Quantum computing isn't merely about speed. It's about tackling problems differently and making the seemingly impossible possible, if not commonplace.

Key takeaways

Making the impossible possible
Quantum computing will be used extensively by new categories of professionals and developers to solve problems once considered unsolvable.

Disruptive life sciences use cases
In the life sciences industry, quantum computing is expected to enable a range of disruptive use cases by linking genomes with outcomes, enhancing drug discovery, and improving protein folding predictions.

The time to act is now
Life sciences could benefit significantly from quantum computing. However, much of the early intellectual property in quantum computing may be proprietary, raising the urgency to get started and engage with partners and ecosystems.

—

Solving the unsolvable

No doubt you've heard it before. Quantum computers can do some things more efficiently than classical computers. Is that a big deal? Why are advanced computational approaches even needed?

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.

Consider drug design. The number of molecules made up of say 50 atoms that can be built using just 10 different types of atoms amounts to around 10^{50}.[1] If we also factor in the number of possible molecular configurations and conformations that can be sampled at room temperature, the total number of molecules that could potentially constitute a valid drug is exponentially greater than the roughly 10^{80} atoms in the observable universe. Tackling this level of complexity is far beyond the capabilities of classical computers; however, quantum computers could make inroads.

The famous physicist, Richard Feynman, suggested back in the 1980s that "if you want to make a simulation of nature, you'd better make it quantum mechanical."[2]
It's about tackling problems differently and making the seemingly impossible possible, if not commonplace.

Insight: Bits and qubits

Quantum computers process information in a fundamentally different way from traditional computers. Previous computer technology advancements—such as integrated circuits–enabled faster computing but were still based on classical information processing. Quantum computers manipulate quantum bits (qubits). These are unlike classical bits, which store information as either a 0 or 1, as they can display uniquely quantum properties, such as entanglement. As a result, it becomes possible to construct quantum algorithms that can outperform their classical counterparts, since they are not able to leverage quantum phenomena.

Quantum computers could be particularly useful in tackling problems that involve:

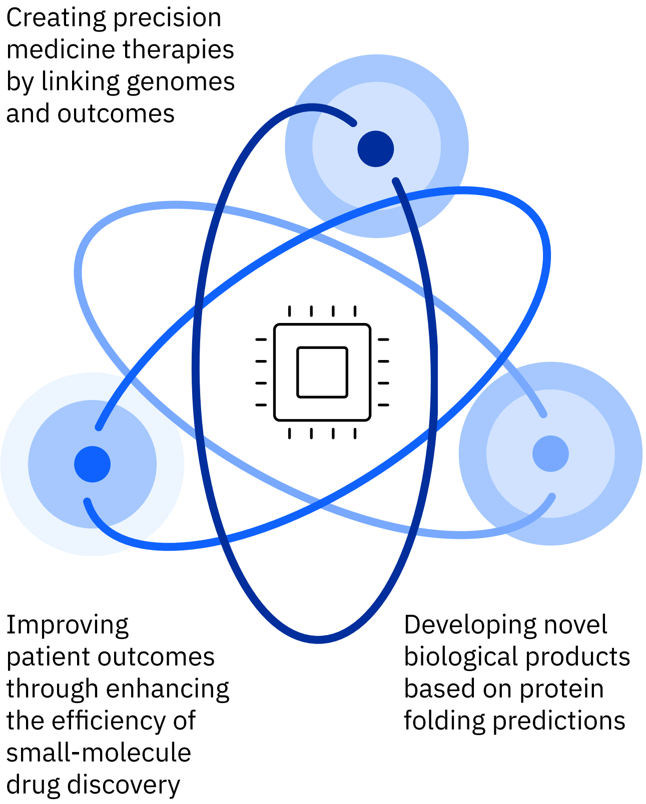
- Chemistry, machine learning/artificial intelligence, optimization, or simulation tasks. In fact, machine learning has shown potential to be enhanced by quantum computing and is already helping drive quantum advances[4]
- Complex correlations and interdependencies among many highly interconnected elements, such as molecular structures in which many electrons interact
- Inherent scaling limits of relevant classical algorithms. For instance, the resource requirements of classical algorithms may increase exponentially with problem size, as is the case when simulating the time evolution of quantum systems.[5]

As a result, there is now a cross-industry 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.[3] In the life sciences industry, quantum computing is expected to enable a range of disruptive use cases. These include:

1. Creating precision medicine therapies by linking genomes and outcomes
2. Improving patient outcomes through enhancing the efficiency of small-molecule drug discovery
3. Developing novel biological products based on protein folding predictions (see Figure 1).

