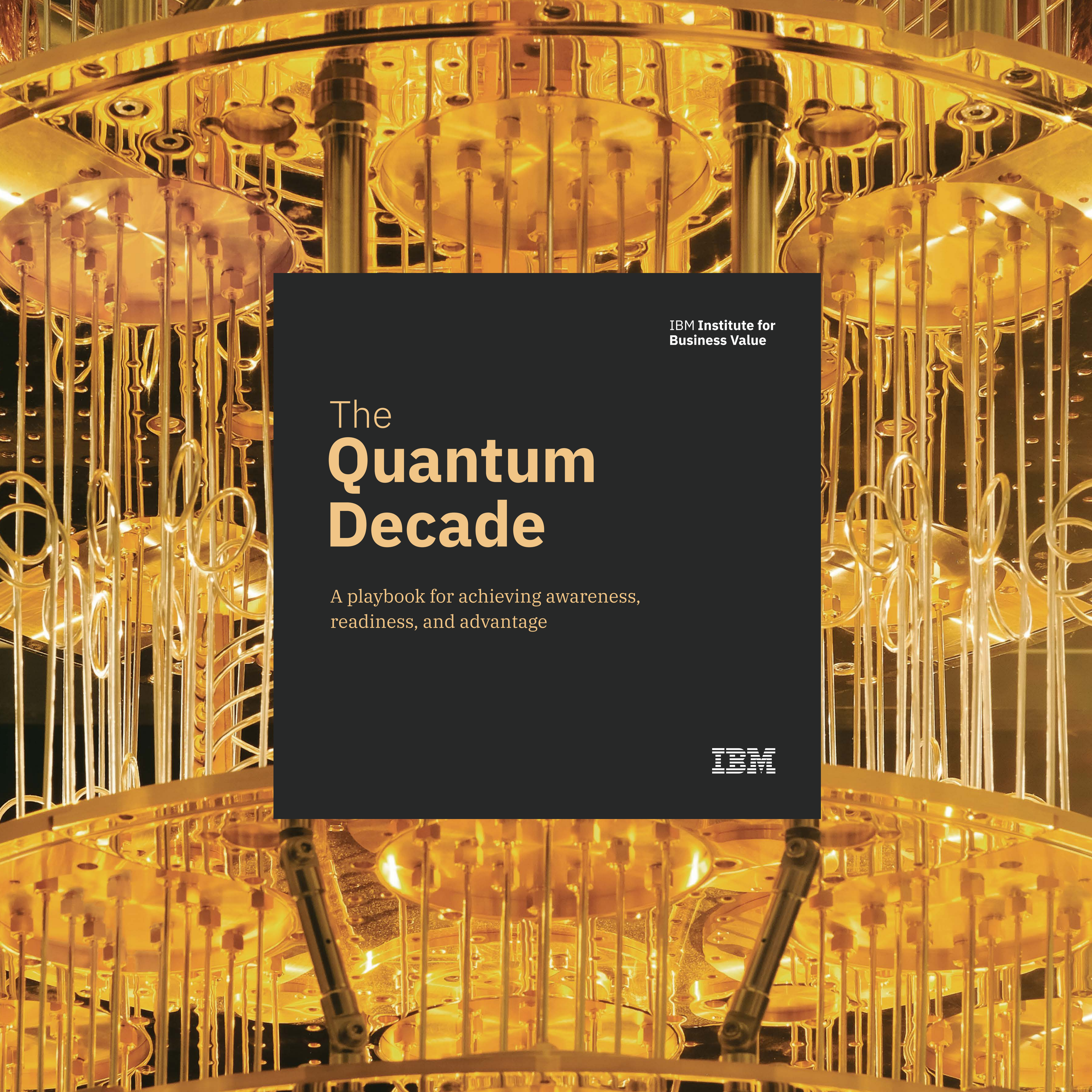

IBM **Institute for Business Value**

The **Quantum Decade**

A playbook for achieving awareness, readiness, and advantage

IBM

How IBM can help

Partnerships in quantum computing between technology providers and visionary organizations are expanding. Their aim is nothing short of developing quantum computing use cases and corresponding applications that solve previously intractable real-world problems. The IBM Quantum Network is a global ecosystem of over 140 Fortune 500 companies, leading academic institutions, startups, and national research labs, enabled by IBM's quantum computers, scientists, engineers, and consultants. Participants collaborate to accelerate advancements in quantum computing that can produce early commercial applications. Organizations that join the IBM Quantum Network can experiment with how their high-value problems map to a real quantum computer. Today, they can access over 20 quantum computing systems, including a 65-qubit IBM Quantum processor via the IBM Cloud. By 2023, we expect a 1,000-qubit quantum computer will be available to explore practical problems important to industries. Visit https://www.ibm.com/quantum-computing/ for more information.

IBM Institute for Business Value

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The Quantum Decade

A playbook for achieving awareness, readiness, and advantage

An IBM Quantum engineer works on the “super-fridge”—a 12-foot-high dilution refrigerator designed and built by IBM Quantum to house quantum systems of 1000+ qubits at a temperature close to absolute zero.

The Quantum Decade

Contents

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The Quantum Decade

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The Quantum Decade
Perspectives from across the field

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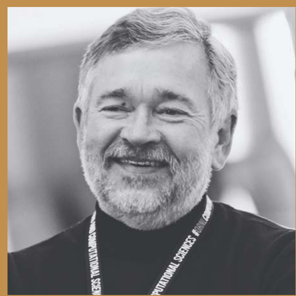

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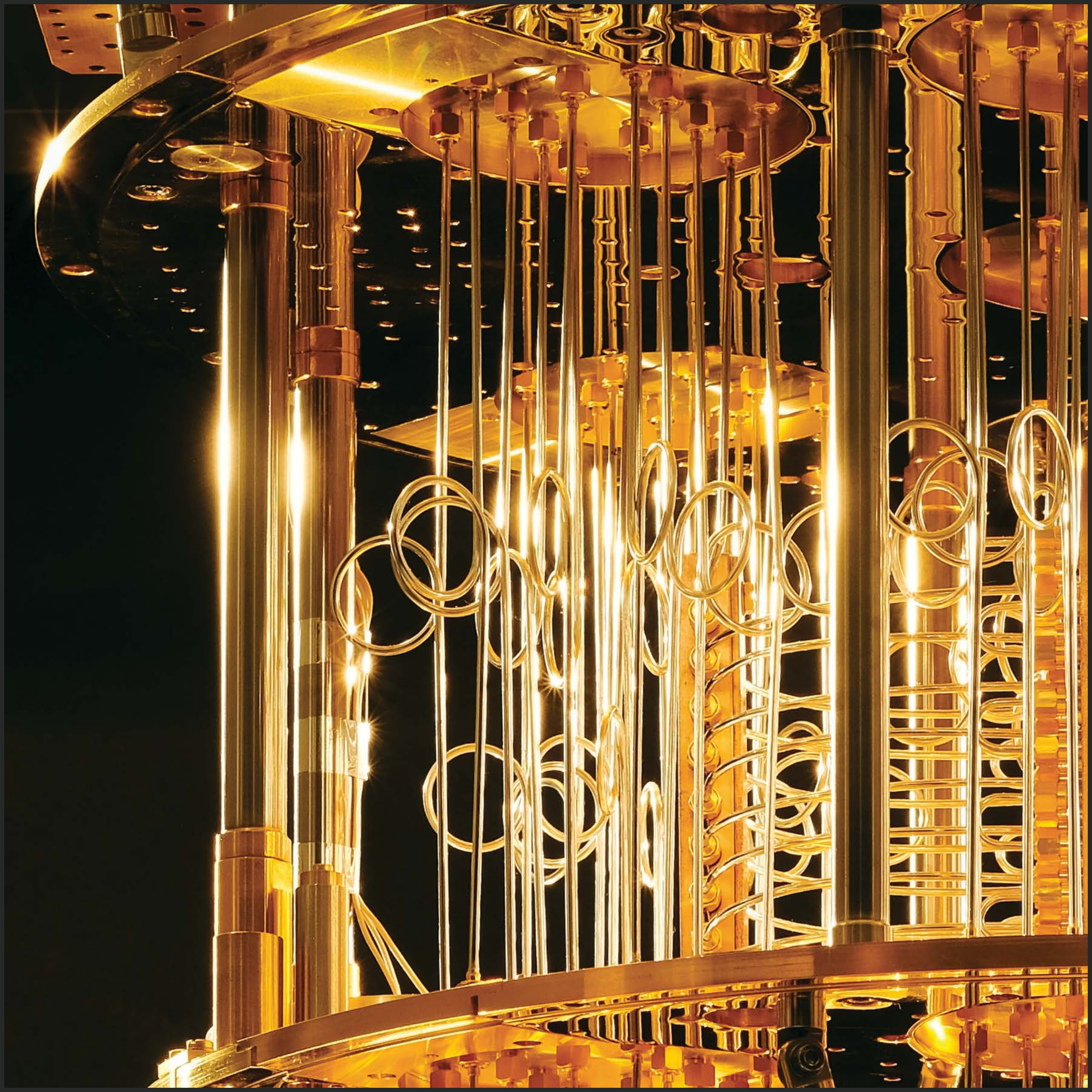


The internal quantum computing components are held at temperatures close to absolute zero. The microwave control lines contain loops to allow for contraction as the device cools down.

Darío Gil

Senior Vice President and Director of IBM Research

Foreword

First, there was theory.

Charlie Bennett first wrote the words "quantum information theory" in his notebook in 1971. Paul Benioff, Richard Feynman, Yuri Manin, and other quantum computing pioneers of the early 1980s used math and theoretical quantum mechanics to argue their case. Their message was clear: to accelerate progress, we had to simulate nature. We had to mimic the weird behavior of atoms and build a quantum computer.

Then came qubits. Just like that, with the first two-qubit quantum computer built in 1998, theory morphed into reality. Qubits are the building blocks of a quantum computer, and today at IBM we make them out of tiny superconducting circuits that behave like atoms. They can be in multiple states at once, can interfere and be entangled—so that when one qubit changes its state, its entangled partner does, too.

Sounds mind-boggling, and it is.

It's the weird but wonderful realm of the small, and we've managed to reproduce its powers. Because it's these odd abilities of qubits to be in multiple states at once, entangle, and interfere that should allow future quantum computers to perform more powerful computations than a traditional classical computer ever could.

We are nearly there. We are living in the Quantum Decade, when quantum computers are getting ready to overperform their classical cousins in a meaningful task, achieving what we call Quantum Advantage. Our qubits are becoming ever more stable, able to stay in their quantum world for longer, and allowing us to run ever more complex computations. For years now, researchers and developers across industry and academia have used IBM's quantum computers through the cloud to create new algorithms that will be crucial in the future. They are getting quantum-ready.

I urge others to join them, too.

By tinkering with quantum computers today, we are shaping the world of tomorrow. Whether you are a bank, a pharmaceutical company, an airline, or a manufacturing giant, quantum computation could give you an edge. Tiny qubits will zip through a myriad of possibilities to find you the best molecular configuration for a new material or a drug, accurately predict your financial risk, or choose the optimal way of shipping your goods from Melbourne to Atlanta.

Read *The Quantum Decade* to find out how you, too, can be quantum-ready—and how this bleeding-edge technology can help you and your business thrive the moment quantum computers come of age.

Because that moment is closer than you think.

The "ceiling" of the "super-fridge" as viewed when standing inside it and looking up

Insights

Priorities of a post-pandemic world

As entire industries face greater uncertainty, business models are becoming more sensitive to and dependent on new technologies. Quantum computing is poised to expand the scope and complexity of business problems we can solve.

The future of computing

The integration of quantum computing, AI, and classical computing into hybrid multicloud workflows will drive the most significant computing revolution in 60 years. Quantum-powered workflows will radically reshape how enterprises work.

The discovery-driven enterprise

Enterprises will evolve from analyzing data to discovering new ways to solve problems. When combined with hyper-automation and open integration, this will ultimately lead to new business models.

The Quantum Decade

Introduction

For decades, quantum computing has been viewed as a futuristic technology: it would change everything, if it ever moved from the fantastical to the practical. Even in recent years, despite billions of dollars in research investment and extensive media coverage, the field is sometimes dismissed by real-life decision makers as too arcane, a far-off, far-out pursuit for academics and theorists. As we enter the Quantum Decade—the decade when enterprises begin to see business value from quantum computing—that perspective is quickly becoming an anachronism.

Because quantum computing is coming of age, and leaders who do not understand and adapt to the Quantum Decade could find themselves a step—or more accurately, years—behind. Over the next few years, we foresee a profound computing revolution that could significantly disrupt established business models and redefine entire industries. Historically, crises have been the impetus for both new technologies and their widespread adoption. World War I ushered in factory processes that are still in place today. The Cold War accelerated the creation of the Advanced Research Projects Agency Network (ARPANET), a predecessor to the internet, in the late 1960s. And now COVID-19 has driven an increased need for agility, resiliency, and accelerated digital maturity. We anticipate quantum computing—in combination with existing advanced technologies—will dramatically impact how science and business evolve. By accelerating the discovery of solutions to big global challenges, quantum computing could unleash positive disruptions significantly more abrupt than technology waves of the past decades.

Perspective
The basics

Understanding the exponential power of quantum computing

Classical computer bits can store information as either a 0 or 1. That the physical world maintains a fixed structure is in keeping with classical mechanics. But as scientists were able to explore subatomic matter, they began to see more probabilistic states: that matter took on many possible features in different conditions. The field of quantum physics emerged to explore and understand that phenomena.

The power of quantum computing rests on two cornerstones of quantum mechanics: interference and entanglement. The principle of interference allows a quantum computer to cancel unwanted solutions and enhance correct solutions. Entanglement means the combined state of the qubits contains more information than the qubits do independently. Together, these two principles have no classical analogy and modeling them on a classical computer would require exponential resources. For example, as the table below describes, representing the complexity of a 100-qubit quantum computer would require more classical bits than there are atoms on the planet Earth.

Qubits	2	3	10	16	20	30	35	100	280
Classical bits required to represent an entangled state	512 bits	1,024 bits	16 kilobytes	1 megabytes	17 megabytes	17 gigabytes	550 gigabytes	more than all the atoms on the planet Earth	more than all the atoms in the universe

To the nth degree
The power of exponential growth

“The time between the first Industrial Revolution and the second was around 80 years, and from the second to the third around 90 years. But the time between the third and the fourth was reduced to about 45 years thanks to disruptions enabled by semiconductors such as the Internet of Things (IoT), artificial intelligence (AI), machine learning, virtual reality, and 4G. I expect the time to Industry 5.0 will be further accelerated to roughly 30 years by quantum computing and many additional disruptions.”

Ajit Manocha
President and CEO
SEMI

The building blocks of quantum computing are already emerging. Quantum computing systems are running on the cloud at an unprecedented scale, compilers and algorithms are rapidly advancing, communities of quantum-proficient talent are on the rise, and leading hardware and software providers are publishing technology roadmaps. The technology's applicability is no longer a theory but a reality to be understood, strategized about, and planned for. And good news: the steps you should take to prepare for future quantum adoption will begin to benefit your business *now*.

Quantum computing will not replace classical computing, it will extend and complement it. But even for the problems that quantum computers can solve better, we will still need classical computers. Because data input and output will continue to be classical, quantum computers and quantum programs will require a combination of classical and quantum processing.

It is precisely the advances in traditional classical computing, plus advances in AI, that are driving the most important revolution in computing since Moore’s Law almost 60 years ago.[1] Quantum computing completes a trinity of technologies: the intersection of classical bits, qubits, and AI “neurons.” The synergies created by this triad—not quantum computing alone—are driving the future of computing (see Figure 1).

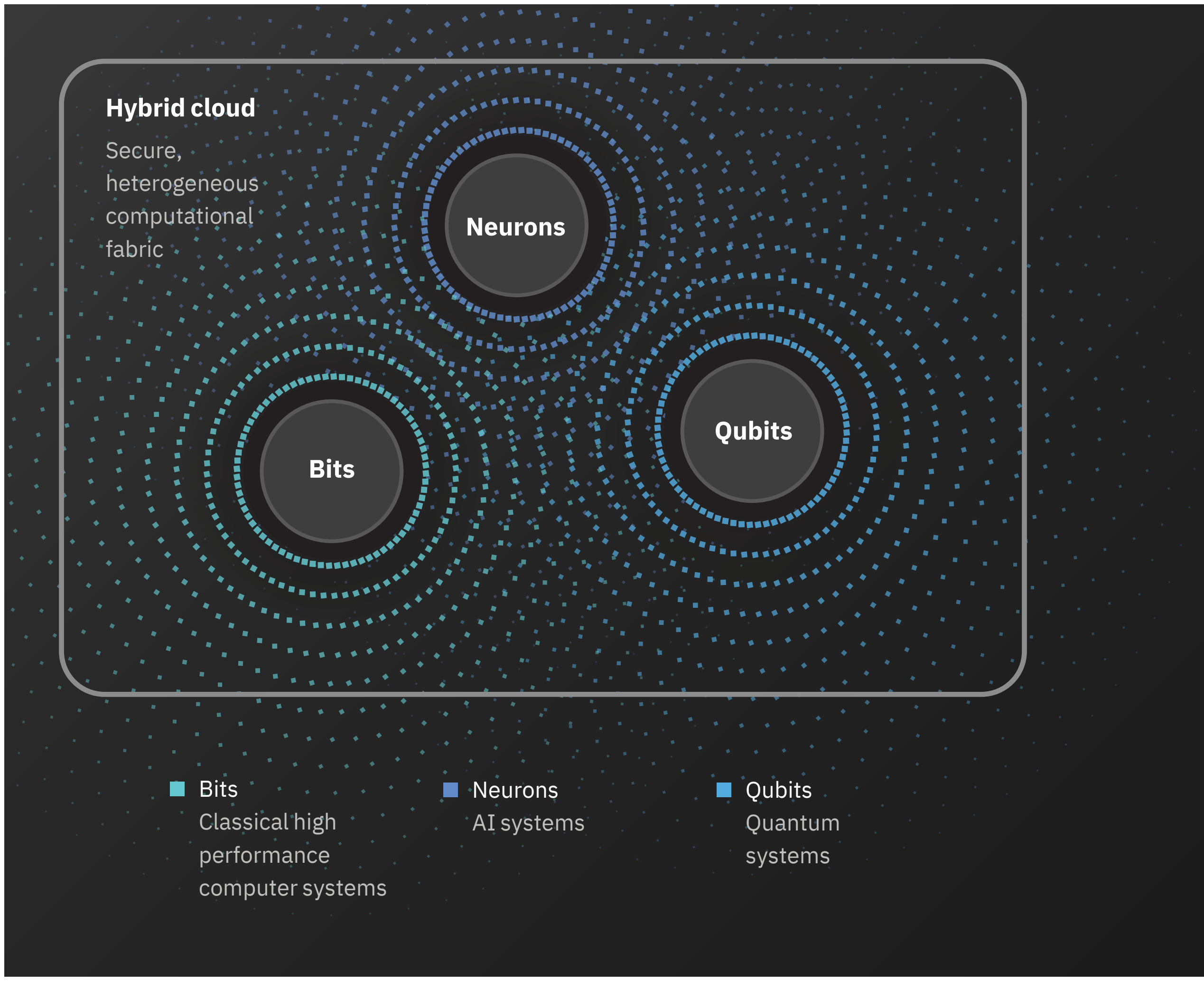


Figure 1

The most exciting computing revolution in 60 years
The convergence of three major technologies

The IBM Institute for Business Value (IBV) has been deeply engaged in conducting more than a dozen industry- and practice-based studies on quantum computing.[2] We've elevated that research here with new insights gleaned from interviews with more than 50 experts, including IBM quantum computing researchers as well as clients, partners, and academics. This report on the Quantum Decade provides executives with strategies to prepare for the upcoming business transformation from quantum computing. It identifies the most important factors, themes, and actions to take at this significant inflection point.

What makes this the Quantum Decade? What will the quantum-powered world look like? And what can and should farsighted leaders and organizations do now to educate and position themselves effectively? The key learnings revolve around three phases of organizational evolution: awareness, readiness, and advantage (see Figure 2).

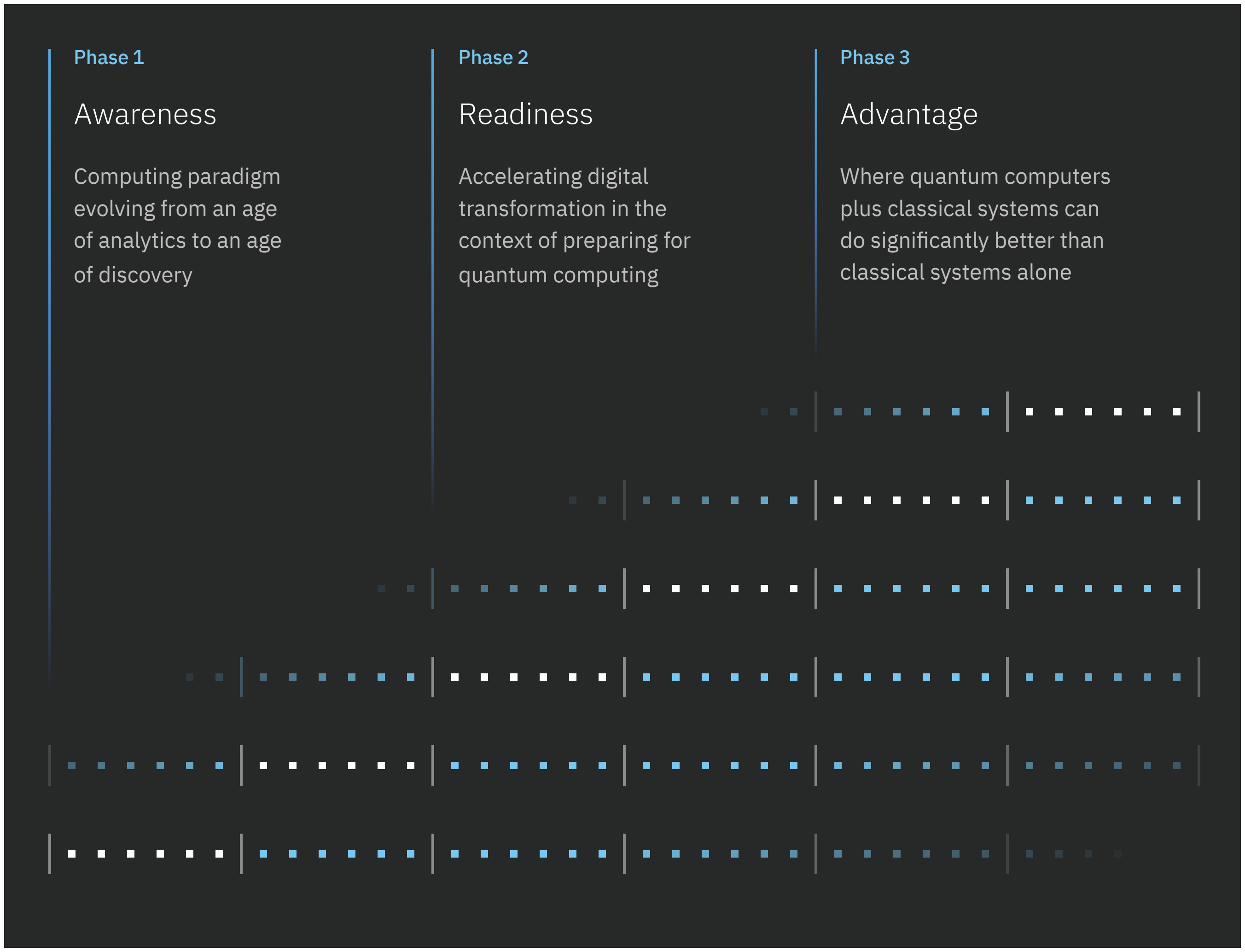


Figure 2

The path to Quantum Advantage

Taking a foundational approach with digital transformation

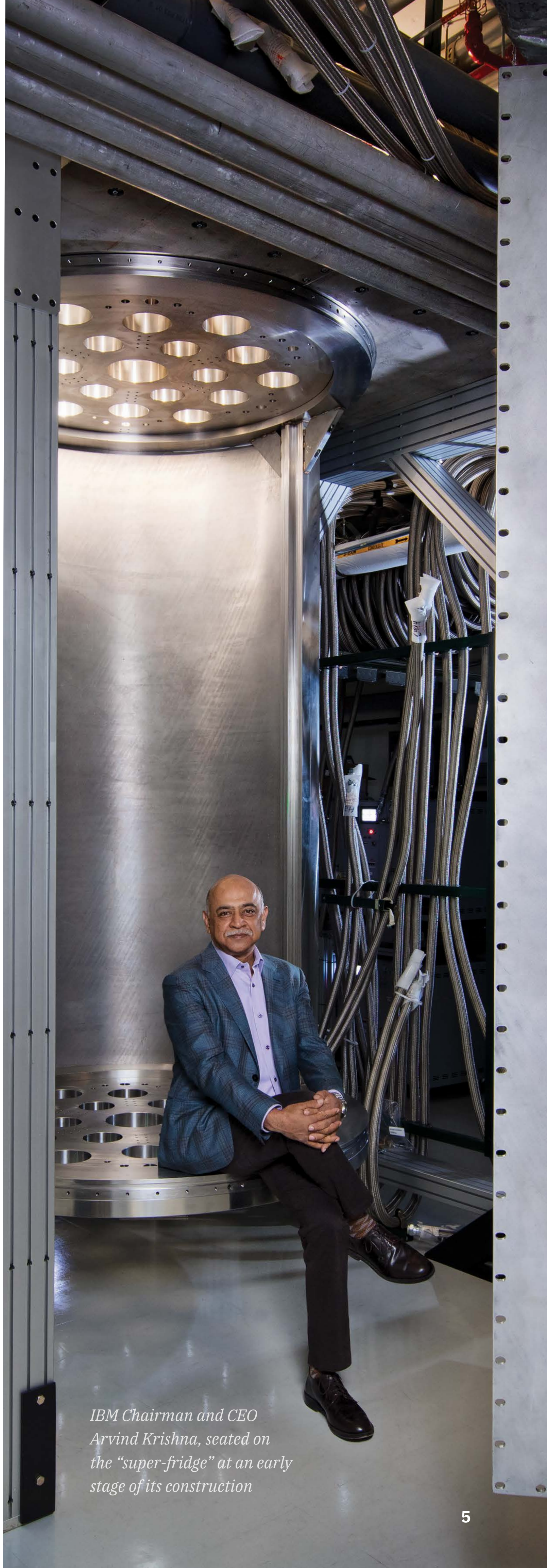
Awareness

According to the IBV's 2021 CEO study, 89% of the more than 3,000 chief executives surveyed *did not* cite quantum computing as a key technology for delivering business results over the next two to three years.[3] For the short term, that's understandable. But quantum computing with 1,000 qubits is projected to be available as early as 2023—just a few years away.[4] Given the technology's disruptive potential this decade, CEOs should start mobilizing resources to grasp early learnings and start the journey to quantum now. CEOs who ignore quantum's potential are taking a substantial risk, as the consequences will be much greater than missing the AI opportunity a decade ago.[5]

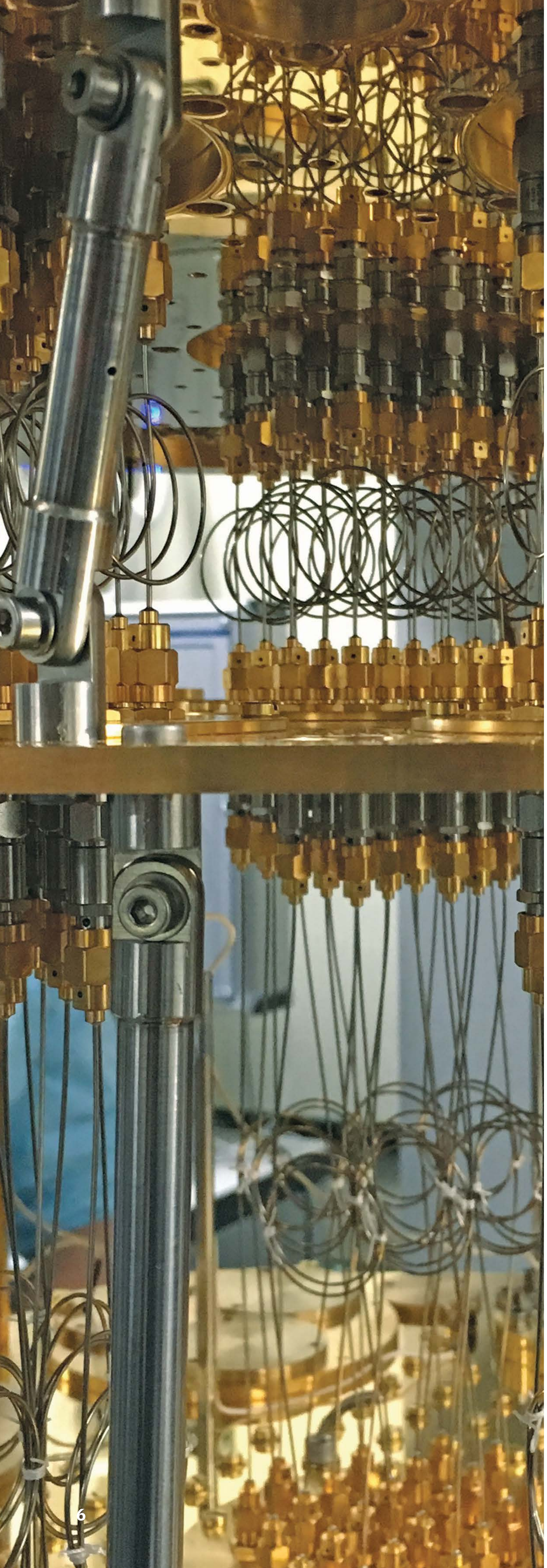
Phase 1 of the quantum computing playbook requires broad recognition that the landscape is changing. The primary shift is a computing paradigm that's evolving from an age of analytics (looking back at established data and learning from it) to an age of discovery (looking forward and creating more accurate models for simulation, forecasting, and optimization). There's real potential for uncovering solutions that were previously impossible.

"CEOs of Fortune 500 companies have a once-in-a-lifetime opportunity. They cannot afford to play catch-up. It's time to break tradition and educate themselves about what quantum computing can do for them."

Ilyas Khan
Founder and CEO
Cambridge Quantum Computing



IBM Chairman and CEO Arvind Krishna, seated on the "super-fridge" at an early stage of its construction



Readiness

Enterprises cannot use quantum computing to solve big problems yet. But quantum computing has shattered timelines and exceeded expectations at every phase of development. It's not too soon for organizational leaders to explore how the advent of this new technology could alter plans and expectations. Phase 2 involves investigating big questions: How could your business model be disrupted and reshaped? How could quantum computing supercharge your current AI and classical computing workflows? What is the quantum computing "killer app" for your industry? How can you deepen your organization's quantum computing capabilities, either internally or through ecosystems? Now is the time to experiment and iterate with scenario planning. Find or nurture talent who is fluent in quantum computing and capable of educating internal stakeholders about the possibilities, and partner for "deep tech" quantum computing resources.

