NEW GROUNDS FOR BOOSTING PHARMACEUTICAL R&D WITH QUANTUM COMPUTING

How quantum computing can be leveraged to accelerate translational research and clinical development

EXECUTIVE SUMMARY

In the next decade, drug discovery and clinical development could be drastically accelerated by quantum computing. To secure future benefits from this technology, pharma companies need to consider its potential when making tactical decisions as of now.

The **lengthy and uncertain R&D process**, one of the key challenges faced by the pharmaceutical companies, mostly stems from the **complexity inherent to life sciences**. Indeed, understanding only partially the intricacies of metabolic pathways, gene regulation, or patients' behavior slows down pharmaceutical R&D. Whilst great progress in modelling and decoding this complexity has been made lately, the current computing capabilities are limiting the pharmaceutical industry in making further breakthroughs.

$1.5 + BLN dollars

Bringing a new molecule to the market costs over 1.5 billion dollars (Wouters, McKee, & Luyten, 2020)

7 %

The probability of launching the drug when starting phase 1 clinical trials is 7% (Dowden & Munro, 2019)

The advent of **quantum computing**, more **performant** than classical computing and leveraging different types of **algorithms**, opens new horizons for the industry. Indeed, the computing based on the principles of quantum mechanics could help solve complex problems better and faster thanks to quantum optimization, quantum simulation, and quantum machine learning. Quantum computing is not only powerful, but also well adapted to **modeling complex chemical and biological phenomena**, from molecular structures to patient medical history.

1.5 BLN times faster

A quantum computer is reported to perform some tasks 1.5 billion times faster than a classical computer (Google, 2019)

While hardware and software challenges persist, the quantum computing field is moving quickly. Indeed, in the **next 3-10 years** pharma companies will likely be able to leverage quantum computing. And if leveraged to the fullest, quantum computing will help bring the right medicine to the right patient much faster, while significantly decreasing the R&D cost.

Quantum computing will likely accelerate drug discovery

QUANTUM COMPUTING USE CASE OF TOMORROW	EXPECTED IMPACT
Quantum chemistry **simulation of small molecules** or their fragments would help identify new promising drug candidates	- Going to clinical phase in less than one year (instead of 3-4 years) - Having a vast choice of promising candidates

EXAMPLE OF SOLUTION TO TEST TODAY	Quantum-inspired solutions (based on using classical computers to simulate quantum effects) for molecular modelling

Speeding up drug discovery with quantum computing would imply changes in the **portfolio management** strategies, as well as potential **re-internalization of research activities**.

We also believe that quantum computing will be leveraged to increase the probability of clinical trials success

Modelling disease and treatment effects at gene, cell, tissue, organ, patient, or population level with quantum computing will lead to:

- Enhanced clinical trials design
- Obtaining generalizable results with reduced patient cohorts

QUANTUM COMPUTING USE CASE OF TOMORROW	EXPECTED IMPACT
Digital twins of patients developed by leveraging medical knowledge and real-world data with quantum machine learning	- De-risking the clinical trials and thus diminishing the costs associated with trial failures - Faster clinical development process - Facilitated shift to precision medicine

EXAMPLE OF SOLUTION TO TEST TODAY	Machine learning models leveraging clinical and real-world data to define the optimal inclusion and exclusion criteria for a clinical trial

Precision medicine paradigm concretized via quantum-powered analysis, which could help to **de-risk phase 3 clinical trials**, would impact the decisions concerning **drug positioning**, as well as the **trial design** and **patient recruitment**.

The pharma industry has already started its journey towards **investing in quantum computing** by teaming up with tech giants, startups specialized in the development of quantum computing software, and research institutions. Yet, the regulatory constraints, the absence of in-house expertise, and the disconnect between technical and business teams would **slow down** quantum computing adoption, as was the case with the adoption of **Big Data, Big Data analytics, and AI**.

To prepare the future use of quantum computing in pharmaceutical R&D starting today, pharma companies need to build **small teams of experts** in quantum computing and or dedicate resources to **scanning the progress** within the ecosystem. Quantum computing potential should also be considered when conceiving **AI-driven projects**. On the **IT infrastructure** side, it would be relevant to consider a hybrid approach, which would progressively include using high-performance and quantum computers, including via cloud.

