by Ernest Granson

# Quantum Leap

## How IBM is partnering with the oil industry to develop quantum computing

**IBM Q System One, the industry's first fully integrated quantum computing system, is assembled for mechanical testing for the first time at Goppion headquarters in Milan, Italy in July 2018. Goppion is a world-renowned manufacturer of high-end museum display cases that protect some of the world's most precious art including the Mona Lisa at the Louvre, and the Crown Jewels at the Tower of London. Photos courtesy IBM**

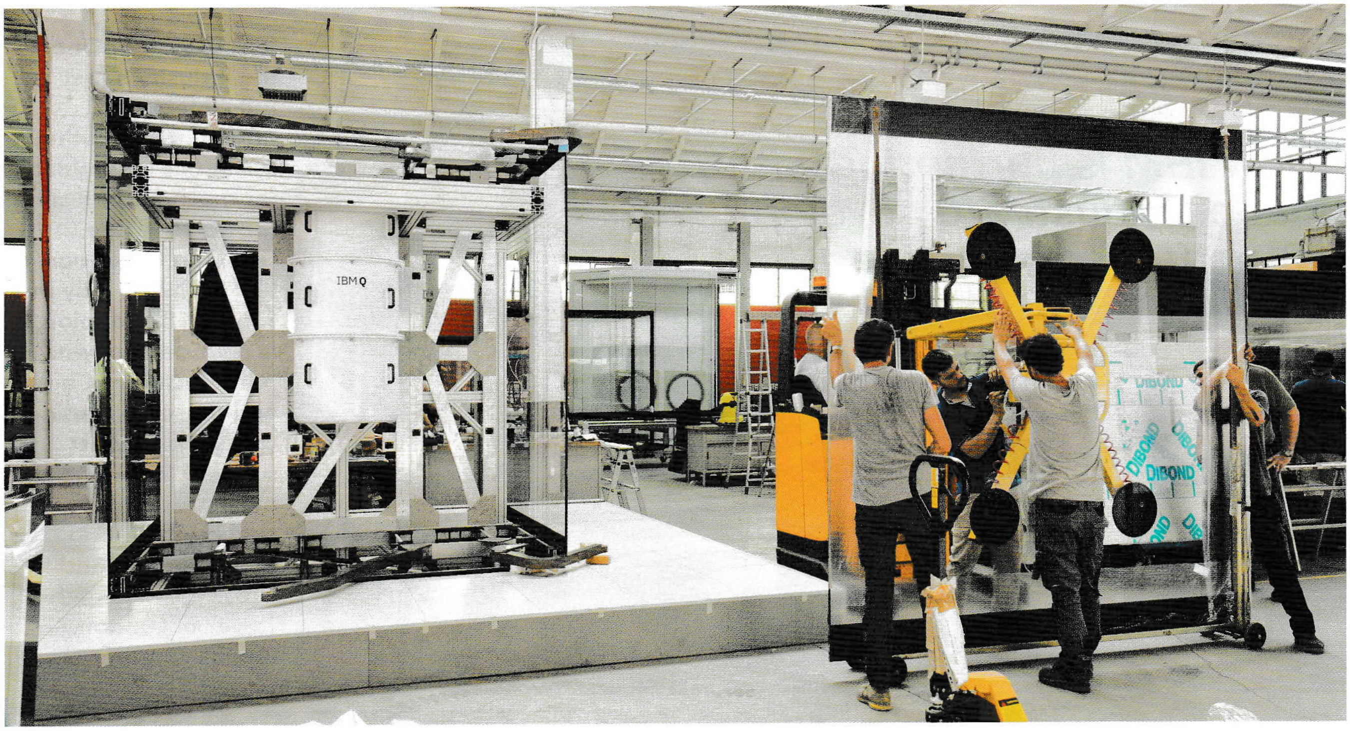
As you might expect, IBM Corp. is heavily involved in the development of quantum computing, particularly through its IBM Q Network. This global network consists of Fortune 500 companies, start-ups, academic institutions and national research labs to advance quantum computing as well as exploring its practical applications.

Earlier this year, IBM and ExxonMobil Corp. signed a partnership agreement which will expand ExxonMobil's efforts to develop an array of new energy technologies, improving energy efficiency and reducing greenhouse gas emissions.

Vijay Swarup, vice president of research and development for ExxonMobil Research and Engineering Company, says the scale and complexity of many challenges faced in the energy business surpass the limits of today's traditional computers.

"Quantum computing can potentially provide us with capabilities to simulate nature and chemistry that we've never had before," Swarup says. "As we continue our own research and development efforts in the areas of energy and chemical manufacturing, our agreement with IBM will allow us to expand our knowledge base and potentially apply new solutions in computing to further advance those efforts. Advances in quantum computing could provide ExxonMobil with an ability to address computationally challenging problems across a variety of applications, including the potential to optimize a country's power grid, perform more predictive environmental modeling and highly accurate quantum chemistry calculations to enable discovery of new materials for more efficient carbon capture."