But just as important is another critical question: What does your organization need to establish now to apply quantum computing when it's production-ready? Indeed, laying the foundation for quantum computing also means upping your classical computing game. Enhanced proficiencies in data, AI, and cloud are necessary to provide the required fertile ground for quantum computing. Accelerating your digital transformation in the context of quantum computing readiness will provide a pragmatic path forward while delivering significant benefits now. After all, quantum computing doesn't vanquish classical computing. The trinity of quantum computing, classical computing, and AI form a progressive, iterative partnership in which they're more powerful together than separately.

"When people think of quantum computing now, they think of researchers trying to figure out how to apply quantum computing. Ten years from now, those questions will be answered. At that point, it will be about whether you are using quantum computing in ways others are not."

Prineha Narang
Assistant Professor of Computational Materials Science
Harvard University

"There is a huge competition in the 'big problem' space in the energy industry. Whoever gets there first will have a significant advantage."

Doug Kushnerick
formerly with Technology Scouting and Ventures
ExxonMobil Research and Engineering

Advantage

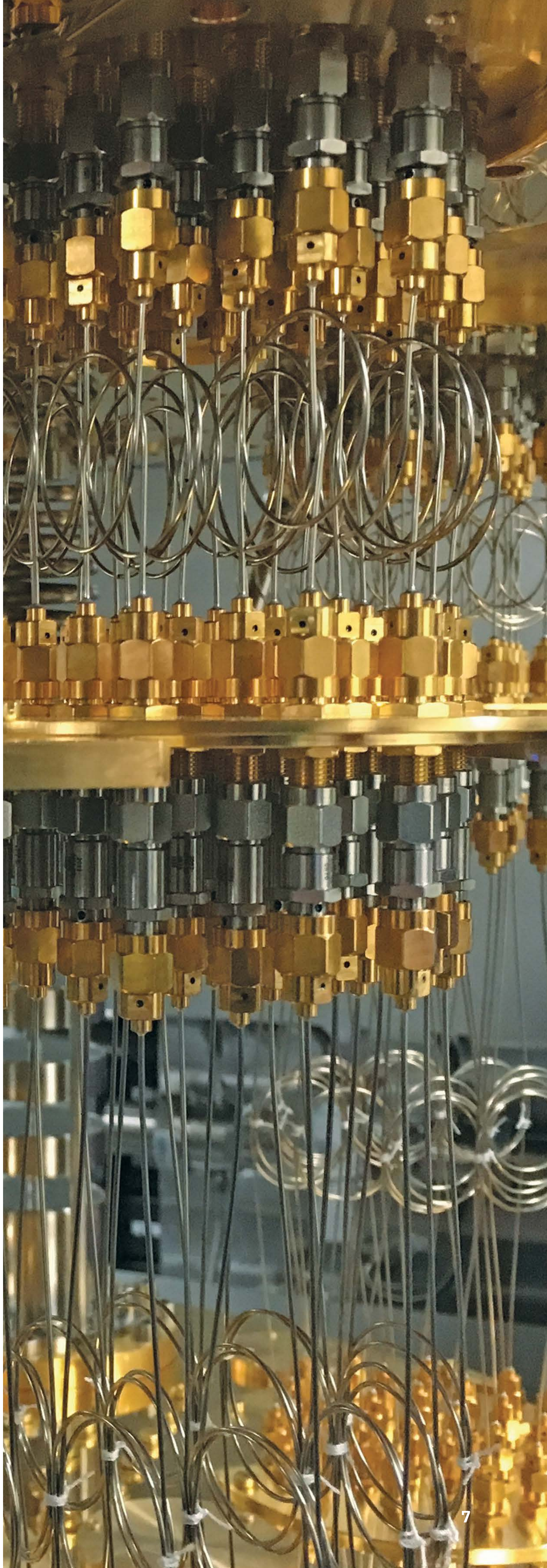
Phase 3, Quantum Advantage, occurs when a computing task of interest to business or science can be performed more efficiently, more cost effectively, or with better quality using quantum computers. This is the point where quantum computers plus classical systems can do significantly better than classical systems alone. As hardware, software, and algorithmic advancements in quantum computing coalesce, enabling significant performance improvement over classical computing, new opportunities for advantage will emerge across industries. But prioritizing the *right* use cases—those that can truly *transform* an organization or an industry—is critical to attaining business value from quantum.

Getting to Quantum Advantage will not happen overnight. But while that advantage may progress over months and years, it can still trigger exponential achievements in usage and learning. From exploring the creation of new materials to personalized medical treatments to radical shifts in business models across the economy, change is coming. Organizations that enhance their classical computing capabilities and aggressively explore the potential for industry transformation will be best positioned to seize Quantum Advantage.

"The best of quantum computing is yet to come. There are applications where we presume Quantum Advantage will play out. And there is a vaster space of quantum computing applications that we don't know yet. That's what will redefine what's possible."

Irfan Siddiqi
Director of the Advanced Quantum Testbed
Lawrence Berkeley National Laboratory

Professor of Physics
University of California, Berkeley



IBM Quantum System One—one of the world's most powerful commercially available quantum computers

Insights

Tackling the world's problems

From discovering new drugs to managing financial risk to re-engineering supply chains, there is an urgency to accelerate solutions to increasingly complex societal, macroeconomic, and environmental problems on a global scale.

The 1,000-qubit milestone

Quantum computing hardware is on a trajectory to scale from 127 qubits in 2021 to 1,000 qubits by 2023 to practical quantum computing, characterized by systems executing error-corrected circuits and widespread adoption, by 2030. Cloud-based open-source development environments will make using quantum computers "frictionless."

The hybrid multicloud future

Many quantum programs involve interactions between classical and quantum hardware. But these interactions introduce latencies, or delays, which must be reduced to optimize capacity. This makes hybrid multiclouds the most viable future for quantum computing.

The power of ecosystems

Quantum computing ecosystems—with opportunities for collaborative innovation and open-source development—are fast becoming fertile grounds for training users to apply quantum computing to real problems.

Chapter One

Quantum awareness and the age of discovery

When new technologies emerge, they can be daunting to comprehend fully—especially when they're as complex as quantum computing. But developing a base understanding is critical for appropriately aligning both technology and business strategy.

In this chapter, we explain the case for quantum computing—what is happening now to create an inflection point—and then explore how the triad of classical computing, AI, and quantum computing will move us from an age of analytics driven by mining data for insights to one defined by accelerated experimentation and discovery. We also outline the implications for enterprises in a discovery-driven environment.

The case for the Quantum Decade

The Quantum Decade will be driven by mounting pressure to solve the biggest business and societal computational problems, a trajectory toward 1,000 qubits by 2023 and practical quantum computing by decade's end, and ecosystems of developers that can unleash this power onto real, intractable problems (see Figure 3).

An increased urgency to solve big problems

Imagine discovering new materials for solar panels that help us obtain clean energy more efficiently. Or accurately simulating aircraft parts in minutes as opposed to years. Envision drug development that can sometimes grind on for a decade coming to fruition in months.

Increasingly, these problems fall into ambitious, industry-altering, data-driven science. In this realm, enterprise discovery builds on data and AI, accelerating cycles of exploration that allow organizations to aggregate knowledge, resolve questions, and enhance operations and offerings.[6]

Planetary-scale issues such as climate change, world hunger, and the possibility of more pandemics require powerful new tools to achieve breakthroughs. Quantum computing can help expedite solutions to these complex computational problems that face business and society.

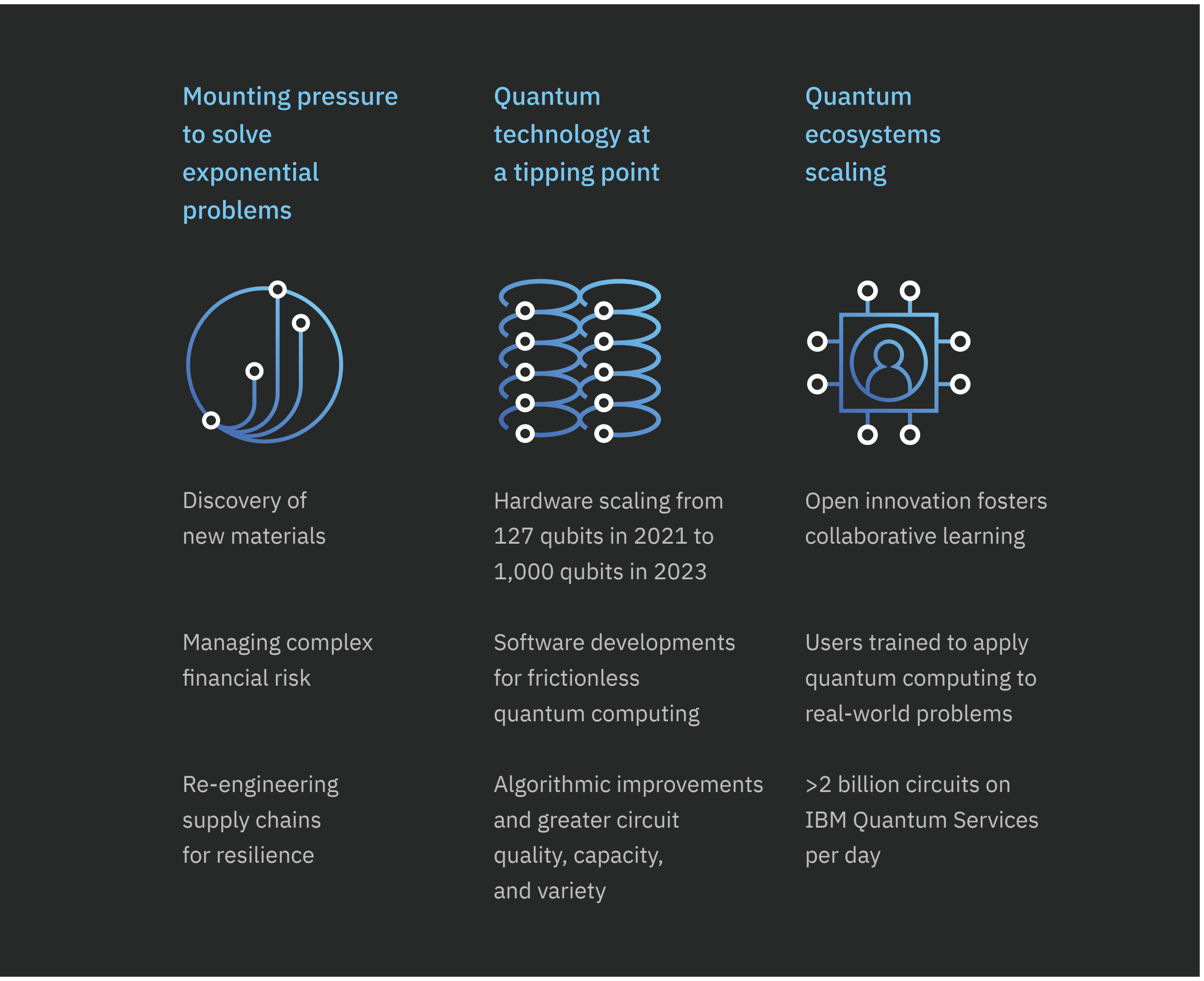


Figure 3

What makes this the Quantum Decade?

Three factors propelling us forward

"We must apply quantum computing to improve human life. The next generation needs to benefit from quantum computing."

Ching-Ray Chang
Distinguished Professor
Department of Physics
National Taiwan University

The information we need for significant breakthroughs on global problems may exist—but we lack the computing power to harness and use it productively. To understand why requires some background. Classical computing has long enabled an age of analytics. Existing systems rely on storing and manipulating individual computing bits—saved in binary form as either 1s or 0s—that help us process vast volumes of data. Quantum computers work in a fundamentally different way via so-called quantum bits or qubits, which can represent information using more dimensions (see Perspective, "Head-spinning facts about quantum computing" on page 15). Exploiting the properties of quantum mechanics, quantum computers excel at the challenge of evaluating multitudes of options that lend themselves well to these properties—and exploring problems that have thus far been intractable.

The quantum tipping point

Quantum computing is not new. It's been the subject of theories and experiments since it was first postulated by Paul Benioff, Richard Feynman, and others in the early 1980s.[7] During the 1990s, preliminary mathematical and algorithmic work took place; the 2000s focused on physically representing qubits; and in the 2010s, multi-qubit systems were demonstrated to be viable, as well as accessible on the cloud (see Figure 4).

Figure 4

A quantum leap
Historic milestones in quantum computing

1970
Birth of quantum information theory

1980
Paul Benioff's quantum mechanical model of computers

1984
Quantum cryptography (IBM)

1994
Shor's factoring algorithm

1995
Quantum error correction

2001
Experimentally factoring 15 (IBM)

2007
The transmon superconducting qubit

2016
IBM makes quantum computing available on IBM Cloud

2017
Quantum demonstrations 0(10) qubits

Quantum applications using hardware-efficient quantum circuits (IBM)

Quantum error mitigation developed (IBM)

Provable quantum advantage with short-depth circuits (IBM)

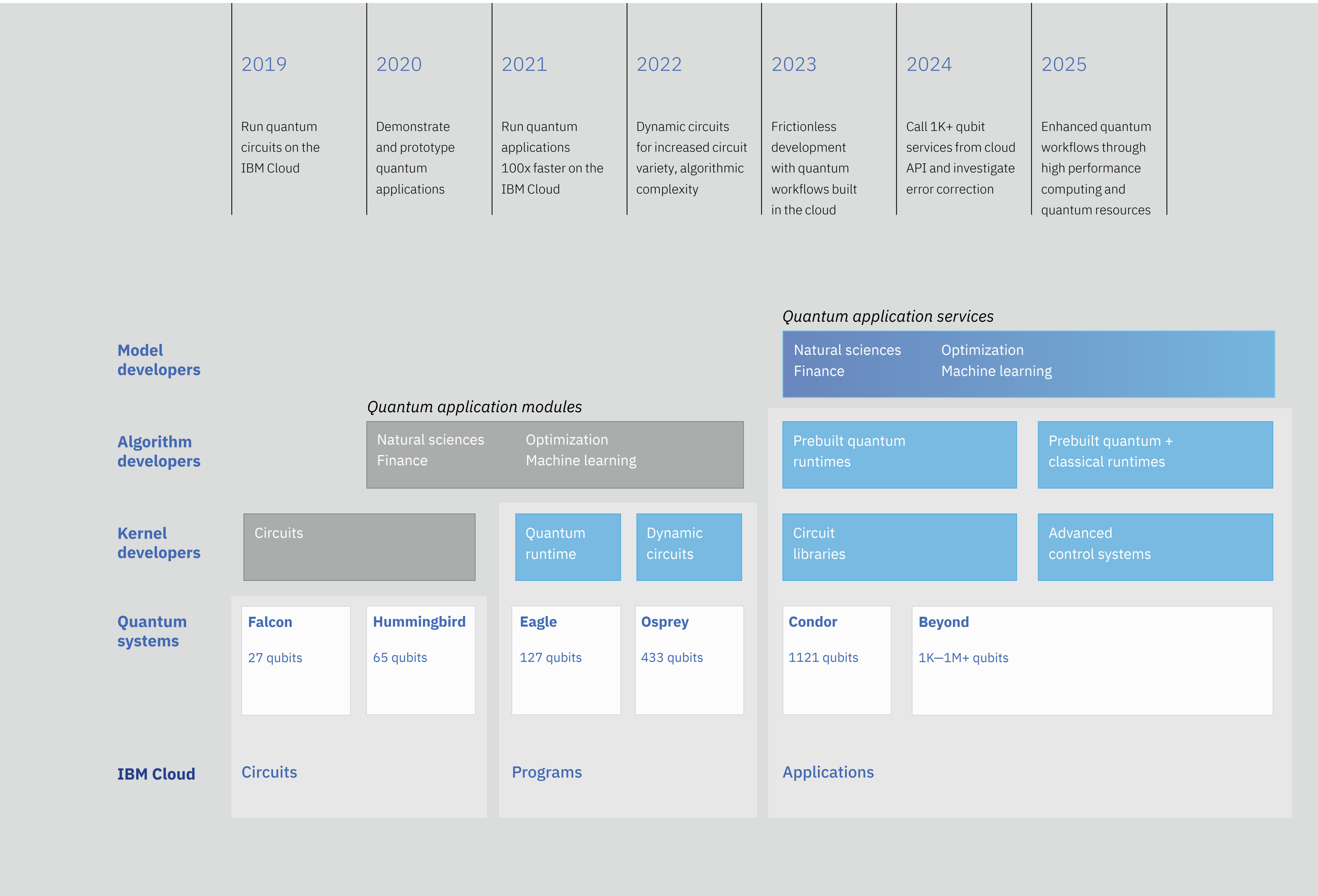


Figure 5

The IBM quantum computing roadmap

Recent progress and looking ahead

So what's happening now? The advance of quantum computing has reached a tipping point. In 2020, the state of the art in quantum computing was an IBM system with 65 qubits. That's expected to nearly double in 2021, triple to more than 400 qubits in 2022, and more than double again to over 1,000 qubits by 2023. Beyond increasing the raw number of qubits, more efficient and denser controls and cryogenic infrastructure will help improve the performance of individual qubits, while limiting noise and footprint. Quantum scientists and engineers will also introduce error correction and mitigation techniques that can increase the variety of problems that can be tackled with quantum computers (see Figure 5).[8]

There are several approaches to creating qubits, such as superconductivity, photons, and trapped ions, each with their respective characteristics and scaling abilities. Qubits are often used as a milestone, but they don't tell the whole story—they're just one component of the bigger picture. For example, the concept of quantum circuits is critical. Similar to a circuit in classical computer science, a quantum circuit represents the set of operations performed on qubits in time.

Three key attributes are required to create quantum computers that can be used productively to solve problems of business value: *quality, capacity,* and *variety.* In 2019, IBM developed the Quantum Volume (QV) metric to measure the computational power of a quantum computer. QV addresses highly technical issues, including gate and measurement errors, crosstalk, device connectivity, and compiler efficiency. Other vendors are starting to report their progress on computational *quality* using QV.

IBM has been successfully doubling QV every year. In fact, IBM doubled it three times in 2020. This is a Moore's Law level of increase, even as Moore's Law itself has been abating for traditional computing (see Perspective, "Classical computing—The trouble with Moore's law on page 16").

"Moore's Law is coming to an end and classical computing is reaching its limits just as our demand is starting to surge."

Richard Debney
Vice President, Digital Technology
BP

Perspective
Three types of problems made for quantum computing

In the near-to-medium term, quantum computing could be especially adept at solving three types of problems:

simulation

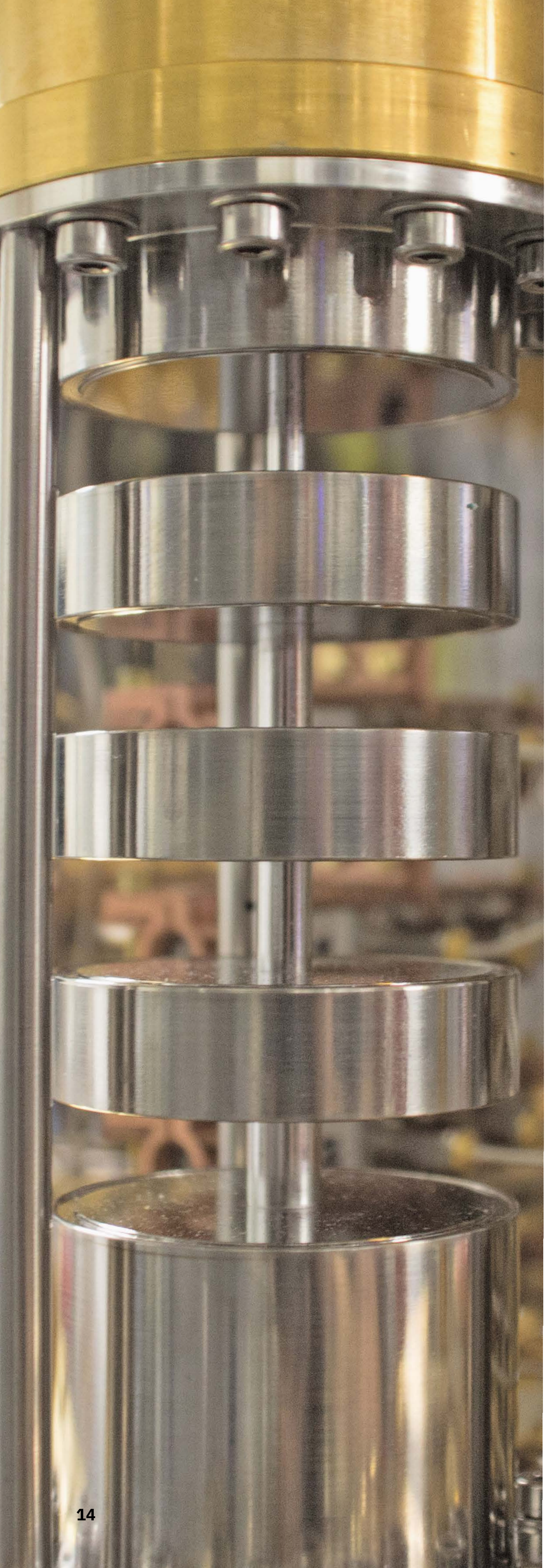
such as modeling processes and systems that occur in nature

search and graph

involving searching for the best or "optimal" solution in a situation where many possible answers exist

algebraic

including applications for machine learning.



The second requirement for productive use of quantum computers is an increase in the *capacity* of the system. The amount of floating-point operations per second (FLOPS) in a classical high performance system is an example of a classical capacity metric. The capacity for a quantum computer is a measure of how many quantum circuits a system can execute per unit time. Quantum programs are a combination of classical instructions and quantum circuits that rely on classical memory. As a result, a quantum computer is a combination of classical resources and quantum computing resources that are brought close together to efficiently run quantum programs. When the program calls across the classical-quantum boundaries, these calls introduce latencies, or delays, which must be reduced to optimize capacity. The capacity of the system also depends heavily on the underlying qubit technology and can likely determine which technology will be successful in delivering business value.

The third requirement for productive use is *variety*, the ability to create more complex and dynamic circuits. Dynamic circuits use very low latency classical instructions that can input within quantum circuit measurements to define the next operations of the quantum circuit. This enables the construction of more efficient quantum circuits and is a fundamental capability needed for quantum error correction. Quantum error correction can protect quantum information by using multiple physical qubits to encode information in a single logical qubit. In terms of variety, quantum computers must be able to run a diversity of circuits to effectively solve a variety of problems (see case study, “Woodside Energy” on page 17).

Perspective
Head-spinning facts about quantum computing

(that you may not need to know)

To say the least, much about quantum computing is counterintuitive. While you do need to understand quantum computing's power and potential to develop strategies and evaluate use cases, the good news is you don't need to be a quantum physicist or theorist—that's what your partners and ecosystems are for. Still, interesting facts to ponder:

Fact one. Quantum computing exploits a fundamental principle of quantum mechanics—that a physical system in a definite state can still behave randomly. The system is in a *superposition,* which is a linear combination of two or more states.

Fact two. Classical computing bits are either a 0 or a 1. But in quantum computing, quantum bits, or qubits, can be in an infinite number of states all at the same time, a superposition of both 0 and 1. Think of a coin. If you flip a coin, it's either up or down. But if you spin a coin, its dimensional possibilities increase exponentially.

Fact three. Along those same lines, in binary logic, things either "are" or they "are not." Quantum computers don't have this limitation, allowing a more accurate reflection of reality.

Fact four. Superpositions are not inherently quantum. For example, when several music tones create sound simultaneously, the surrounding air is in a superposition. What's unique to quantum mechanics is that in some circumstances when you *measure* a quantum superposition, you get random results, even though the state of the system is definite.

Fact five. Measuring a classical bit doesn't change it. If a bit is a 0, it measures as a 0, and the same for a 1. But if the qubit is in a quantum superposition, measuring it turns it into a classical bit, reflecting a 0 or 1.

Fact six. *Entanglement* is a property of a quantum system in which two qubits that are far apart behave in ways that are individually random, yet are inexplicably correlated. Two entangled qubits individually measured can give random results. But when you look at the system as a whole, the state of one is dependent on the other. The combined system contains more information than the individual parts. Hard to wrap your head around? Einstein himself called it "spooky action at a distance."[9]

Fact seven. Quantum computers can use *interference* to cancel paths that lead to incorrect solutions and enhance the paths containing the correct solution.

Fact eight. Noise causes qubits to lose their quantum mechanical properties, hence they must be kept isolated from any source of noise. There are different ways to build qubits. A leading way is leveraging superconductivity to build devices with quantum mechanical properties that can be controlled at will. But for the qubits to work, they have to be kept in a "super-fridge" at extremely cold temperatures of 10 to 20 millikelvins—colder than the vacuum of space.[10]

Perspective
Classical computing

The trouble with Moore's Law

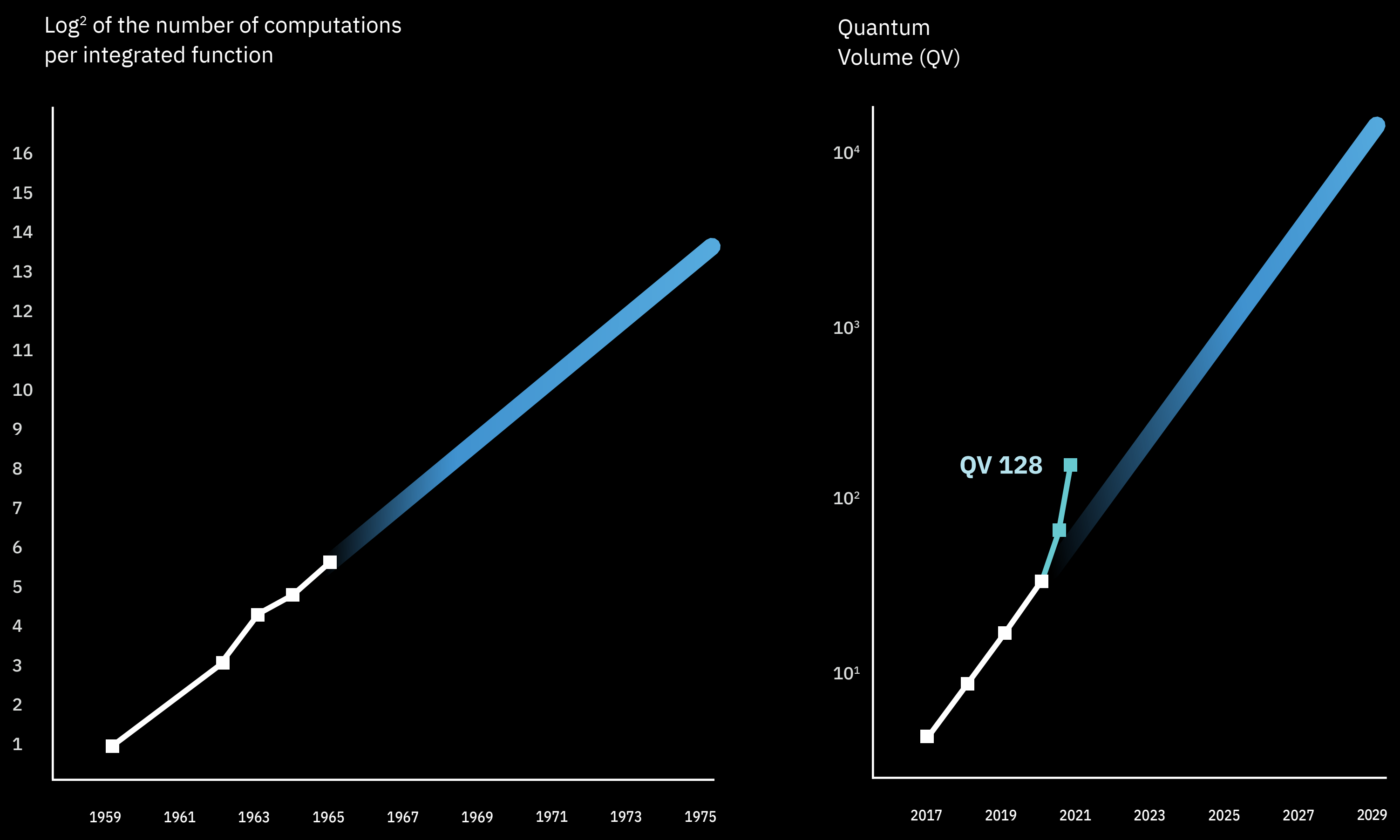
In 1965, Gordon Moore observed that the number of transistors on a given area of a silicon computer chip was doubling every year. He predicted this doubling of density would continue well into the future, though the timeframe was later revised to 18 to 24 months.[11]

For Moore's Law to survive this long, chip designers and engineers have consistently shrunk the size of features on chips. The most advanced laboratories today are experimenting with chip features that measure only 5 nanometers. (A nanometer is 1 billionth of a meter.) These features are so small that some need to be measured in individual atoms.

But now, physical limits are creating serious headwinds for Moore's Law. Some chip industry leaders point to the massive expense and effort required to sustain it. One estimate is that the research effort to keep Moore's Law on track this far has increased by a factor of 18 since 1971. And the facilities needed to build modern chips will cost $16 billion apiece by 2022.[12]

What all this indicates: the slowdown of improvements in classical computing only escalates the importance of integrating quantum computing with classical systems.

Doubling up
Scaling Quantum Volume by 2x per year



Woodside Energy

Introducing quantum kernels into classical machine learning workflows[13]

In classical machine learning, algorithms sometimes use kernels (similarity measures between two pieces of data) to solve classification or regression problems. Usually, kernels are used to increase the dimensionality of the data to separate it, thereby boosting accuracy of the algorithm. Recently, IBM researchers proved the existence of quantum kernels providing a super-polynomial advantage over all possible classical binary classifiers and requiring only access to classical data.

