HPC User Forum Update

Advanced Scientific Discovery with Quantum Computing, Santa Fe, New Mexico

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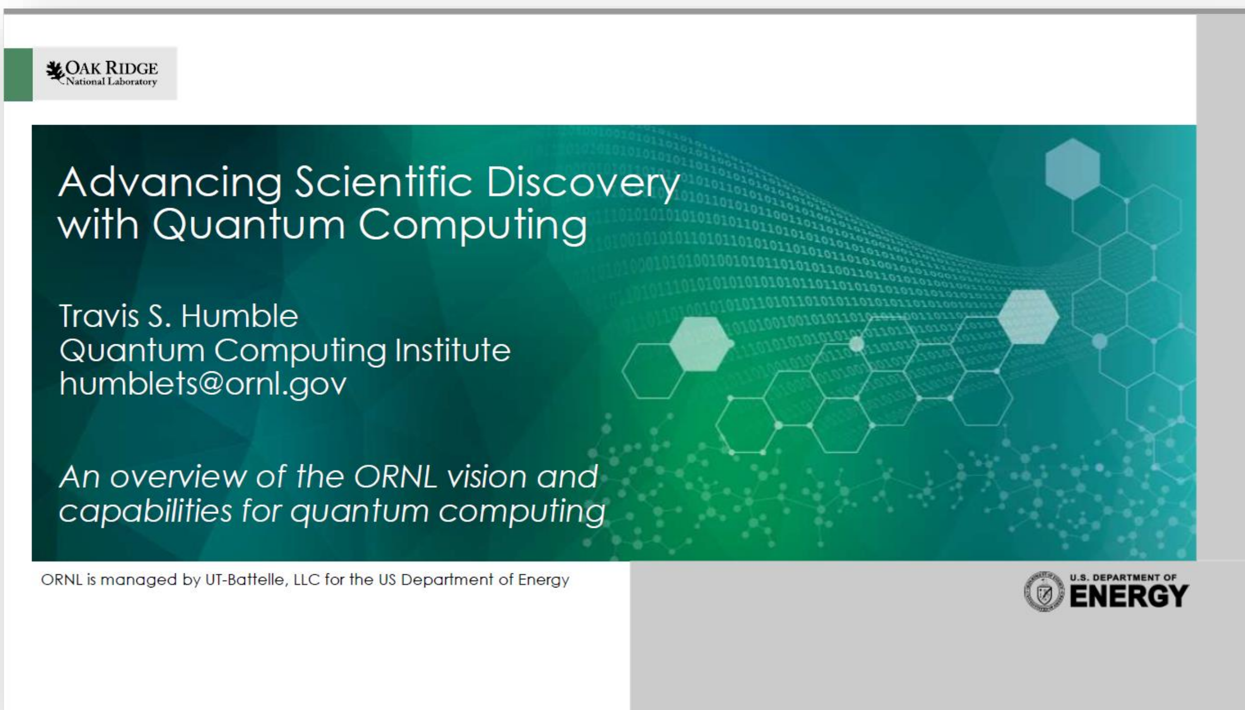
IN THIS UPDATE

The HPC User Forum was established in 1999 to promote the health of the global HPC industry and address issues of common concern to users. In April 2019, the 72nd HPC User Forum took place in Santa Fe, New Mexico. This update summarizes a presentation from that meeting entitled, *Advanced Scientific Discovery with Quantum Computing*, presented by Travis Humble, Quantum Computing Institute, ORNL.



