilbert-space simulation of multi-qubit systems is computationally expensive—each extra qubit doubles the simulation effort. Since 2010, the world record for the quantum circuit simulation by a supercomputer was 42 [3]. Only recently (April, 2017, after the workshop completed), has this increased to 45, using the supercomputer ranked #5 on the Supercomputing Top 500 list, *Cori* [4]. When the effects of general Markovian noise and decoherence are incorporated into the simulation, this record drops down to closer to 20 qubits. With companies such as Google planning to demonstrate a 49-qubit quantum computer before 2017 ends, it will not be long before supercomputers are no longer able to keep up. New modes of quantum computing simulation and emulation are needed.

By following ideas developed for simulating classical computers, several possibilities exist. These include doing analytical calculations, Monte Carlo numerical studies, and multi-scale simulations. The challenge with any non-exact method is building accuracy and trust. This is an area in which expertise in emulating complex classical hardware could be helpful. Eventually, just as classical computers are used to design and evaluate advanced classical computers, the expectation from the

group was that small quantum computers would be used to design and evaluate advanced quantum computers.

Leveraging early-generation classical computing design and evaluation tools. It has been many decades since classical computers were at the 5-10 *logical* gate level, and few remember what design and evaluation tools were utilized at that time. Quantum computers, on the other hand, currently consist of a relatively small number of physical qubits that have yet to demonstrate error-corrected operations. To overcome this, it was observed that an effective design and evaluation tool for a quantum testbed might productively center on the various error mitigation strategies one might employ. These include optimal and quantum control methods, dynamical decoupling and pulse-sequence methods, and quantum error-correction methods.

Benchmarking a quantum testbed. Because benchmarking suites have been influential in steering the development of classical computers; it is natural to ask about developing a standard suite of quantum algorithms to serve as benchmarks for a quantum testbed. Because relevant applications for DOE will likely involve many *logical* qubits, quantum algorithms on *physical* qubits will probably not provide a path for architects to design for these large-scale applications of interest. It was suggested that perhaps the most important benchmarks would measure how well logical qubits perform at relevant tasks.

Related to benchmarking is the need to establish relevant specifications for quantum computers. Because quantum-computing technologies can differ substantially from classical, determining the right tangible properties to compare is unclear, and developing those is likely to be an organic process as the quantum testbed develops, and not one that can be proscribed ahead of time.

## **4.2 Hardware Characterization, Verification and Validation**

One of the important reasons to build a quantum testbed is to use it to learn about issues relevant to the design of larger, DOE mission-scale machines. This includes learning about failure modes, controllability, and challenges to scalability. For this reason, an important task for a quantum testbed is to execute protocols for characterization (“What did we build?”), verification (“Did we build it correctly?”) and validation (“Did we build the right thing?”). Only when a quantum testbed passes these protocols can we trust it to provide us with the information we seek.

The discussion of hardware quantum characterization, verification, and validation (QCVV) was initiated by speakers from the University of Sydney, LANL, and SNL. Take-away points from the discussion included:

1. One of the important near-term testbed applications is fault-tolerant quantum error correction (FTQEC). Some mission-scale algorithms will only run on *logical* (error-corrected) qubits.
2. One valuable testbed objective would be to develop control and error models. If this objective were achieved, the understanding of the science and engineering path to achieve larger machines will be greatly improved.
3. Low-level QCVV tools play an important role in debugging FTQEC. These tools are needed to troubleshoot and learn *why* FTQEC fails if/when it does.
4. Analog simulators and quantum annealers have significantly different QCVV issues than digital quantum information processors. QCVV for these three types of QC systems must be considered separately. A digital QC component to a testbed will be essential for exploring QCVV for science and energy applications of QC.

Learning control and error models with a quantum testbed. One of the primary applications for a quantum testbed scale system could be to develop a path from understanding the performance of *physical* qubits assemblies to the development of error-corrected *logical* qubit building blocks. Each error-corrected logical qubit, comprised of multiple physical qubits, is the analog of a logical bit in a conventional electronic computer that reliably processes or stores digital data. Because quantum computers are not just extremely powerful but also extremely fragile, FTQEC processes are required to fully understand and then optimize a QC at the physical qubit level. The panel discussion showed that many FTQEC codes are under consideration, each with their own pros and cons, but no clear leader has emerged. Hence, a quantum testbed would be an excellent crucible within which to determine which quantum codes work best in the realistic noisy environments of the technologies employed in that testbed, or that it can simulate faithfully. Moreover, to indicate how the performance of FTQEC might scale to mission-scale machines, it is essential that multiple FTQEC codes and protocols be investigated, at different sizes. Learning the control model and the error model for one or more quantum devices would be a significant testbed accomplishment.

There is no substitute for direct testing of multiple QEC protocols. While a handful of QEC experiments have been demonstrated to date, none have run *fully fault tolerant* QEC (including preparation and measurement), and none have done so in an iterated fashion that could sustain a logical qubit for a user-specified amount of time. Because of this, virtually all of the work on FTQEC has been theoretical, and has assumed numerous things about what kinds of control capabilities will be available in a real quantum computer and what kinds of errors will afflict the hardware executing FTQEC in a real quantum computer. Building an actual quantum testbed would reveal the “ground truth” for both the control and error models studied by theorists. Many of the discussion participants suggested that the models currently used by most theorists are probably too “simple,” and that real data are needed from a quantum testbed to assist theorists in generating more valuable and practical FTQEC solutions, as well as developing error suppression strategies that could even be implemented in the physical layer of a QC device. Examples of errors whose parameters are not necessarily well known for all technologies or whose error-mitigation strategies would benefit from further development include non-Markovian errors, burst errors, and leakage errors.

Additional QCVV, FTQEC research will be required as QC devices advance. Looking deeper at FTQEC, there was an expectation that the current tools will fail at some point and will then require finer-grained QCVV tools for debugging qubit performance. The group discussed several options, including randomized benchmarking, gate-set tomography, and Hamiltonian identification. This is a very active area of research, and there is no consensus in the field about which method might be best. There was good discussion about how fine-grained the models needed to be. For example, on the one hand, while noise independence between quantum gates and qubits in time and space at some scale was generally expected to hold, QCVV protocols would need to be executed at larger and larger scales to prove out what that scale is. Because the cost of tomographic characterization protocols scales exponentially with system size, this is expected to be an arduous task. On the other hand, it may not be necessary to know the details of the noise model at such a fine scale. There could be many aspects of the noise model to which the key quantum testbed application—FTQEC—is insensitive. From an operational viewpoint, the only aspects of the noise model that need to be known are those that impact FTQEC. The upshot of this discussion was that there is a need to better connect low-level QCVV tools with FTQEC.

Analog quantum simulators and quantum annealers. The panel discussed how QCVV would work on a testbed operated in an analog quantum simulation mode. The view of many participants in this discussion was that there is no general-purpose QCVV methodology known, and whether it is possible to develop one is an open research question. A lack of QCVV would limit (but not eliminate) the value of these types of QC devices for some domain science applications.

### 4.3 Analog Simulation

The idea of using one controllable quantum many-body system to simulate the properties of another many-body system goes all the way to Feynman’s original ideas on quantum computation [5]. Since then it has been often argued [6, 7] that in the short term it would be considerably easier and faster to construct a quantum simulator targeted at a set of important, but classically inaccessible, problems than to pursue a universal (digital) quantum computer.