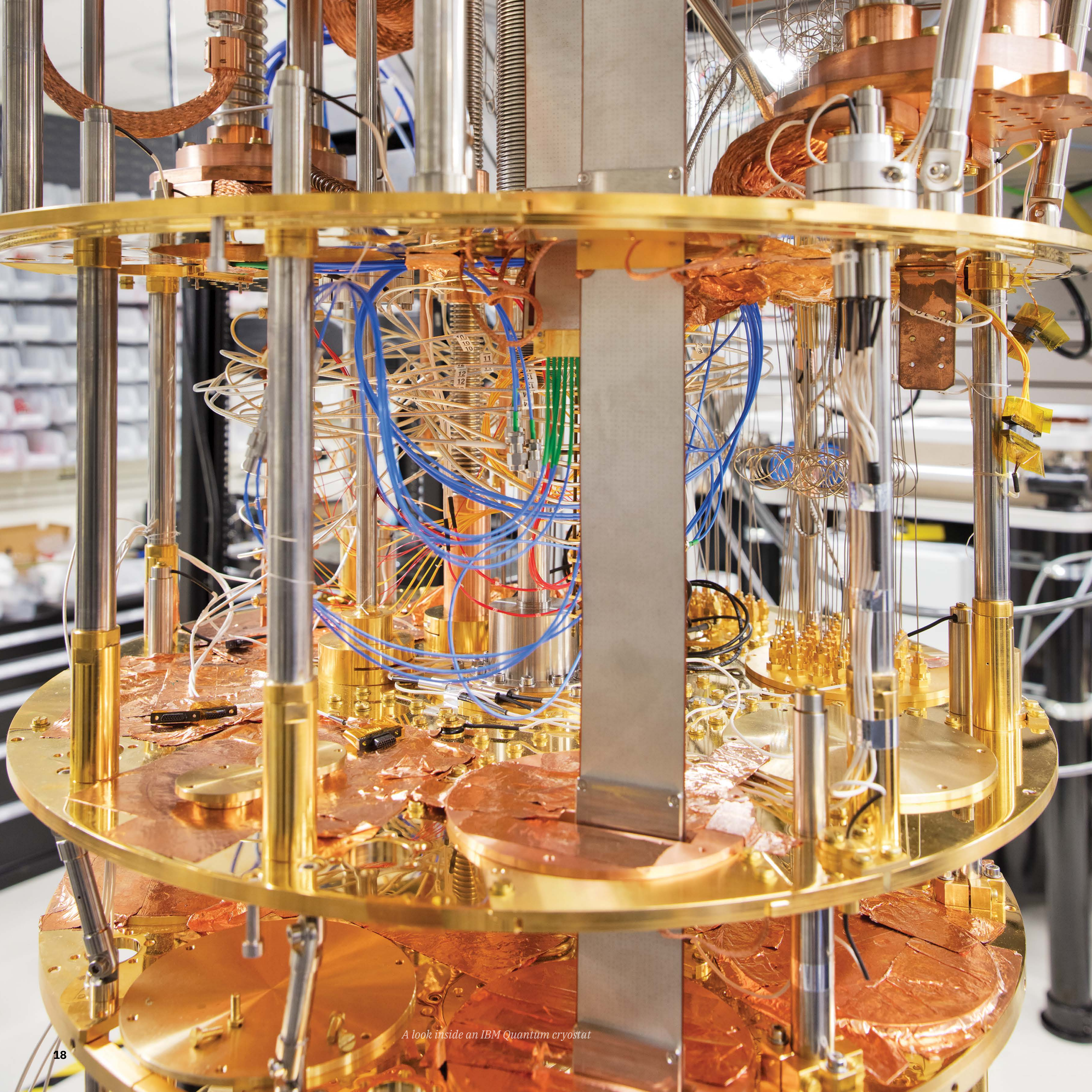
Researchers from Woodside Energy, a leading natural gas producer in Australia, saw an interesting opportunity to collaborate with IBM's quantum researchers. Could quantum kernels be practically deployed in industry-relevant classical machine learning workflows?

As part of their exploration of quantum computing, the teams wanted to understand how to define those kernels using quantum circuits and reduce the amount of quantum computing resources required to evaluate them. This involved connecting properties of quantum circuits to properties of kernels and assessing how well those kernels worked.

The commonly understood way of using quantum kernels in classical machine learning workflows requires one query to a quantum processor for every kernel value to be calculated. Instead of evaluating every value this way, to reduce the calls to the quantum computer and make it more practical, the team began research combining quantum kernels with classical algorithms for matrix completion that answers the following question: Taking a collection of kernel values calculated using a quantum computer, could the researchers use that information with the classical algorithm to accurately predict what an uncalculated value might be?

Investigating this approach raised some essential questions, including: Could leveraging state-of-the-art completion techniques lower the number of queries required, thereby making the use of quantum kernels more practical, more quickly? Do these kernels provide useful benefits to Woodside Energy, such as enhanced classification accuracy in their industry data sets? Can predictions be made relating properties of quantum circuits to the ease with which quantum kernels can be completed?

Woodside Energy considers this research a "pathfinder project" that establishes a foundation for subsequent experimentation. The company is continuing this line of thinking by researching literature about other quantum circuit families used as building blocks for other applications. Going forward, the additional data can help Woodside refine its predictions about the tractability of quantum kernels and where they could be most useful. One potential use case: applying this technology to petrophysical analysis of well log data.



A look inside an IBM Quantum cryostat

"Quantum computing is not just an expansion of classical computing. We can't just port problems to quantum computers. We need to break them down and build communities that can effectively apply this technology to the right problems."

Richard Debney
Vice President, Digital Technology
BP

But the speed and power of quantum computing alone do not define the Quantum Decade. The exponential increase of qubits is impressive, but if that brute computing force is inaccessible and inapplicable to real problems, we're back to abstract theory.

Fortunately, the power of quantum is accessible. Historically, if you wanted computing power, you had to build or install and maintain the machines yourself. But now, thanks to the cloud, even highly sophisticated quantum computers are attainable.

In fact, a programmer can sit at his or her laptop and create a quantum circuit using quantum gates. When the software sends the circuit via the cloud to a quantum computer, the machine converts those gates into microwave pulses. In turn, the pulses control the physical qubits, which work their magic on the problem at hand. The results are returned—translated back into classical bits—to the programmer.[14] This frictionless interface is what will unleash quantum computing to today's developer communities.

Open ecosystems are scaling

A decade ago, quantum computing experts were predominantly Ph.D. physicists in labs—a valuable commodity that's still in short supply. But communities of developers, not necessarily Ph.D.s or other physicists, are beginning to appear. These communities include chemists, electrical engineers, and mathematicians, among others. They're learning and applying quantum concepts, even in classical computing environments.

Ecosystems fostering open innovation have sprung up and are training software developers to apply quantum computing to real problems. IBM started one such open-source community, Qiskit, to build the necessary code development tools and libraries for quantum developers. The community also offers skills development for thousands of quantum students. Over 2 billion quantum circuits are run per day over IBM Quantum Services using real quantum computers.[15]

From analysis to discovery

The advances in quantum computing have been significant, but what are their practical implications? How will they impact our ability to address complex problems at scale?

In its early days, science was empirical and theoretical. People observed and measured phenomena, such as the motion of objects; made hypotheses and predictions about why they happened; and tested them repeatedly. Computers—and eventually AI and supercomputers—changed that, ushering in the age of analytics. We can now ingest massive amounts of data and develop models for how systems will behave. We can also now model chemical systems, move individual atoms, and simulate how some materials will perform or react over millions of uses.

But some challenges remain beyond our reach. While we may be able to model a chemical system, these classical models work well for problems where we already have data. These models are not based on the underlying physics of how molecules behave and are therefore imprecise. We don't have the toolset to address these shortcomings. As powerful as it is, classical computing has fundamental limitations in the face of exponential problems (see Figure 6).

Figure 6

Progress through the ages
The road to quantum-accelerated discovery

1st paradigm	2nd paradigm	3rd paradigm	4th paradigm	5th paradigm
Empirical science	Theoretical science	Computational science	Big data-driven science	Quantum-accelerated discovery
Observations Experimentation	Scientific laws Physics Biology Chemistry	Simulations Molecular dynamics Mechanistic models	Big data Machine learning Patterns Anomalies Visualization	Scientific knowledge at scale AI-generated hypotheses Autonomous testing
Pre-Renaissance	**~1600s**	**~1950**	**~2000**	**~2020**

Increasing speed, automation, and scale

IBM and Cleveland Clinic
Using the power of quantum to tackle key healthcare challenges[16]

IBM and Cleveland Clinic, a nonprofit academic medical center that integrates clinical and hospital care with research and education, have announced a planned 10-year partnership to establish the Discovery Accelerator. Cleveland Clinic and IBM will strive to advance discovery in healthcare and life sciences through high performance computing using hybrid multicloud, AI, and quantum computing technologies.

Through the Discovery Accelerator, researchers anticipate using advanced computational technology to generate and analyze data to help enhance research in the new Global Center for Pathogen Research & Human Health. Research is expected to focus on areas such as genomics, single-cell transcriptomics, population health, clinical applications, and chemical and drug discovery.

As a critical component, IBM plans to install an on-premises, private-sector IBM Quantum System One on the Cleveland Clinic campus—the first installation in the US. This quantum program will be designed to engage with universities, government, industry, startups, and other organizations. It will leverage Cleveland Clinic's global enterprise to serve as the foundation of a new quantum ecosystem for life sciences, focused on advancing quantum skills and the mission of the center.

In addition to the on-premises IBM Quantum System One, Cleveland Clinic will have access to IBM's current fleet of more than 20 quantum systems, accessible via the cloud. IBM is targeting the unveiling of its first next-generation, 1,000+ qubit quantum system in 2023, and Cleveland Clinic is slated as the site of the first private-sector, on-premises system.

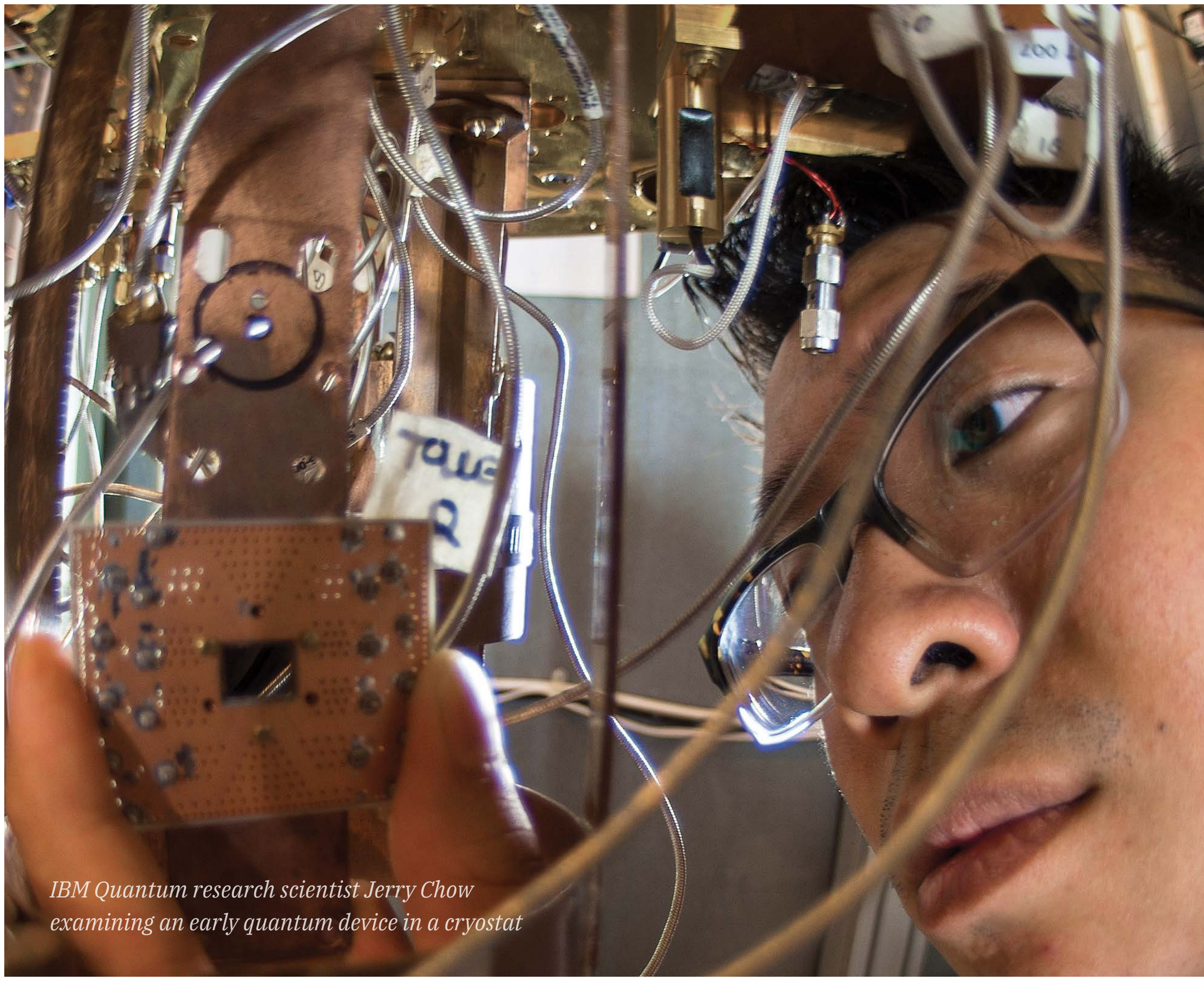
"This will be the Quantum Decade if we can apply quantum computing to discover one thing, heretofore unimaginable, that progresses our line of inquiry into the future."

Todd Hughes
Technical Director, Strategic Projects and Initiatives
CACI

That's where quantum computing, in combination with classical computers and AI, comes in. This triad is poised to generate discovery at a radically faster pace. Consider the amazing impact of research involving mRNA, a single-stranded RNA molecule that is complementary to one of the DNA strands of a gene.[17] This research expedited COVID-19 vaccine development: decoding the virus to vaccine creation took only a few weeks, followed by months of clinical trials and broad release in a year.[18] Yet this was only possible because we already had a decade's worth of mRNA research to leverage.

With quantum computing, that kind of discovery might itself be compressed, especially when starting with a blank slate, vastly accelerating vaccine development and efficacy and easing the pain of future pandemics.

So many of our best practices in healthcare remain approximations: extrapolating information from large data pools and applying it to individuals. In many ways, we are still using trial-and-error techniques—more sophisticated, certainly, but hardly treatment tailored to each specific individual. Quantum computing's step-change capabilities hold the promise of eventually creating personalized medicine, matching therapeutics to an individual's genome (see case study, "IBM and Cleveland Clinic").



IBM Quantum research scientist Jerry Chow examining an early quantum device in a cryostat

"The materials discovery process is unbearably slow. Companies don't have time to experiment endlessly. Quantum computing can give us an exponential leap in discovery."

Doug Kushnerick
formerly with Technology Scouting and Ventures
ExxonMobil Research

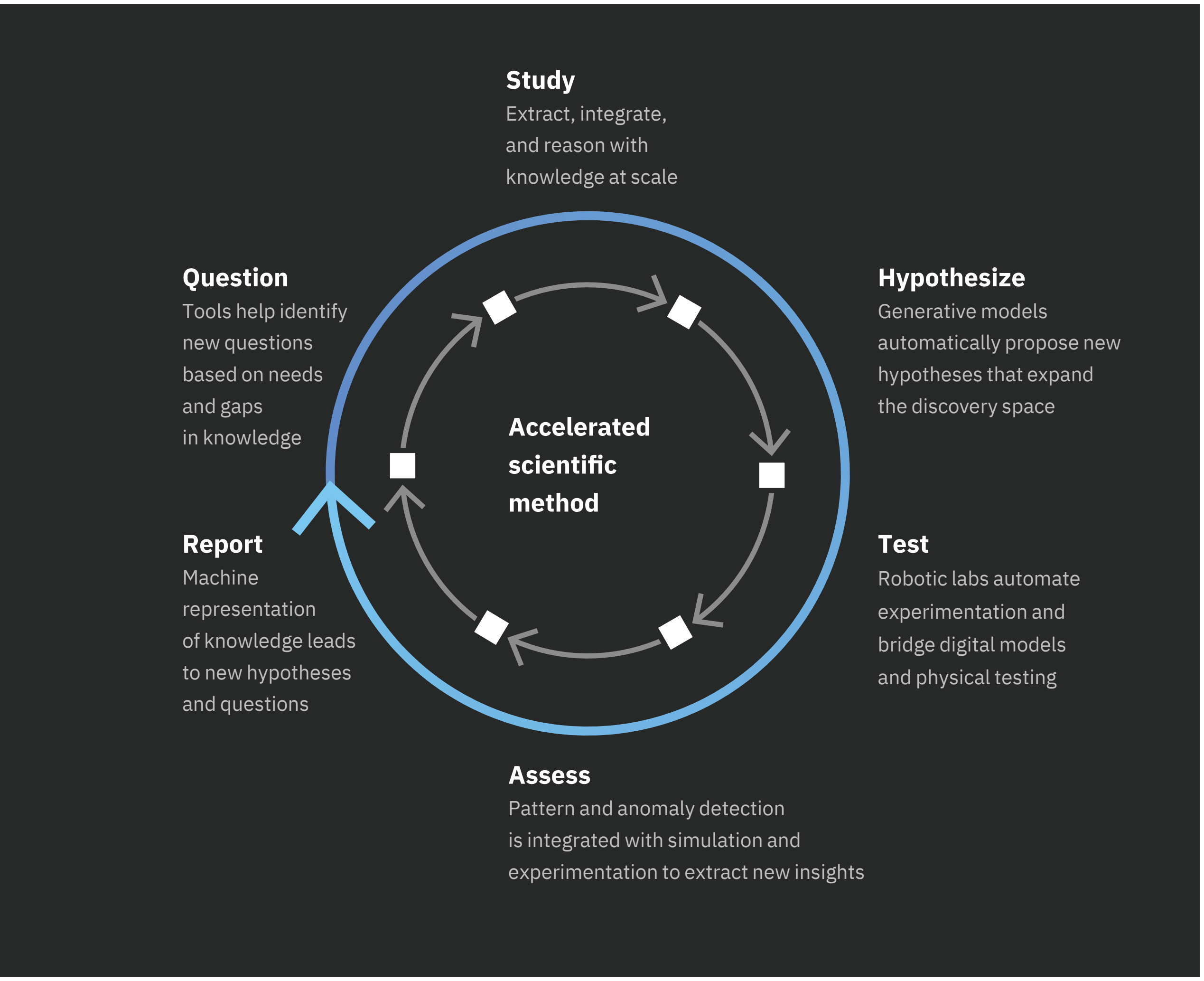


Figure 7

Scaling the scientific method
From questions to hypotheses to reports

This dream can become a reality by supercharging how experimentation is done. You may recall learning about the basics of the scientific method as a child: a sequence that runs from observation, to question, hypothesis, experiment, results, and finally, conclusion. With classical computing, we've been able to speed up that process. The triad of classical, AI, and quantum computing can supercharge the scientific method (see Figure 7).

The unprecedented ability to model complex systems will accelerate the ability to extract, integrate, and validate so that we can draw conclusions. We are already using AI to generate hypotheses automatically and using robotic labs to automate physical experimentation. The greater ability of quantum computing will expand the possibilities that can be evaluated before moving to physical experimentation, and accelerate the entire discovery process as a result. "For the first time, the loop in the scientific method is closing," as the *2021 Science and Technology Outlook* from IBM Research puts it. "Each breakthrough is a step toward realizing the dream of discovery as a self-propelled, continuous, and never-ending process."[19]

By accelerating discovery and more rapidly translating knowledge into practice, all kinds of new leaps will be possible. Healthcare is only one area of application. Another scenario: quantum computing can be put to work on finding new materials. These capabilities may improve the efficiency of solar panels, wind turbines, and battery life. As we will explore in the Industry Guides on page 69, the applications to specific industries are myriad.

The discovery-driven enterprise

In organizational terms, what will emerge from the Quantum Decade is a new kind of discovery-driven enterprise (see Figure 8). Just as cloud has increasingly virtualized the traditional enterprise, the injection of quantum will open new possibilities.

The computing triad will revolutionize how businesses manage and operate market-making business platforms enabled by *intelligent*—or AI-driven—workflows. By examining how people work, AI can already help determine the most efficient or effective workflows. Tasks can then be routed to traditional or quantum systems—one or more quantum computers working with a classical computing system—depending upon which is the best option. Once information technologists establish a workflow, a user need not know where or how the computation is being done. No specialized knowledge of quantum computing would be required.

Just a decade ago, those who appreciated the potential of AI—and took steps to prepare for it and implement what they could along the way—are now the outperformers.[20] Today, we are in the Quantum Decade, and as we accelerate the pace of discovery, enterprises of all kinds need to pay close attention.

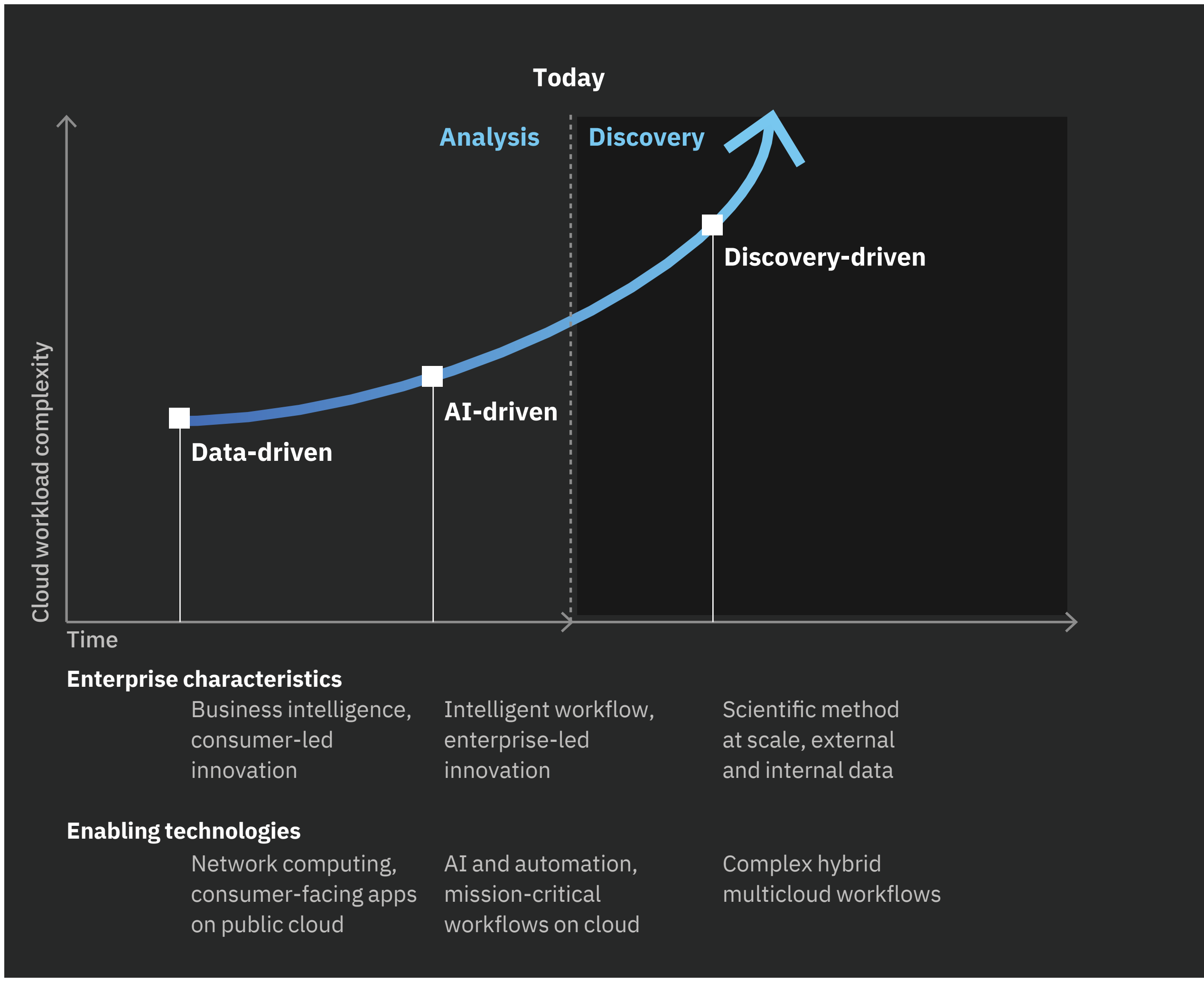


Figure 8

A new normal
The emerging discovery-driven enterprise

A view from below an IBM Quantum cryostat

Questions to ask

Question One

How would your team, your executives, and your board define the case for quantum computing?

Question Two

What steps are you taking to become—or compete with—a discovery-driven enterprise that includes quantum computing?

Question Three

How are you educating yourself and your key talent on quantum computing possibilities?

Question Four

What are some viable ecosystems through which you can access powerful, scalable quantum computing capabilities on the cloud?

Insights

The power of quantum literacy

You can develop partnerships and join ecosystems for "deep tech" quantum know-how. What you do need on your team is literacy in quantum computing potential—a fluency that can help you conduct experiments and scope out the advantages for your organization.

The hidden workflow opportunity

Getting more value from quantum computing requires examining workflows for quantum computing opportunities and modes of interaction with classical systems. But readiness will take more than quantum computing literacy and experimentation. It requires preparing your classical enterprise to integrate quantum computing deeply into new ways of working and new business models.

Don't go it alone

The speed at which quantum computing is improving and expanding makes it difficult for many companies to keep up. Being part of a quantum computing ecosystem can provide access to technology and talent that might not be accessible otherwise.

Chapter Two

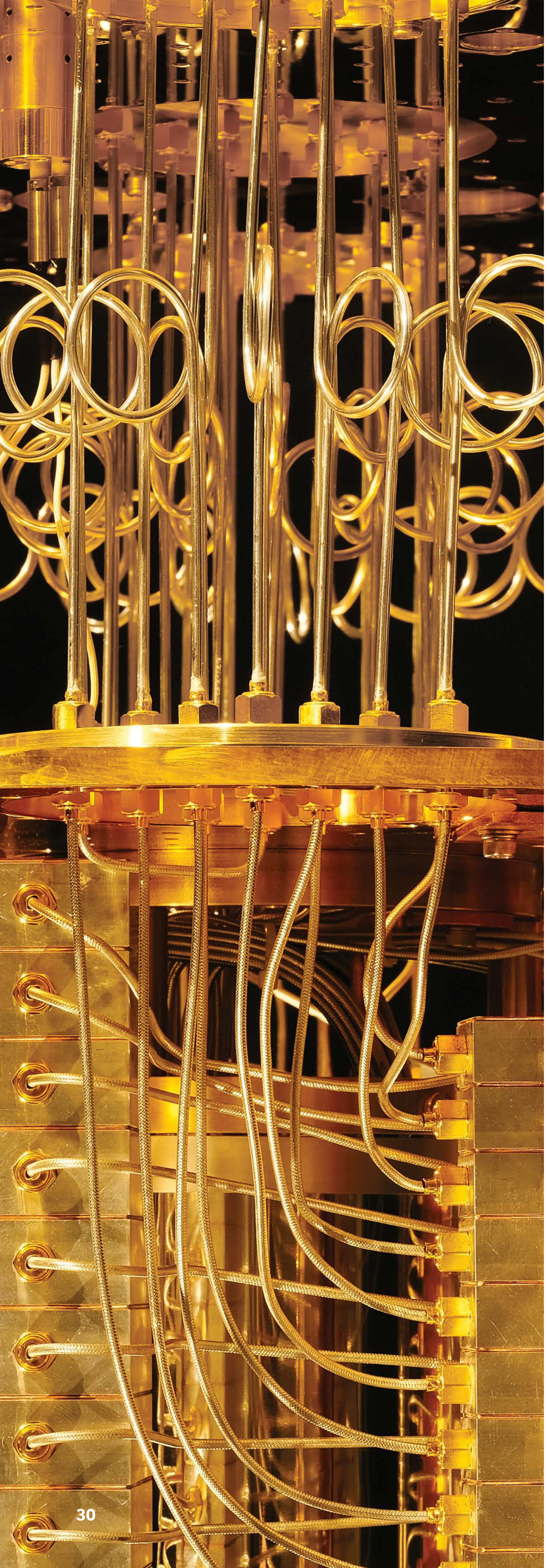
Quantum readiness and the power of experimentation

“There is no doubt that quantum computing technology will be ready for business this decade. There will be multiple million-qubit quantum machines by 2030,” says Christian Weedbrook, CEO of Xanadu Quantum Technologies. *“The question is, are you ready?”*

The short answer is, “maybe—if you act now.” Quantum computing readiness is a continuously evolving state that depends on your general approach to, and investment in, innovation, as well as new talent and skills, and overall digital maturity. This readiness includes your adoption of enabling technologies such as automation, AI, and hybrid multicloud; your willingness to analyze, experiment, and iterate with evolving computing capabilities; the sophistication of your workflows; and your organizational skillset.

Your industry and location factor in as well. Industries fluctuate in their quantum computing readiness based on competitive pressure and concentration, growth and innovation requirements, and quantum computing’s potential for solving industry-specific computational problems. Countries and regions can vary by geographical context, mainly with respect to investment, education and skills, regulation, and ecosystem availability. And ecosystems themselves must achieve readiness to provide viable support. But still, partnering with the optimal ecosystem can be an astute way to alleviate fluctuations in readiness, regardless of your location or industry.

Think of it like this: Getting a head start in a technology such as quantum computing is analogous to the power of compounded interest. Waiting a couple of years and letting early adopters pull away can give them an exponential lead.



Experiments by design: Applying quantum literacy to real problems

Encouraging news: You don't need on-staff Ph.D.s in quantum computing to get started. Yes, the world of qubits, superposition, and entanglement can be a slippery slope best left to quantum experts, and it does take Ph.D.-level proficiency to create novel intellectual property. But by developing partnerships and joining ecosystems for "deep tech" quantum computing know-how, that can be surmountable. What you do need on your team is literacy in quantum computing potential—a fluency that can help scope out the advantages for your organization.

The exciting—and challenging—part is applying that literacy to business problems. What are the current limitations in your industry? Dig deeper. What limitations are causing those limitations? How would dissolving these seemingly intractable barriers reshape your industry? Where are the stumbling blocks in how you mobilize computing and design workflows today? Where are your industry and organization headed in 10 years?

Complex real-world problems may not be solvable until we progress toward fault-tolerant quantum computing—the Quantum Decade's culmination. This is a class of quantum computing where you can run general-purpose quantum programs compiled across both quantum and classical resources. Fault-tolerant computers incorporate procedures that help prevent errors from multiplying and spreading, allowing them to run quantum circuits arbitrarily close to correct even when their physical components are faulty.

We are already learning how quantum computing can contribute to our understanding of problems—big problems, at that. It's helping researchers explore the development of new materials. Over time, it can contribute to developing earth-friendly, efficient fertilizers to support the global food supply chain. On a genuinely cosmic level, it could be a key player in investigating the mysteries of how our universe is stitched together.[21]

"Executives need to understand what quantum computing can solve in the next decade. They need to look across the stack, evaluate the cost, and determine the advantage."

Jeff Nichols
Associate Laboratory Director
Oak Ridge National Laboratory

“It’s not just decomposing, but rethinking and recomposing problems for quantum computers.”

Christopher Savoie
Founder and CEO
Zapata Computing

But let’s think shorter term. To achieve quantum readiness, you need to define the art of the possible *now* through problem scoping, experimentation, and iteration. This can involve one—or a combination—of several approaches used independently or together (see Figure 9).