So, what is it about the quantum computing concept which allows it to work at such a higher level than the traditional binary or "classic" computer? As Chris Schnabel, director for IBM Q Offering Management says, classic computers are highly capable of solving certain problems, and as the amount of information or size of a problem grows, the runtime of the classic computer also grows proportionately.




"But there are other problems in which the runtime can grow exponentially," Schnabel says. "If I'm continuing to add data points, the runtime can double each time those data points are added and you can get ridiculously large numbers very quickly. The concept behind quantum computers means those types of problems can be solved by the quantum computer using polynomial runtime instead of the more time-consuming exponential runtime."

Schnabel emphasizes that a comparison between a classic computer and a quantum computer is not a black and white issue in which the quantum computer is simply the "fastest." Rather, there are certain problems for which a quantum computer has a noticeable advantage. One of those types of problems would be those related chemistry.

"For instance," Schnabel says, "quantum computing is very applicable to simulating a molecule. In trying to find a molecule's ground state, in other words, its most stable configuration, you have to simulate how the electron will interact with other atoms and their protons and neutrons that make up the nucleus. If I'm using a classic computer algorithm, every time I increase the size of the molecule by adding an electron orbital to the simulation, it interacts with every other electron orbital and multiplies the runtime. A quantum computer, on the other hand, is able to solve that problem more efficiently because a molecule is, essentially, a quantum system itself. With the current available classic computing, chemistry problems are being solved through approximation."

Because quantum computing is in its early stages, actual application for industrial use is still limited.

"When we talk to a business that is interested in the potential for quantum computing, we begin with asking, 'what are the hard problems you are trying to solve with classic computing that have strategic business value?'" Schnabel says. "It's

**The System One includes a hinged glass door engineered to open effortlessly using a motor-driven rotation around two displaced axes. The door design simplifies the process of performing maintenance and upgrades to the system.**

**The enclosure is built using half-inch thick borosilicate glass that is reminiscent of the display case Goppion devised for the Mona Lisa to protect it from damage by human and environmental causes.**

critical that we go through that list first to isolate the problems that aren't suitable for resolution by quantum or problems that won't be solved using quantum for the foreseeable future. For any problems outside of the chemistry space, we have to be able to show that use by a quantum computer will be more efficient than what current high-level classic computers are capable."

A practical example of an issue in which quantum computing could help an energy company such as ExxonMobil is the development of catalysts for use in the petroleum sector. Cobalt is used as a catalyst to remove sulfur from natural gas and from refined petroleum products like gasoline, diesel, kerosene, jet and other fuel oils. Cobalt catalysts are also used to synthesize precursors in the production of polyester which is used for polyester fibres and polyester resin to make recyclable plastic. Catalyst compounds cannot be modeled accurately by using a classic computer and so it is difficult to confirm the viability of other potential catalysts. Quantum computers, however, could provide a realistic model of yet undeveloped catalysts.

Schnabel says quantum computers are in the early stages, with the first commercially viable computers years away.

"We're in what is known as the 'quantum ready' phase, that is, getting ready for production," he says. "We're proving the systems and getting ready to build out more robust hardware. I should point out that a bigger investment for companies is developing people and their skills to operate in that environment. We expect this state of first use cases will take place over a five-year horizon, after which we'll move quickly into the 'quantum advantage' stage to extract real business value. But we are actually building the quantum centres of the future and once we understand the mapping of problems to quantum computing we believe it will transform the industry."

In great part, that rapid transformation will take place because of open source ecosystems like the Q Network and its cloud which provides access to quantum computing for many parties.

"There have been more than 10 million experiments by non-IBMers because we are giving them the tools," Schnabel says. "The cloud lowers the barriers for what people are able to develop and that's the power of community. We recognize we're not the only game in town, that there's an incredible amount of global talent and we want to enable that talent. Do you remember those old black and white photos of the first classic computers? That's where we are at now. Someday soon, we'll be pointing back at the companies and people who are driving this new transformation just as we have for those who developed those first classic computers." 

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## What is Quantum mechanics?

To leap into the world of quantum physics and its subset, quantum mechanics, is to subject yourself to a mental enigma. Quantum mechanics describes the properties of matter like molecules, atoms and their components, quarks, gluons and other particles. It also describes how these particles interact with one another and with electromagnetic radiation, which is the flow of photons. Because they take place at that scale, some of those interactions and the concepts behind them, are hard to visualize or perceive.

Two of the major quantum mechanics concepts that are incorporated into quantum computing are known as "superposition" and "entanglement." Superposition is a property which says that a quantum system can exist in a number of states simultaneously while entanglement means two quantum particles can be linked and synchronized to each other even if separated by vast distances. For most people, even physicists, these concepts are hard to comprehend. Even Einstein described entanglement as "spooky action at a distance."

What a quantum computer does is to utilize these two "spooky" concepts to supercharge processing capabilities. The traditional computer operates on a binary system using strings of bits composed of ones and zeros while a quantum computer incorporates not only ones and zeros but also the superpositions of ones and zeros that are called quantum bits or qubits. This distinction will enable a quantum computer to drastically accelerate the processing of information, leading to advancement in many areas such as energy, chemistry and pharmaceuticals.