COMPUTING

Quantum leap for oil and gas

ExxonMobil and IBM recently announced a partnership to advance energy sector application of quantum computing. Here, *Dr Jeannette M Garcia*, Senior Manager, Quantum Algorithms, Applications and Theory, IBM Research, and *Dr Bob Parney*, IBM Quantum Industry Consultant for Chemicals and Petroleum, IBM Global Business Services, outline the realities of quantum computing that are relevant to the oil and gas sector.

A quantum computer is any device that leverages a physical quantum mechanical system to do calculations. The basic memory units in a quantum computer are qubits (quantum bits), which are an extension of the bits used in classical computation. A classical bit can take two distinct values, 0 and 1. At any given time, a bit has exactly one of these two values. As such, a bit is similar to a coin sitting on a table – it can be either in a head-up state (which we can consider to be the equivalent of a bit set to 0) or in the head-down position (bit set to 1). In contrast, a qubit can take complex amplitudes for each of its 0 and 1 states; this allows the qubit to exhibit wavelike properties. At a given time, the state of a qubit can be a combination of 0 and 1, called superposition. It's like the qubit is a continuous wave and the state of a qubit is distributed across both of its 0 and 1 states simultaneously.

In universal quantum computing, qubits are manipulated by a series of gates that are the quantum equivalent of 'AND' and 'OR' gates etc that operate on classical bits. These quantum bits can be constructed by engineering circuits out of super-conducting materials (which must be kept at temperatures approaching 0° Kelvin (K)) or other methods such as using photons on trapped ions. All approaches are built around maintaining a physical quantum mechanical system that can be manipulated several times in its quantum states and doesn't collapse to 0 or 1 until measured.

Scaling quantum devices continues to be a significant engineering challenge with the power of a quantum computer measured not just by the number of qubits it contains, but the number of gates that may be implemented before errors overwhelm the accuracy of the calculation or the qubits themselves spontaneously collapse to classical state of 0 or 1 and quantum based calculations can no longer be applied.

Oil and gas applications

Where might a quantum computer apply in oil and gas? Indications are that early applications are likely to be in chemical simulation; followed by optimisation, risk analysis and artificial intelligence (AI).

Research in applications related to reservoir simulation and seismic imaging have already begun, but as the largest commercially available quantum computing hardware is IBM's 53-qubit universal hardware, the ability to address commercial-scale seismic imaging and reservoir simulations that are often run on cloud compute environments will likely require larger machines that could be 10 or more years out.

Chemistry use cases

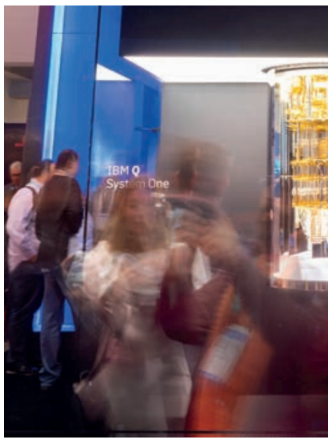
The renowned US theoretical physicist Richard Feynman originally envisioned using quantum computers to simulate quantum systems, and the modelling of chemical interactions that are inherently quantum mechanical in nature with quantum algorithms, is showing great promise. Determining the electronic structure of molecules is imperative to understanding the reactivity of molecules. In this way quantum computers could simulate chemical reactions between water, rock and oil to speed up the search for customised surfactants to recover a greater volume of trapped hydrocarbons, and also to develop new classes of petrochemicals – potentially including catalysts that could reduce greenhouse gas (GHG) emissions.

Prototype quantum computers, supported by classical computers, are already performing quantum chemistry simulations. In 2017, the cover story in *Nature*[1] by IBM scientists showed depictions of the small inorganic salts lithium hydride (LiH) and beryllium hydride (BeH_2) whose potential energy surfaces were modelled on IBM's publicly available quantum computers. Application of these same hybrid methods to challenges in the chemicals and petroleum industry may soon be possible, leading some to consider chemistry the 'killer app' for quantum computing.

The reason chemistry is such a good fit for quantum computing has to do with scaling – how quickly the compute resources required increase as the number of electron-electron interactions (essentially the size of the problem) increases. To get a sense of the relative scaling, the simple hydrocarbon, naphthalene ($C_{10}H_8$), could be represented exactly with approximately 116 fault-tolerant qubits, but it would require a classical computer with 10^{34} bits to do the same. For perspective, 10^{34} bits is 7.1bn times the total volume of data predicted to be stored electronically by 2025 – perhaps 175 zettabytes. While modelling naphthalene in this manner may or may not be of commercial interest, this example illustrates the potential scaling advantage of using quantum computers for chemical simulation.

Optimisation, risk analysis and AI

Quantum computers may potentially find the best solution among varying weighted options more efficiently than classical computers, and could provide advantage in areas such as portfolio optimisation, risk



The IBM Q System One, as shown at CES 2020. The cryostat measures about 3-ft tall – pictured here is the internal wiring and cooling components that all connect to and cool the quantum processor (square) at the bottom; when the system is running, all of these components are enclosed by the silver canister

Photo: IBM

analysis and Monte-Carlo-like applications (which are used to model the probability of different outcomes in a process that cannot easily be predicted due to the intervention of random variables).