- **The pyramid approach.** Industry-essential problems, by their nature, are complex. This approach involves experimenting and learning in an iterative way, using classical decomposition and heuristic techniques to deliver an abundance of potential solutions. Then, quantum processes identify a subset of optimal solutions that rise, in this analogy, to the top of the pyramid. In other words, classical approaches can provide a good set of solution options, then quantum systems can optimize. This enables refining larger solution sets and transcending smaller, theoretical options that are not of any robust consequence.

- **The analyze-and-extract approach.** Solving a complex problem in its entirety could require a million qubits. For now, the strategy needs to involve extracting the parts that are solvable with classical computing and reserving the other segments for quantum computing and its extreme computational power. It’s like a dissection. The problem undergoes analysis at various stages: preparation, deconstruction, then resolving each deconstructed part.

For now, this usually shakes out to align classical computation with data understanding, decomposition, and the computation it can handle; quantum capabilities align with specialized computation. Additionally, this process of deconstructing and reconstructing the problem in different ways helps to *see* it differently—perspectives that can ascertain even greater eventual value from quantum computing.

- **The benchmarking framework approach.** Both classical and quantum computing are far from static. They’re improving and evolving constantly, especially quantum computing. Experiments can benchmark problems against classical and quantum capabilities at one time and then re-run them against improved hardware, software, algorithms, error correction capabilities, and so forth. Isolating and identifying those specific quantum computing improvements and strategically applying them to broader problem sets can help advance quantum readiness and the path to Quantum Advantage.

The potential for quantum computing is tremendous, even if the concepts themselves are esoteric. But experimenting and iterating with quantum computing can demonstrate the power of conceptualizing outside the box (see case study, “IBM Services Supply Chain” on page 32). As you evaluate scenarios and develop experiments for your industry, creating a tangible roadmap for quantum readiness can bring the esoteric very much down to earth. What’s critical is experimenting with state-of-the-art quantum computing hardware, most likely through an ecosystem.

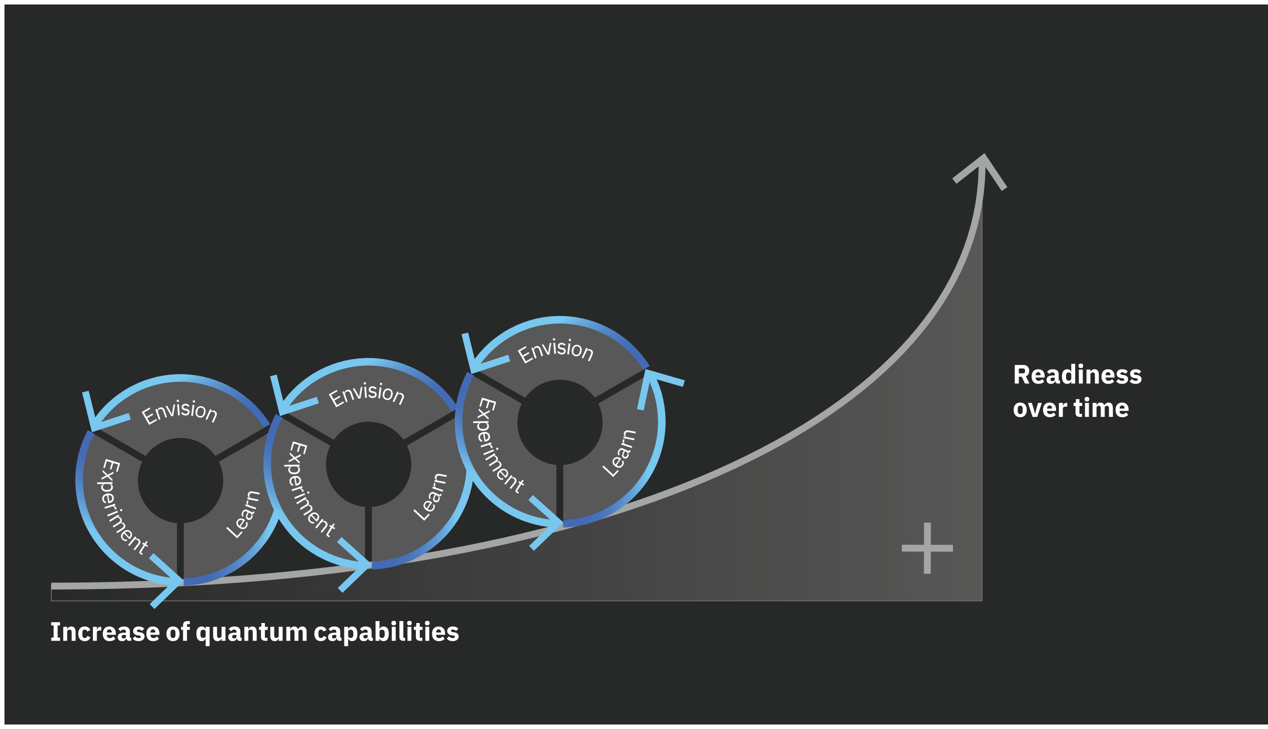


Figure 9

Envision, experiment, learn
Experimental approaches for applied learning

IBM Services Supply Chain[22]

A quantum-fueled search for more accurate demand forecasting

Predicting the future—is it possible? Across industries, organizations give it their best shot in multitudes of areas: demand forecasting, inventory forecasting, capacity forecasting, and more.

But classical computing forecasting techniques can suffer from low accuracy. As an example, for demand forecasting, the challenge of aligning supply chains with quickly changing demand is daunting. Even consistent forecast improvements of just 1% can have a significant financial impact. In services, there is a larger component of independent demand driven by variable failure characteristics. With that in mind, IBM researchers are preparing a demonstration that pairs quantum and classical computing techniques to make demand forecasting more efficient.

To that end, researchers are working with IBM Services Supply Chain (SSC), an organization responsible for servicing data centers by storing and delivering field-replaceable service parts. IBM SSC's millions of dollars of inventory encompass more than 2,000 different parts housed in 114 warehouses located around the US. Depending on the severity of the issue, delivery needs to occur within one of four specific timing windows: two hours, four hours, one day, or two days. As a result, IBM SSC's forecasting challenge is to predict how many parts are needed when and where.

The researchers used a two-step approach to the scenario. The first was to apply demand pattern classification with example patterns that include:

Fast

Demand is continuous

Slow

Demand is intermittent, with time periods that have zero demand

Inactive

Demand becomes inactive

Rare

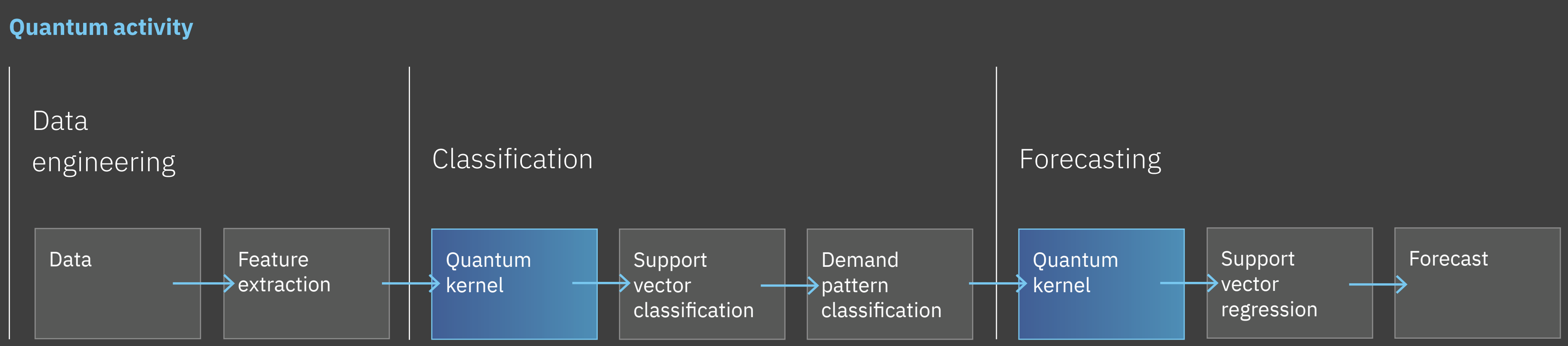
Few orders or one-time order

Then, the researchers executed the appropriate forecasting algorithm for the demand pattern. Both classification and forecasting could be done using a combination of classical and quantum (see figure below). Classical and quantum computing work together as a team, with quantum doing the computational heavy lifting part of the workflow.

Quantum machine learning models have the potential for greater generalizability, which means forecasting algorithms could achieve greater accuracy with new data. While classical computing can complete these workflows without quantum computing, as the researchers refine their techniques, they're getting closer to understanding the role quantum computing can play. This is going to be essential in areas such as predictive maintenance, in which IoT sensors are increasingly a source of data. And for safety-related maintenance, such as airplane parts, the increased performance and accuracy of quantum machine learning models could become a necessity.

As with many quantum computing experiments, this classification and forecasting work is both foundational and evolving, providing IBM researchers the platform to explore quantum algorithms and capabilities for business forecasting. Upon completion, researchers will have a tangible demonstration that maps a business problem to quantum computing. And it will help to illustrate a critical point: Classical and quantum computing are not competitors. Rather, they are complementary technologies that, together, can be more effective.

Combining classical and quantum
The forecasting workflow



Quantum-fueled process workflows

Thinking small and incrementally can be an expeditious route to Quantum Advantage, especially when integrating quantum computing into your workflows.

A workflow is essentially a tree of tasks, with functionalities spanning adaptive customer and vendor interactions, proactive executive decision support, targeted employee training, and other AI applications.[23] However, workflows can encounter difficulty in comprehensively computing large amounts of complex data in a timely manner. As a result, businesses may be forced to employ computed approximations even in the face of pressing market demands. Examples could include workflows involving complex networks such as distribution, transportation, communications, or logistics.

Applications of quantum computing are almost always in terms of accelerating a process or sub-process within a workflow. Getting more value from quantum computing requires examining workflows for quantum computing opportunities and modes of interaction with classical systems (see case study, "OLED screens" on page 36).

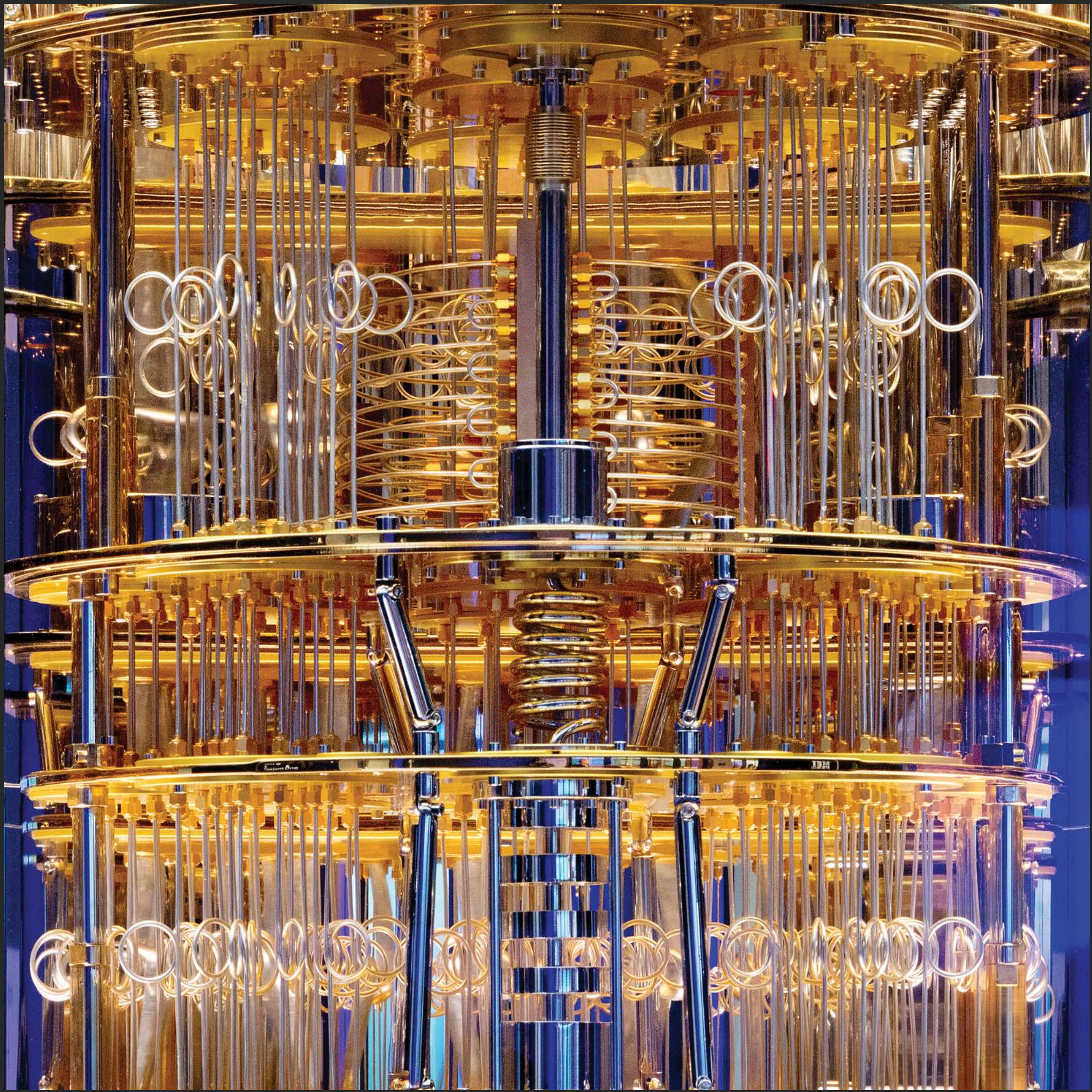
Evaluating quantum computing in this way requires a broad focus on industry transformation. How can quantum computing partner with classical computing within a particular context? What workflow subsections are best suited for quantum computing? The intellectual analysis required in assessing workflows for classical versus quantum computing can result in a fresh perspective on the workflow itself—as can the potential range of results that quantum computing provides. Quantum computing can be conducive to computation that generates unexpected breakthroughs—yielding new efficiencies, sharper methodologies, and more meaningful modes of engagement with both internal and external stakeholders.

"Quantum computers won't cannibalize classical computers. Quantum computers will help with certain difficult optimizations that exist in workflows. It will be additive."

Christopher Savoie
Founder and CEO
Zapata Computing

"We need to spend more time on what part of the workflow quantum computing can address. Not mysterious physics, but the mission and business problems that it can solve in a transformative manner."

Glenn Kurowski
Senior Vice President and Chief Technology Officer
CACI



OLED screens

Brighter, more efficient displays through quantum-driven simulation[24]

What's the one thing that comes between humans and their phones? The screens, also known as flat panel displays. But these displays are one of the highest power-consuming components in smartphones, often limiting battery lifetimes.

New, advanced materials can produce brighter displays that are more efficient and less power hungry. But developing these new materials requires labor- and time-consuming traditional lab research methods. The process spans several development stages, including material identification, process development, device prototyping, and qualification testing.

Traditionally, progress in this realm has been slow. For organic light-emitting diode (OLED) displays, 34 years passed from the first reported observance of electroluminescence in an organic molecule (1963) to the first OLED display commercially available on the market (1997).[25]

But quantum computers can contribute to a brisker pace. Quantum computing can help commercialize new materials with faster, more accurate molecular modeling of both the materials as well as their interactions with manufacturing processes and operating conditions. These new materials can produce brighter, lower-power, lower-cost displays that may expedite their commercialization, enabling companies to offer more compelling, more competitive products sooner.

Materials simulation with classical computing currently has limited application in the development of new materials. The time required to accurately simulate molecular scenarios of sufficient complexity quickly expands beyond practical time frames. As a result, without accurate computer simulations, laborious and costly experimental methods must be employed.

With the quantum computing approach, quantum simulations can be used across the workflow to more realistically simulate materials and their interactions with device operation, manufacturing processes, and the operating conditions. More complex and more accurate molecular-level materials simulations can enable productive experimentation on the computer, reducing costly, cumbersome lab research and manufacturing development.

These quantum computing-driven material simulation workflows can create strategic, competitive product advantages such as brighter, lower-power displays. And the potential financial rewards are considerable. Just a 1% revenue increase per year could mean an additional $320 million for the OLED display market.[26]

The intelligent workflow: Adding the power of quantum

"Process workflows alone miss the complexity of real-world work. Quantum computing will change the relationship among people, technology, and work."

Colonel (Retired) Stoney Trent, Ph.D.
Founder and President
The Bulls Run Group

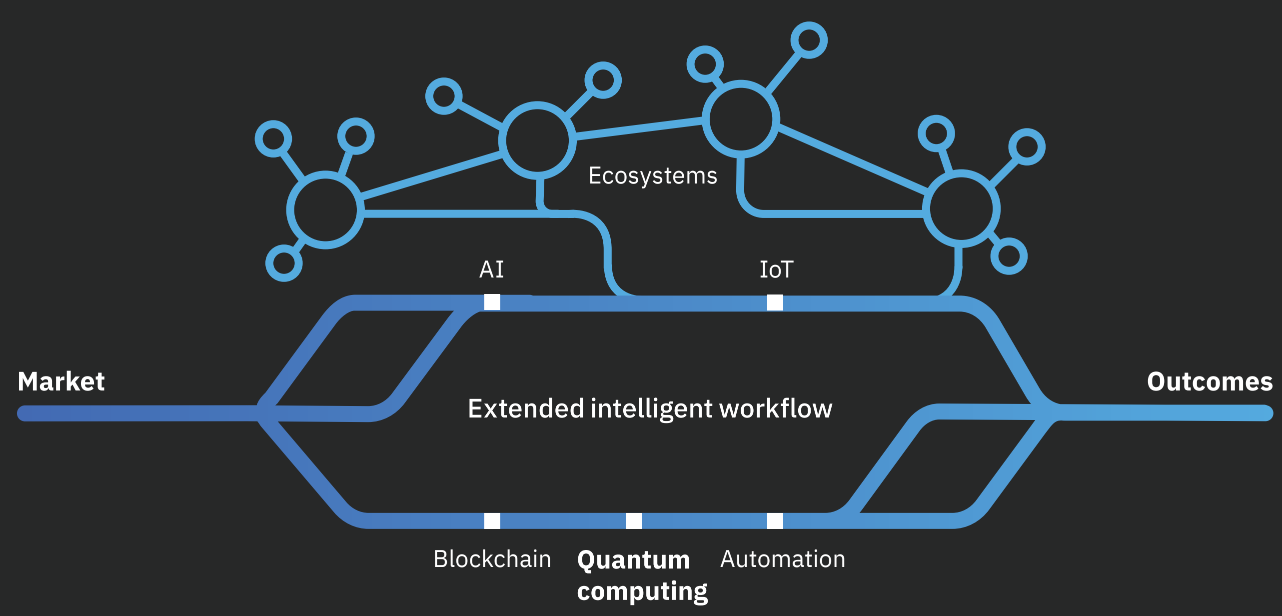
At IBM, we define intelligent workflows as extended end-to-end systems that, through the application of technology at scale, define the customer experience and influence economic results.[27] These workflows are more expansive than simple processes and traditionally have used technologies such as automation, blockchain, AI, 5G, cloud, and edge computing to contribute to exceptional outcomes. IBM research shows that using these classical computing technologies in workflows can triple the benefits.[28] Incorporating the power of quantum computing has the potential to improve on that exponentially (see Figure 10).

In fact, we're approaching a revolution that's driving computing toward highly heterogeneous environments. Increasingly, classical, AI, and quantum computing will be integrated into intelligent workflows managed on a hybrid multicloud.

As you evaluate quantum computing in the context of intelligent workflows, here's an analogy. Processes function as an organizational backbone. But intelligent workflows serve as the organization's nervous system—in short, they're interconnected and interdependent. These workflows differ from simple processes because they extract information from the ecosystem, sense and determine the appropriate response, and send feedback to other workflows.[29] Quantum computing, with its ability to evaluate many options, excels here.

Figure 10

The booster shot
Intelligent workflows powered by quantum computing



"It would be very strange if any major cloud platform in 2030 does not have a quantum play. Quantum is going to be more impactful than AI or supercomputers."

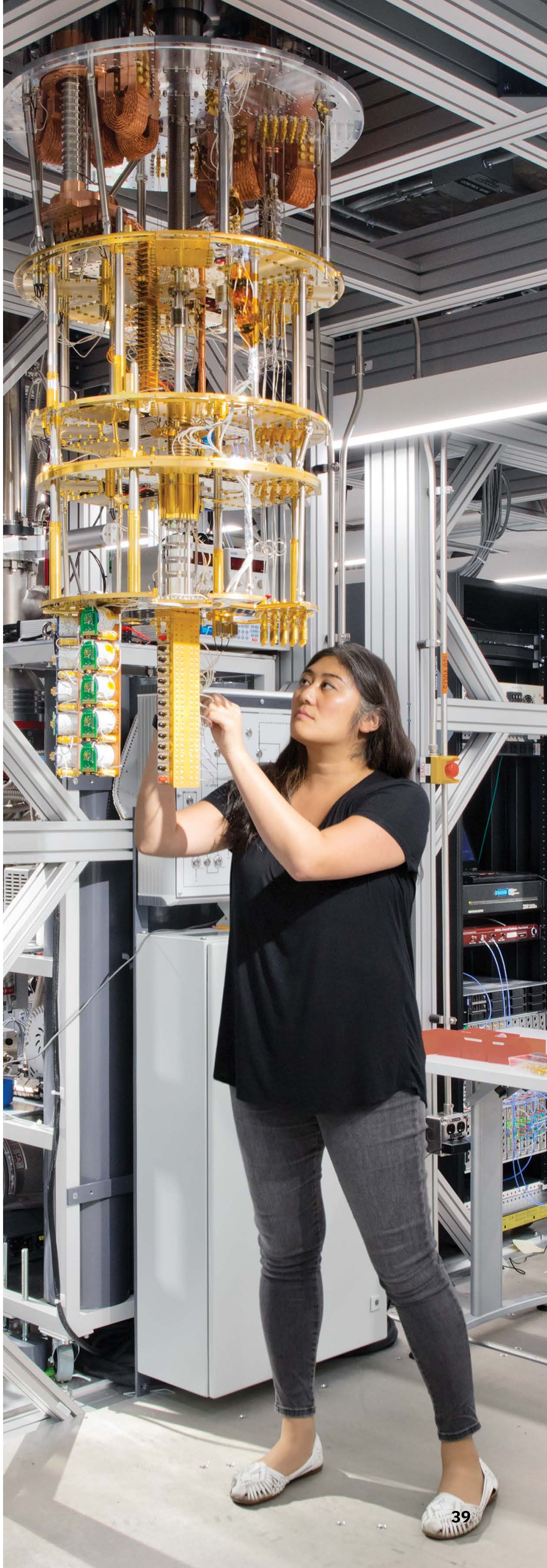
Christian Weedbrook
CEO
Xanadu Quantum Technologies

Intelligent workflows are creatively crafted models with a fresh approach to both data and innovative technology. Establishing these workflows—and enhancing the requisite AI, data, and cloud capabilities—can benefit your business now, while you're laying the groundwork for quantum (see Perspective, "Intelligent workflows" on page 40). Other considerations include the reality of quantum computing breaking Rivest-Shamir-Adleman (RSA) and elliptic curve crypotgraphy (ECC) encryption, and the need to migrate to existing quantum-safe cryptography.[30]

By their very definition, intelligent workflows are inherently based on a mix of technologies—and that mix can and should include quantum computing. Intelligent workflows thrive in an open, loosely coupled architecture, for starters, that *connects* applications and technical approaches. Their ability to leverage hybrid environments is critical, given most organizations are accessing quantum computing on the cloud versus developing the infrastructure themselves. Even if your organization uses a more simplified process approach, establishing some foundational intelligent workflows can be an excellent segue into quantum computing.

In the intelligent workflow framework, quantum computing may be intuitively thought of as an accelerator at first—a booster technology to supplement classical computing where extra power is needed. But in reality, quantum computing is a *catalyst* for deep industry business model revolutions that can spawn disruptive services and modes of consumption.

For these revolutions to happen, enterprises need to develop a strategic compass that guides them toward optimal opportunities. They also need to shore up the ability to apply quantum computing within classical business environments from technology, process, and people perspectives. In short, enterprises need to establish a quantum-receptive infrastructure—and when the technology fully comes to fruition, they'll be ready.



Perspective
Intelligent workflows as a foundation for quantum computing acceleration[31]

Developing intelligent workflows can help you prepare for quantum computing—and their business-enhancing properties can create organizational benefits now. The four steps below outline a broad framework for incorporating emerging technologies, curating data, and embracing a hybrid multicloud environment. With that infrastructure in place, organizations can progress to analyzing sub-workflows for quantum computing acceleration opportunities.

1. Embed emerging technologies, including AI and machine learning, to change ways of working.

Apply other emerging technologies to build highly dynamic and intelligent workflows that radically change how work gets done and new experiences are designed. In particular, strengthen AI and machine learning capabilities, which partner exceptionally well with quantum computing.

2. Drive value from data.

Leverage curated data across intelligent workflows to mine the most important value pools. Establish robust governance to engender trust in your data and AI models so decisions can be pushed out to the front lines of the organization. Identify sub-workflow components of exceptional complexity that would benefit from quantum algorithms.

3. Deploy through hybrid multicloud.

Use the journey to a hybrid multicloud to access data and put it to new use, house intelligent workflows, and modernize applications in an open and de-risked manner. Use this flexibility to seek out opportunities for experimenting with cloud-based quantum computing.

4. Evaluate sub-workflows best suited to quantum computing acceleration.

Explore options relating to quantum emulators, or better yet, join an open-source quantum computing ecosystem. Such a community provides access to quantum computing on a manageable scale, providing a low-commitment “laboratory” for experimentation. Classical and quantum computing usage should be choreographed for quantum computing to most effectively augment classical functions.

To get to this point requires key capabilities (see Figure 11). None of them are about mastering quantum technology itself. Rather, they're about enhancing enterprise skills, technical capabilities, and forward-looking strategies that will enable the quantum computing revolution to take root and thrive.

The good news: Taking a pragmatic, agile, and iterative approach to quantum computing now isn't just about reaping future rewards. This strategy can start to deliver significant business benefits today. For example, setting up a modern dynamic delivery model and open innovation platform through a hybrid multicloud can yield its own significant returns in your classical enterprise.[32] In parallel, they advance your ability to seamlessly integrate quantum computing when it is production-ready.

By enhancing your classical computing environment now while also investing in experimentation and quantum-ready workflows, you are better positioned to accelerate your path to Quantum Advantage.

Figure 11

On solid ground
Laying the foundation for quantum computing

Strategy

Ability to convert quantum computing market information into actionable insights on opportunities and threats

Proficiency to capture business value from quantum-triggered strategies, capabilities, and innovation initiatives

Expertise to secure and protect intellectual property (IP) or quantum computing technologies

Influence of regulations and standards related to intended use of quantum computing

Technology

DevSecOps framework to build, test, deploy, and update quantum computing applications

AI and other advanced computational model maturity for supporting quantum computing-addressable workflows

Hybrid multicloud architecture that enables orchestration and interoperation of quantum-classical workloads

Operations

Governance and oversight to help ensure successful execution of the quantum computing roadmap

Talent strategy and culture to build a high performing team

Innovation processes that create a quantum-enabled solution that meets business needs

Agile practices that result in high velocity of R&D and iterative solution design

The quantum computing ecosystem talent track

In this global, complex economy, no business can do everything itself. We rely on partners, specific expertise, and ecosystems to leverage the best of what is available—and to exploit and demonstrate our own differentiating value-add.

The speed at which quantum computing is improving and expanding makes it difficult for many companies to keep up, and the cost of "going it alone" could be prohibitive. Being part of a quantum computing ecosystem can provide access to that technology when it might not be possible otherwise. And these ecosystems also provide a window into better understanding quantum computing's implications and how they relate to your business issues.

Determining exactly what those business problems are, and how quantum can play, requires expertise. Organizations can strive to build their own in-house quantum computing team, and to an extent that could be necessary. But ecosystems provide valuable supplementation—or even substitution—for in-house quantum computing talent, especially of the deeply technical sort.

Due to limited availability, attempts to build or bring quantum computing skills in-house are very challenging. But the most advanced ecosystems are already stockpiling talent.

Keeping the following questions in mind can help effectively align ecosystems with talent needs.[33]

What is your type of business problem? You may not yet possess the expertise to explain your issue in terms of quantum capabilities, but you undoubtedly have a broader-brush perspective. Is your problem a simulation problem based in chemistry? Or are you looking for quantum algorithms that enhance machine learning? Maybe your primary concern is security in the quantum era? Prospective ecosystems are most effective when they're already working on use cases relevant to your specific issue and include experts who understand your industry problems.

Who are the world's leading organizations and thinkers related to quantum computing and your business issues? Because of the rapid pace of quantum computing innovation, you need partners who are at the forefront of scientific breakthroughs and their application to business problem-solving (see Figure 12). The difference between partnering with Tier 1 and Tier 2 players could mean the difference between being part of a "winner-takes-all" competitive scenario and being left behind.

"At this point, partnering for quantum skills makes much more sense than acquiring them."

Doug Kushnerick
formerly with Technology Scouting and Ventures
ExxonMobil Research

"I'm managing intellectual capital that's not even formed yet."

Irfan Siddiqi
Director of the Quantum Systems Accelerator
Department of Energy (DoE)
National Quantum Information Science (QIS) Research Center

What is the optimal mix of consultants versus in-house staff?
The right quantum computing ecosystem for you contains the right mix of ecosystem participants concentrating on your business problems alongside your industry and technical professionals, including:

— **A quantum computing technology provider** that offers easy access to cloud-based quantum computing systems, an open-source programming framework, educational resources such as tutorials and research papers, quantum computing researchers, quantum computing consultants, technical support, and a collaborative community actively engaged in addressing quantum computing challenges.

— **Quantum computing developers** who understand quantum computing application development using open-source code and access to application development libraries, and have access to real quantum computing hardware.

— **Academic partners and universities** conducting relevant quantum computing research and developing budding quantum computing experts that you may ultimately hire onto your team.