Figure 1

Quantum computers may enable three key life sciences use cases that reinforce each other in a virtuous cycle



Research focus has shifted to taking advantage of new computational tools to deepen our understanding of how genomic sequences translate to function.

Use Case 1: Creating precision medicine therapies by linking genomes and outcomes

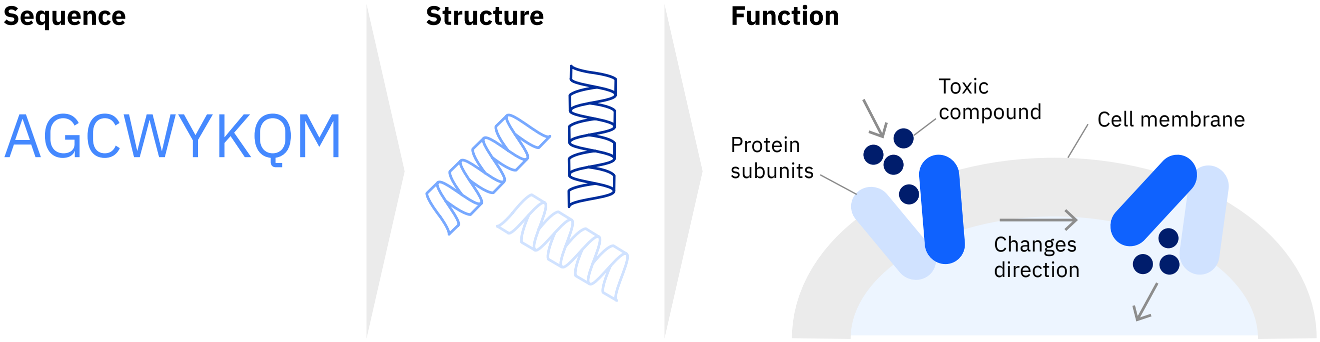
The 15-year, USD 2.7 billion investment to accurately sequence the human genome and subsequent reductions in sequencing costs helped launch the "-omics" era.[6] Accordingly, understanding primary sequences is no longer a major limitation for scientists. Instead, research focus has shifted to taking advantage 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.[7]

Potential opportunities at the intersection of genomics and quantum computing include:[8]

- *Motif discovery and prediction*[9]*:* 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. New insights from quantum computing could further our understanding of transcription factor binding and de novo genome assembly.
- *Genome-wide association studies (GWAS)*[10]*:* 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, which may significantly narrow the typically long 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*[11]*:* 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 2). Despite sophisticated methods, such as homology models, classical approaches to predict structure de novo often scale poorly.[12] For instance, the search space of potential protein configurations increases exponentially with the size of the protein (see Use Case 3). Quantum computing has the potential to drastically improve structure predictions for RNA molecules, proteins, DNA-protein complexes, and other constructs.

Figure 2

Sequence-structure-function dogma, which is at the heart of biology research



Quantum computing has a diversity of potential applications in drug discovery.

Such advances could eventually help realize the vision of powerful digital twin models.[13] 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.

Use Case 2: 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.[14] 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.[15] 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 the high-throughput task of 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 explore more molecules is important since the number of possible small molecules is enormous. Normally only a small fraction is considered. In fact, the total number of possible carbon-based compounds whose molecular masses are similar to those of living systems is around 10^{60}.[16] Effectively exploring this chemical space is an area of great potential. It opens the door to better assessing ultra-large libraries of small organic molecules now available for purchase with synthesis "on demand."[17]

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 applications as well as developing the underlying parameters of the classical force field. Such advances would apply to both lead optimization as well as the growing field of computational process chemistry, such as in modeling enzymatic reactivity and stereoselectivity to support biocatalysis in drug manufacturing.[18]