Why? The ground state energy of a molecule requires the optimisation of a quantum mechanical system expressed as a Hamiltonian.[2] Similarly, one approach that many other non-quantum optimisation problems have – ranging from investment portfolios to feedstock routing, or transportation and supply chain logistics – can also be solved on a quantum computer by mapping them to a Hamiltonian. The current state-of-the-art is that while the potential for quantum advantage in the scaling of chemical modelling is recognised, the quantum advantage for optimising non-quantum problems is intriguing but the path to large-scale advantage is a little less clear.

However, this is an area of significant research, particularly in the financial sector with JP Morgan Chase and Barclays among banks experimenting with quantum computing to accelerate risk mitigation and improving performance modelling.

Meanwhile, quantum computing holds promise for improving results in AI. In a March 2019 *Nature* cover article[3], IBM, MIT and Oxford scientists demonstrated that classification of artificial data-sets could be improved over classical-only compute results alone by implementing a quantum-classical hybrid support vector machine.

Reservoir simulation, seismic imaging and cryptography

Peter Schor, a US professor of applied mathematics at MIT, developed a quantum algorithm that can efficiently factor a larger integer into two prime numbers in a short enough time that when implemented would effectively break asymmetric RSA encryption – but only when the technology matures and stable machines significantly larger than current technology become available.

There are also algorithms in development for solving large sets of linear equations and computational fluid dynamics, but it is generally believed that practical applications of these algorithms will also require large and mature quantum computers. Even after the first industrial applications of quantum computing come online there are likely to be decades or more of further development after the initial breakthroughs that seem likely in chemical simulation.

Quantum computing today

Quantum computers are currently available through the cloud. Machines currently are small and noisy (which means they cannot reliably run large algorithms), but research and investment has been ramping up significantly. Ground work is actively being implemented on real hardware that is accessible through the cloud, and many algorithms are being developed now in areas applicable to oil and gas.

IBM recently announced a new quantum computing centre with 15 quantum computers accessible over the cloud, including a 53-qubit machine that is the largest commercially available universal gate model quantum computing system to date.

Getting quantum ready

With the major impact of quantum computing still on the horizon, why is it so important for chemical and petroleum companies to take action now?

Industry-specific applications that show quantum advantage are likely to be proprietary for the companies that develop them first. In oil and gas, companies like ExxonMobil are collaborating with IBM Quantum experts to advance quantum computing.

Embracing quantum computing as an emerging technology necessitates a different way of thinking, a new and highly sought-after set of skills, hybrid IT architectures, and novel corporate strategies. Companies must look at their risk profile and where technology fits within their portfolio. They need to evaluate what level of quantum readiness they are comfortable with, including what is the potential that they or their competitors will find a competitive advantage in the quantum space.

So, how can an oil and gas company get started evaluating quantum computing now – while standards, strategies, use cases and ecosystems are still being developed?

Explore applications: Identify quantum champions in your organisation to experiment with actual quantum computers and explore the potential applications of quantum computing relevant to your company. Cloud access and opensource software and training (such as Qiskit.org) make this readily available. To help focus on your highest-value problems, have your quantum champions report to a quantum steering committee that includes line-of-business executives and market strategists.

Prioritise use cases: Understand and prioritise quantum computing use cases specific to your industry according to their potential for attaining business advantage – given your organisation's business strategy, associated customer value propositions and future growth plans. Keep an eye on progress in quantum application development to stay in the vanguard of which use cases might be commercialised sooner rather than later.

Leverage an ecosystem: Consider partnering with a world-class leader in quantum and an ecosystem of like-minded research labs and academic institutions, quantum technology providers, quantum application developers and coders, and start-ups with supporting technologies. Include organisations with similar challenges to gain immediate access to an entire quantum computing stack capable of developing and running quantum algorithms specific to your business needs. Look for breakthroughs in quantum technology that might necessitate a change in ecosystem partners.

Quantum computing offers some exciting potential business applications for oil and gas. While there continues to be uncertainty about the final impact of the technology, the time to start getting ready is now. ●

Footnotes

1 'Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets', Abhinav Kandala, Antonio Mezzacapo, Kristan Temme, Maika Takita, Markus Brink, Jerry M Chow and Jay M Gambetta, *Nature*, September 2017.

2 The Hamiltonian of a system specifies its total energy, ie the sum of its kinetic energy (that of motion) and its potential energy (that of position).

3 'Error mitigation extends the computational reach of a noisy quantum processor', Abhinav Kandala, Kristan Temme, Antonio D Corcoles, Antonio Mezzacapo, Jerry M Chow and Jay M Gambetta, *Nature*, March 2019.

Jeffrey Cohn, postdoc for Quantum Applications in Quantum Chemistry and Science at IBM, also contributed to this article