With this long history of thinking about quantum simulators, speakers from LBNL and Boston University initiated a discussion that included the following key points:

QC platforms capable of performing both digital and analog simulation may be impractical. Most currently available qubit technologies have been used for analog quantum simulations, for example superconducting qubits, trapped ions, ultracold atoms or molecules, and photons. Of these, superconducting qubits and trapped ions have also shown promise for scalable gate-based digital quantum simulation. In principle, it would be possible to deploy a testbed comprising either of these technologies for both analog and digital simulation paradigms. However, the specifics of qubit connectivity and other hardware details required for gate-based computing might prevent easy switching from one mode of operation to another and render this dual use impractical. In the case of quantum computing using ultracold atoms or molecules, particularly those using optical lattices for confinement and a high numerical aperture lens for imaging, the use has been exclusively in analog simulation.

Analog simulation may have high-impact, near-term applications. For some kinds of simulation challenges, analog simulation results have been very impressive. For example, Choi *et al.* have characterized 2D many-body localization transitions using ultracold Rb atoms [8] in a regime inaccessible to simulation on classical computers. Dynamical properties of Fermi- and Bose-Hubbard models in higher than one dimension are also hard problems for classical simulation, but are amenable to analog simulation devices. Indeed, the analog simulation of their ground and thermal states was a major goal of past work, and was largely achieved in the bosonic case, with verification against solvable limits. As an example where a quantum simulator would have an immediate impact, the Fermi-Hubbard model is believed to underlie high-temperature superconductivity, but pump-probe experimental measurements of its dynamics are difficult to model by any existing classical simulation method. In the longer term, the Fermi-Hubbard model is a first step toward simulation of lattice models with additional complexity, such as lattice QCD, and possibly toward verification of circuit-based approaches to these models.

Verification and validation remains a challenge. Some authors [7] have speculated that error correction required for analog simulators may not be as stringent as that needed in circuit based approaches, based partly on useful results from analog simulation studies where QEC was not used. Turning to QCVV for analog simulation, and noting that verification and validation is difficult in the general case, discussion participants suggested that a number of indirect approaches

could be tried: comparing two distinct analog simulators targeting the same problem; comparing two results of known accuracy obtained from classical simulation techniques, or perhaps related results obtained from classical simulation techniques. Similarly, evaluating the major sources of error in an analog quantum simulator emulating a many-body Hamiltonian is a very difficult task. Typically, the Hamiltonian used to describe the dynamics of the laboratory (simulator) system is an approximation, introducing errors compared to that of the simulated system; ideally there should be enough classically tractable limits or special cases to diagnose possible errors in the simulator.

Overall, discussion participants had mixed opinions about the appropriate role for analog quantum simulation in a testbed. Analog simulation could be a powerful testbed component, provided that QCVV concerns are adequately addressed and the simulator hardware is sufficiently flexible to address several computationally well-defined and broadly interesting classes of problems.

#### 4.4 Tools for Making a Testbed Useful

While quantum algorithms [9], quantum complexity [50], and programming quantum computers [10-12] have been active topics of research for more than 20 years, only recently have software architectures or workflows to implement quantum programs on actual devices been studied [13-14]. Figure 4.1 provides an illustration of what such a system could look like, detailing a software stack with tools available to help with all steps required in going from a simulation described at a level of abstraction accessible to a domain scientist to being able to run on quantum, or simulated quantum, hardware.

Speakers from GTRI, LBNL, and ORNL initiated a discussion that yielded the following key points:

A testbed both needs and is needed to create QC software. A modular software architecture is an important element for creating a usable testbed and is a necessary part of being able to execute hardware/software co-design for more effective next-generation systems. In parallel, a testbed could provide both an environment to evaluate tools in the software stack and a community to guide the development of standards between software layers. Such standards would allow the development of additional software components that could provide users with higher levels of abstraction and guarantee interoperability with middleware components and multiple hardware platforms.

Many gaps exist in the hardware / software stack. One of the gaps identified in many current implementations of quantum computing workflows is modular software to control hardware devices at a fundamental level. These systems tend to be specific to the laboratory where the device is built, and disconnected from other tool chains. There is also a lack of software in the community to enable specification of problems at the top level of Figure 4.1, e.g. of describing a simulation in terms an application scientist would intuitively grasp, e.g. specifying a Hamiltonian. Similarly software allowing of mapping one Hamiltonian (of the simulation) to another (that which describes the device) is largely absent.

Modular software tools and standard APIs encourage development. It is likely that in the next two to five years, progress in physical hardware will enable the deployment of systems that we are not currently able to emulate or simulate, and improved tools will help prepare users for future systems. It is important to keep the software and tools ecosystem as flexible as possible to encourage a broad community and shared software ecosystem development.

While the list of relevant software is growing, a comprehensive catalog is lacking. There is active work in describing a software stack at a conceptual level [14], but there are few current comprehensive assessments of the usability, utility, etc., of current QIS software and tools from application developer to qubit control. The following list of computer science tools that could be useful for testbed implementation was developed during and after the session. The list is meant to be illustrative rather than comprehensive.

- XACC (ORNL) – Programming framework for hybrid quantum/classical applications
- Circuit Scheduler and Target Translator (GTRI) – Scheduling and mapping instructions to quantum hardware
- ProjectQ (ETH, *et al.*) – Embedded Domain Specific Language; Simulation/emulation; Compiler with interface to multiple gate-based intermediate representations
- Scaffold (U Chicago, *et al.*) – C-like language and compiler
- Quipper (Applied Communication Sciences, *et al.*) – Functional language and compiler
- ARTIQ (NIST) – Embedded Domain Specific Language for control for trapped-ion qubits
- FermiLib (Google / LBNL) – Library to facilitate fermion simulations with ProjectQ
- PyQuil, Quil & Forest (Rigetti Computing) – Embedded Domain Specific Language; Intermediate Representation; Instruction Set Architecture and Simulation
- LIQ*Ui*> (Microsoft) – Embedded Domain Specific Language (in .NET); Simulation/emulation; compiler & runtime
- QCoDeS (Copenhagen / Delft / Sydney / Microsoft) – Python-based data acquisition framework
- QX, QISKit (IBM) – Visual user interface, open quantum assembler language specification

Software Validation and Verification is also important. Several workshop participants pointed out that verification and validation for software tools is just as important as the hardware V&V discussed in previously. Established techniques such as formal methods, satisfiability modulo theories (SMT), etc., may need to be extended.