Source: ORNL and Hyperion Research, 2019

PRESENTATION: ADVANCED SCIENTIFIC DISCOVERY WITH QUANTUM COMPUTING, PRESENTED BY TRAVIS HUMBLE, QUANTUM COMPUTING INSTITUTE, OAK RIDGE NATIONAL LABORATORY

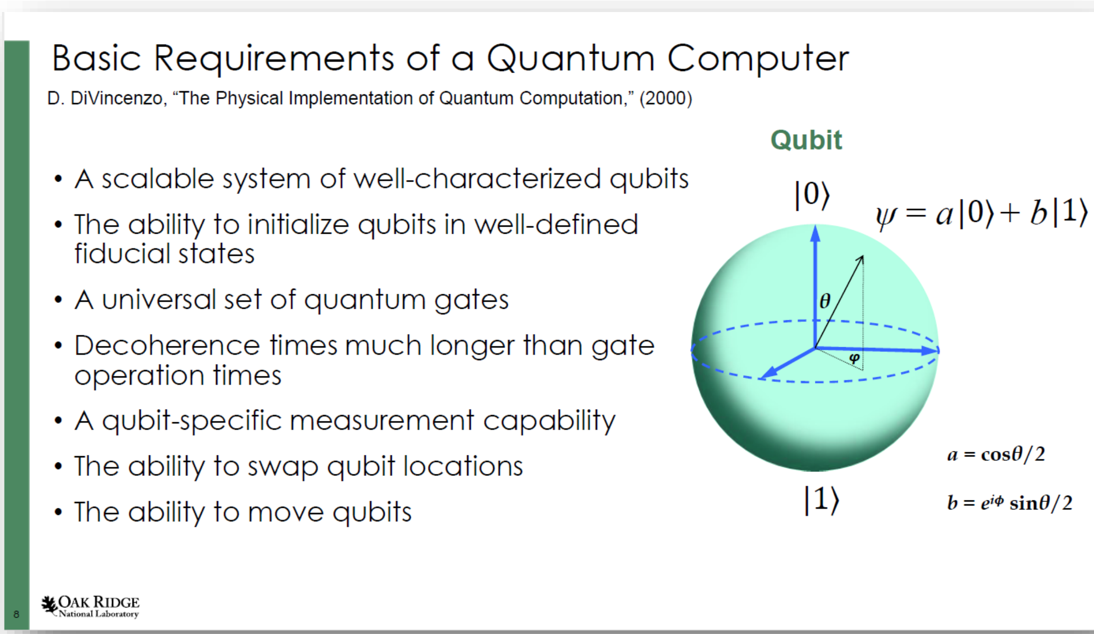
Travis S. Humble from the Quantum Computing Institute of Oak Ridge National Laboratory (ORNL) described his role in imagining quantum computing systems in the 2025 time frame and beyond. Humble began by outlining some of the fundamental requirements of a quantum computer, starting off with a discussion of a system of well-characterized qubits.

Qubits are the quantum version of bits, the notional amount of information that can be represented. As shown in Figure 1, qubits can be envisioned as spheres where the north and south poles represent the values of zero and one, much like normal binary logic. A qubit can exist on any point on the surface of this sphere, and there is an infinite number of those points. As a result, quantum computing gives more access to new states of information than users have never had access to before.

Next, Humble stated that to build a quantum computer there needs to be system of qubits with features such as registers and the ability to address those registers using operations. These registers must be initializable to start a calculation. Humble also noted the need for a set of operations that can be used to implement the necessary logic functions.

- In conventional computing, Humble thinks of the logic in terms of Boolean algebra. In quantum computing it's an operator algebra. So, again, it's a more complex system of equations but it's performing something very similar.