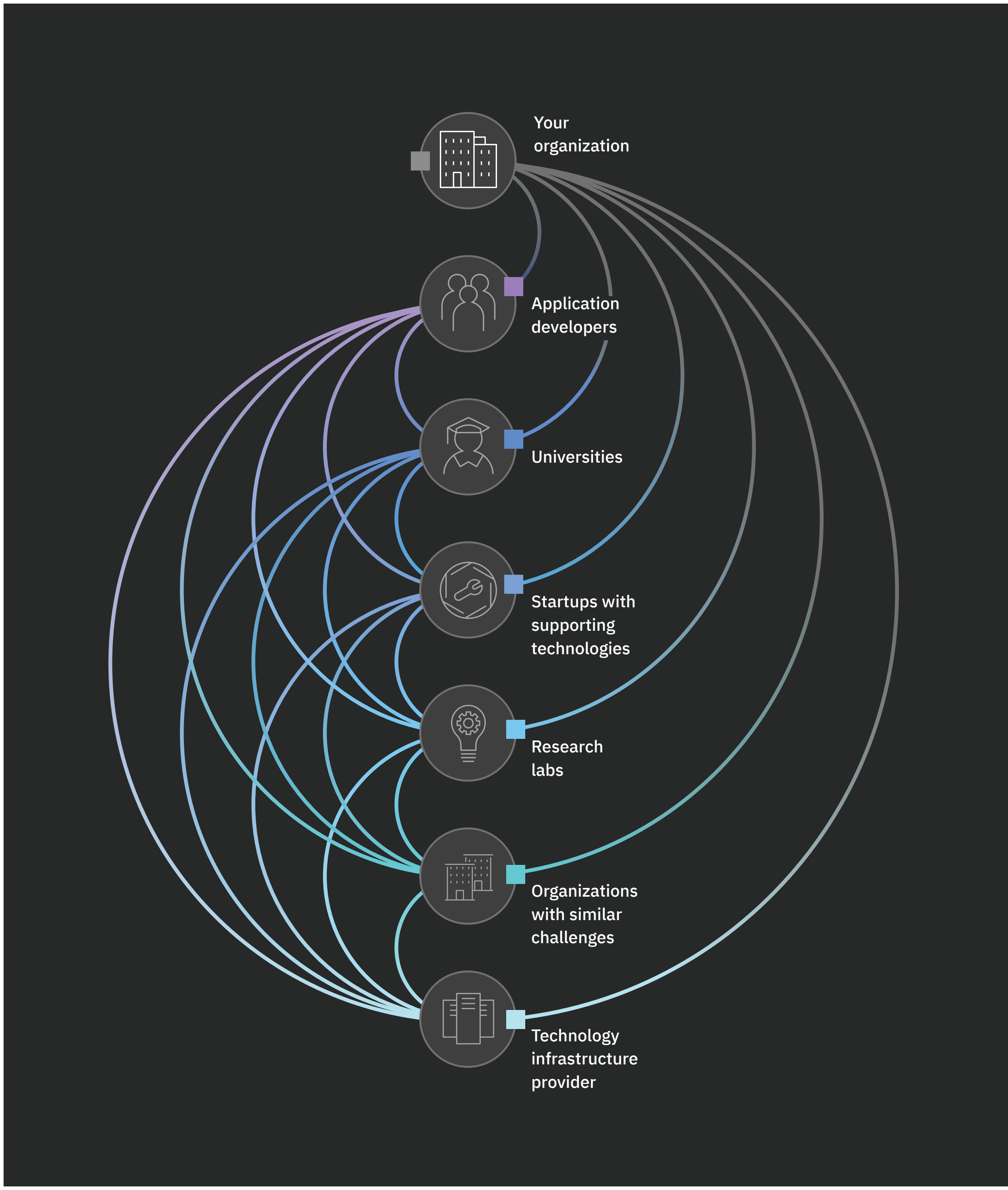


Figure 12

Who are your superpowers?
Assembling the right mix of ecosystem constituents

Quantum stack components	Skills required
Technical services	General technology expertise
Applications	Application architecture and development
Use case-specific libraries	Industry/domain knowledge
Performance libraries	Quantum computing system algorithms
Compilers, optimizers, simulators	Advanced math, quantum computing system expertise
Assembly language and drivers	Quantum physics, quantum computing system expertise
Quantum computing hardware	Quantum physics, chemistry, engineering

Figure 13

Stacked for success
What components and skills can help you achieve quantum computing literacy?

If developing at least some in-house talent is a priority, a first step can involve seeking out community platforms. These "hands-on" ecosystems give developers access to tools to create and run quantum computing algorithms on actual quantum computing hardware or simulators. For example, the IBM quantum computing community offers the open-source Qiskit framework. Such platforms are open to both students—a critical constituency—and organizational IT teams.

A less "deep tech" option is to form small teams to start identifying problems—whether industry-changing breakthroughs or workflow accelerators—in which quantum computing can play a role. Team members don't need Ph.D.-level quantum computing expertise, but they do need enough quantum computing literacy to assess quantum computing capabilities against industry and organizational needs (see Figure 13).

When you're hiring for quantum computing, what's the optimal talent? Researchers from the Rochester Institute of Technology and the University of Colorado Boulder provided some interesting insights. They interviewed managers at more than 20 quantum tech companies based in the US, and the responses yielded two common paths.

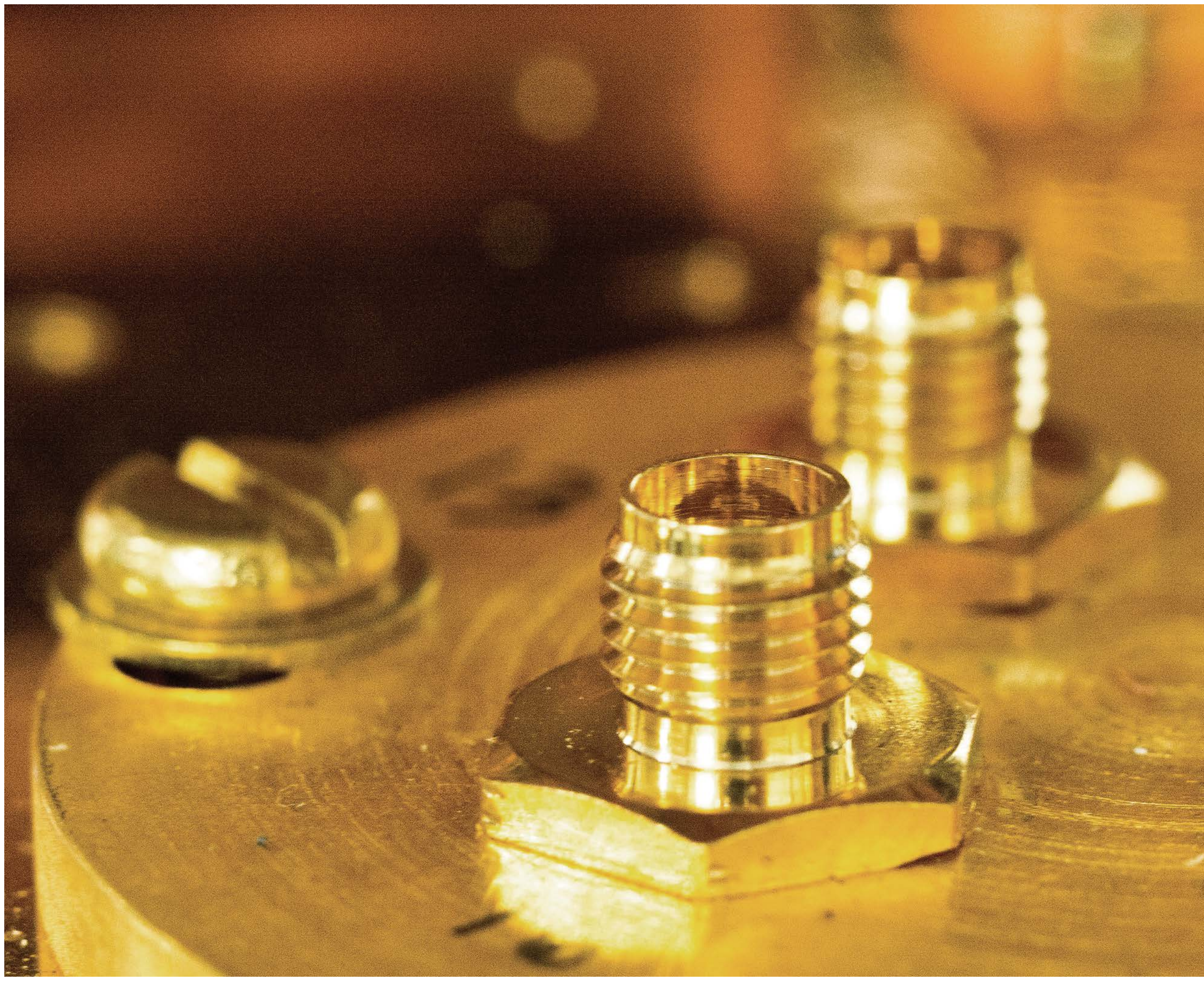
“The semiconductor industry and quantum computing in the US face challenges acquiring STEM graduates—first from having to compete for engineers with more well-known software and social media companies, and second from having a shrinking pool of STEM graduates compared to other countries over the past 30 years.”

Ajit Manocha
President and CEO
SEMI

First, the organizations said they were seeking candidates who were quantum “aware.” This encompassed a broad understanding of quantum computing concepts and the ability to discuss and apply those concepts—what we call quantum literacy. The prospects didn’t necessarily need an in-depth knowledge of equations and theory.[34] Our IBM experts point out that this quantum literacy can often be a re-skill, a case of learning enough quantum computing to augment domain expertise and figure out how to integrate quantum computing in that area.[35]

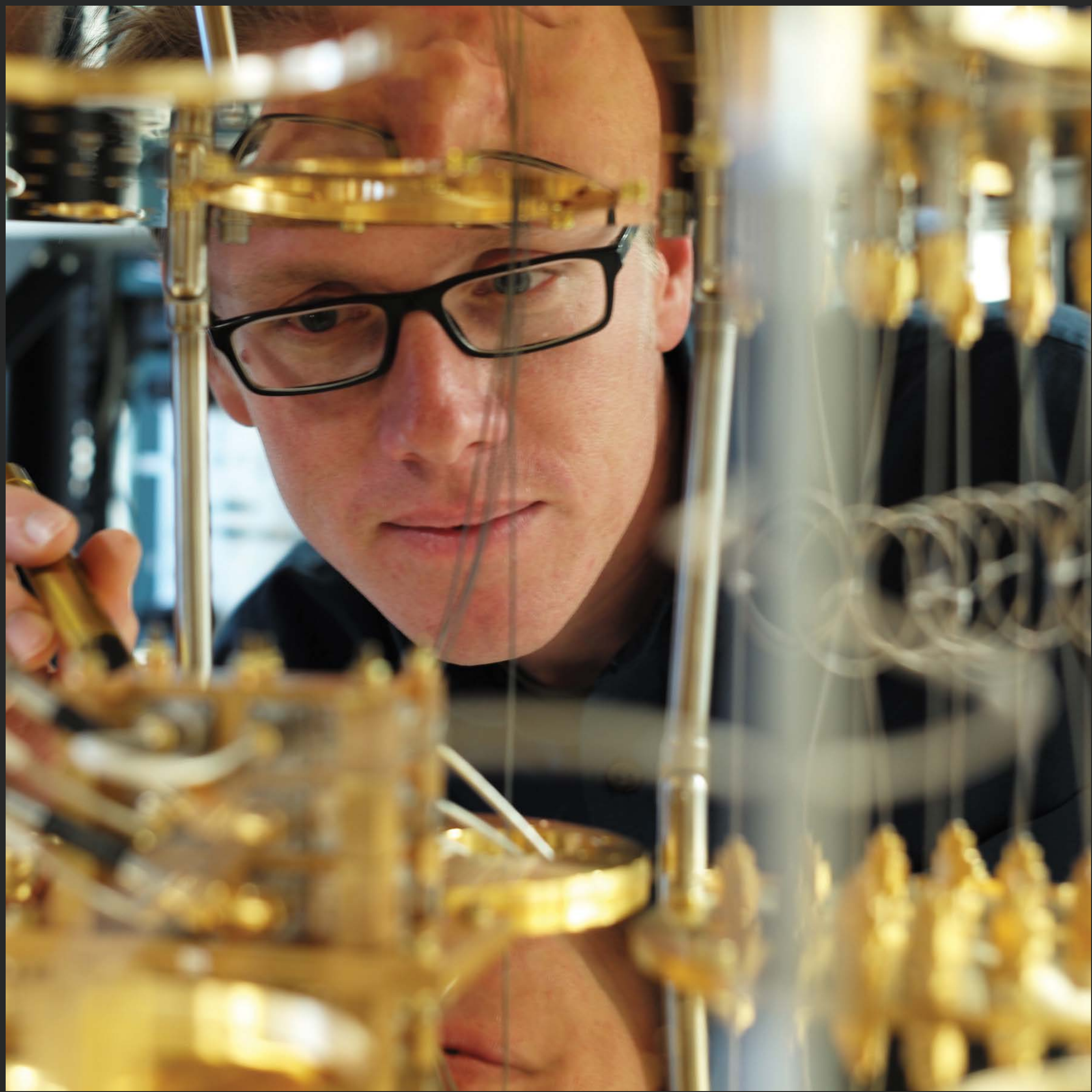
Second, candidates who had hands-on lab skills were favored over those with none.[36] One IBM industry expert estimates only about 3,000 skilled quantum workers exist today, and that base needs to be doubled or quadrupled.[37] As recently as October 2018, *The New York Times* reported that fewer than 1,000 people globally were doing leading research in the quantum computing field.[38]

Acquiring this level of deeply technical skill can be challenging, especially when competing against universities, startups, and vendors. This “talent drought” can boost the appeal of up-and-running ecosystems with their own talented quantum teams.



“If anything slows down the Quantum Decade, it’s unlikely to be the technology. It will be the talent. There’s access to capital, a lot of interest, and we will have the technology. It’s the people that we need.”

Prineha Narang
Assistant Professor of Computational Materials Science
Harvard University



Questions to ask

Question One

How can dissolving seemingly intractable barriers reshape your industry?

What types of quantum computing experiments could you be conducting now, in pursuit of those goals?

Question Two

How can quantum computing partner with classical computing within a particular workflow?

Which workflow subsections are best suited for quantum computing?

How does this assessment alter perspectives and possibilities related to your processes?

Question Three

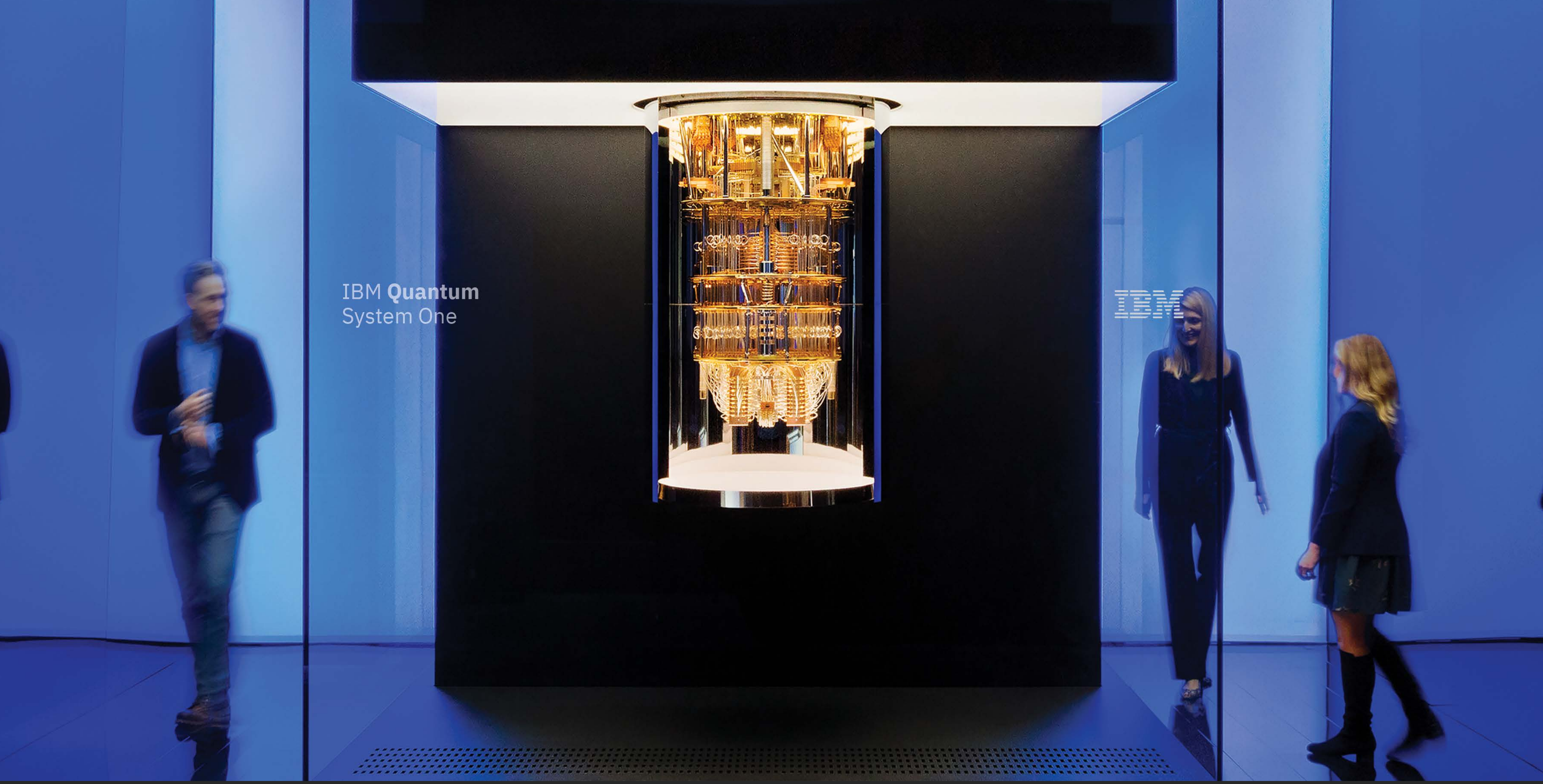
Intelligent workflows that use technologies such as automation, blockchain, AI, 5G, cloud, and edge create an ideal environment for quantum computing to plug into.

How can establishing this foundation benefit your business now?

Question Four

What steps can you take to foster quantum computing literacy within your organization?

What ecosystems can you partner with for "deep tech" quantum computing expertise?



Insights

A process, not a destination

When quantum demonstrates its superiority over traditional computing for a specific problem, that's Quantum Advantage. It's gradual, coming in waves that both progress and pause, but ultimately move the technology forward.

Three classes of problems at which quantum excels

Quantum computing is especially astute at simulations of nature; algebraic problems, including machine learning, differential equations, and dealing with matrices; and quantum search-and-graph problems.

The quantum computing "prioritization matrix"

Evaluating the potential business impact of quantum computing applications can be challenging. We show you how to evaluate which potential quantum computing applications are better positioned to deliver optimum business benefits.

Chapter Three

Quantum Advantage and the quest for business value

Quantum Advantage—as introduced on page 7—occurs when a computing task of interest to business or science can be performed more efficiently, more cost effectively, or with better quality using quantum computers. This is the point where quantum computers plus classical systems can do significantly better than classical systems alone.

But Quantum Advantage is not a dramatic, all-at-once event. It will be more ambiguous, coming in waves that both progress and pause, but ultimately move the technology toward achieving concrete business value. Each use case has its own unique timeline for Quantum Advantage. The particular quantum computing system or ecosystem partner you're engaging can influence that timeline and advantage as well. Fortunately, Quantum Advantage can benefit from a domino effect in which successes in one use case can cascade to others.

"Exponential acceleration can occur after an initial use case. What we learn from those early use cases can be applied to others."

Sabrina Maniscalco
Professor of Quantum Information and Logic, University of Helsinki
CEO, Algorithmiq Oy

As we evaluate the time it will take to attain Quantum Advantage, it's helpful to understand a bit about the current systems and where we are heading. Today's qubits are subject to errors from hardware limitations and "noise" from the surrounding environment. If superconducting qubits—which live at a temperature close to absolute zero—aren't protected from noise by keeping them in a vacuum, vibrations or stray photons hitting the device could ruin a computation. The same goes for heat and ambient effects. Remember, quantum computing is built on the physics of quantum mechanics, and that is the model for interactions at the atomic, electron, and photon level. Coupling to the environment could disturb what we are doing in our system.

More precisely, qubits in quantum hardware are called *physical qubits*. Currently, quantum computing use cases are enabled by the types of algorithms available to us but we are limited to implementing them using noisy physical qubits. While we expect it may be possible to reach the earliest Quantum Advantage examples with physical qubits, we will need to move to logical qubits to achieve quantum computing's full value. Logical qubits are created by combining software with hundreds of physical qubits to implement error-correction. With this type of qubit, errors coming from noise affecting the underlying hardware can be both detected and corrected. Implementing quantum error correction is a crucial goal for this decade.

As we progress through the Quantum Decade, one important question needs hashing out: As the results from quantum computing truly transcend those of classical, how do you evaluate them? They're well past validation from traditional techniques and traditional computers. When conducting theoretical research, the issue might not be as consequential. But in scenarios that impact real-world health and safety, it's a daunting question.

Out of necessity, we need to veer away from classical validation—it simply won't keep up—to using multiple "flavors" of quantum computing. This could mean benchmarking across different modes of quantum computers themselves, or even different ecosystems. Validation and quantification of results could ultimately elevate some systems over others in terms of reliability and accuracy. It's yet another factor that can influence waves of Quantum Advantage.

"In order for quantum computing to be an advantage, you have to have confidence in and trust the results. Look at it this way. If a quantum computer designed a parachute for you, would you be willing to wear it and jump out of a plane?"

"For example, would three different quantum facilities come up with the same answers, with similar error rates and answer sets? It's through consensus that you get confidence."

Peter Tsahalis
CIO of Strategic Services and Advanced Technology
Wells Fargo

At IBM, we see those waves aligning into three phases (see Figure 14).

- **The first wave is low tide and low key.** There may be murmurs in some industry and academic research corners, but overall results are not heavily publicized. Those with the foresight to experiment with the technology may see value, followed by ways to improve, then applications for other areas and new algorithms.

- **The second wave is high tide.** Breakthroughs are more structured and commonplace. Conversations about quantum computing are gaining currency. More organizations are aligning with ecosystems, experimenting with cloud-based quantum computing services environments, and test-driving quantum computing with increasing success.

- **The third wave? Here comes the tsunami.** Much can change, and industries are transformed. Quantum machine learning comes to the forefront, and breakthroughs grow more complex and revolutionary. This is where the Quantum Decade reaches a crescendo, with a strong surge into error-corrected quantum computations.

Ultimately, the third wave confers Quantum Advantage to organizations, end users, and society overall. How can airplanes be manufactured with less corrosive metals—and fly more safely with less maintenance? How can the medical industry better personalize diagnoses, treatments, and pharmaceuticals (see case study, “IBM and Cleveland Clinic” on page 22)?

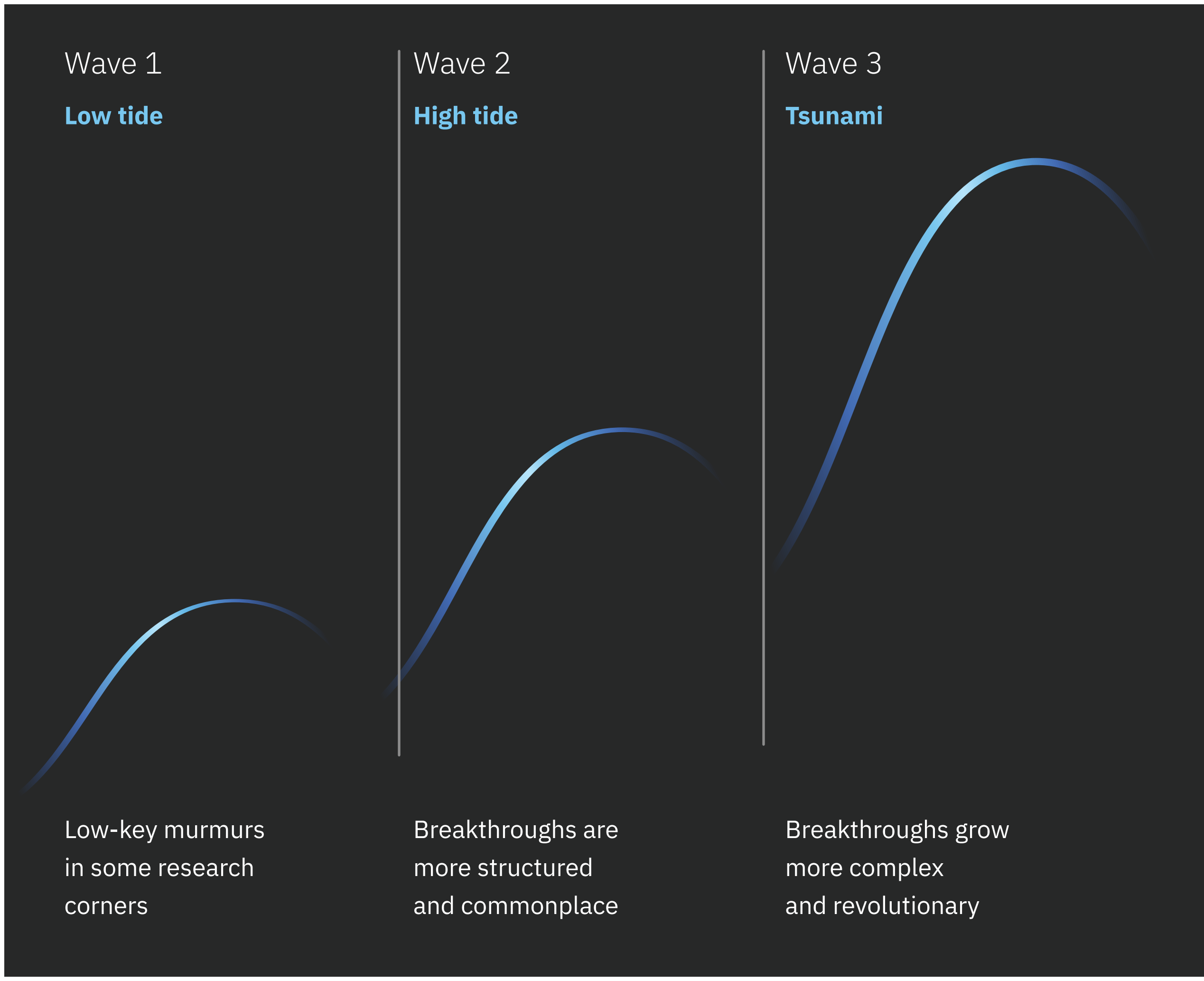
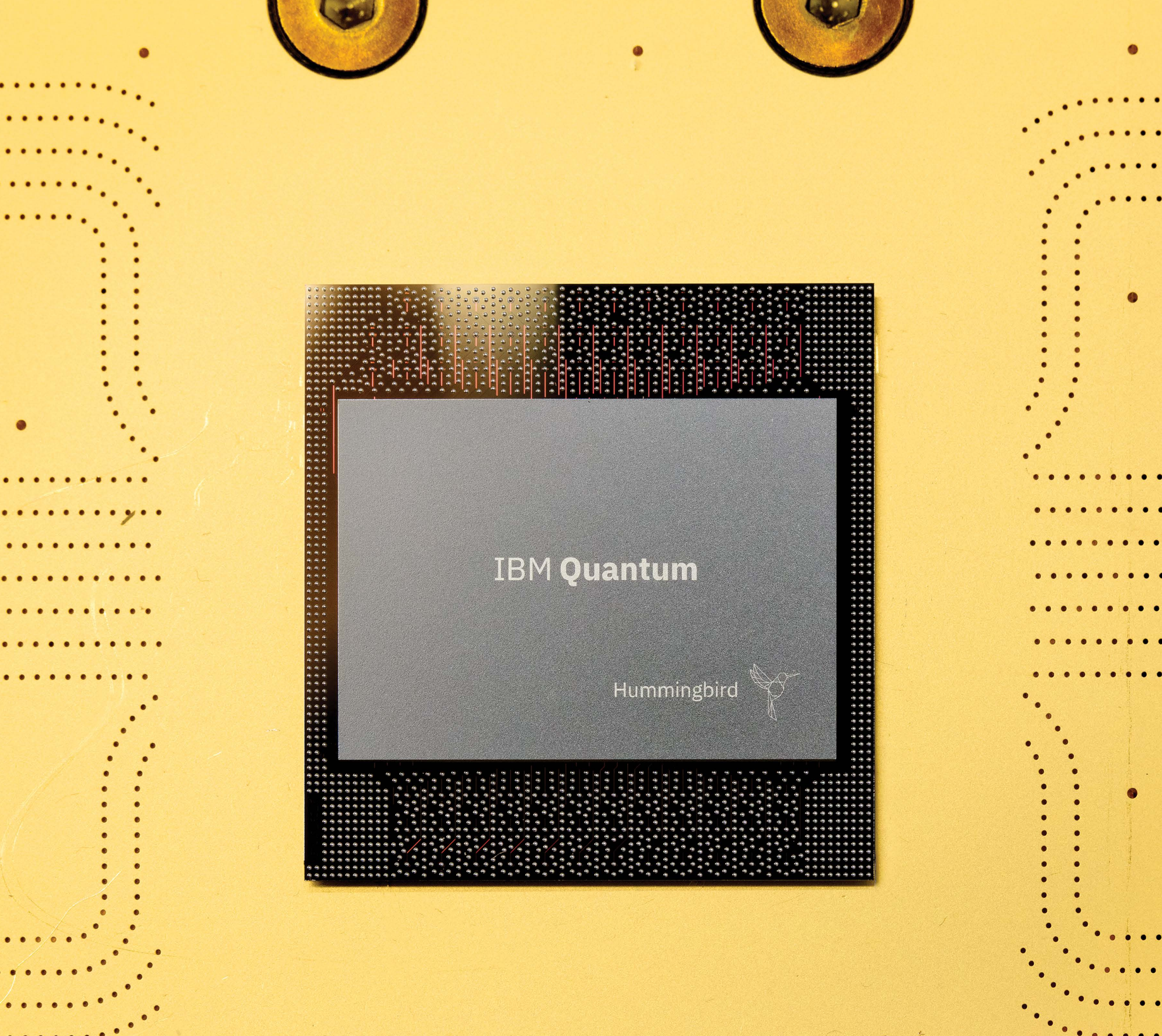


Figure 14

The three waves

From low tide to tsunami



The 65-qubit IBM Quantum Hummingbird quantum processor, slightly larger than a US penny coin

To put it in perspective, some experts believe that quantum computing is where AI was in 2010. By virtue of the exponential nature of the technology, quantum computing has the potential to take off even faster.

"In 10 years, we will have achieved what took 40 to 50 years in classical computing. In the '60s, '70s, and '80s, computer science was niche, almost a dark art. But by 2030, we will have figured out how businesses can use quantum computing—with no in-depth knowledge of how it actually works."

Ilyas Khan
Founder and CEO
Cambridge Quantum Computing

However, it will take investments in carefully considered use cases to reveal quantum computing "killer apps" by industry domain. To get a grasp on evaluating quantum computing's commercial potential for your industry, we'll jump into how quantum computing can help specific classes of problems, and from there, a methodical approach to prioritizing use cases. We've also included an extensive set of Industry Guides outlining industry-aligned use cases and scenarios on page 69—detailed guides to what quantum computing could mean for you.