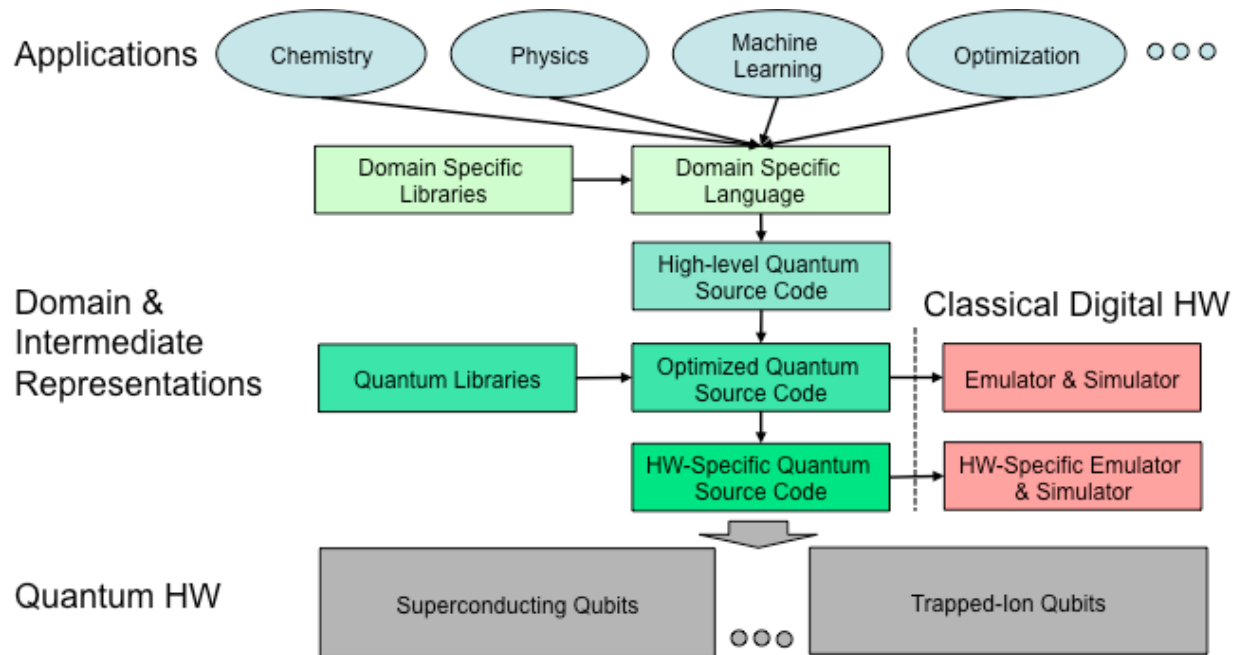


Figure 4.1. Illustrative Sketch of Key Components for an End-to-end Software Stack

#### 4.5 Superconducting Qubits

Macroscopic superpositions in cryogenic ( $T \sim 20$  mK) electronic circuits form the basis of the superconducting qubit [15]. Although many variations of the qubit have been investigated, such as charge, flux, or transmon devices, they all crucially leverage superconducting metals to realize ultra-low-loss linear elements that are combined with one or more Josephson junctions operating as a nonlinear element to realize a tunable artificial atom. Superconducting qubits have now been demonstrated by many groups, with applications including factoring [16], quantum annealing [17, 18], and quantum simulation [19]. Moreover, the applicability of many traditional semiconductor manufacturing and high speed electrical signal processing techniques support the idea of a scalable quantum processor architecture using these qubits.

Superconducting qubit technology was discussed at length in this breakout session, which began with presentations from LBNL and MIT Lincoln Laboratory, addressing advantages and disadvantages, enabling technologies, and scaling challenges. Key points include:

Movement of quantum information is a technical challenge to scaling to larger numbers of interconnected qubits. Current iterations of superconducting qubit technology have shown impressive results in systems ranging from 2-9 qubits, and technological developments are in progress that will allow scaling beyond this point. A crucial step for scaling this architecture is related to the movement of large quantities of both classical and quantum information, and in particular the challenge of resource efficient and robust quantum/classical interfaces on the control and readout lines in a many qubit architectures. For example, measurement and back action, both due to engineered circuitry and the uncontrolled electromagnetic environment, play a crucial role in determining processor coherence and operation fidelity. Maintaining such quantum application imposed constraints in a scalable device is a topic of active research.

Circuit topology affects scalability. Depending on the circuit used, limitations may arise from the fundamental topology of the qubits. Devices thus far have essentially been limited to 1D

connectivity, or have had too few elements for this to be considered. Without the move to a 2D qubit topology, implementations of leading quantum error correcting codes may not be possible, and other simulation algorithms may also suffer from unnecessary overhead in qubit swap operations. An enabling technology to overcome this technological gap that is currently being pursued by many research groups is 3D integration. This integration process can include a number of steps and components, including through-silicon-vias (TSVs), bump bonds, and thermo-compressive bonding. A fully controlled 2D lattice with flexible connectivity has yet to be experimentally demonstrated.

Cryogenic electronics are a mid-to-long-term need. As the number of qubits grows, some suspect a move in the control electronics from room temperature hardware to cryogenic electronics may be required. However, others believe this is beyond the timescale of the testbed, perhaps 5-10 years out, and these electronics could be introduced only as needed and not before. It was speculated that current control and fridge electronics will be sufficient for up to 100 or 100s of qubits, but that fundamentally new solutions may be required to reach the level of 1000s. Some work has already been done to integrate other quantum technologies with cryoelectronics and the difficulties were not insurmountable; however, more research is required to evaluate the specific impact on superconducting technology.

A testbed may yield critical insight into mitigating crosstalk. A potential challenge in the scalability of superconducting qubits using microwave control is crosstalk between the qubits. Some work has been done on 3D integration for the past decade in attempt to reduce the amount of crosstalk to reasonable levels, and some believe that a potential path for mitigating this crosstalk is local shielding structures. Planar architectures may always suffer from some degree of crosstalk, but it is an open question as to how much of an impact this will have at the level of 100 or 1000 qubits. There is concern that it may increase correlated errors within systems that are not fully compatible with current error correcting codes.

The concern with respect to crosstalk is closely related to the attendees' view on the optimal outcomes of a testbed system within the next few years. In particular, the construction of a system with 100-1000 qubits will allow, for the first time, a glimpse into the types of errors we expect in a scalable implementation of superconducting qubits. This information will be essential both for engineering future devices and for theoretical algorithmic development. Ideally, these devices would allow theorists to more rapidly prototype algorithmic innovations, such as those needed to realize simulation of quantum systems on near term devices with real noise.

In summary, the attendees felt positive about the scalability of superconducting qubits in both the short- and long-term, and that current implementations were well suited for a test-bed system. The challenges to overcome, such as 3D integration, scaling of electronics, and crosstalk would be made more accessible through the development of a testbed device, and its ideal outcome would provide widespread applicability for both experimentalists and theorists alike.

#### **4.6 Trapped Ion Qubits**

It has long been recognized that qubits can be encoded in the clock states of trapped ions. These states are well isolated from the environment resulting in long coherence times [20] while enabling efficient high-fidelity qubit interactions mediated by the Coulomb coupled motion of the ions in the trap. Quantum states can be prepared with high fidelity and measured efficiently using fluorescence detection. State preparation and detection with 99.93% fidelity have been realized in multiple systems [20, 21]. Single qubit gates have been demonstrated below rigorous fault-

tolerance thresholds [20, 22]. Two qubit gates have been realized with more than 99.9% fidelity [23,24]. Quantum algorithms have been demonstrated on systems of 5 to 15 qubits [25-27].

