The Big Read **Quantum technologies**

Quantum computing: the power to think outside the box

With potential uses in healthcare and finance, the technology promises to revolutionise computing

Richard Waters in San Francisco and John Thornhill in London SEPTEMBER 3, 2018

As a keen player of the board game Go, Mark Griswold was enthralled by the 2016 contest between the world's top player and a computer — a milestone in the history of artificial intelligence. He still recalls move 102 in the opening game with awe. The computer, developed by the Alphabet subsidiary DeepMind, placed a white piece in a position that surprised even the experts.

It turned out to be a stroke of genius that human players would have had trouble planning, and a key moment in a contest that resulted in the victory of machine over man.

People are limited in the range of possibilities they can perceive and analyse, forcing them to think inside "boxes", he says now. "We humans are innovative — we do get outside our boxes. But we can't do it at the rate that computers can."

A professor of radiology in Cleveland, Ohio, Mr Griswold has just had his own encounter with a computer that thinks outside the box. The machine in question: one programmed to simulate the behaviour of a quantum computer, a technology that could revolutionise computing.

Humans rely on a mix of experience and intuition when tackling a problem too complex for them to analyse completely, he says. In his case, that involves adjusting the settings on an MRI machine to get the best possible scan from any particular situation — something he compares with coaxing the best sound from a musical instrument.

After only a few weeks of experimenting with quantum technology, however, Mr Griswold says he has already seen a computer come up with MRI results that have exceeded those of his own expert "feel" — much as the DeepMind machine came up with the unexpected on the Go board.

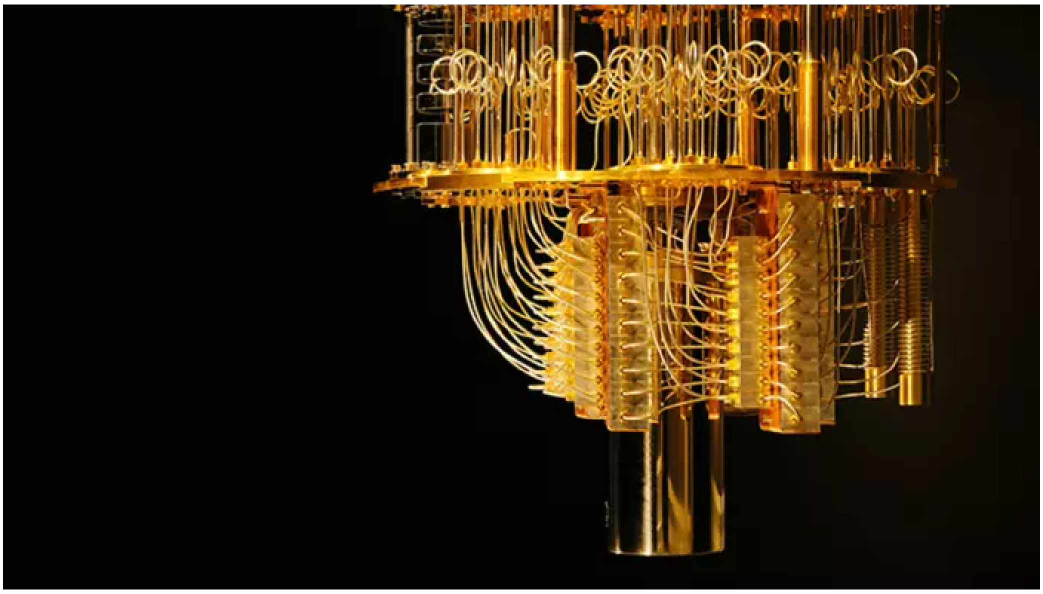
The IBM Q quantum computer, which can be accessed by companies via IBM's cloud operation © Connie Zhou/IBM

It is, he claims, an intimation of a new era, when quantum computers challenge much of what we think we know about the world: "We're going to see these things all the time, that are against our intuition. It's so overwhelming we can't understand it, we don't know how much power is there," says Mr Griswold.