Ultimately, Quantum Advantage comes down to results.

"At the end of the day, executives need capabilities. They care about the business answer. They're agnostic as to how that gets done, and that won't change. You don't go to business leaders with quantum solutions per se. *You go to them with ways to better optimize their business."*

Christopher Savoie
Founder and CEO
Zapata Computing

Quantum computing at its best: Three classes of problems[39]

What could the commercialization of quantum computing mean for your organization? What types of problems are the best candidates for Quantum Advantage?

In the near-to-medium term, quantum computing could confer business benefits in three areas: simulation, search, and algebraic problems (see Figure 15).

Quantum simulation of natural processes
Because quantum mechanics describes how nature works at a fundamental level, quantum computing is well-suited to model processes and systems that occur in nature (see case study, "IBM Researchers: Exploring the molecular simulation of water").

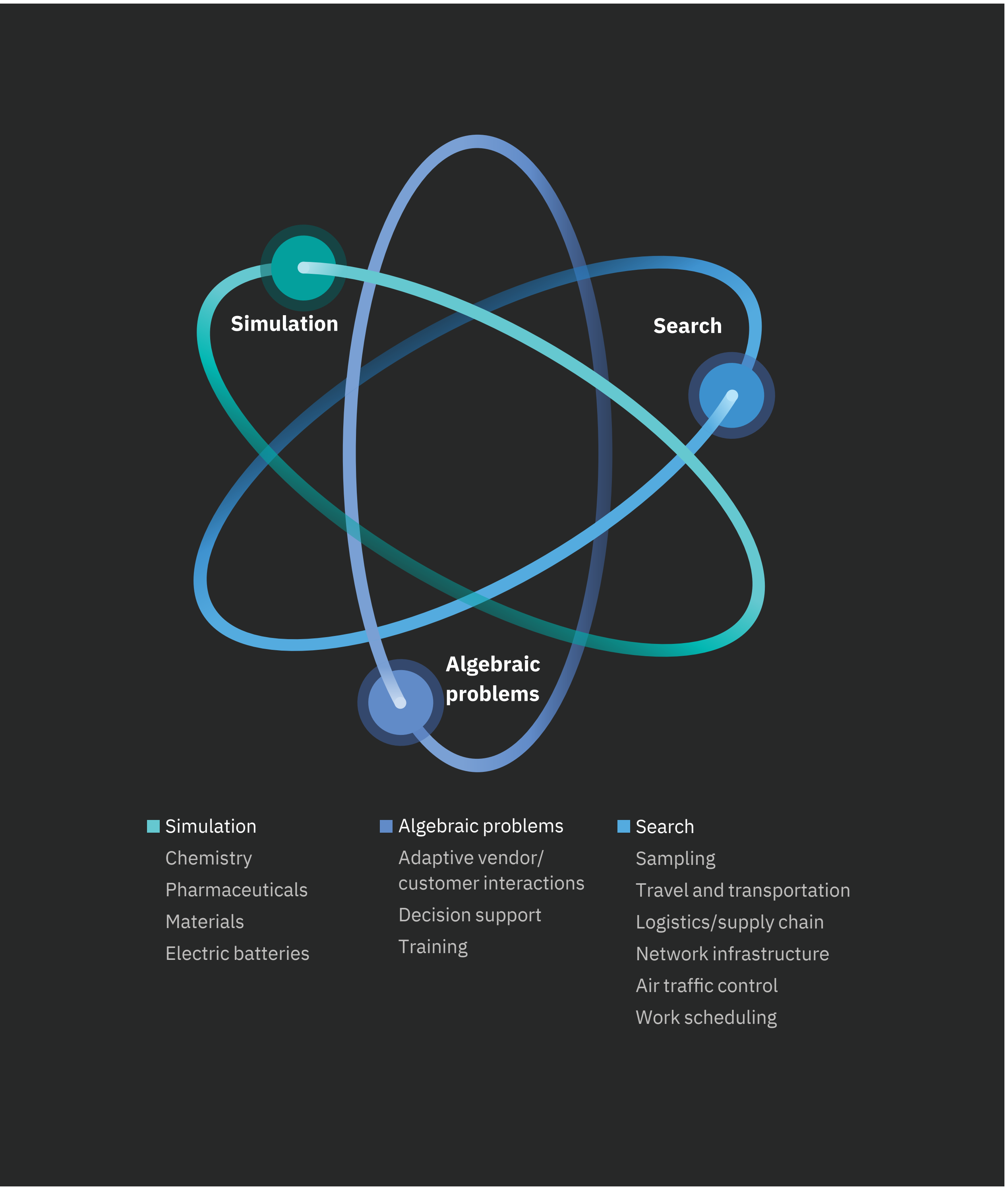


Figure 15

Where the rubber meets the road
Anticipated uses of quantum computing

IBM researchers
Exploring the molecular simulation of water[40]

The future is not quantum computing alone. Rather, it's the convergence of quantum computing, classical computing, and AI that has the power to transform. Combining classical and quantum computations in nontrivial ways, trading off one for the other, can enhance the capabilities of any one on its own and increase what is possible with the resources available.

The methods described here harnessed classical and quantum resources to capture quantum correlations and *double* the size of the system that can be simulated on quantum hardware.

Exploiting the symmetries of the problem, IBM researchers developed a technique to split the quantum circuits into smaller ones, capturing the most challenging aspects of the computation and requiring only half as many qubits as the full circuit. This strategy allowed them to not only reduce the number of qubits needed but also to make the quantum circuits required shallower. Each smaller circuit was run separately on a quantum computer and the outputs combined using classical post-processing techniques.

The researchers tested this method in a molecular simulation of water. In this case, the parts of the problems difficult to simulate could be reduced to 10 orbitals, or wave functions. These orbitals could be represented on five qubits of an IBM Quantum processor to compute the ground state energy of the molecule in the most accurate simulation to date.

Methods like this have the potential to scale by doing twice as much with the resources available, trading off quantum and classical computations to expand the computational reach of the quantum computing systems. This method can prove productive in materials discovery workflows.

Search and graph problems

The art of solving optimization problems involves searching for the "best" or optimal solution in a situation where many possible answers exist. Take the example of building a package delivery schedule. Mathematically, more than 3.6 million possible combinations exist for scheduling 10 deliveries in adjacent time slots.[41] But which schedule represents the optimal solution, given variables such as timing requirements of the recipients, potential delays, and the shelf life of transported goods? Even when applying approximation techniques, the number of possibilities is still far too large for a classical computer to explore (see case study, "ExxonMobil").

As a result, classical computers today take extensive shortcuts to solve optimization problems of significant size. Unfortunately, their solutions are often suboptimal. Businesses that could benefit from quantum search-and-graph optimization include:

- Telecommunications companies upgrading their network infrastructure
- Healthcare providers optimizing patient treatments
- Governments improving air traffic control
- Organizations developing employee work schedules
- Universities scheduling classes.

While no one has yet delivered a mathematical proof confirming that quantum computing will confer an exponential speed-up for search-and-graph problems, researchers are working on demonstrating this heuristically. Forward-thinking companies are already exploring solving optimization problems using quantum computing in their quest to leap ahead of competitors. Their foresight may prove warranted after the first demonstrations of Quantum Advantage in optimization are confirmed.

Algebraic problems

Algebraic problems include linear systems of equations, differential equations needed for industry problems, problems relevant for machine learning, and operations on matrices. Mathematical problems like some methods of machine learning and options pricing in finance involve the mapping and evaluation of functions over a multidimensional parameter space.

The state of qubits in a quantum computer is itself a complex high-dimensional space capable of exploring aspects of data inaccessible to classical computers. In fact, a symbiosis between AI and quantum computing is beginning to spawn a virtuous cycle of advancement in both fields. For example, quantum algorithms can enhance machine learning in the area of data clustering.[42] But machine learning can be used to better understand quantum systems.[43] Other businesses that could benefit in this area include consumer products and retail companies tailoring marketing offers (see case study, "IBM Quantum and University of California, Berkeley researchers" on page 58).

ExxonMobil
Investigating the use of quantum computing to help optimize global journeys[44]

How do you orchestrate tens of thousands of merchant ships traversing the oceans to deliver the consumer goods we use in our daily lives? Roughly 90% of world trade is dependent upon maritime shipping. More than 50,000 ships, carrying as much as 200,000 containers each, move around every day, transporting goods worth $14 trillion.

On an international scale, optimizing this magnitude of shipping routes is intractable for classical computers. Research teams from ExxonMobil and IBM are using this scenario to investigate how to effectively map optimization problems to quantum computers.

In 2019, ExxonMobil was the first energy company to join the IBM Quantum Network, a consortium of organizations that are provided access to advanced quantum computing systems and tools. ExxonMobil has used the network's capabilities to explore methods that map the routing of merchant ships globally to quantum computers.

The advantage of quantum algorithms is rooted in their ability to reduce incorrect solutions while amplifying correct solutions. Using the Qiskit quantum optimization module, ExxonMobil set out to test various quantum algorithms. Depending on the aspects of the problem, some heuristic quantum algorithms performed slightly better than others, and Variational Quantum Eigensolver (VQE)-based optimization performed better depending on the choice of the ansatz (in physics terms, this is an educated guess or assumption).

These investigations could easily apply to other industries and use cases that involve time constraints. Scenarios could include goods delivery, ride-sharing services, or urban waste management.

IBM Quantum and University of California, Berkeley researchers

A winning algorithm for quantum machine learning[45]

Machine learning in a quantum computing environment is intriguing to researchers. Over the past few years, they have proposed quantum machine learning algorithms that promised quantum speed-ups over their classical counterparts.[46] Most of these learning algorithms assumed access to the data as coherent quantum mechanical states—*yet the world operates with classical data.*

Researchers from IBM Quantum and the University of California, Berkeley explored the possibility of finding circuits that are hard for classical computers and using them to provide an advantage in machine learning tasks requiring only access to classical data.

In the case of supervised machine learning, the researchers in this case study map data to spaces in higher dimensions, or feature spaces, to work with it, and the space of the state of multiple qubits is itself rich and high dimensional. In other words, a quantum environment takes data to those high dimensions naturally.

The researchers used quantum circuits to map classical data to the higher dimensional space of multiple qubits, and to estimate the quantum kernel, which is a similarity measure between the pieces of data. The estimated kernel was then used in a classical support vector machine to calculate the support vectors that separate the data.

In late 2020, the researchers provided rigorous proof of quantum advantage for a quantum feature map circuit over all possible binary classical classifiers, requiring access to just classical data. This may be useful in applications such as forecasting, prediction of properties from features in data, or risk analysis. For the first time, we have formal theoretical proof of Quantum Advantage in machine learning.

Prioritizing use cases for business value[47]

"It all comes down to the 'killer app' and what problem quantum computing can solve for your industry. It may not be obvious, just as in the early days of the internet, but it's about realizable use cases, not outlandish or esoteric problems."

Todd Hughes
Technical Director, Strategic Projects and Initiatives
CACI

Evaluating the potential business impact of quantum computing applications can be challenging, particularly given the complexity of this emerging technology. Your organization needs a way to evaluate which potential quantum computing applications are better positioned to deliver optimum business benefits.

A quantum computing "prioritization matrix" helps address this dilemma. Executives from various disciplines in your organization—including strategy, operations, innovation, IT, and risk—can evaluate the potential impact of quantum computing on their domains, prioritize quantum computing applications, and subsequently measure Quantum Advantage as your organization moves from early adoption to mainstream quantum computing.

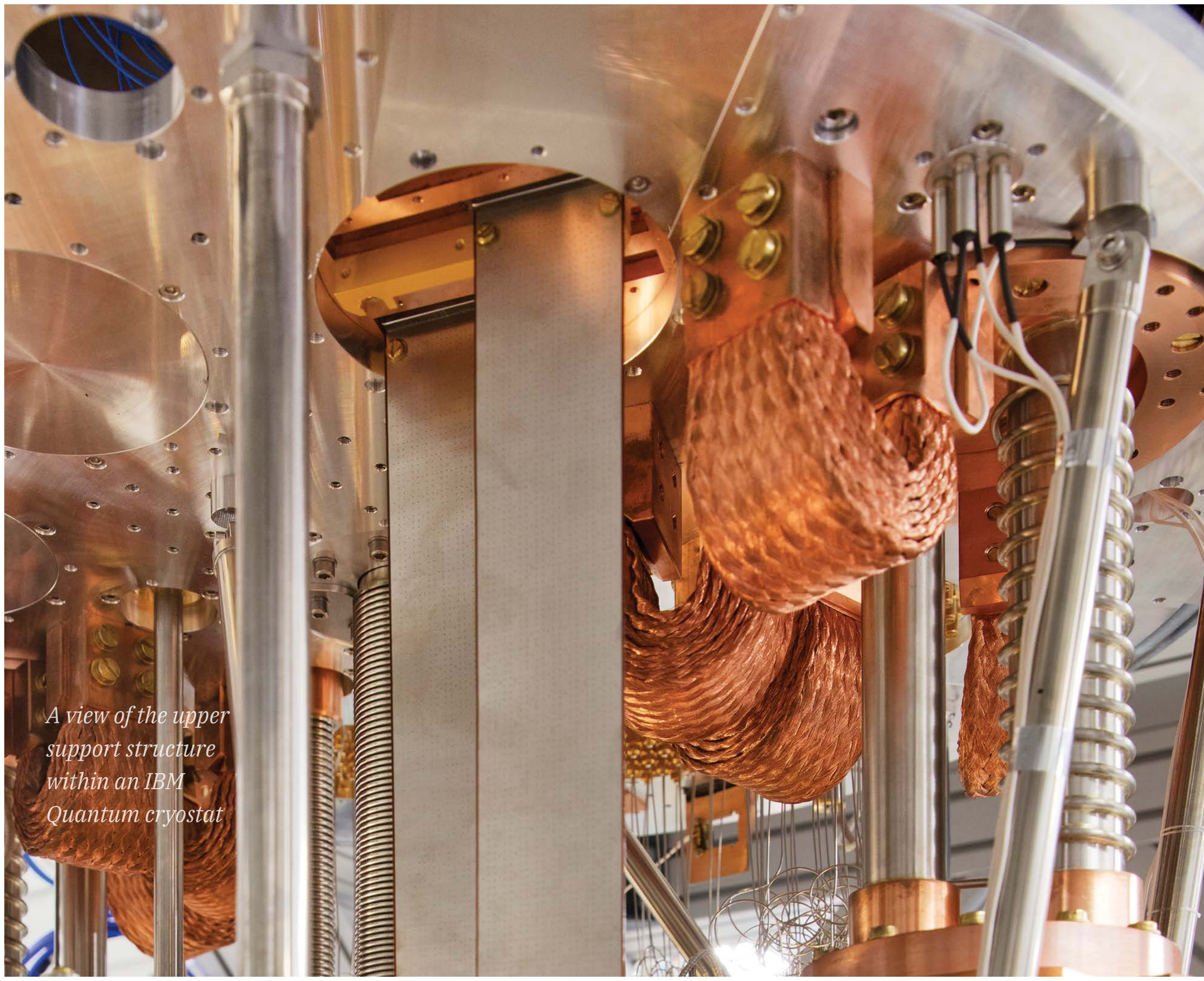
Our prioritization matrix categorizes quantum computing applications into four distinct categories:

"Early Bloomer"
applications are the most feasible to implement today.

"Late Bloomer"
applications promise significant Quantum Advantage in the future.

"Wild Card"
applications may or may not ultimately deliver clear business advantage.

"Mature Industry"
applications can deliver competitive advantage on a business scale.



A view of the upper support structure within an IBM Quantum cryostat

A tested prioritization framework[48]

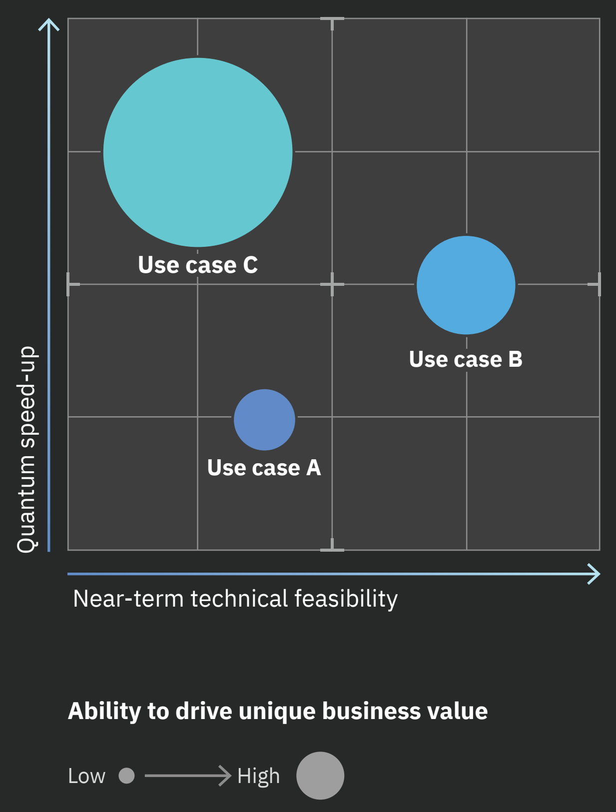


Figure 16

The quantum prioritization framework
A visual representation of decision trade-offs

Our quantum computing prioritization matrix helps executives evaluate each application in three dimensions (see Figure 16):

Quantum speed-up
Theoretical capacity to deliver technological advantage over classical computing solutions (Y-axis).

Near-term technical feasibility
Operational readiness (X-axis).

Relative potential business impact by use case
Ability to drive unique business value for a specific enterprise (bubble size).

Prioritizing quantum computing applications in this way provides a comprehensive portfolio overview, visually graphing an organization's decision trade-offs. As a result, you can make more informed decisions about your organization's quantum computing adoption based on strategic priorities, such as following a first-to-market strategy, a cost-optimization approach, or acting as an industry disruptor.

The Y-axis: Quantum speed-up

Overall, the promise of Quantum Advantage is to efficiently solve particular business problems that are not currently feasible (or are prohibitively expensive) to resolve due to today's computational constraints.[49] Correspondingly, where an application sits on the quantum computing prioritization matrix's Y-axis is dependent upon the theoretical magnitude of improvement a specific quantum computing algorithm is expected to deliver over a classical solution.

An individual application's Quantum Advantage may manifest in different ways. One example is a faster runtime to find a desired solution or a better approach to solving a problem that achieves greater accuracy.

The X-axis: Near-term technical feasibility

The quantum computing prioritization framework's X-axis depicts the technical requirements for quantum hardware and software needed to successfully execute each identified application. A key aspect of this is the expected qubit and performance requirements. Placement on the X-axis is also impacted by further quantum computing hardware and software considerations, such as chip and algorithm design, qubit interconnectivity, number of gates and qubits used in the code, and the compiler's efficiency.

Even though quantum computing technologies are in a nascent state, some algorithms, such as quantum approximate optimization algorithm (QAOA) or quantum support vector machines (QSVM), have shown potential to run better on near-term quantum systems due to their shorter circuit-depth requirements, while other algorithms will need mature quantum computing systems to run more sophisticated problems.[50]

Bubble size: Business impact

The third dimension of the quantum computing prioritization matrix is tailored to the size of the business impact each application is predicted to have for a specific enterprise. This dimension incorporates business metrics exclusively chosen by each organization. As part of each individual company's selection process, it is important to realize that assessing business impact is more than merely measuring economic outcomes.

Metrics should be a blend of market outcomes and competitive consequences, as well as financial impact. For example, depending on an organization's strategic objectives, this dimension may include measures of value chain enhancement, operational improvement, market disruption and/or innovation, market share growth, revenue generation, cost reduction, and/or risk mitigation.

Quantum computing application classification[51]

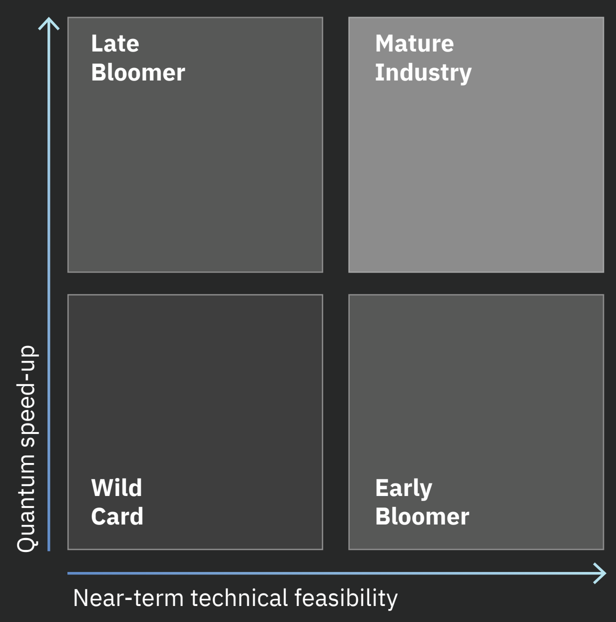


Figure 17

Quantum computing application categories
Rapid responses through diversified applications

As noted earlier, employment of the quantum computing prioritization matrix elucidates four quantum computing application categories: Early Bloomer, Late Bloomer, Wild Card, and Mature Industry (see Figure 17). Identifying a diverse mix of these types of applications prepares your organization to respond rapidly to breakthrough advances in quantum computing technology (see Perspective, “Applying the quantum computing prioritization matrix” on page 64).

Early Bloomer

Early Bloomer applications are the "no-brainers." Because their solutions are heuristic, businesses can experiment with and use them to help build talent. Since Early Bloomer applications operate using existing technology, their adoption is a profound step for organizations learning how to use quantum computing. The use of these applications helps clarify how to integrate quantum computing into your current business processes and build momentum for additional quantum computing adoption. Adopting Early Bloomer applications initially may be critical to sustaining marketplace relevance, as they may establish the basic requirements necessary to remain competitive.

Late Bloomer

Late Bloomer applications pose the "innovator's dilemma." They promise the greatest Quantum Advantage, but they require more advanced quantum computing technology to solve meaningful business problems. Late Bloomer applications can potentially transform competition in particular industries through their potential to significantly impact business value in the future. Because it is less clear when Late Bloomer applications will become technically feasible, your organization needs to keep a close watch on advancements in quantum computing. A new quantum computing algorithm or hardware approach could cause a Late Bloomer to leapfrog into technical feasibility. Due to their expected impact on company value chains, competitive success can accrue disproportionately to those companies that are first to recognize and implement Late Bloomer quantum computing applications.

Wild Card

Wild Card applications do not currently exhibit a straightforward path to deliver the substantial Quantum Advantage of Late Bloomers, nor are they as technically feasible as Early Bloomer applications are today. While they may or may not ever pan out, evaluating them helps you to better understand how quantum computing's attributes could apply to your organization's future success. These long shots are not to be completely counted out. As quantum technology evolves, some Wild Cards may transform into Early or Late Bloomers.

Mature Industry

Mature Industry applications are the ultimate goal for businesses leveraging quantum computing. Although no application has yet demonstrated Quantum Advantage at business scale, in the future—if quantum computers achieve sufficient scale and quantum computing applications demonstrate competitive value—some will confer business advantage, transforming company operating models and industry value chains. Some applications already in development may be placing their creators on the path to significant marketplace success even now.

Perspective
Applying the quantum computing prioritization matrix[52]

To illustrate how the quantum computing prioritization matrix works, let's take the actual quantum computing application investigation undertaken by a financial services trading organization. This financial institution identified four potential uses of quantum computing that are computationally challenging for conventional machines:

1. Value-at-risk analysis

Strengthening risk mitigation by developing more accurate risk-simulation models.

2. Derivative pricing

Improving the pricing of financial assets using market-scenario simulations.

3. Fraud detection

Enhancing the detection of irregular patterns to flag fraudulent transactions and imposters.

4. Credit/asset scoring

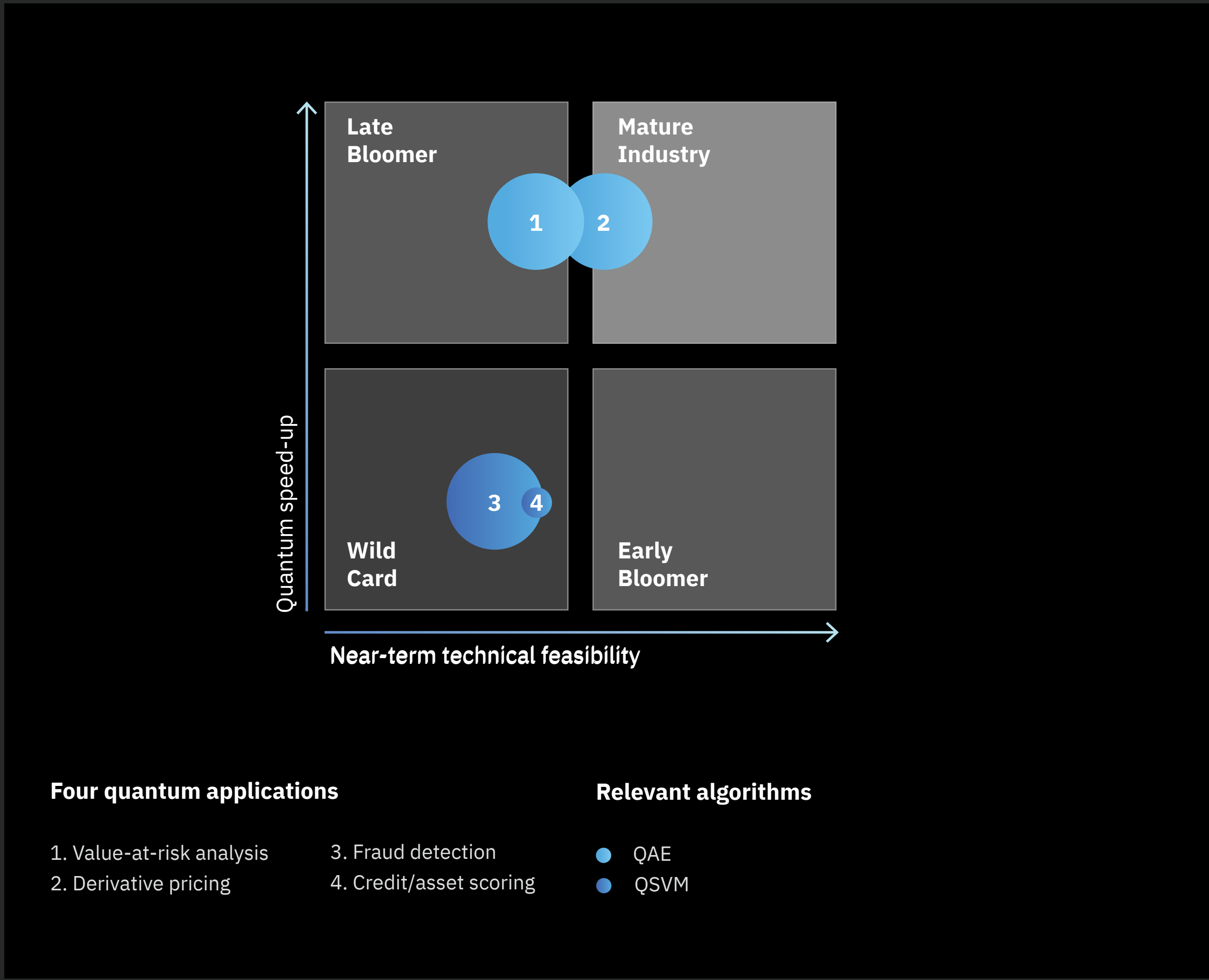
Strengthening the statistical analysis that segments customer financial solvency and bond ratings.

Each of these potential applications can be solved by a specific quantum computing algorithm that helps designate its level of quantum speed-up and its stage of technical feasibility (see figure):

—Value-at-risk analysis and derivative pricing are solved with a simulation algorithm, called quantum amplitude estimation (QAE), to estimate scenarios. This type of algorithm delivers a quadratic speed-up while improving the quality of the solution, even though quantum error correction could diminish the advantage. However, it requires mature quantum computing systems. Applications associated with this algorithm are usually identified as Late Bloomers.

—Fraud detection and credit/asset scoring are solved with machine-learning algorithms for classification and prediction (QSVM). This type of algorithm can run on near-term quantum systems and may bring increased accuracy. However, the benefit needs to be proven as quantum system capacity increases, typically placing associated applications as Wild Cards.

The business value these applications might collectively bring to the financial services industry could surpass $10 billion in the first year of their launch.[53] Enhancing fraud detection and reducing monetary losses from money laundering could deliver more than half of the total.



Quantum prioritization in practice
Four financial applications

Perspective
Charting a path to business value[54]

We have outlined five steps to developing a quantum computing portfolio for your organization.

Step One

Identify the quantum computing skills your organization needs.

Determine whether to acquire them directly, hire a consultant, and/or join an existing quantum computing ecosystem to access them.

Step Two

Identify potential quantum computing applications.

Select business problems or opportunities likely to benefit from the unique capabilities of quantum computing, such as those constrained by resources or huge optimization calculations.

Step Three

Position each application on the quantum computing prioritization matrix.

Evaluate the technology profile of each proposed application, both in terms of potential quantum speed-up and near-term technical feasibility, based on state-of-the-art quantum computing hardware and algorithms.

Step Four

Determine the expected business impact.

Assess the size of the projected business impact by analyzing each application's potential competitive advantage and expected financial benefits specific to your organization.

Step Five

Plan for quantum adoption.

Determine whether you will purchase a quantum computer or access the latest quantum computing technology through a partnership arrangement. Plan for quantum computing's impact on your internal workflows, including potential process redesign and resource allocation adjustments.

Questions to ask

Question One

Where do you see your organization positioned during each of the "three waves" of Quantum Advantage?

Question Two

Think about your intractable industry problems we discussed in Chapter Two.