Speakers from MIT Lincoln Laboratory, Innsbruck, and SNL initiated a discussion to explore the current status, challenges and promise of trapped ion based quantum computing that yielded the following key points:

There are multiple paths to increasing the number of interconnected qubits. A hierarchy of approaches can be used to scale trapped ion quantum processors [28]. First, ions can be trapped and manipulated in chains of moderate length. Even though these are 1-dimensional chains, interactions between any pair of ions can be realized leading to a fully connected graph [25]. Second, on a single trap chip, larger systems can be realized by shuttling ions, and thus qubits, in microfabricated trap structures [29]. Shuttling not only enables larger systems, but allows one to realize dynamically reconfigurable systems that can then be adapted to the requirements of different quantum algorithms. Finally, using the optically active ion qubits and remote entanglement, trapped ion systems can be scaled beyond a single chip [30]. This approach enables the assembly of a large quantum information processor from identical elementary logic units.

Technical challenges to be addressed to realize scaling are: the anomalous heating of ions in close proximity to trap electrodes [31]; realizing an excellent vacuum to achieve long lifetime of ion chains; mastering the control complexity in shuttling ions between different sites with minimal heating of their motion and directing the necessary control laser beams on individual ions; and realizing a sufficiently strong atom light interaction for efficient generation of remote entanglement.

Integrated photonics, electronics, and systems engineering are critical enablers. Realizing ion traps capable of trapping ions in multiple locations and shuttling ions between different locations relies on microfabrication. Current fabrication technologies enable one to build almost any surface ion trap [32]. Important next steps will be the integration of light delivery [33] and detection systems with the traps. While this is a challenging task, a good balance between monolithic and hybrid integration techniques will make these integrated devices possible. Finally, integration of voltage generation and optical modulations systems would enable one to reduce the number of necessary control lines per qubit and thus be of great value for increasing system size while keeping control complexity manageable. Systems engineering will be an important aspect in balancing monolithic and hybrid integration and achieving best system performance.

Trapped ion systems are flexible and reconfigurable. In small systems, fully connected interaction graphs can be realized with important advantages for algorithm performance [34], while shuttling of ions can provide a means of dynamically reconfiguring the system for optimal performance of a quantum algorithm. With the same system, analog quantum simulation as well as fault tolerant digital quantum computation can be achieved.

Clock speed is a potential limiting factor. While trapped ion systems offer large coherence time to gate time ratios and high fidelity operations, the currently achieved clock speeds are considerably slower than in superconducting qubit systems. While the clock speeds might be sufficient to realize algorithms, the statistics necessary to calibrate and characterize a trapped ion quantum processor will take much longer due to these slow clock speeds.

In summary, a trapped ion testbed could take immediate advantage of the high coherence time to gate time ratios, high fidelity operation, and reconfigurability. As discussed elsewhere, a testbed could also facilitate overcoming technical challenges to scalability.

#### 4.7 Emerging Qubit Technologies

While there was significant focus at the workshop on superconducting cavity and trapped ion technologies, there are a number of emerging qubit technologies that may overcome some of the possible scaling issues with these more mature technologies. Speakers from Stanford and SNL guided a discussion about the status, promise, and challenges of these alternative qubit technologies that yielded the following key points:

There is inherent value in maintaining diversity among qubit technologies. Many of the session participants felt that it is too early to choose a winning qubit technology, and that precompetitive basic research into a variety of approaches should continue. Of the, admittedly non-exhaustive, emerging technologies reviewed during this session, silicon quantum dots were considered to be moving very quickly because two qubit gate constructions have become more reliable in only the past couple of years. Trapped neutral atoms have very simple and scalable two qubit gate implementations. Finally, a third technology, photonics, was considered to be emerging as both a qubit candidate and as an interconnect between separated qubits.

Other qubit technologies discussed included:

1. Various quantum dot systems, including alternatives to silicon. Silicon-based qubits with bismuth donors in place of phosphorus promise to solve the problem of nondeterministic defect placement, potentially leading to scalable manufacturing [35].
2. Nitrogen vacancy centers in diamond, which offer long coherence times and a route towards scalable quantum memories [36].
3. Other spin donors [37].
4. Trapped electrons on liquid helium [38].
5. Photonic quantum annealers [39] were discussed in the context of non-universal QC, in which a coprocessor can be used to accelerate a certain task, such as machine learning, without the need for a universal gate set. These devices could also lead to a general quantum Hamiltonian simulation paradigm [40], but more research is needed on where the quantum speedup occurs in order for quantum annealers (optical or otherwise) to be truly useful.

Each of these qubits have inherent limitations and potential advantages that will require additional research to explore more thoroughly. It is likely that some of them will be particularly suited to certain classes of applications. The group generally considered photonic qubits the most mature of the technologies discussed, with a larger number of algorithms and error correction schemes demonstrated to date (including Grover's algorithm [41] homomorphic encryption [42], machine learning [43], a surface code demonstration [44], and various simulators [45-47]). However, progress on all of them should be monitored for possible inclusion into future testbed architectures.

#### 4.8 Interconnects

Speakers from the University of Illinois and Raytheon BBN initiated a discussion of the importance of connecting qubits, interconnect technologies, and technical challenges. Key points included:

Optical interconnects could be an important element of a fault tolerant quantum computer. This need arises from the belief that only a certain number of physical qubits will fit into a single vacuum chamber/dilution refrigerator, likely far fewer than required to carry out a fault tolerant quantum operation. Since fault tolerant qubits require entanglement between many qubits in a stabilizer state in order to carry out quantum error correction, connections between qubits in different chambers will be required if such codes are to be implemented across the number of qubits required to make a fault tolerant device useful for a meaningful computation. The need can be reduced by placing as many qubits as possible within one device, but stakeholders present at the session, and more broadly at the workshop, stated that somewhere between a few dozen and one hundred qubits could likely be expected to fit into a single device, depending on the technology.

The appropriate interconnect technology depends on distance. For the long distance interconnects between two separate chambers, photonics-based interconnects may be the appropriate technology. However, it was also noted that over short distances, and within the same physical device, microwaves are good interconnects for qubits such as superconducting current loops, owing to the fact that microwaves are a natural way to address such qubits and control them.

Scalability remains a challenge. In either case, interconnect technology has obstacles to overcome before becoming scalable. Current first generation interconnect proposals based on schemes such as entanglement swapping and joint Bell measurements have very low success probabilities, making them inadequate for scaling. With a low chance of successfully mediating entanglement between two distant qubits, a computation that requires more than one chamber/qubit device is itself unfeasible. This is an active area of research and the technology for scalable interconnects is expected to emerge.

## **5 Industry Perspectives**

The development and demonstration of operational quantum computing systems will require the close coupling of industry, academia, national labs, and government within a common framework. Each player brings strengths to the challenge, and leveraging these is one of the key tenets of the co-design practice. To begin to build understanding between these players, industry representatives from large and small companies were invited to share their perspectives on the near-term promise of quantum computing, the major challenges to developing this technology, and the role government might play in advancing the development of quantum computers.

The panel included representatives from IBM, Google, Rigetti Computing, IonQ, ColdQuanta, and Quantum Circuits. Each of these companies has made significant internal investments to develop quantum computing systems. In addition, Sandia National Labs shared their experience on partnering with industry to develop high-performance computing architectures.