Quantum machines, which tap into the weirdness of quantum mechanics — a branch of physics that deals with the behaviour of sub-atomic particles — are a long-held dream in the tech world. By harnessing properties that extend beyond the limits of classical Newtonian physics, they hold the promise of exponential gains in computing power.

After decades in the labs, the technology is starting to make the transition from science experiment to rudimentary prototype sparking interest in fields as diverse as chemicals and banking, and prompting research efforts at companies stretching from Samsung to Daimler-Benz and JPMorgan Chase.

"It takes as much as 30 years for this basic research to become viable — in the case of quantum computing, that time really has passed," says Mladen Vouk, a computer science professor at North Carolina State University. The result is that researchers at universities like NC State are now getting their first chance to try the technology out.



A dilution refrigeration unit used to supercool qubits so that they can function reliably © Graham Carlow/IBM

According to tech groups such as IBM and Microsoft, as well as specialist start-ups such as Rigetti Computing, the first real benefits from quantum computing could be seen within five to 10 years — a timeframe that raises tantalising possibilities for the companies that hope to be first to harness the technology.

JPMorgan Chase began committing some of its research effort to quantum computing two years ago. Asked if being one of the first in the field would bring clear advantages over rivals, Bob Stolte, a managing director at JPMorgan's corporate and investment bank, says: "I think there could be, potentially" — though he cautions: "It's too early to say that."

The results could far exceed even the most high-powered AI systems of today. Referring to the specialised chips, called graphics processing units, used in many of today's most advanced machine learning systems, Mr Stolte says: "If you weren't limited to the number of GPUs you can get in a data centre, what problems would you be able to solve, and what products would you be able to offer customers?"

Researchers trying to harness the power of the new hardware are homing in on three main types of problem that quantum machines are expected to be particularly well suited to handling.

The first involves analysing the natural world, using computers to model the behaviour of molecules with the kind of precision that today's computers could never match.

"Nature is quantum mechanical so, if you have a computer that worked on quantum principles, it would be mapping apples to apples," says Bob Sutor, a researcher at IBM. Compared to current computers, which have to make approximations when trying to model the behaviour of sub-atomic particles, quantum machines could do it precisely.

Ilyas Khan, chief executive of Cambridge Quantum Computing, a start-up that is designing applications for the technology, suggests that one of the first sectors to benefit will be the chemicals industry. The massive increase in computing power will enable the discovery of new materials, he says.

“Computational chemistry is the single biggest area right now. Over the past two years quantum computers have been increasingly valuable replacing guesswork with more and more empirical evidence,” he adds.

Traditional computers could never handle this kind of task. Modelling a relatively basic molecule such as caffeine would require a traditional computer with 10 to the power of 48 bits, says Mr Sutor — or about 10 per cent of the number of atoms in planet Earth. Penicillin, meanwhile, would require 10 to the power of 86 bits — more than all the atoms in the observable universe.

In the quantum realm, calculations like these suddenly become possible. In theory, a quantum computer with 160 quantum bits (or qubits) could model caffeine, according to Mr Sutor, while it would take 286 qubits to handle penicillin.