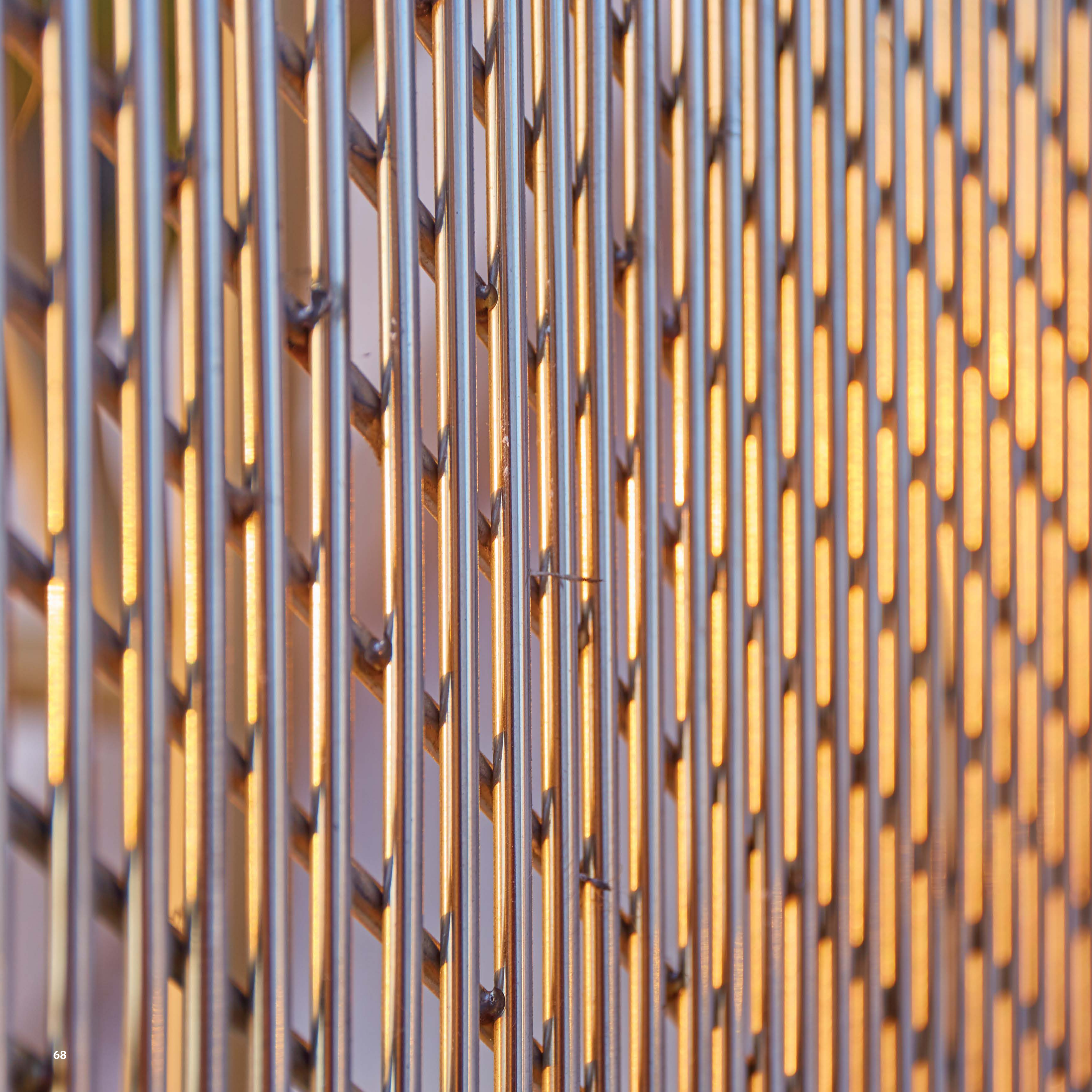
How do simulation, search, and algebraic use cases play in their resolution?

Question Three

Take the quantum computing prioritization matrix for a test drive.

What were the results?

Were there any surprises?



Industry Guides

As we've discussed, Quantum Advantage occurs when a computing task critical to science or business can be performed more efficiently, more cost effectively, or with better quality using quantum computers. This is where quantum computers plus classical systems can transcend what classical systems can do alone.

As hardware, software, and algorithmic advancements in quantum computing converge, enabling significant performance improvement over classical computing, new opportunities for advantage will emerge across industries.

In this section, we provide quantum adoption information across five specific industries: airlines, banking and financial markets, chemicals and petroleum, healthcare, and life sciences. Each section contains industry-specific observations and use cases to help guide your quantum journey.

While attaining Quantum Advantage can take some time, it can still trigger exponential achievements in usage and learning that can benefit your business—and industry—now.

Quantum computing applications

Airlines

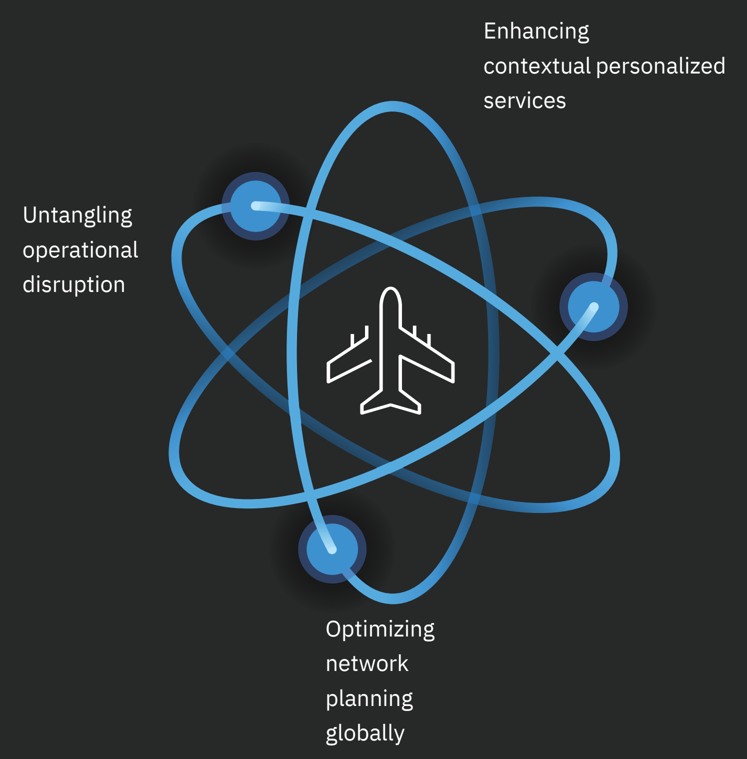
Organizations in the travel and transportation sector took some of the worst hits from the COVID-19 pandemic. Record losses are expected in the airlines and hotel industries, with a return to growth not expected until 2023 or 2024.[55] Resuming global travel and work requires embracing financial, health, and safety measures amid the uncertainty of a post-pandemic recovery.

Some organizations view the crisis as an opportunity not only to survive, but to evolve and emerge stronger. A winning strategy involves looking beyond survival to anticipate future pent-up demand and prepare for growth by exploring new technologies and solutions for first-mover advantages. Quantum computing is one of these technologies.

Quantum computing opens the door to new opportunities across industries, mainly through higher computational speed, greater accuracy of data-driven actions, and the creation of new algorithms and systems capabilities to address challenges that classical systems cannot solve. Quantum computing capabilities could play a crucial role in solving airlines' complex business problems.

Following are three use cases where Quantum Advantage may transform how airlines seek to optimize operations and improve customer experience.

Quantum computing use cases for airlines



Use case

Untangling operational disruption for airlines (IROPS)

Pandemics, storms, earthquakes, operational issues, technical problems, and other challenges can wreak havoc on airline schedules and staffing. Recovering from such disruptions is one of the most difficult problems that airlines manage. Current solutions are fragmented and primarily focused on operational information, with less consideration given to inventory, profit maximization, or even the impact on customer service and satisfaction.

Airlines currently work through these disruptions—known as irregular operations (IROPS) management—using suboptimal algorithms on classical computers. Due to the limitations of current computers, each specific element, such as crew, slots, and equipment, is managed in a sequential and siloed manner. System-wide recovery can take a week or more, threatening passenger satisfaction, and second-order effects on other flights and airports can drive higher costs for an airline.

The technical limitations of current IROPS solutions are primarily linked to:

1. Lack of data visibility to incorporate all relevant inputs into the resolution of the disruptions.
2. Fragmentation of solution development. Different parts of the IROPS problem—fleet, crew, passengers, look-ahead impact—are solved separately in multiple steps with different tools, which leads to suboptimal and inefficient solutions.

It's the second limitation—fragmentation of solution development—where quantum computing could help. Due to the massive scope of IROPS and the resulting complexity of the underlying global mathematical optimization problem, solving a single operational disruption on today's computers could take years—or even centuries. With improvements in quantum algorithms and better error-correction schemes, airlines may be able to:

— Improve the accuracy and speed of scenario simulations that quantify the impact of potential solutions on future flights and passengers—and do it in time to respond to a disruption. Quantum computing algorithms have already proven effective in choosing the best scenarios in Monte Carlo simulations used in banking and finance.[56]

— Provide a simulation tool to operation control center analysts so they can proactively test scenarios before a major event that may disrupt operations, such as air traffic control or crew work stoppages or aircraft delivery delays. Due to the complexity of these issues, today they can only be solved for each functional area separately, thwarting the development of integrated solutions.

— Deliver advisory tools to customer service agents and automated customer care systems using quantum machine learning to advise on best approaches to IROPS resolution. For example, a quantum computing algorithm could advise agents on how to best compensate each specific customer whose travel has been disrupted based on personal preferences for cash, accommodations, upgrades, or other amenities. Imagine how customer satisfaction might improve if you could do this today.

In these ways, quantum capabilities could dramatically shorten recovery time and reduce the cost of irregular operations while mitigating their negative impact on passengers.

Use case

Enhancing contextual personalized services for airline customers

For the global travel industry, one of the pivotal actions for survival and recovery is to restore customer trust and confidence by creating personalized services that emphasize health and safety measures. For airlines specifically, it's key to differentiate services, improve customer experience, and drive incremental revenue though individualized offerings. Providing personalized customer engagement and services requires four specific steps:

1. Collecting and extracting data, including customer data and transactional data.
2. Performing data engineering to build customer data features.
3. Training customer segmentation models based on customer and journey context features.
4. Scoring and identifying the best offers depending on customers' individual travel contexts.

Today's personalized offering systems often fall short of living up to their promises, mainly because of limitations in the customer segmentation step. Current segmentation methods often rely on basic customer features, such as demographic and sales data, but do not include contextual data, reducing the pertinence of the recommended offer. Current systems also lack multidimensional segmentation to effectively capture contextual differences in preferences, intent, and behavior of travelers. One reason for the absence of contextual features is insufficient computing capacity and scale to handle the high number of data elements required to build complex segmentation models.

The "segment-of-one" is a personalization strategy for which scalability is probably the biggest challenge. As sophistication in digital marketing grows, organizations are likely to see increases in the number of users for whom they need to create personalized experiences. It is one thing to personalize a landing page for one customer segment, but it's a completely different challenge when you have hundreds of personas, multiple geographies, a dozen sites, and thousands of places where personalization is needed. At that point, personalization strategies need to scale in order to be feasible.

Quantum computing may solve these problems, enhancing the personalization process by:

—Supporting richer customer segmentation, incorporating more complex customer features for multidimensional passenger segmentation, and allowing for higher specificity in contextual profiling to improve personalized offerings.[57]

—Improving the accuracy of machine learning models that deliver insights and interpretability of results to help marketers or customer service agents better understand the causality links between customer data and delighted passengers.

—Potentially enabling the identification of a dramatically greater number of finely tuned customer segments that is unmanageable for classical computers through better machine learning capabilities.

If airlines can leverage quantum computing to unlock the promise of contextual and dynamic personalization, that personalization can then help increase ancillary revenue, provide better customer experience, and support service differentiation.

Use case

Optimizing airline network planning globally

In addition to the steep decline in global travel demand due to the COVID-19 pandemic, airlines are also facing major shifts in customer preferences for new routes, close-to-departure bookings, and no-fee itinerary changes. Addressing such challenges requires dynamic and flexible network planning processes that can no longer depend on historical demand data.

Network optimization, from flight planning and fleet allocation to crew scheduling, is at the heart of airline operations, significantly impacting operational costs. But, despite substantial efforts dedicated to streamlining this process, there are still important limitations. They are mainly linked to a step-by-step approach that leads to local optimization of the sub-processes deployed with isolated decision support tools. These tools generate suboptimal, local, and uncoordinated solutions.

For example, aircraft route planning often does not incorporate crew scheduling. Similarly, crew scheduling does not include block times, and block-time planning does not factor in fuel planning, often with detrimental consequences. Additionally, network planning typically does not coordinate its solution optimization with revenue management (RM) and pricing, resulting in two major processes happening daily with the same objective—profit optimization—but with separate models and parameters.

This out-of-sync approach leads to inferior solutions in terms of total cost, profit, and adapting to change. It also causes confusion during key operational updates, such as the introduction of new types of aircraft or the opening of new routes. While RM or pricing is optimizing offers based on schedule, capacity, and aircraft configuration, network planning may be inadvertently changing these parameters based on profit optimization. The main reason for airlines taking this distributed solution path is the complexity required to solve a global network optimization problem in a single step. It is practically impossible to solve with current classical computers alone.

In the future, quantum computers, working in concert with classical computers, should enable an airline network to co-optimize fleet, schedule, block/gates, crew, and fuel, while dynamically coordinating with RM, pricing, cost targets, sales, and customer relationship management (CRM). This is because quantum optimization algorithms can search the universe of solutions more widely and efficiently.[58] In order to make the best use of future quantum capabilities, airlines need to change the way they manage network operations, with more centralized operating models and tighter data integration. The expected results could be a proprietary competitive advantage for the airlines that embrace quantum technology.

Quantum computing applications

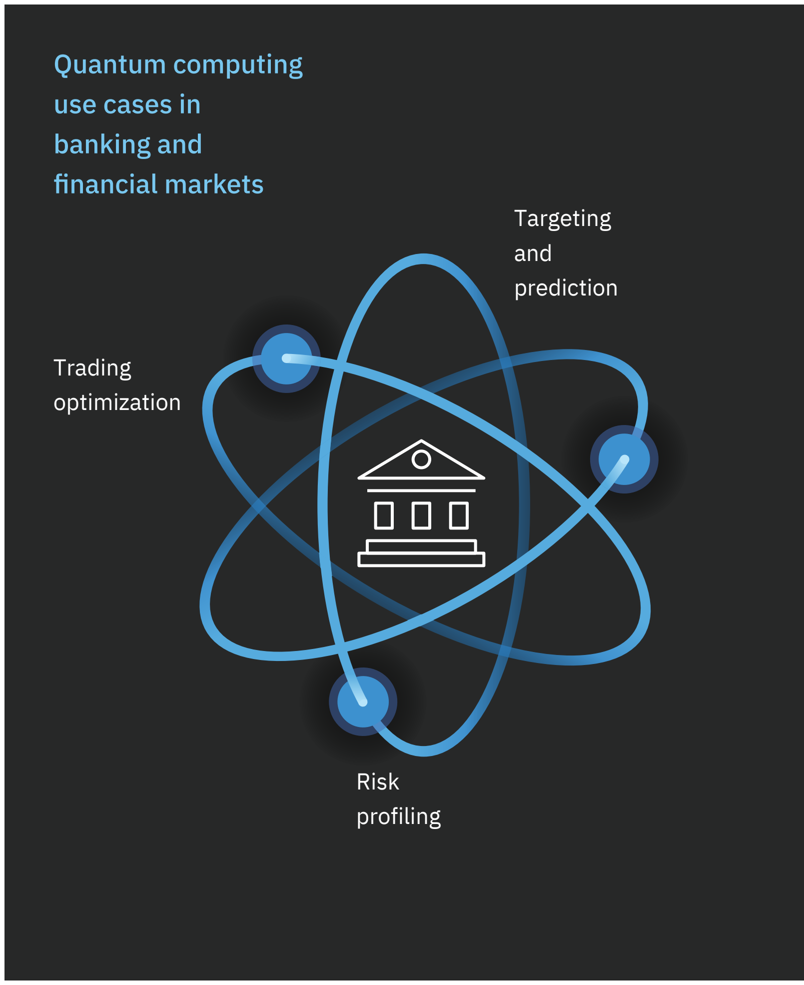
Banking and financial markets

The financial services industry has a history of successfully applying physics to help solve its thorniest problems. The Black-Scholes-Merton model, for example, uses the concept of Brownian motion to price financial instruments—like European call options—over time.[59]

Applying emerging quantum technology to financial problems—particularly those dealing with uncertainty and constrained optimization—should also prove hugely advantageous for first movers. Imagine being able to make calculations that reveal more profitable arbitrage possibilities that competitors are unable to see. Beyond that, employing behavioral data to enhance customer engagement and enabling faster reactions to market volatility (for example, intraday versus overnight risk calculations) are some of the specific benefits we expect quantum computing to deliver.

While broad commercial applications may remain several years away, quantum computing is expected to produce breakthrough products and services that will likely solve very specific business problems within three to five years.[60] Quantum computing can also enable financial services organizations to re-engineer operational processes, such as front-office and back-office decisions on client management; treasury management, trading, and asset management; and business optimization, including risk management and compliance.

Quantum computing's specific use cases for banking and financial markets can be classified into three main categories: targeting and prediction, risk profiling, and portfolio optimization.



Use case

Targeting and prediction

Today's financial services customers demand personalized products and services that rapidly anticipate their evolving needs and behaviors. 25% of small- and medium-sized financial institutions lose customers due to offerings that don't prioritize customer experience.[61] Customer behavior patterns are complex, and missing aspects of these relationships can prevent financial institutions from providing preemptive product recommendations with optimal feature selection. This can lead to failure to grasp opportunities to expand current customer share of wallet or reach the 1.7 billion adults worldwide who are unbanked.[62]

A similar problem exists in fraud detection. According to some estimates, financial institutions are losing up to $10 billion a year in revenue due to poor data management practices, and total losses from fraud were as high as $56 billion in 2020.[63] Fraud detection systems remain highly inaccurate, returning in the vicinity of 80% false positives, causing financial institutions to be overly risk averse.[64] To help ensure proper credit scoring, the customer onboarding process can take as long as 12 weeks.[65] In today's digital age, where 70% of banking takes place digitally, consumers are just not willing to wait that long.[66] Financial institutions too slow in engaging effectively with new customers are losing them to more nimble competitors.

For customer targeting and prediction modeling, quantum computing could be a game changer. The data modeling capabilities of quantum computers are expected to prove superior in finding patterns, performing classifications, and making predictions that are not possible today because of the challenges of complex data structures.

Use case

Risk profiling

Financial services institutions are under increasing pressure to balance risk, hedge positions more effectively, and perform a wider range of stress tests to comply with regulatory requirements. Liquidity management, derivatives pricing, and risk measurement can be complex and calculations difficult to perform, making it hard to properly manage the costs of risk on trades. Today, Monte Carlo simulations—the preferred technique to analyze the impact of risk and uncertainty in financial models—are limited by the scaling of the estimation error. Simulating all of the risks in a financial institution can be prohibitive and may include portfolios of many options, requiring numerous samples and hours to complete.

Looking forward, we expect continual waves of overlapping amendments to regulations, directives, and standards, such as Basel III and its revisions.[67] They will require a much larger array of risk-management stress scenarios. As a result, compliance costs are expected to more than double in the coming years, including regulatory penalties and remediation in cases of non-compliance.[68]

In the face of more sophisticated risk-profiling demands and rising regulatory hurdles, research and breakthroughs in quantum computing capabilities may speed up these very long risk-scenario simulations with higher precision, while testing more outcomes.

Use case

Trading optimization

Complexity in financial markets trading activity is skyrocketing. For example, the valuation adjustments model for derivatives, the X-Value Adjustment (XVA) umbrella, has greatly increased in complexity, now including credit (CVA), debit (DVA), funding (FVA), capital (KVA), and margin (MVA).[69]

Due to greater transparency requirements from regulations, stricter validation processes are applied to trading, impacting risk-management calculations that need to align counterparty credit exposures with credit-limit utilization of derivatives portfolios.[70] Furthermore, significant investment frameworks and vehicles have changed. For example, bond exchange traded funds (ETFs) are projected to reach $2 trillion by 2024, and environmental, social, and government (ESG) investments are gaining traction, with $35 trillion invested in this asset taxonomy in 2019.[71]

In this complicated trading landscape, investment managers struggle to incorporate real-life constraints, such as market volatility and customer life-event changes, into portfolio optimization. Ideally, money managers would like to simulate large numbers of potential scenarios and investment options to validate sensitivities when estimating expected returns. Currently, finding the best rebalancing strategy that keeps up with market movements is significantly constrained by computational limitations and transaction costs.

Quantum technology could help cut through the complexity of today’s trading environments. Quantum computing combinatorial optimization capabilities may enable investment managers to improve portfolio diversification, rebalance portfolio investments to more precisely respond to market conditions and investor goals, and more cost-effectively streamline trading settlement processes for large portfolios.

Quantum computing applications

Chemicals and petroleum

The chemical industry has a hand in about 7%—or $5.7 trillion—of global domestic product, along with approximately 120 million jobs.[72] Developing new chemical products requires expensive and time-consuming lab work. Today, classical simulations of chemistry can help guide lab testing, but the accuracy of calculations decreases as the complexity of molecular interactions increases.

When attempting energy calculations in a quantum mechanical system such as large molecules, calculating all the different parameters, including the movement of electrons, becomes intractable on conventional computers. As a result, modeling many industrially important molecules becomes increasingly inexact—or simply too time consuming to wait for an exact solution.

Determining the electronic structure of molecules is imperative to understanding the reactivity of the molecule. As molecules increase in size beyond hydrogen (H_2), the mathematical descriptions of molecules that accurately capture electron-electron interactions, nuclear effects, etc. become increasingly complex. In fact, when a full configuration interaction calculation is performed classically, the algorithms have exponential scaling. However, due to the nature of quantum algorithms, chemistry calculations have been predicted to scale polynomially, a promising step toward the ability to perform exact calculations on molecules that are currently out of reach.

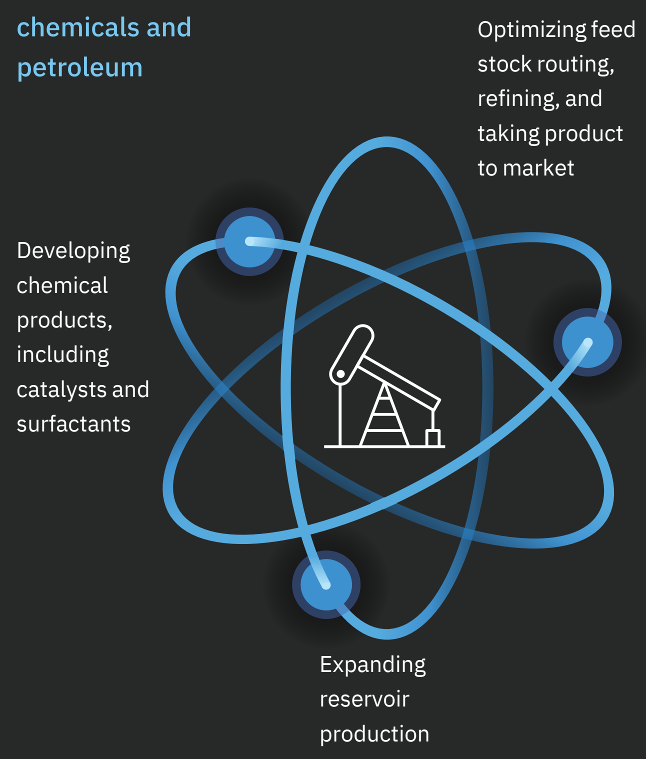
For example, the simple hydrocarbon Naphthalene ($C_{10}H_8$), could be modeled with ~116 qubits, but it would require a classical computer with 10^{34} bits to do the same.[73] For perspective, 10^{34} bits is 7.1 billion times the total volume of data predicted to be stored electronically by 2025—perhaps 175 zettabytes.[74]

Quantum computing may change the way chemicals are designed, hydrocarbons are refined, and petroleum reservoirs are located and produced. In the next few years, it may accelerate the go-to-market cycle in the development of new chemical products, refine investment strategies in light of tightening environmental regulations, and optimize complex systems that directly impact profits, such as transportation, refinery, and chemical plant processes.

Eventually, quantum computers may be able to tackle reservoir simulation and seismic imaging. Consequently, quantum computing is expected to fundamentally disrupt the landscape of the chemicals and petroleum industry. We have identified three powerful quantum computing use cases already being explored by chemicals and petroleum companies:

—Developing chemical products, including catalysts and surfactants
—Optimizing feed-stock routing, refining, and taking product to market
—Expanding reservoir production.

Quantum computing use cases in chemicals and petroleum



Use case

Developing chemical products, including catalysts and surfactants

In this use-case scenario, chemical and petroleum companies use quantum computers to accelerate the discovery and development of new chemical methods and materials. Prototype quantum computers, supported by classical computers, are already performing quantum chemistry simulations.

In 2017, a cover story in *Nature* showed depictions of the small inorganic salts lithium hydride (LiH) and beryllium hydride (BeH_2) modeled on IBM's publicly available quantum computers.[75] Application of these same variational methods to challenges in the chemicals and petroleum industry may soon be possible—such as applying insights to new catalysts for emissions reduction or surfactants to improve subsurface recovery. These possibilities, among others, have led some to consider chemistry the "killer app" for quantum computing.[76]

Use case

Optimizing feed-stock routing, refining, and taking product to market

Perhaps surprisingly, similar approaches (using Hamiltonians) employed in molecular modeling can be repurposed to address a wide range of optimization problems, from transportation and supply chain logistics to optimizing investment portfolios.[77]

In this use-case scenario, quantum computing could improve the profit margins of chemicals and petroleum businesses by determining optimal combinations of feed-stock routing, refining, and taking product to market. The impact on a refinery can be viewed as the estimated annual loss of business due to octane giveaway. Octane and vapor pressure giveaways result in an annual loss of more than $4.9 billion in the US and more than $4.2 billion in the European Union.[78]

Use case

Expanding reservoir production

In 1856, Henri Darcy, a French engineer trying to design water filtration systems for the city of Paris, created a simple experiment by flowing water through a tube filled with sand. His observations led to Darcy's law, which has formed the basis of the entire field of reservoir simulation and production engineering.[79]

However, modern developments in nanoporous unconventional reservoirs are causing Darcy's law to break down. One outcome is that the global oil hierarchy has been reordered, with the US becoming the world's top energy producer. Quantum computing may usher in a new generation of subsurface understanding and reservoir simulation by allowing the exploration of molecular-scale physics in tight reservoirs.

In unconventional reservoirs, liquid oil flows as if it has a high permeability, similar to a gas, with preferential production of short-chain hydrocarbons and leaving long chains behind. The physics is inconsistent with conventional understanding of subsurface flow dynamics.

Using quantum computers to do molecular scale modeling of the interactions among oil, water, and gas molecules with the surface of rocks could help explain the physics behind the disconnect between Darcy and non-Darcy flow. If so, the benefits would be substantial.

For example, if the number of wells could be reduced by only 10%, the net cash flow of the top 32 North American unconventional oil producers would shift from a net loss of $1 billion (January to September 2018) to a positive cash flow of $8 billion (based on an estimate of $6 million per well).[80]

Quantum computing applications

Healthcare

Healthcare data—such as information from clinical trials, disease registries, electronic health records (EHRs), and medical devices—is growing at a compound annual growth rate of 36%.[81] Increasingly, this data helps address challenges associated with the "quadruple aim" of healthcare: better health, lower costs, enhanced patient experiences, and improved healthcare practitioner work lives.[82] At the same time, healthcare consumers are making more decisions and have to navigate an increasingly complex system.

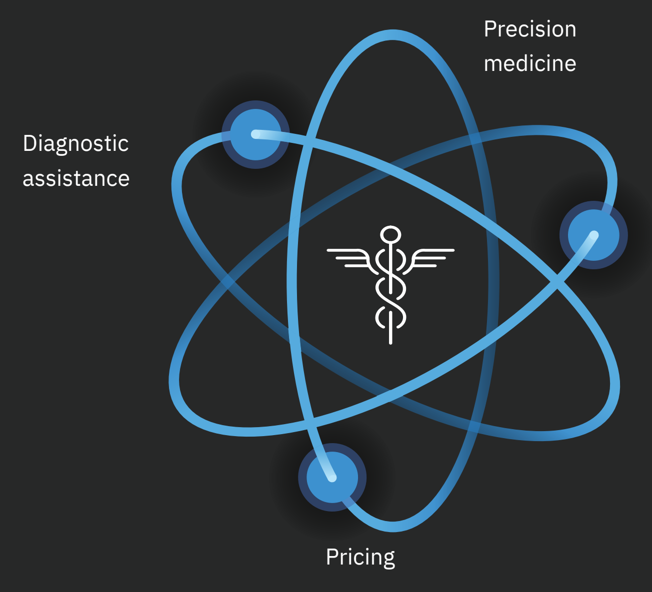
Significant investments are being made to deliver the right data and powerful insights at the point of care. Industry incumbents and new entrants alike are trying to create digital experiences that reinforce healthy, preventive behaviors. Despite that, accounting for the exponential possibilities from this diversity of new data is stretching the capabilities of classical computing systems.

Quantum computing has the potential to provide both more computing power and speed. However, it necessitates a different way of thinking, a new and highly sought-after set of skills, distinct IT architectures, and novel corporate strategies. The technology also has immediate implications for security.[83] Security is an area of particular relevance for healthcare, given the sector's data privacy responsibilities and challenges.

In healthcare, as in other industries, using quantum computers in concert with classical computers is likely to bestow substantial advantages that classical computing alone cannot deliver. As a result, there is now a race toward quantum applications.

Three key potential quantum computing use cases are central to the healthcare industry's ongoing transformation: diagnostic assistance, insurance premiums and pricing, and precision medicine.

Quantum computing use cases for healthcare



Use case

Diagnostic assistance

Early, accurate, and efficient diagnoses usually engender better outcomes and lower treatment costs. For example, survival rates increase by a factor of 9 and treatment costs decrease by a factor of 4 when colon cancer is diagnosed early.[84] At the same time, for a wide range of conditions, current diagnostics are complex and costly.[85] Even once a diagnosis has been established, estimates suggest that it is wrong in 5 to 20% of cases.[86]

Medical imaging techniques, such as CT, MRI, and X-ray scans, have become a crucial diagnostic tool for practitioners over the last century. Computer-aided detection and diagnosis methods for medical images have been rapidly developing. At the same time, many of these images are impacted by noise, poor resolution, and low replicability.

One of the reasons for these challenges is the need to adhere to strict safety protocols. Quantum computing has the potential to improve the analysis of medical images, including processing steps, such as edge detection and image matching. These improvements would considerably enhance image-aided diagnostics.

Furthermore, modern diagnostic procedures may include single-cell methods.[87] In particular, flow cytometry and single-cell sequencing data typically require advanced analytical methods, especially when considering combining data sets from the different techniques.[88]

One challenge is the classification of cells based on their many physical and biochemical characteristics. These cause the feature space, that is, the abstract space in which the predictor variables live, to be large (high dimensional). Such classification is important, for example, in distinguishing cancerous from normal cells. Quantum-enhanced machine learning approaches, such as quantum support vector machines, may enhance classification and could boost single-cell diagnostic methods.

Moreover, discovering and characterizing biomarkers may necessitate analysis of complex “-omics” data sets, such as genomics, transcriptomics, proteomics, and metabolomics.[89] These can entail a large feature space, as well as many interacting features leading to interdependencies, correlations, and patterns that are challenging to find with traditional computational methods.[90] Further extending biomarker insights down to the level of the individual naturally requires even more advanced modeling. These characteristics suggest that quantum computing could help discover biomarkers, perhaps even for individuals.