FIGURE 1

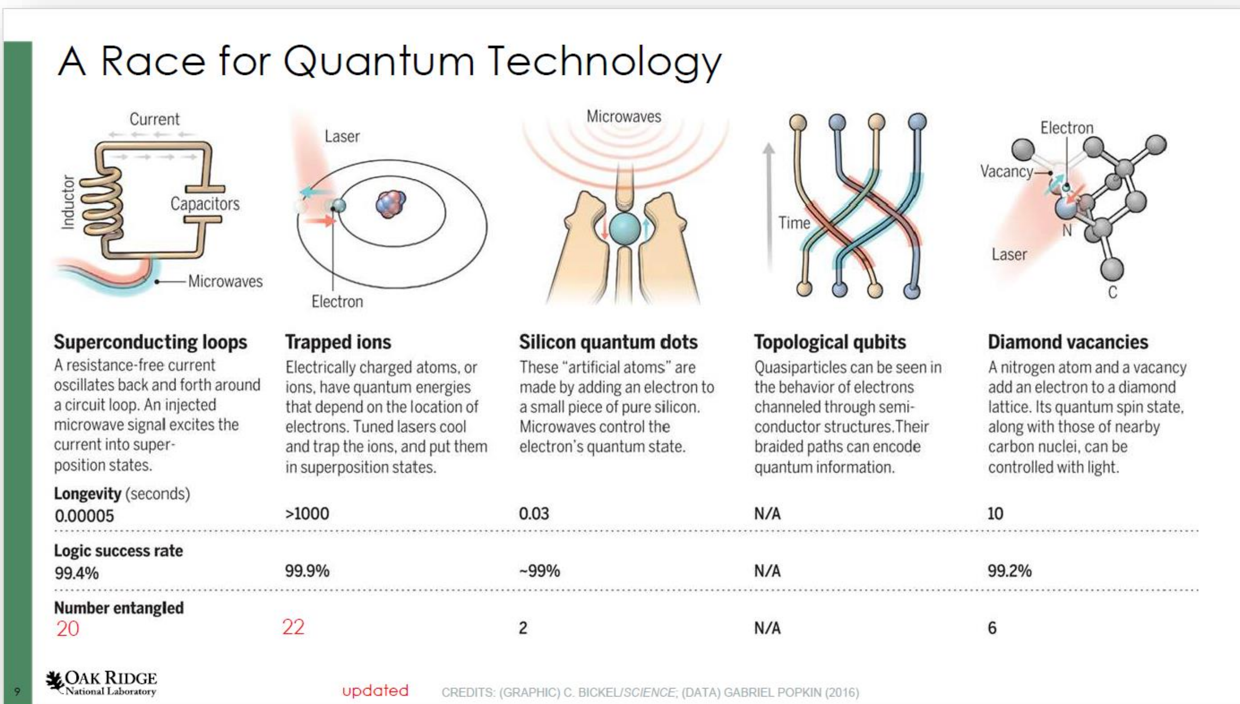


Source: ORNL and Hyperion Research, 2019

Another critical requirement, Humble noted, is that one must be able to maintain the state of this qubit-based information long enough to complete a calculation. This, Humble said, is where QC get gets difficult. Demonstrating true quantum computing requires control of the qubits and a way to measure the system. Finally, Humble noted there are significant architectural concerns about moving data around.

Humble then went on the explain that there is currently a race for quantum technology to try and realize these ideas in many different implementations. As shown in Figure 2, two of the leading candidates now are superconducting electronics operating at cryogenic temperatures and individual trapped ions, typically using electromagnetic fields. There are also demonstrations using silicon in which the individual electrons within the silicon substrate are manipulated and other, more exotic forms which are not yet realized. This is a worldwide endeavor, and there are many diverse efforts striving to be first to demonstrate a scalable approach to realizing quantum computing.

FIGURE 2



Source: ORNL and Hyperion Research, 2019

Humble noted the US National Quantum Initiative signed into law late last year, intended to accelerate quantum research in the United States. The DoE is expected to start up its own programs in this area. There is a national quantum coordination office to manage efforts across government agencies, subcommittees of the national science and technical council and, finally, a quantum economic development consortium recently established through NIST to provide stability within the supply chain.