Decide on the overarching goal and initial applications. A number of common themes emerged from both the presentations and subsequent discussions. One of the first themes to emerge, even before this focused industry session, was that a clear definition of the overarching goals and the application space of a quantum testbed was needed. By having general community agreement on the objectives of an initial 6 - 10 physical qubit system, possible partners can see how their technologies can integrate into a system. There was recognition that general community agreement will never equate to complete agreement, but that significant forward momentum can be generated and sustained by the establishment of a community practice to share and debate ideas. This initial community understanding can then be used to roadmap the future to define the

technologies and major application space that subsequent QC systems will fill. Further expanding on the need for specific goals, one of the common points of discussion was the quest for succinct articulation of the major problems a QC might solve. In the context of this DOE-sponsored workshop, participants discussed DOE-centric applications of QC such as materials design, molecular structure, and possibly material subjected to extreme environments. This was balanced by the comment that this focus does not need to preclude other applications, even though there is a need to focus efforts in the early stages of QC system development to achieve early program wins, and thereby build a broad base of support.

Define the metrics for measuring progress. Another theme to emerge from the panel and discussion was determining the role the testbed would serve in fostering an ecosystem where the technical language to properly describe QC technologies and their performance can grow. One of the major goals of industry is to sell QC systems to a wide variety of users, including the US government. However, at this early stage in the technology development, there are neither tools nor even a common language to describe system performance analogous to the commonly used HPC benchmarking standards. These benchmarks are important because they provide one basis for making the myriad technology and architecture co-design tradeoffs that will likely be required to develop specialized QC systems. They also serve as a way to make fair and balanced comparisons between technologies, including between conventional HPC and QC. One way to foster the development of a comparison language is by forging a closely coupled workforce in a work ecosystem wherein to be successful, individuals must develop a common language to describe the technology, architectures and performance of these currently underdeveloped systems. In addition, the ecosystem provides a training ground for people that will eventually move to industry.

The importance of standards and transparency. One possible outgrowth of a common benchmark language is the development of appropriate interface standards. Standards are recognized to lower the price for entry of new ideas and technology into existing systems. The innovation of smaller technology firms, or academia, can be supported because they are not required to have a complete operational QC system to test their building block ideas. Another positive aspect of standards is that they encourage transparency and open source solutions. A number of the companies present noted that open source efforts and transparency will be important to engage the broader community and share the cost of system development. It is believed that transparency will also encourage the development of unique applications for which QC systems are the only viable solution. Finally, standards, like the relationships between institutions that generated the need for standards, need to be flexible and time dependent. A testbed could facilitate this by opening up options to test new ideas and enable a user to fail fast so that they can quickly recover and try again—and eventually succeed.

## **5.1 Roles for Government and Industry in a National Ecosystem**

Historically, industry and government have teamed to accomplish significant goals that increase national economic competitiveness, ensure national security, and improve citizens' lives. The goal of this session was to understand some of the elements of a successful partnership. Speakers from the DOE partnerships office and Intel helped guide the discussion with the following take-away:

DOE is committed to providing a flexible organizational framework that ensures that the legal needs of all the participants are recognized and protected while not stifling the technical interactions that are at the heart of the envisioned testbed community. There are a number of possible agreement mechanisms that can be mixed and matched to provide the level of IP

protection and federal program oversight required. There is not one particular model for user facilities that was viewed as most appropriate, but rather a suite of tools that could be used and changed as needs evolve. For example, Memorandums of Understanding (MOUs) can be combined with Cooperative Agreements and Cooperative Research and Development Agreements (CRADAs) in a flexible structure, which can also be modified as needed. DOE also has experience with a number of management models, such as the hub model and various user facility models. In addition, there are models for international interactions, such as those with CERN. The upshot of the discussion was that DOE can establish a legal construct for collaboration among stakeholder groups appropriate to the goals and changing needs of a quantum testbed and its user community.

Industry works best when needs are clear. The representative from Intel shared philosophical insight on what makes for high performing government/industry interactions. Those comments were prefaced by the understanding that this perspective was one company's perspective, although several of the other industry representatives in the room also agreed in principle. One key tenet was that the industrial sector works best when it has a clear understanding of the needs of government. Thus, one of the roles that government can play is to set strategy, assemble the larger team, and define roles and responsibilities. This is critically important when the technology is immature and the timeline is decadal, like in the field of QC. The vision for a quantum testbed could help catalyze this type of long-term planning. Industry would be both a user of the technology advances produced by the testbed team and an active participant in providing technology to the quantum testbed.

There was discussion about the places that various industries would contribute in the context of the hardware/software stack. The lower layers are hardware-centric, and composed of individual qubits, qubit assemblies, memory elements, error corrected logical qubits, and finally the architecture of logical qubits. Interwoven through this stack are control layers to drive individual physical qubits and build the logical qubit architectures. Sitting above the hardware layer(s) are a number of as yet undefined software interface levels culminating in a traditional high level programming interface layer that could look, for example, like Python. One often-mentioned role for government is to help develop these upper layers, including standardized tests to compare machines and stress test them on challenging applications. There was a recognition that government also has an interest in understanding how the hardware layers function and in funding basic research on those topics.

## **5.2 Constructing Functional Quantum Computers**

The coupling of industry, academia and government engenders a successful ecosystem in which to develop a functional quantum computer. Since quantum computers are today at a low technical readiness level, the design and delivery of a system that can tackle DOE-relevant problems becomes both an exciting research opportunity and a challenging path toward functionality. Working together, industry, academia and the national laboratories have ideas for the initial objectives but after that the path forward becomes less clear. The goal of this session was to explore the near term objectives and look for common themes. Speakers from D-Wave and QxBranh were invited to share their perspectives and lead a group discussion that led to the following observations:

Hurdles depend on the hardware. For example, the D-Wave representative noted that control of the annealing cycle and a need to increase connectivity among qubits remains an important challenge. Another hurdle identified during this session involves the control of correlated errors which are relevant to atomic and superconducting instantiations of a quantum computer. In

classical Monte Carlo algorithms, the control of bias and error correlation must be handled with care. In quantum computing, we do not yet have a clear understanding of how errors correlate or propagate on larger systems and we cannot extrapolate from current few qubit systems. One clear objective of a QC testbed could be to explore this important problem and quantify how errors affect answers.

Application and algorithm development will be an important aspect of a QC testbed. The construction of algorithms will depend on the underlying technology, at least at the early stages of quantum computing. Different hardware platforms could enable the testing of multiple algorithms that we know work classically and provide a way to engage a broad community to utilize the platform. Questions for users might be: my algorithm works on a classical machine; can a QC provide a time-to-solution that is faster, or enable a larger problem to be solved? Classically, we know what to expect from certain algorithms; what will be the quantum analogue, and how does one validate results from a QC simulation? This user-driven approach to the testbed can also enable an early adopter model within DOE which has a similar feel to the early user programs at Leadership Computing Facilities.

Discussion of how the response to technical challenges and the unpredictable outcome of current scientific research might influence the future of the field pointed toward several other considerations. A carefully constructed and managed feedback loop should be developed so that hardware can be improved upon to solve problems of interest to the DOE scientific community. While industry is a willing partner, at some point QCs will need to generate profit. This also argues for a multiple testbed approach as the government needs to consider level playing fields as QC technology matures. For the DOE, the determining factor for the future of the field will be whether specific mission relevant problems can be solved. Success for industry involves turning a research opportunity into a profitable business.