Even though quantum technology still needs to mature, we advise pharmaceutical companies **to consider the potential of quantum computing** in their operational and tactical decisions, starting today.

FOREWORD

We have provided the first insights on the actions to take by life sciences organizations to enable a scalable quantum computing strategy in our recent Point of view: *The Future of Quantum in Life Sciences*.

In this paper we are developing the topic further and drilling down to **concrete use cases of quantum computing in pharmaceutical R&D** to help pharma companies prepare the launch pad for quantum computing adoption.

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1 KEY STAKES OF PHARMA R&D

The key challenges of pharmaceutical R&D are anchored in the complexity of both, the underlying science and the operational models. Breakthrough technological solutions will be crucial to unravel it.

The traditional pharma business model relies on massive R&D investments, with high uncertainty of success and lengthy times to market leading to a short opportunity window for profit generation.

The pharmaceutical sector is characterized by tremendous R&D expenses as constant heavy investment is needed to identify new relevant therapeutic options.

On average, bringing a new molecule to the market costs over **1.5 billion dollars**, when considering the costs of failed trials (Wouters, McKee, & Luyten, 2020).

As clinical development advances, the accumulated investments are steeply growing, while the risk of failure remains high.

Thus, the probability of launching the drug is as low as **7%** when starting phase 1 clinical trials, it doubles by phase 2, and grows to 62% by phase 3 (Dowden & Munro, 2019).

Patents for new drugs have a validity of 20 years. So, once the drug is approved, the time left for generating profit is limited to approximately **10 years**, while exclusivity can last for only up to 7 years (FDA, 2020).

After the patent expires, pharmaceutical companies can be faced with competition from generics or biosimilars, leading to price pressure and a drop in sales.

Today we are reaching a **patent cliff**, with 15 drugs with the highest sales going to lose their patent in the next 8 years (FiercePharma, 2021). Thus, it is crucial to accelerate both research and drug development to secure revenues and to maximize patent validity post market authorization.

The drug blockbuster model is highly challenged, with the future being shaped by the quest to decipher and address patients heterogeneity and the complexity of disease sub-populations.

The past years were marked by the advent of **precision medicine**. Indeed, patients' heterogeneity in terms of environment, clinical history, and genetic background affects the body's biological response to drugs, including the pharmacokinetics, pharmacodynamics, and bioavailability. "High resolution" snapshots of the underlying biology can be analyzed using omics data. For example, it was demonstrated that the response to breast cancer treatment depends on the baseline characteristics of the tumor ecosystem, including its multi-omics landscape (Sammut, et al., 2022).

The last decades in pharma business were marked by the success of **blockbusters**, drugs with total annual sales over US$1 billion, usually indicated for diseases with high prevalence (Schumacher, Hinder, Boger, Hartl, & Gassmann, 2022).

However, the number of personalized drugs, including cell and gene therapies, is growing. Thus, **personalized medicines** account for **35% of approvals by the FDA in 2021**, and for over a quarter of all approvals in the past 7 years (Personalized Medicine Coalition, 2021).

The overall financial performance of a molecule is shaped by the patients pool and the price. And while the target populations for personalized therapies are often limited, payers appear willing to approve high list prices, especially for one-time treatments. Thus, the most expensive drug marketed today is Zolgensma, a gene therapy approved in May 2019 for pediatric spinal muscular atrophy (Fierce Pharma, 2019).

Breakthrough technological solutions are awaited to tackle challenges faced by the pharma industry.

We observe the multiplication of available real-world data (RWD), such as electronic health records, case report forms, patient-reported outcome surveys, and insurance billing and claims. RWD contains the information on patient demographics and medical history (comorbidities, procedures and treatment history, healthcare services utilization, etc.), population coverage, and prescribing patterns. In parallel, more and more health-related data from connected objects is being accumulated. Finally, the genomic data volume is skyrocketing with genomic research projected to generate 2 to 40 exabytes of data (National Human Genome Research Institute, 2022).

This data is increasingly exploited to address the stakes of the pharmaceutical R&D.