FIGURE 3

Source: ORNL and Hyperion Research, 2019

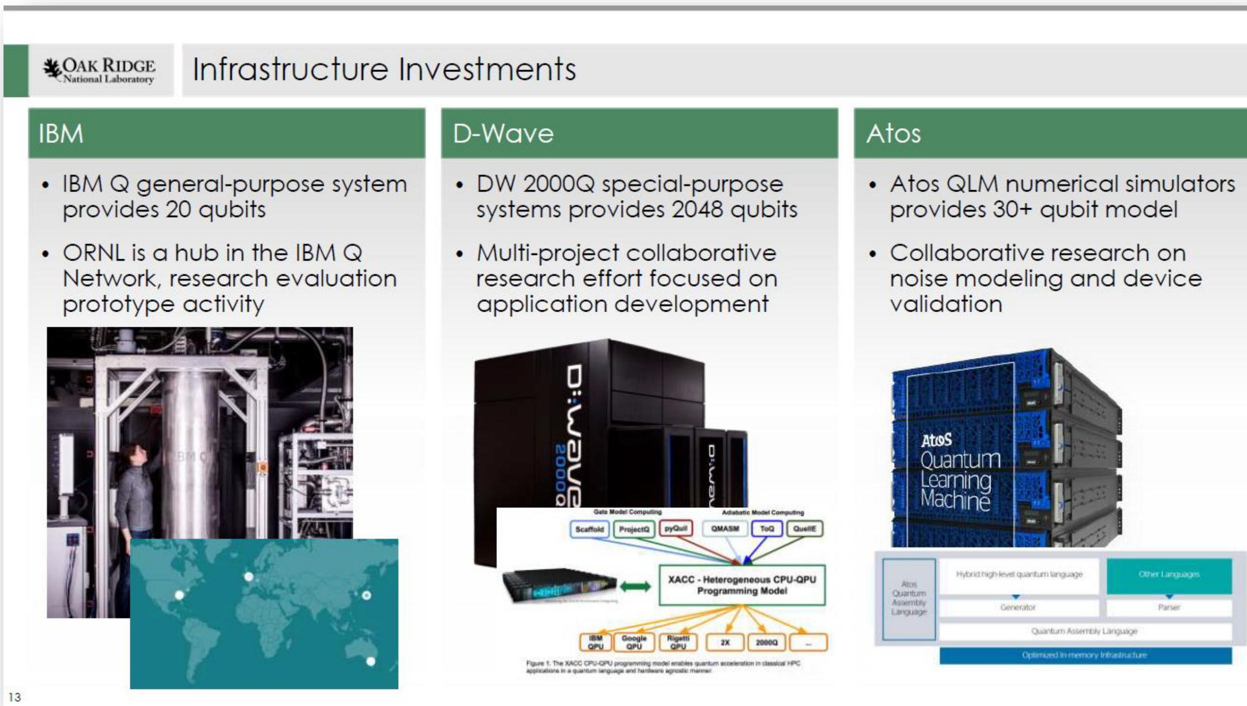
Closer to home, Humble outlined how the role of ORNL wants to be an international leader in the field of quantum computing. Humble went on to explain that means ORNL must advance the technology itself, all the way from the atoms up to the applications. Those applications are important for their scientific discovery. ORNL must be able to figure out how quantum computing is going to integrate into existing work flows and how ORNL can leverage it with problems that researchers are not yet able to tackle with conventional approaches. This ties into national priorities, including discovery and innovation and energy security, and ORNL wants to be able to transfer this knowledge for the public good.

One important way to support these activities is that ORNL is making investments in infrastructure. Humble highlighted three QC systems currently at the lab.

- One of these is in partnership with IBM to gain access to their general-purpose quantum processor, the IBM Q (ORNL is a hub within that network). ORNL is also partnering with other DoE laboratories to develop applications on this gate-based model of quantum computing that they can then apply to scientific discovery.
- Similarly, they are partnering with D-Wave, who makes a special-purpose processor tailored to optimization problems. Using access to that system, ORNL is partnering with outside collaborators to develop applications for scientific discovery.

- And, finally, there are numerical simulations, which are basically conventional, numerical analyses of how quantum systems work. ORNL bought a system from Atos, which developed a numerical simulator.