## 6 Summary

The Quantum Testbed Stakeholder Workshop brought together a broad constituency of practitioners from industry, academia, national laboratories, and government to explore the critical program elements that are required to realize the promise of quantum computing. The goals of the workshop included identifying individual institutional capability in quantum computing hardware, assessing its use for near term applications, and then identifying those critical elements that will be needed to advance the goal of advancing quantum computing for scientific applications in the next five years. Equally important to assessing the technical state of the field was the sharing of best practices for the organization and management of a testbed system, including elements of workforce development and building stronger relationships within the broader research community. With input from presentations and discussion, this workshop report provides a summary and assessment of the many elements that will need to be incorporated into a testbed to effectively weave together a diverse, high performing team to advance the state of the art in quantum computing and realize the long term economic and scientific promise of QC.

The US government, and the ASCR office in particular, has a leading role to play in providing a framework for intentional development of quantum computing systems. A testbed could serve as a catalyzing force to bring the community together and focus it on the challenges of blending cutting edge science with the systems engineering to enable the application of QC to solve problems of interest to DOE. Those problems, in areas such as quantum chemistry, materials science, or matter at extreme environments, and more fully discussed in prior ASCR workshops

[48, 49], are far beyond the capability of any envisioned HPC machine and rely on the unique entangled processing of a QC. The testbed can also serve as a bridge between industry and academia to encourage transparency while these precompetitive technologies are being developed, lower the barriers for entry into the field by medium and small sized companies or academic research groups, and foster the establishment of metrics and standards to effectively compare the performance of engineering design tradeoffs. This extends to the development of a common language to characterize performance, as well as the obvious training of the next cadre of quantum computing scientists and engineers that will carry the field forward.

One of the major barriers that was identified was the immaturity of not only the individual QC technology building blocks (including hardware and software), but also the system architectures and general infrastructure required to make effective design choices. The implication of this current state-of-the-art is that the principle of co-design arguably becomes even more important than it might be for conventional HPC design. Current QC technologies are working at the individual physical qubit level and have yet to demonstrate the robust, error-corrected logical gates that will be required for future architectures. Thus, a quantum testbed will require an extension of the principles of co-design.

The development of a quantum testbed and the realization of the many economic and scientific benefits of having an operational system are well aligned with the long-term nurturing of advanced computing technologies within the ASCR office. It is fully expected that the problems that can be addressed by a QC will find applications in many of the other offices of DOE/NNSA. The demonstration and growth of a quantum computing ecosystem is a long-term undertaking, with a time horizon of a decade or more, which will require the close coupling of many diverse skills, and entities. This is precisely the type of challenge that ASCR is effectively structured to bring to completion.

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## Appendix A: Program Committee

The workshop agenda was developed by a program committee from Industry, National Laboratory and Government stakeholders.

|                 |                                                            |
|-----------------|------------------------------------------------------------|
| Jonathan Carter | Lawrence Berkeley National Laboratory                      |
| David Dean      | Oak Ridge National Laboratory                              |
| Greg Hebner     | Sandia National Laboratory                                 |
| Jungsang Kim    | Duke University                                            |
| Andrew Landahl  | Sandia National Laboratory                                 |
| Peter Maunz     | Sandia National Laboratory                                 |
| Raphael Pooser  | Oak Ridge National Laboratory                              |
| Irfan Siddiqi   | Lawrence Berkeley National Laboratory and<br>U.C. Berkeley |
| Jeffrey Vetter  | Oak Ridge National Laboratory                              |

## Appendix B: Workshop Agenda

### Tuesday, February 14, 2017

|             |                                                                |                                        |
|-------------|----------------------------------------------------------------|----------------------------------------|
| 8:00-9:00   | Continental breakfast and registration                         |                                        |
| 9:00-9:30   | Welcome and Introduction – DOE Perspective                     |                                        |
| 9:30-10:00  | Plenary 1: Quantum Processors Based on Ion Traps               | Chris Monroe<br>University of Maryland |
| 10:00-10:30 | Plenary 2: Quantum Processors Based on Superconducting Qubits  | Will Oliver<br>MIT/Lincoln Labs        |
| 10:30-11:00 | Break                                                          |                                        |
| 11:00-11:30 | Plenary 3: Near-term Practical Applications of Quantum Devices | Jarrod McClean<br>LBNL                 |
| 11:30-12:00 | Plenary 4: Evaluating the Efficacy of Quantum Hardware         | Robin Blume-Kohout<br>SNL              |
| 12:00-1:00  | Working lunch                                                  |                                        |
| 1:00-2:15   | Lab Presentations 1                                            | ANL, FNAL, LANL                        |
| 2:15-2:30   | Break                                                          |                                        |
| 2:30-3:45   | Lab Presentations 2                                            | LBNL, LLNL, ORNL                       |
| 3:45-4:00   | Break                                                          |                                        |
| 4:00-5:15   | Lab Presentations 3                                            | PNNL, SLAC, SNL                        |
| 5:15-5:30   | Wrap-up, instructions for Day 2                                |                                        |

### Wednesday, February 15, 2017

|             |                                                                                                                                                                                                                                                                                            |  |
|-------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| 8:00-9:00   | Continental breakfast                                                                                                                                                                                                                                                                      |  |
| 9:00-9:30   | Introduction to Day 2                                                                                                                                                                                                                                                                      |  |
| 9:30-10:30  | Breakout Sessions: <ol style="list-style-type: none"><li>1. Best practices for management of and access to a quantum testbed</li><li>2. Staffing and workforce considerations for a quantum testbed</li><li>3. User community development and interactions for a quantum testbed</li></ol> |  |
| 10:30-11:00 | Break                                                                                                                                                                                                                                                                                      |  |
| 11:00-12:00 | Breakout Sessions Resume                                                                                                                                                                                                                                                                   |  |
| 12:00-1:00  | Working lunch                                                                                                                                                                                                                                                                              |  |
| 1:00-2:30   | Co-design for Quantum Computing: Presentations and Discussion                                                                                                                                                                                                                              |  |
| 2:30-3:45   | Breakout Sessions: <ol style="list-style-type: none"><li>1. Models for system design and testing</li><li>2. Analog quantum simulation</li><li>3. Superconducting qubits</li><li>4. Emerging qubit technologies</li></ol>                                                                   |  |
| 3:45-4:00   | Break                                                                                                                                                                                                                                                                                      |  |
| 4:00-5:15   | Breakout Sessions Resume: <ol style="list-style-type: none"><li>1. Validation and verification</li></ol>                                                                                                                                                                                   |  |

- 2. Tools for making a testbed usable
  - 3. Trapped ion qubits
  - 4. Interconnects
- 5:15-5:30      Wrap-up, instructions for Day 3

**Thursday, February 16, 2017**

- 8:00-9:00      Continental breakfast
- 9:00-10:30     Review and Discussion of Day 2 Breakout Sessions
- 10:30-11:00    Break
- 11:00-12:30    Industry Panel
- 12:30-2:00     Working lunch and Industry Breakouts:
- 1. Roles for Government and Industry in a National Quantum Computing Ecosystem
  - 2. Constructing Functional Quantum Computers
- 2:00-2:45      Review and Discussion of Industry Breakout Sessions
- 2:45-3:00      Summary and Conclusions
- 3:00             Adjourn

## Appendix C: Breakout session guidance

The following is the guidance that was provided to the breakout session leaders to aid in leading their sessions.