Through quantum computing, care providers may be able to improve diagnoses while simultaneously eliminating the need for repetitive invasive diagnostic testing. They may be able to continuously monitor and analyze the health of individuals. In addition to helping patients, such improvements could also benefit health plans and providers via reduced treatment costs as a result of earlier diagnoses. It might even become possible to carry out meta-analyses for more elaborate diagnostic procedures in order to determine which procedure should be performed and when. This could help further cut costs and enable more data-driven decisions by health plans and governments for providers and individuals.

Use case

Insurance premiums and pricing

Determining health insurance premiums is a complex process. A number of factors need to be taken into account by a health plan in the process of developing a general pricing strategy (recognizing that regulations in some countries, such as the US, may limit the number of factors used to calculate premiums).[91] These include complex interdependencies, such as population health levels and disease risks, treatment suitability and costs, and the risk exposure a health plan is willing and able to accept based on corporate strategy and regulations. While health plans have already made considerable progress in this space by applying classical data science methods, achieving more granular models with lower uncertainties remains difficult.

One key area in which quantum computing may help optimize pricing is risk analysis. Leveraging insights about disease risk at the population level and combining them with quantum risk models that can compute financial risk more efficiently could allow health plans to achieve improved risk and pricing models.[92]

Another important lever through which quantum computing may support pricing decisions is enhanced fraud detection. Currently, healthcare fraud costs hundreds of billions of dollars in the US alone.[93] Classical data mining techniques already help with detecting and reducing healthcare fraud; nevertheless, more computationally efficient methods are needed.[94] Quantum algorithms could enable superior classification and pattern detection and thus help uncover anomalous behavior and eliminate fraudulent medical claims.[95] This is expected to allow health plans to further optimize pricing strategies and offer reduced premiums as a result of having lower costs associated with fraud loss and prevention schemes.

Enhanced pricing computations would enable lower average premiums as well as better-tailored premium options. The complexity of healthcare is reflected in the challenges associated with making pricing strategies easily understood. New regulations that require transparency and lower average healthcare costs make it even more important to optimize pricing models.[96]

Use case

Precision medicine

Precision medicine aims to tailor prevention and treatment approaches to the individual.[97] Due to the complexity of human biology, individualized medicine requires taking into account aspects that go well beyond standard medical care. In fact, medical care only has a relative contribution of 10 to 20% to outcomes; health-related behaviors, socioeconomic factors, and environmental aspects account for the other 80 to 90%.[98] Computationally, the interdependencies and correlations among these diverse contributors create formidable challenges with regard to optimizing treatment effectiveness.

As a result, many existing therapies fail to achieve their intended effects due to individual variability. For example, only a third of patients respond to drug-based cancer therapies. In some cases, consequences of drug therapies can be disastrous; in Europe alone, up to 200,000 people die each year due to adverse drug reactions.[99]

A key aspect of tailoring medical approaches is proactivity. As mentioned, early treatments and preventive interventions tend to drastically improve outcomes and optimize costs. Classical machine learning has already shown some promise in predicting the risk of future diseases for a range of patient groups based on EHRs.[100] Nevertheless, challenges remain due to the characteristics of EHRs and other health-relevant data, including the level of noise, size of the relevant feature space, and complexity of interactions among the features. This suggests supervised and unsupervised quantum-enhanced machine learning techniques could allow earlier, more accurate, and more granular risk predictions.[101] Eventually, medical practitioners might even have the tools to understand how an individual's risk for any given condition changes over time, enabled by continual virtual diagnostics based on ongoing data streams from individuals.

Knowing an individual's disease risk is not sufficient, however. Just as important is knowing how to effectively medically intervene for any given individual. One avenue in this endeavor is the study of drug sensitivity at the cellular level. For example, by taking into account the genomic features of cancer cells and the chemical properties of drugs, models that can predict the effectiveness of cancer drugs at a granular level are already being investigated.[102] Quantum-enhanced machine learning could support further breakthroughs in this area and ultimately enable causal inference models for drugs.

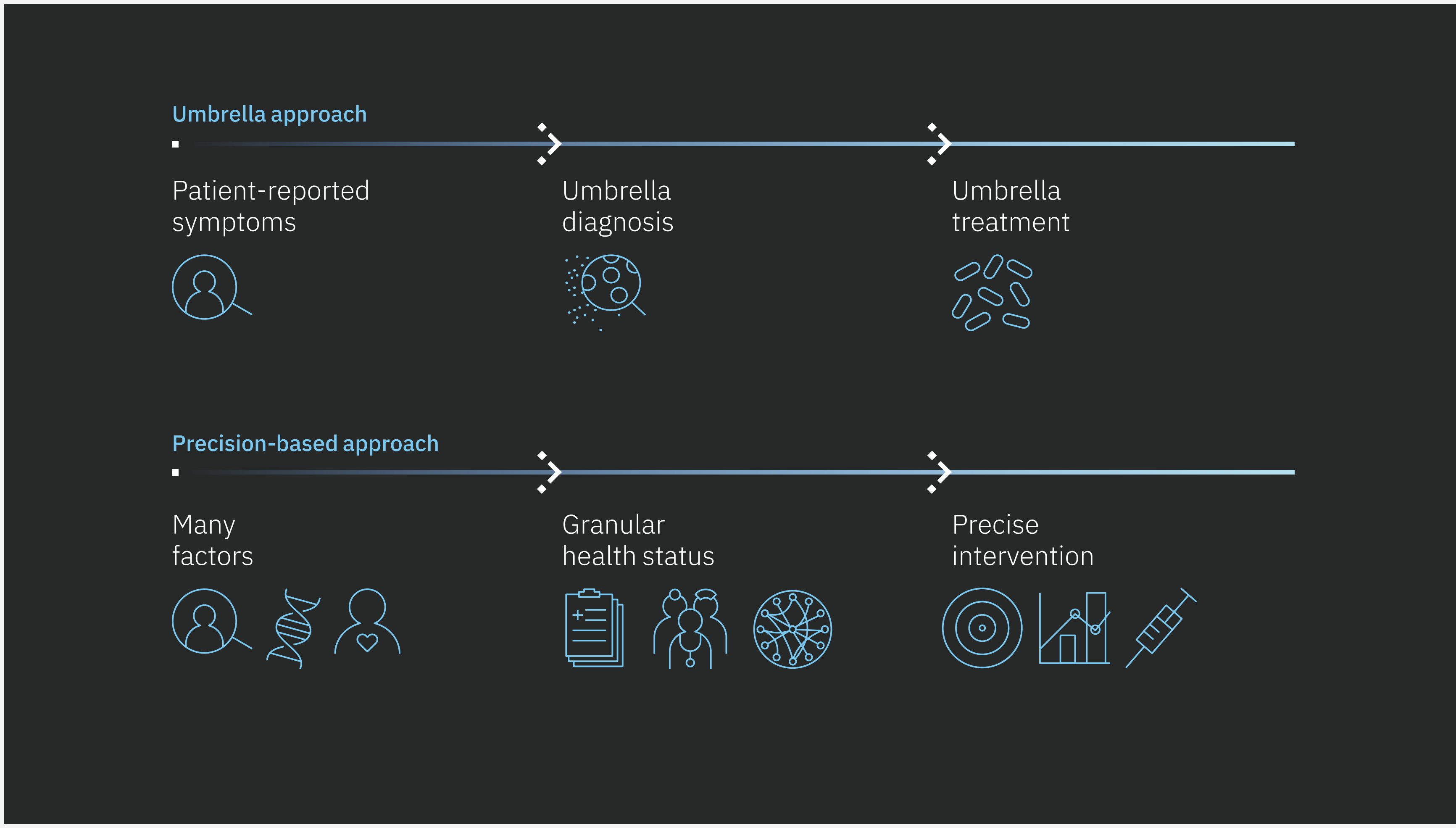
The goal of precision medicine is lofty: identifying and explaining relationships among interventions and treatments on the one hand and outcomes on the other to provide the next-best medical action at the individual level. Traditionally, diagnosing a patient's condition has been based heavily on patient-reported symptoms, which is time consuming and results in an umbrella diagnosis and associated treatment that frequently fail.

We are now moving toward a setting where insights from additional health-relevant data can be obtained to efficiently arrive at a continuous and precise health status, along with personalized interventions (see Figure 18). While we are still a long way from realizing this, quantum computing may be able to accelerate our progress toward such a new framework.

This framework would allow healthcare organizations to optimize and personalize their services throughout the continuum of care. Moreover, adherence and patient engagement are also key considerations in decisions about the next-best medical action for a given individual. Advanced computational modeling can address this area too.[103] For instance, adherence data analysis allows the timing of interventions to be optimized for individuals.[104] Eventually, population health management at this level of granularity could become possible.[105]

Figure 18

Quantum computing has the potential to accelerate the transition *from umbrella diagnosis and treatment to precision health status intervention.*



Quantum computing applications

Life sciences

In life sciences, major challenges include understanding the relationships among sequence, structure, and function and how biopolymers interact with one another, as well as with small organic molecules that are native to the body or designed as drugs. Such problems are computationally complex and are at the heart of genomic analysis, drug design, and protein folding predictions.

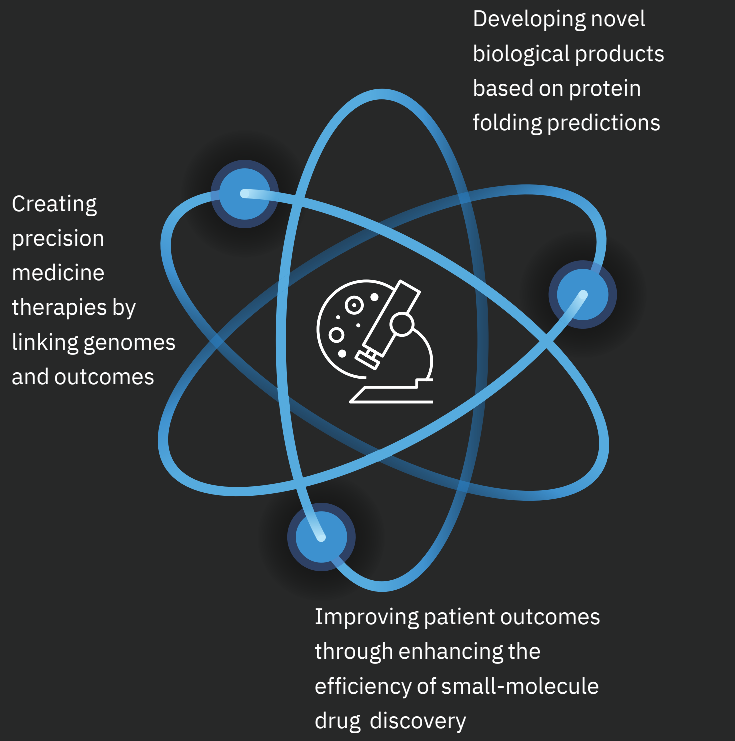
As a result, there is now a cross-discipline race toward quantum applications. Within five years, it is possible quantum computing will be used extensively by new categories of professionals and developers to solve problems once considered unsolvable.[106]

Trends such as the spread of efficient low-cost sequencing and the advent of the "-omics" era result in life sciences companies exploring ways to take advantage of the diversity of novel data sources. Further, the life sciences industry is among those in which people could most directly experience future quantum computing benefits.

Exploration and implementation of quantum computing use cases, paired with further scientific progress in quantum computing hardware and algorithms, are expected to enable the transition from potential to reality over the coming years. Quantum computing has the potential to enable a range of disruptive use cases in life sciences. These include:

— Creating precision medicine therapies by linking genomes and outcomes
— Improving patient outcomes through enhancing the efficiency of small-molecule drug discovery
— Developing novel biological products based on protein folding predictions.

Quantum computing use cases for life sciences



Use case

Creating precision medicine therapies by linking genomes and outcomes

The 15-year, $2.7 billion investment to accurately sequence the human genome and subsequent reductions in sequencing costs helped launch the "-omics" era.[107] Accordingly, understanding primary sequences is no longer a major limitation for scientists. Instead, research focus has shifted to taking advantage of new computational tools to deepen our understanding of how genomic sequences translate to function. However, this task is extremely difficult with traditional methods due to the size of the human genome (about 3 billion DNA base pairs), the variation that exists across populations, and the wide range of health outcomes.[108]

Potential opportunities at the intersection of genomics and quantum computing include:[109]

—Motif discovery and prediction:[110] DNA, RNA, and amino acid sequences have all been shaped through evolutionary pressures. One bioinformatic challenge is identifying motifs in these sequences, such as patterns that activate or inhibit gene expression and, thereby, help us better understand mechanisms of gene regulation. Classical algorithms to identify motifs are computationally expensive because they require exhaustively searching all possible arrangements for a given length. The application of quantum optimization algorithms could further our understanding of transcription factor binding and de novo genome assembly.

—Genome-wide association studies (GWAS):[111] The goal of GWAS is to find associations between a selected trait or disease and single mutations in DNA. Current methods are inherently high dimensional and computationally challenging. This highlights the potential for quantum computing to significantly narrow the lists of candidate genes that need to be experimentally validated. Quantum computing may also enable progress in gene network and graph models.

—De novo structure prediction:[112] With the explosive growth of sequencing information and technology, an increasing gap exists in understanding how sequence translates to structure and, ultimately, function (see Figure 19). Despite sophisticated methods, such as homology models, classical approaches to predict structure de novo often scale poorly.[113] For instance, the search space of potential protein configurations increases exponentially with the size of a protein, making brute-force approaches infeasible. Quantum computing has the potential to drastically improve structure predictions for RNA molecules, proteins, DNA-protein complexes, and other constructs.

Such advances could eventually help realize the vision of powerful digital twin models.[114] Organic digital twins might be used in pharmacogenomic testing to predict an individual's response to specific drugs over time, aiding the development of precision medicine therapies. Additional inorganic digital twins could be created to optimize research or care facilities by comparatively stress-testing aspects such as procedures, staffing levels, facility layout, and equipment. Reaching the day when a medical team can tell a patient, "Based on your genome, we have confidence that this will be the specific result of your treatment," may someday no longer seem like a purely utopian goal.

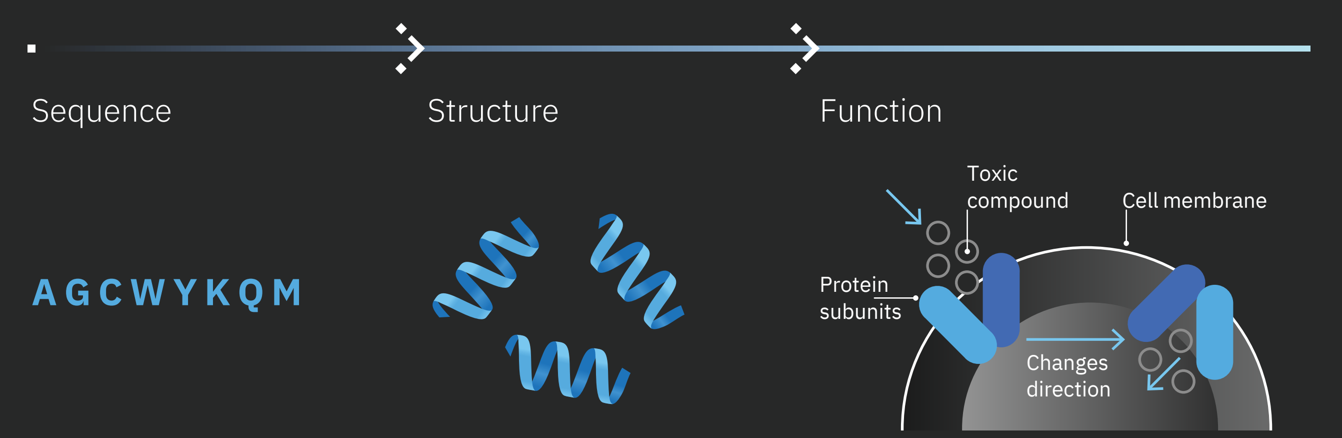


Figure 19

Sequence-structure-function dogma
at the heart of biology research

Use case

Improving patient outcomes by enhancing the efficiency of small-molecule drug discovery

Small-molecule drug design and discovery has always been a complex optimization process. Its goal: improving patient outcomes by designing a novel molecule active against the disease-related target while simultaneously reducing activity against the thousands of other targets in the body to avoid side effects and dangerous toxicities. In pursuit of this goal, typically 200,000 to >10^6 compounds are screened in experimental and computational workflows, and a few thousand are produced and tested in the necessary battery of assays.[115] Here, computing has long played a role, largely through similarity and classification approaches to support screening and detailed 3D structure, as well as energy calculations to support more precise target-based design.

Quantum computing has a diversity of potential applications in drug discovery.[116] The technology could help assess a greater number of candidate molecules and evaluate them more accurately using, for example, classification methods such as those employed in lead-finding and off-target screening. And it may impact the classification associated with lead-finding and the modeling of off-targets in lead optimization—as well as with the physics-based modeling carried out in lead optimization when a 3D protein structure or good model is available.

The ability to study more potentially pharmacologically active molecules, beyond the roughly 10^7 organic and inorganic substances that have been reported in the scientific literature to date, is important. In fact, the total number of possible carbon-based compounds whose molecular masses are similar to those of living systems is around 10^{60}.[117] There are thus many orders of magnitude of uncharted chemical space left to explore, clearly an area of great potential. This opens the door, for instance, to better assessing ultra-large libraries of small organic molecules now available for purchase with synthesis “on demand.”[118]

Particularly accurate scoring is possible through molecular dynamics simulations of protein-ligand complexes. Here, quantum computing could offer significant advantages for carrying out hybrid quantum/molecular mechanics approaches as well as developing the underlying parameters of the classical force field. Such advances would apply to both lead optimization and the growing field of computational process chemistry, such as in modeling enzymatic reactivity and stereoselectivity to support biocatalysis in drug manufacturing.[119]

Use case

Developing novel biological products based on protein folding predictions

In contrast to small-molecule drugs, in the case of biologics, a protein or other macromolecule is the drug. Biological drugs, such as antibodies, insulin, and many vaccines, have been employed for decades.[120] In recent years, pharmaceutical companies are increasingly targeting biologics to treat a number of diseases. Designing the 3D structure of biologics is important for function, specificity, and stability.[121]

Real-world protein modeling cases involve exploration of the enormous number of possible folding patterns, as illustrated in Levinthal's paradox (see Figure 20).[122] The exponential growth of potential conformations with chain length makes the problem challenging for classical computers. For example, in one model, a chain of 20 amino acids has 109 potential conformations, and chains with 60 and 100 amino acids have 10^{28} and 10^{47} conformations, respectively.[123] Moreover, as part of the US Food and Drug Administration's biological product definition, a protein must comprise more than 40 amino acids.[124]

While many proteins can be modeled adequately by analogy to known structures, an important and challenging design target is the hypervariable H3 loop in the complementarity-determining region of antibodies. This loop typically contains 3–20 residues but is sometimes much longer, and accurate representation has been the subject of much study.[125]

Quantum computing has the potential to overcome many of these computational challenges—for example, scoring the great number of possible structures and identifying the likeliest one. A recent publication demonstrated that quantum computing could score a peptide in two common conformations represented on a lattice—alpha helix and beta sheet—and leveraged a quantum algorithm for the search.[126] It has also been shown that quantum computing may drastically improve the calculation of protein force fields.[127] As Quantum Volume increases, quantum computing's ability to score additional conformations will increase accordingly.[128] Recent progress in predicting protein structure with classical deep-learning networks suggests that quantum algorithms may be particularly valuable when polypeptides with unnatural amino acids are studied, where suitable machine learning training data is quite limited.[129]

Finally, as with all the potential quantum applications previously discussed, quantum computing could enable further use cases in tangential areas. For instance, biologics tend to be much less stable than small-molecule drugs. Optimization of the biologics supply chain itself—from formulation through shipment and, ultimately, transport to pharmacies, hospitals, and even homes—is a complicated process that also may be improved by quantum computing.[130]

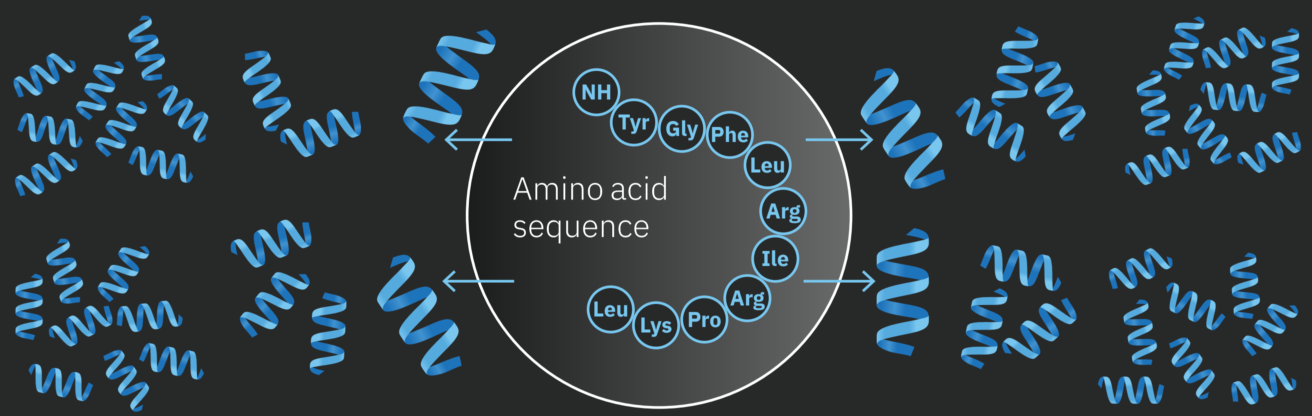
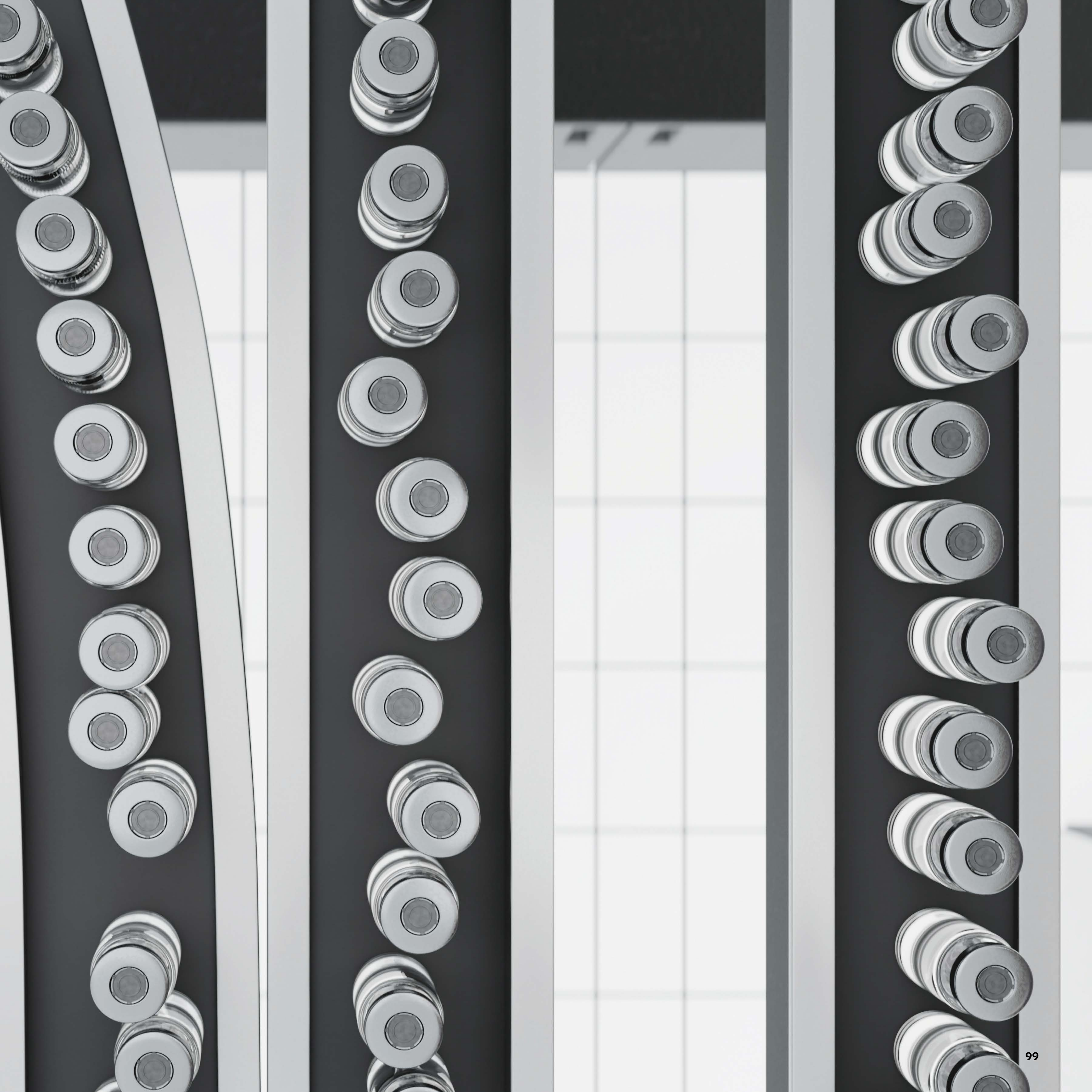


Figure 20

Levinthal's paradox

Even a protein with only 100 amino acids has around 10^{47} potential conformations. In reality, however, many proteins fold to their native structure within seconds.



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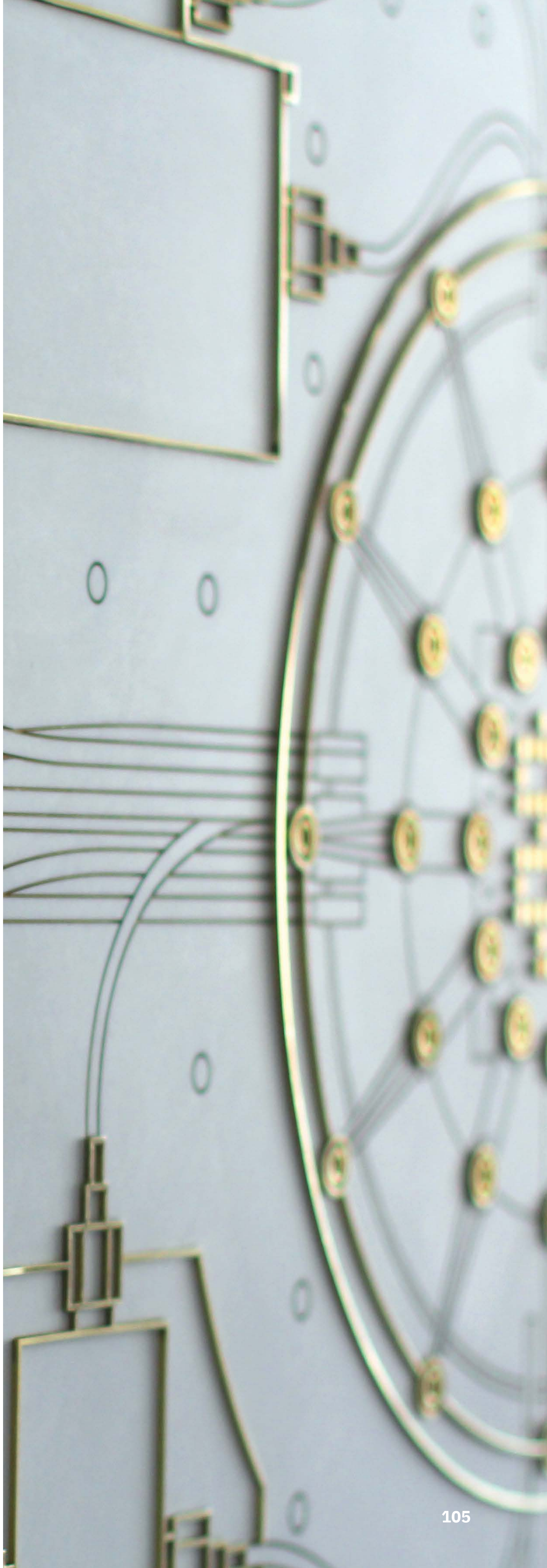

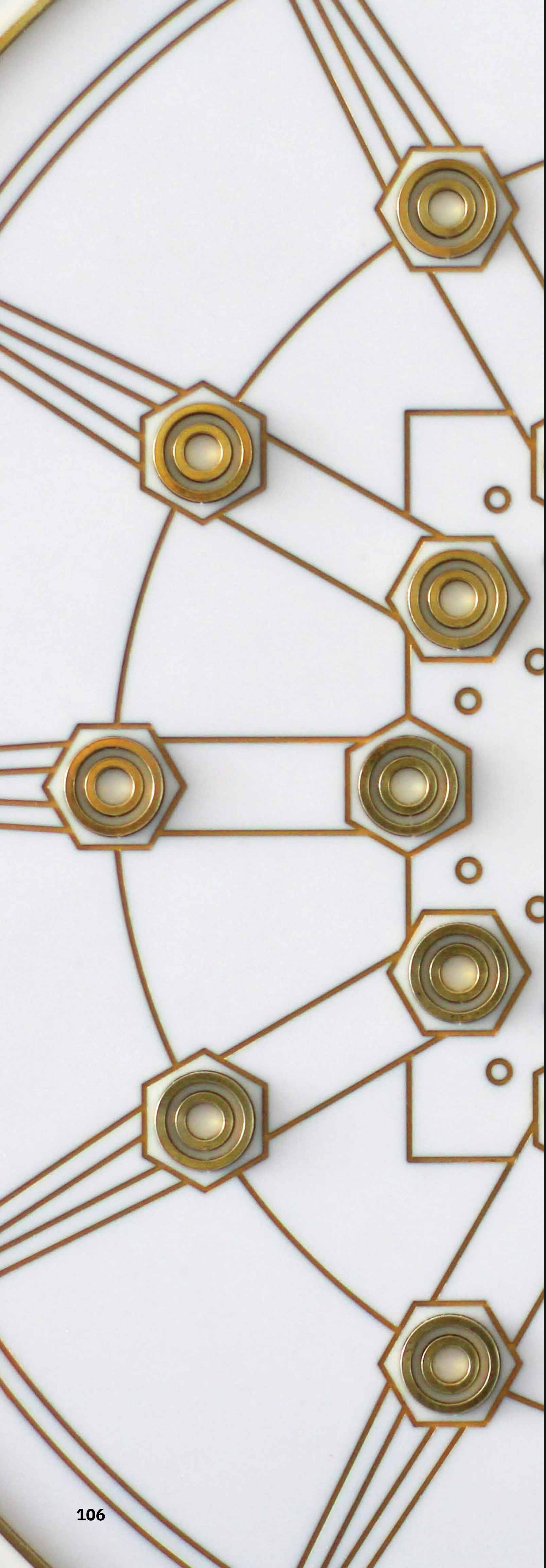

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