FIGURE 4

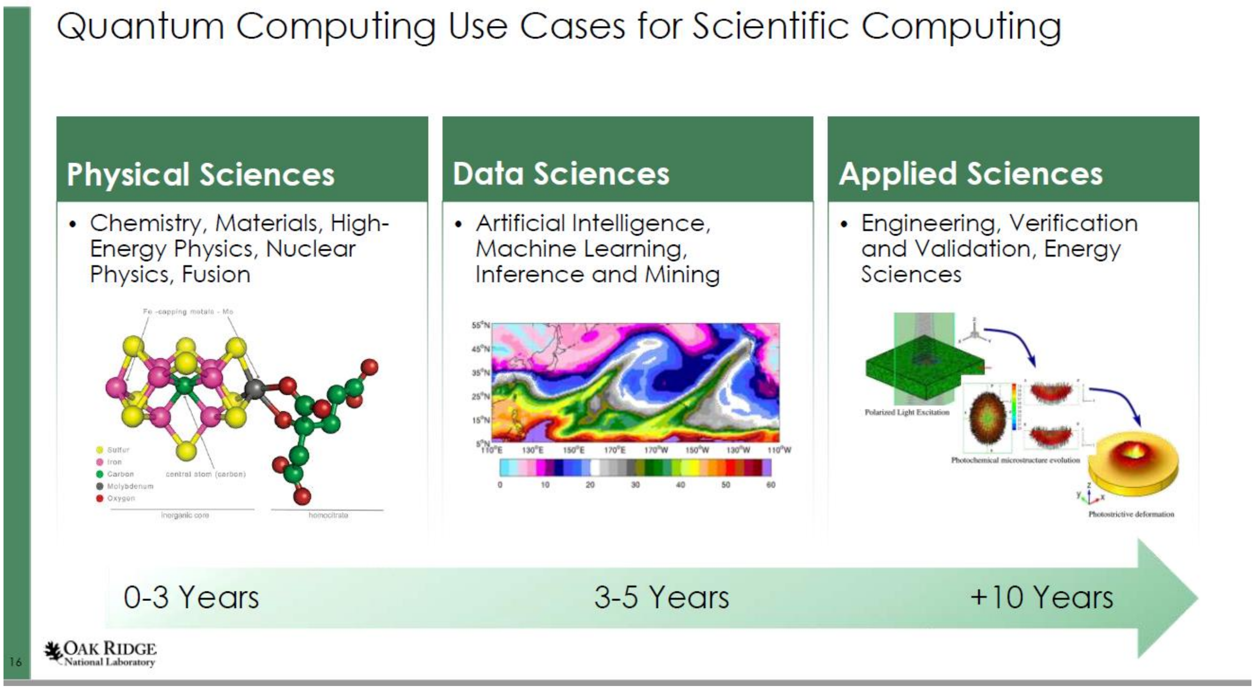


Source: ORNL and Hyperion Research, 2019

Humble outlined where he believes quantum computing is going to be useful, citing three specific use cases relevant to scientific computing, as shown in Figure 5.

- The first is already being done: physical science that covers chemistry, high energy physics, and materials. Current QC methods may not yet be competitive with conventional approaches, certainly not competitive with high performance computing codes, but they are at the point where researchers can start thinking of a path where they could be.
- Next is machine learning, specifically in areas where quantum computing, which is a probabilistic model of computation, can be used for inference problems. Humble cautioned, however, that there is an I/O problem right now that prevents researchers from using QC in real settings where there is a requirement for delivering enough data to the processor in a sufficient amount of time to be competitive.
- Finally, there are applied sciences that include verification and validation of engineering designs, solving partial differential equations and monitoring flows. Humble posits that that's probably in the 10+ years range.

FIGURE 5



Source: ORNL and Hyperion Research, 2019

Humble concluded with a discussion on looming workforce issues in QC. ORNL is trying to train people to get an even better understanding of the issue. They're looking at classes that they've had onsite and are also looking for partnerships with people who have a stake in the development of quantum computing. And then, of course, there are efforts to transfer the technology outside of the laboratory to their partners and others.

Finally, Humble noted that Oak Ridge National Lab has a newsletter that they send out weekly to keep people updated on a wide range of QC topics, noting that anyone can sign up at:

https://elist.ornl.gov/mailman/listinfo/qci-external.

For more information or to view this and other presentations given at HPC User Forums dating back to 2008, visit www.hpcuserforum.com.

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