### Wednesday, February 15, 2017 breakout topics

#### **Programmatic Breakout Discussions (9:30 – 12:00)**

##### Topic 1: Best practices for management of and access to a quantum computing testbed

In this breakout session, we will discuss how existing facility models and practices could be adapted for use by a quantum computing testbed. The session will begin with thoughts from a panel with familiarity of the operation of a number of facilities and then flow into a free discussion of the following questions:

1. How can lessons learned from other facilities and testbeds inform implementation of a quantum computing testbed? Does the management and access model depend on the testbed implementation?
2. What are the advantages and disadvantages of various approaches to implementing a quantum testbed and providing user access?
3. How does the answer to the questions above depend on the technical readiness level of quantum computing technology? Given that quantum computers are not yet off-the-shelf systems, what is the proper balance between efforts in hardware, software, architecture, and systems engineering?
4. If the quantum testbed were to grow beyond its initial implementation, what would be important factors to consider in evaluating and prioritizing future technologies, scaling paths, and possible upgrades?
5. What are the advantages and disadvantages to different processes, including peer-reviewed proposals, to give users access to the testbed?

##### Topic 2: Staffing and workforce considerations for a quantum computing testbed

In this breakout session, we will discuss staffing concerns for a quantum testbed. We will also discuss possible roles for a quantum testbed in developing a workforce to meet future DOE needs in quantum information science. To facilitate discussions, we will flesh out answers to a set of questions.

1. What types of scientific and technical expertise will be required during the first year of testbed deployment and operation? How does this depend on the model chosen for testbed implementation?
2. How will the initial staffing needs evolve over time as qubit technologies mature and commercial devices become available?
3. What staffing models from other facilities or testbeds could be adapted for a quantum testbed and what are their advantages and disadvantages?
4. How could one utilize the testbed for workforce development?
5. How could one design a successful mode of operation that produces both science and well-trained scientists who would then continue R&D in the quantum computing arena?

### Topic 3: User community development and interactions for a quantum computing testbed

In this breakout session, we will discuss the user community for a quantum computing testbed and strategies for successful interaction between the testbed and its users. The session will begin with thoughts from a panel representing a variety of different perspectives and flow into a free discussion of the following questions:

1. Which scientific communities are likely to be the first users of a quantum computing testbed and why? How will the relevance of a quantum testbed to various domain sciences change as technical capabilities of a testbed improve over time?
2. What are different strategies for engaging new user communities and bringing them up to speed? To what extent might different strategies be appropriate for different communities?
3. User groups can serve many functions in keeping a facility or testbed productive. What are the advantages and disadvantages of different user group models?
4. What are the most significant hurdles, technical or otherwise, to making early-stage quantum devices accessible to users who are not themselves hardware experts?

### **Co-design for Quantum Computing (1:00 – 2 :30)**

The objective of this session is to gain understanding of what co-design means in the quantum computing design space. Co-design for classical digital computing takes input from a broad community consisting of end-users through to hardware designers to iteratively refine a computer system design which is optimized for simulation capability versus resources consumed. We expect that there will be similar and additional tradeoffs in the quantum co-design space.

In this session, there will be two talks, one on classical digital co-design and one on some of the first efforts in quantum co-design. This will be followed by a discussion which will attempt to address the following questions:

1. What communities must be brought together for effective co-design of a quantum testbed? How can a testbed help to bring these communities together?
2. What standards, interfaces, etc., for hardware, software, theoretical and mathematical models are needed to enable the co-design community to effectively communicate goals, requirements, tradeoffs, limitations, etc. with each other?
3. What are the elements of testbed operation that will enable rapid and effective iteration and improvement of hardware, software, and simulations?
4. Model and algorithm development; fundamental device engineering; and software (end-user facing, "middleware", and at the device level) are all key for successful co-design. What are some of the key advances required in these areas for the next 2- and 5-years?

## Technical Breakouts (2:30 – 3:45)

### Models for system design and testing

In this breakout session, we will discuss software tools for designing and evaluating the performance of quantum computing hardware. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. What software tools exist for design and evaluation of systems of qubits, quantum simulation algorithms, etc.? What are the inherent limitations of these tools? What problems are they well-suited to address and what problems can only be explored with hardware?
2. To what extent are tools and techniques for design and evaluation of early-stage classical computing technology applicable to quantum computing?

Speakers:

1. Adam Meier, GTRI  
Testbed Modeling and Validation
2. Anastasiia Butko, Lawrence Berkeley National Lab  
Towards Scalable Quantum Architecture Simulation
3. Adolphy Hoisie, Pacific Northwest National Lab  
The CENATE Approach to Testbeds

Session Chair: Robin Blume-Kohout, Sandia National Lab

### Analog quantum simulation

In this breakout session, we will discuss the role analog quantum simulation could play in a quantum testbed. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. What technologies are available for analog quantum simulation and to what extent do these overlap with technology for digital quantum simulation? Can and should a system support both gate- and Hamiltonian-based computation?
2. Are there scientific applications to which analog simulation is particularly well-suited?
3. What verification and validation techniques are available for analog simulation?

Speakers:

1. Dan Stamper-Kurn, Lawrence Berkeley National Lab  
Large-scale Simulation with Ultracold Atoms and Molecules
2. Joel Moore, Lawrence Berkeley National Lab  
Connecting Finite Quantum Networks to Extended Quantum Materials
3. Alex Sergienko, Boston University  
Quantum Simulation of Complex Discrete Hamiltonians

Session Chair: Jonathan Carter, Lawrence Berkeley National Lab

## **Superconducting qubits**

In this breakout session, we will discuss superconducting qubits as a potential technological foundation for a quantum testbed. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. What is the scaling potential for quantum computing devices based on superconducting qubits? What factors limit scalability?
2. What enabling technology will be important for advancing quantum computing with superconducting qubits? Please be specific.
3. What are the advantages and disadvantages of superconducting qubits for a quantum testbed?
4. What computing model, size, performance, and qubit connectivity are of value for a trapped ion testbed?
5. Are there scientific applications to which superconducting qubits are particularly well or poorly suited?

Speakers:

1. Irfan Siddiqi, Lawrence Berkeley National Lab  
Scaling up Multi-qubit Circuits for Quantum Simulation
2. Will Oliver, MIT/Lincoln Lab  
Superconducting Qubit Testbed Facility

Session Chair: Peter Maunz, Sandia National Lab

## **Emerging qubit technologies**

In this breakout session, we will discuss alternatives to ions and superconducting circuits, including promising qubit technologies that could be mature enough for integration into a quantum testbed within the next few years. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. What are the alternatives to trapped ions and superconducting qubits?
2. Are these alternatives sufficiently mature for use in a quantum testbed? If not, what advances would be required to reach testbed level?
3. Are there scientific applications to which these technologies are particularly well or poorly suited? Do any have unique advantages?