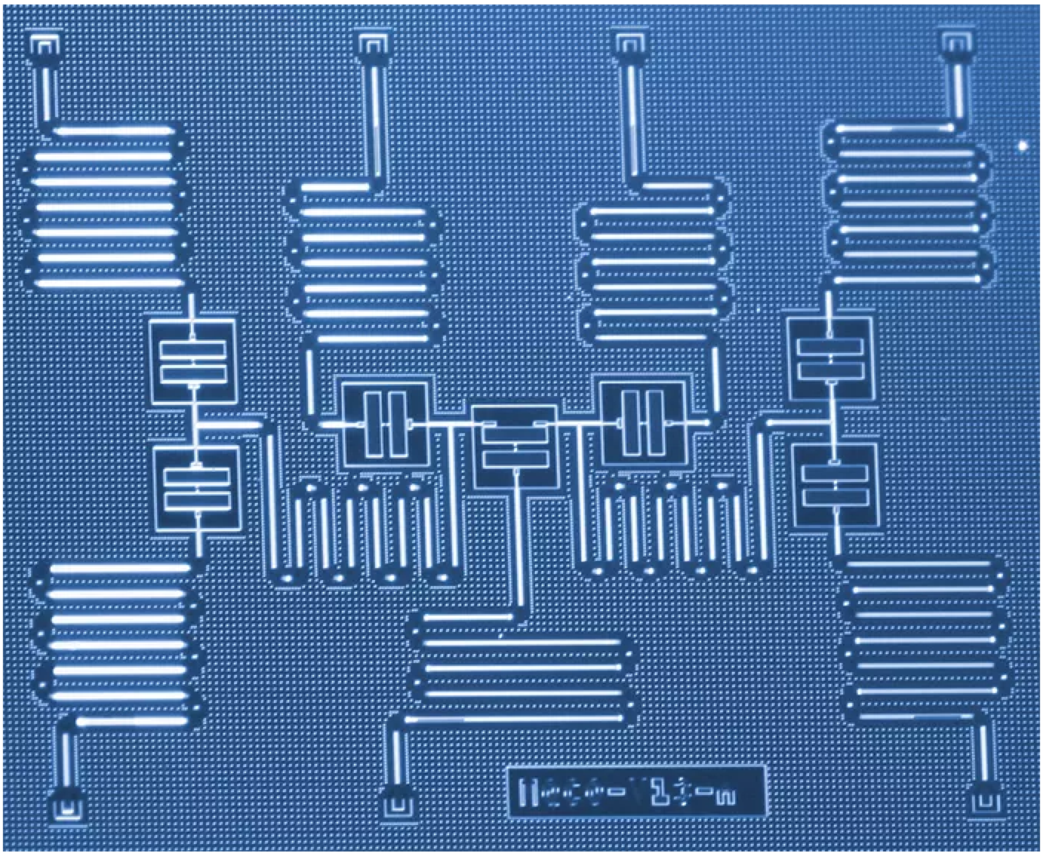
That could make it easier to design new materials, or find better ways for handling existing processes. Microsoft, for instance, predicts that it could lead to a more efficient way of capturing nitrogen from the atmosphere for use in fertilisers — a process known as nitrogen fixation, which currently eats up huge quantities of power.

At first glance, it might appear that the technology is advancing rapidly towards these levels. After stringing together the first basic systems out of a small number of qubits two years ago, companies such as IBM, Rigetti and Google are quickly moving on to computers comprising dozens of qubits.

The numbers, however, do not tell the full story.

Today’s qubits are unstable — they only hold their quantum state for a tiny fraction of a second — and, as increasing numbers are linked together, unpredictable interactions between them lead to high error rates. Learning how to coax results out of these “noisy” systems is already a huge challenge, and scaling them up to computers of 100 qubits is far beyond today’s capabilities.

Quantum computing: real world applications



A 7-qubit device that scientists used to simulate complex molecular reactions in 2017, showing how it could revolutionise materials science © Kandala et al/IBM

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The promise of being able to handle simple molecules is close enough, though, that chemicals companies have been among the first to start experimenting with the technology. They include JSR Corporation, the Japanese materials multinational, which has taken a 5.5 per cent stake in Cambridge Quantum Computing, and is also one of the first companies to work with IBM since the US computer company began trialling its version of the technology with a small number of companies late last year.

Pharmaceutical groups, which might see similar benefits from quantum technology in the long term, are still on the sidelines. “They are trying to understand when we’ll have sufficient qubits to handle the molecules they deal with,” says Mr Sutor, since these are far larger and more complex. He estimates that timeframe, “very broadly”, at five to 10 years.

Quantum computing is also expected to bring early benefits to machine learning. Rather than simply adding more raw computing power to speed up the training of today’s machine learning systems, the technology is well-suited to tackling particular problems that present a challenge for traditional computers, says Peter Wittek, an assistant professor at the University of Toronto.

“The real question is not so much speed-up, but whether they can give you a qualitative advantage with certain models,” he says.

Quantum machines are particularly well suited to certain types of probabilistic algorithms, he and other experts say — calculations that don’t proceed through a logical sequence of steps, like those carried out by today’s so-called “classical” computers, but instead rely on a certain element of chance to alight on the best result.