Use Case 3: 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.[19] 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.[20]

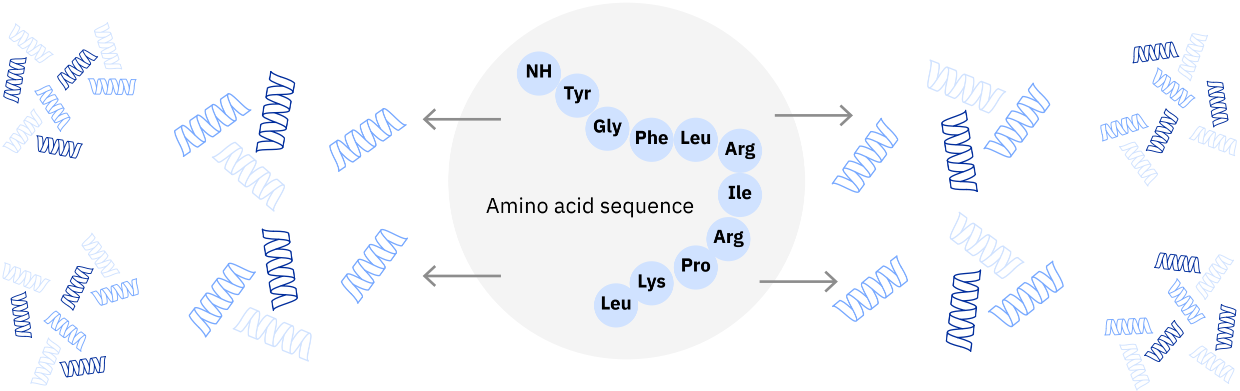
Real-world protein modeling cases involve exploration of the enormous number of possible folding patterns, as illustrated in Levinthal's paradox (see Figure 3).[21] The exponential growth of potential conformations with chain length makes the problem challenging for classical computers. For example, in one model, a chain of 20 amino acids has 10^9 potential conformations, and chains with 60 and 100 amino acids have 10^{28} and 10^{47} conformations, respectively.[22] Moreover, as part of the FDA's biological product definition, a protein must comprise more than 40 amino acids.[23]

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.[24]

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.[25] It has also been shown that quantum computing may drastically improve the calculation of protein force fields.[26] As quantum volume increases, quantum computing's ability to score additional conformations will increase accordingly.[27]

Figure 3

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.



Finally, as with all the potential quantum applications discussed in this report, 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.[28]

From bench to bedside

The life sciences sector has the potential to benefit significantly from quantum computing. 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 this diversity of novel data sources. Further, it is among the industries in which people could most directly experience future quantum computing benefits.

Exploration and implementation of quantum use cases, paired with further scientific progress in quantum hardware and algorithms, is expected to enable the transition from potential to reality over the coming years. Leading life sciences and pharmaceutical companies have started this journey toward quantum advantage.

Action guide

Exploring quantum computing use cases for life sciences

Quantum computing necessitates a different way of thinking, a new and highly sought-after set of skills, distinct IT architectures, and novel corporate strategies. Imagine some of the capabilities and benefits described in this report in the hands of your top competitors, particularly as much of the early IP in quantum computing may be proprietary. That's why the time to get started with quantum computing is now—when standards, strategies, use cases, and ecosystems are being developed.

So how can life sciences organizations get started with quantum computing? There are three key initial steps:

1. Identify and enable quantum champions in your organization to experiment with actual quantum computers and explore potential applications for your specific industry. To help focus on your highest-value problems, have your quantum champions report to a quantum steering committee that includes line-of-business executives, innovation and technology leads, and market strategists.

2. Prioritize quantum use cases according to their potential for attaining business advantage—given your organization's therapeutic focus areas, business strategy, associated customer value propositions, and future growth plans. Keep an eye on progress in quantum application development to stay in the vanguard of which use cases might be commercialized sooner rather than later.

3. Consider partnering with an emerging quantum ecosystem of like-minded research labs and academic institutions, technology providers, application developers, and start-ups. Obtain access to an entire quantum computing stack capable of developing and running quantum algorithms specific to your business needs. Look for breakthroughs in quantum technology that might necessitate a change in ecosystem partners.

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