Speakers:

1. Dwight Luhman, Sandia National Lab  
A Multi-qubit Testbed using Silicon Quantum Dots
2. Michael Martin, Sandia National Lab  
Scaling Neutral Atom Qubits for Quantum Information and Simulation
3. Peter MacMahon, Stanford University  
Computing Using Networks of Optical Parametric Oscillators and Measurement Feedback

Session chair: Raphael Pooser, Oak Ridge National Lab

## **Technical Session 2 (4:00 – 5:15)**

## **Characterization, validation, and verification**

In this breakout session, we will discuss the characterization, verification, and validation needs of a quantum testbed as well as the role a testbed could potentially play in developing validation and verification capabilities. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. What verification and validation protocols are available for use with a quantum testbed? To what extent are these able to predict the performance of quantum algorithms on a testbed system?
2. What characterization capabilities will a quantum testbed need? How does this depend on the specific hardware instantiation?
3. How might a testbed be used to advance research in validation and verification? What are the hardware requirements for a testbed capable of advancing this research?
4. What are the quantum control capabilities needed for calibration, verification, and validation? Do these differ from control capabilities needed to implement algorithms?

Speakers:

1. Andrew Landahl, Sandia National Lab  
Demonstrating Fault-Tolerant Quantum Error Correction with a Small Testbed
2. Michael Biercuk, University of Sydney  
Quantum Control Engineering for Quantum testbeds
3. Scott Pakin, Los Alamos National Lab  
Physical Characterization of Quantum testbeds

Session Chair: Robin Blume-Kohout, Sandia National Lab

## **Tools for making a testbed usable**

In this breakout session, we will discuss the technical challenges associated with making early-stage quantum computing hardware available to external users. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. What software infrastructure, programming tools, applications, etc. are currently available for use in a quantum testbed? How might a testbed be used to advance the development of these tools?
2. Given the current state of the tools in the previous question, what support will testbed users require?

Speakers:

1. Bert de Jong, Lawrence Berkeley National Lab  
End User and Developer Software Framework
2. Kelly Stevens, GTRI  
Quantum Machine Compilation
3. Alex McCaskey, Oak Ridge National Lab  
Software Framework for Interfacing Classical HPC with Quantum Accelerators

Session Chair: Jonathan Carter, Lawrence Berkeley National Lab

## Trapped ion qubits

In this breakout session, we will discuss trapped ions as a potential technological foundation for a quantum testbed. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. What is the scaling potential for quantum computing devices based on trapped ions? What factors limit scalability?
2. What enabling technology will be important for advancing quantum computing with trapped ions? Please be specific.
3. What are the advantages and disadvantages of trapped ions for a quantum testbed?
4. What computing model, size, performance, and qubit connectivity are of value for a trapped ion testbed?
5. Are there scientific applications to which trapped ions are particularly well or poorly suited?

Speakers:

1. Thomas Monz, Innsbruck  
Technical Considerations for an Ion-trap-based Quantum testbed
2. Jeremy Sage, MIT/Lincoln Lab  
Technologies for a Robust, Scalable Trapped-ion Quantum testbed
3. Matthew Blain, Sandia National Lab  
Micro-fabricated Ion Traps for Scalable Quantum Information Processing

Session Chair: Peter Maunz, Sandia National Lab

## Interconnects

In this breakout session, we will discuss the connections between qubits in a quantum testbed. The session will begin with a few brief presentations that lead into a discussion of the following questions:

1. Connections between qubits are as important as the qubits themselves, especially as the number of qubits in a device increases. Are the interconnects used in current-generation quantum devices adequate for scaling up? If not, when will new interconnects be required?
2. What alternatives exist for connecting components within a quantum processor and for connecting separate processors? What are their advantages and disadvantages? What are the technical challenges to developing them and integrating them into a quantum testbed?

Speakers:

1. Saikat Guha, Raytheon BBN
2. Quantum Computing Using Photons
3. Paul Kwiat, University of Illinois  
Optical Quantum Interconnects and Photonic Qubits

Session chair: Raphael Pooser, Oak Ridge National Lab

## Thursday, February 16, 2017 Breakout Topics

### Industry Panel

Representatives from large and small companies engaged in developing quantum computing and related technologies will share their individual views on the near-term promise of quantum computing, the major challenges to developing this technology, and the role government agencies might play in advancing the development of quantum computers. The panel will also address questions from the audience.

The panel will include representatives from: IBM, Google, Rigetti Computing, IonQ, ColdQuanta, and Quantum Circuits, as well as a representative from one of DOE's labs with significant experience partnering with industry in the classical digital computing space.

### Industry Breakouts:

After the initial industry panel, workshop participants will take lunch to one of the following breakout sessions. Each breakout will begin with one or two presentations that will lead to general discussion on the breakout theme.

#### **Topic 1: Roles for Government and Industry in a National Quantum Computing Ecosystem**

Speakers and Discussion Leaders: Anne Matsuura (Intel) and Brian Lally (DOE)

The discussion will focus on two areas:

1. Ways individual workshop participants envision government getting involved
2. Specific examples of government-industry partnerships that could be developed and what these partnerships could accomplish.

Additional discussion topics could include (but are not limited to): industry interactions with DOE testbeds, IP management, and government role in transitioning technology.

#### **Topic 2: Constructing Functional Quantum Computers**

Speakers and Discussion Leaders: Steve Reinhardt (D-Wave) and John Kelly (QxBranch)

The discussion will focus on three questions:

1. What are the key technological hurdles to be overcome?
2. What are the most important hardware or algorithmic problems to tackle first?
3. What basic scientific or technological aspects of a quantum computer are still uncertain or debated, and will likely determine the future of this field?

Additional discussion topics could include (but not limited to): system design and operating system development, collaboration between system integrators and key component vendors, and roles of national labs and government agencies.

## Appendix D: Acronym List

|       |                                                            |
|-------|------------------------------------------------------------|
| ALCF  | Argonne Leadership Computing Facility                      |
| ANL   | Argonne National Laboratory                                |
| AP    | Advisor Panel                                              |
| API   | Application Program Interface                              |
| ASCR  | Advanced Scientific Computing Research Program             |
| BES   | Basic Energy Science                                       |
| CINT  | Center for Integrated Nanotechnologies                     |
| CMOS  | Complementary Metal Oxide Semiconductor                    |
| CRF   | Combustion Research Facility                               |
| DOE   | Department of Energy                                       |
| FNAL  | Fermi National Accelerator Laboratory                      |
| FTQEC | Fault-Tolerant Quantum Error Correction                    |
| GST   | Gate Set Tomography                                        |
| GTRI  | Georgia Tech Research Institute                            |
| HPC   | High Performance Computing                                 |
| LANL  | Los Alamos National Laboratory                             |
| LBNL  | Lawrence Berkeley National Laboratory                      |
| LLNL  | Lawrence Livermore National Laboratory                     |
| MESA  | Microsystems and Engineering Sciences Applications Complex |
| NSF   | National Science Foundation                                |
| ORNL  | Oak Ridge National Laboratory                              |
| OS    | Office of Science                                          |
| PNNL  | Pacific Northwestern National Laboratory                   |
| QC    | Quantum Computer                                           |
| QCVV  | quantum characterization, verification, and validation     |
| QTSW  | Quantum testbed Stakeholder Workshop                       |
| SLAC  | Stanford Linear Accelerator National Laboratory            |
| SNL   | Sandia National Laboratories                               |
| STEM  | Science, Technology, Engineering and Math                  |