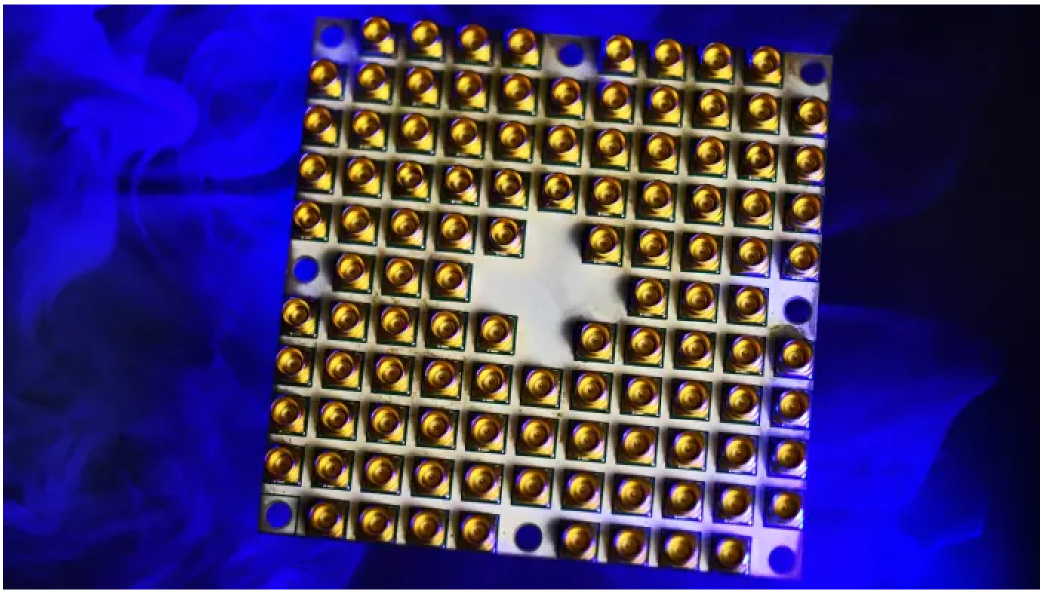
A third area of focus involves complex optimisation problems that have too many variables for today’s computers. This is the case with Mr Griswold’s MRI machines. Using a technique known as quantum annealing, optimisation problems are turned into the equivalent of a 3D landscape, comprising mountains and valleys: the challenge is to find which point is the lowest.

Though each of these classes of quantum calculation seems narrow, together they could cover a range of real-world problems, making the technology more broadly applicable in its early years than might at first seem apparent. The new systems should be able to tackle any difficult mathematical problems that can be translated into a form that the specialised quantum algorithms can handle, says Mr Sutor.

“The future quants” on Wall Street for instance will “map financial problems to similar problems in physics and then map them back”, he says.

That helps explain why a handful of banks have been among the first to dip their toes into the water.

Lee Braine, from the Investment Bank CTO office at Barclays, says that the bank is already actively investigating potential uses for quantum computing. He suggests the technology is in a similar place to where blockchain, which many banks are looking to exploit, was 10 years ago.



A 49-qubit test chip built by Intel and unveiled at this year's Consumer Electronics Show in Las Vegas © Walden Kirsch/Intel Corporation

He predicts its first uses for the bank will be to build ever better models of financial markets, strengthen cryptography by inventing new numbers, and improve operational efficiencies in messy and complicated areas, such as clearing and reconciliation of trades. “We are playing at toy solutions at the moment,” he says.

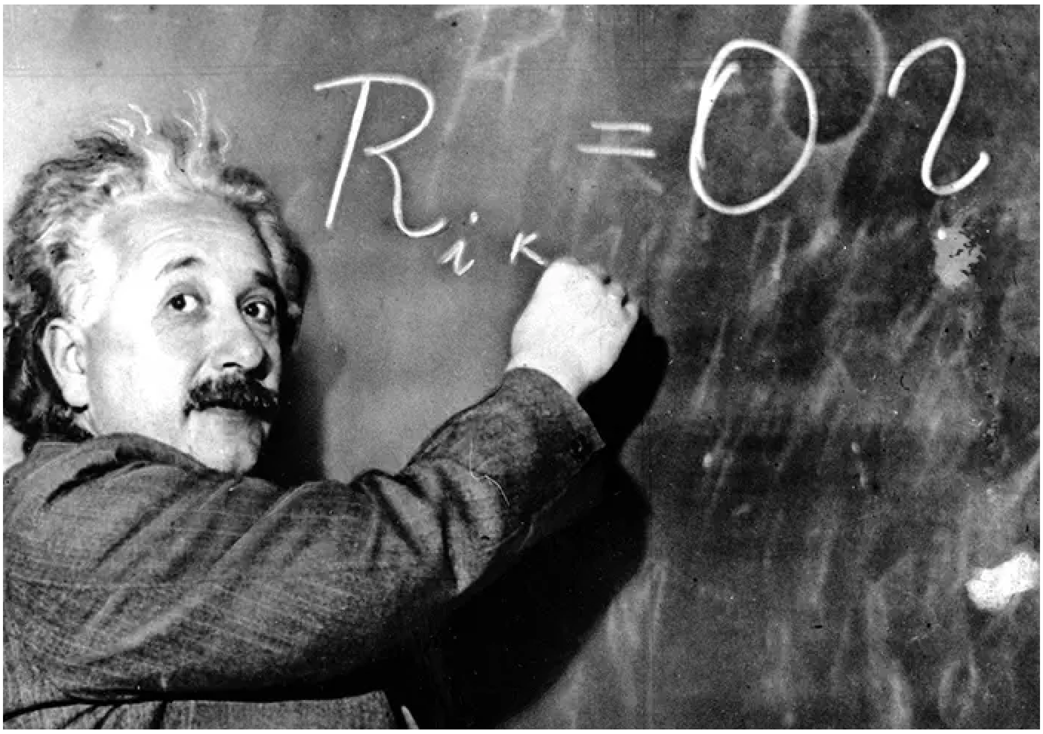
Mr Stolte adds that pricing derivatives, optimising investment portfolios and managing risk in highly complex and constantly shifting situations are all things that quantum systems could handle.

“When you look at what financial services is, and quantum computing promises — which is essentially a significant increase in the availability of processing power for probabilistic algorithms — that matches really well,” he says.

Yet the technology is in its infancy, and the entirely new field of computer science needed to harness the power of the machines has yet to be developed. Alex McCaskey, a researcher at the US energy department’s Oak Ridge National Laboratory, compares the current state of the art to the first efforts to program classical computers in the 1950s and early 1960s — though he adds that “the field is moving very fast”.

“It’s not as universal as classical computing,” he adds, echoing a cautious view held by others in the field. “Personally I think this will be a technology that will be available for very specific problems.”

Qubits v bytes: how quantum computing works



Albert Einstein

Quantum computing taps into the quirky behaviour of sub-atomic particles, which bend our normal understanding of physics.

One of these properties, called **superposition**, involves a particle being in two states at the same time. So unlike the most basic binary elements, or bits, in a classical computer, which represent either ones and zeros, quantum bits — or qubits — can be a 1 and a zero at the same time.

By stringing together dozens or even hundreds of these qubits, the number of states they could represent would rise exponentially, making it possible to compute millions of possibilities instantly.

A second quantum property these machines draw on is **entanglement**: two quantum bits can influence each other, even when they aren't physically connected, something Albert Einstein called "spooky action at a distance".

In theory, by harnessing this property, it will be possible to write algorithms that take short-cuts around the usual sequential logic processes in computers, making it possible to rule out incorrect answers and home in on the correct ones far more quickly.

Harnessing this computing power will require an entirely new form of programming.

"The way you think about algorithms is wildly and completely different," says Bob Sutor of IBM. Unlike "classical" computing, where each step in a calculation follows logically from the one before it, quantum programming is "much more three-dimensional", he says. "There are very unusual correlations and linkages between qubits." As a result, "you can figure out solutions that don't work, and things that could solve the problem are magnified."

Letter in response to this report:

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