Artificial intelligence (AI) solutions are being adopted to cut down the time and cost of discovering new medicines and bringing them to the market, as well as to personalize the therapies. Yet, the algorithmic and technological solutions we have at hand are not always precise and powerful enough to fully decode the complexity of human health based on the multitude of biological and clinical data. For instance, to fully leverage spatially-resolved transcriptomic data (the information of gene activity within a tissue) new computational solutions would be needed (Atta & Fan, 2021)

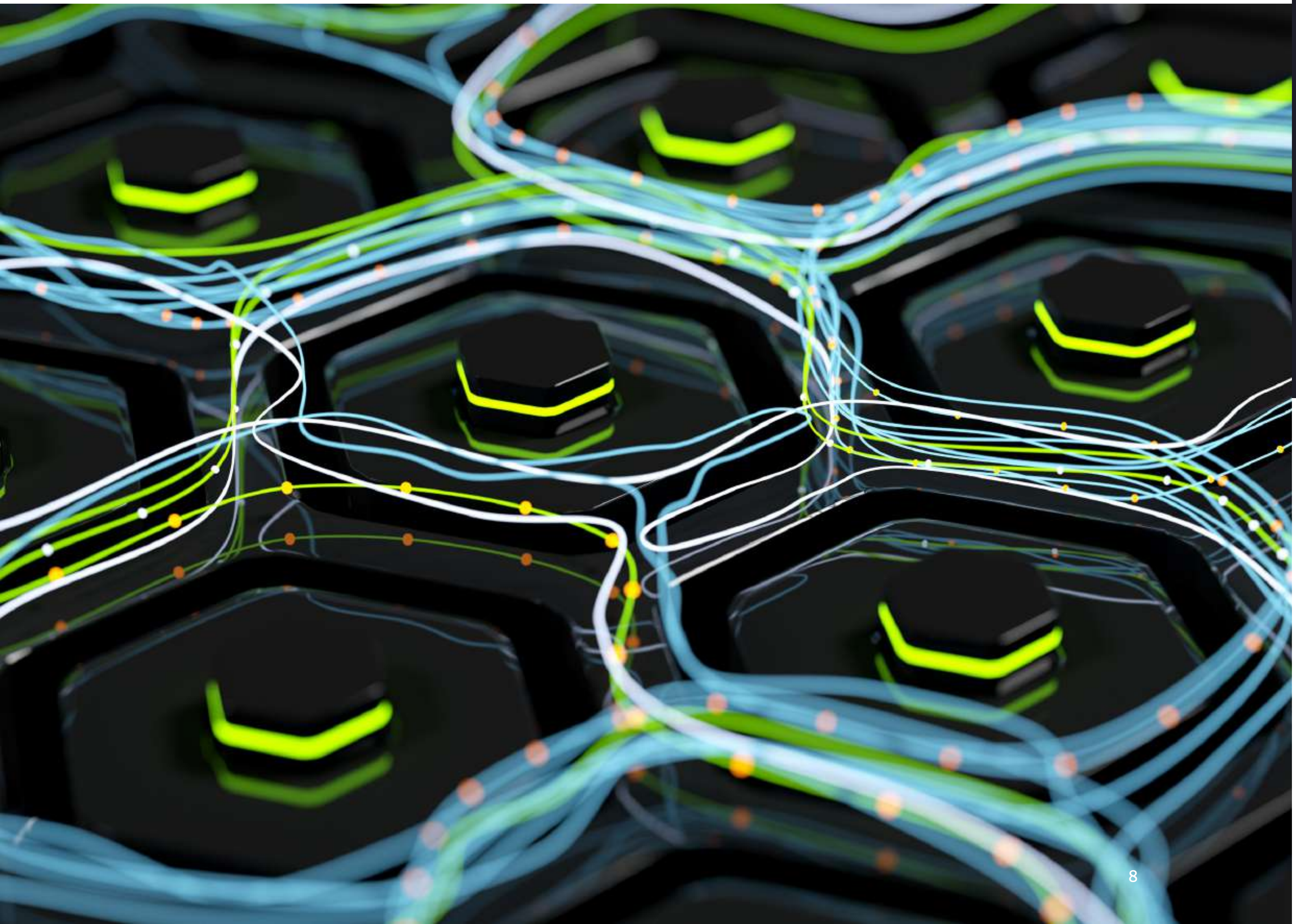
In this context, quantum computing could accelerate pharmaceutical R&D by better simulating and predicting the biological and clinical phenomena linked to human health.

2 QUANTUM COMPUTING: THE FUNDAMENTALS

Quantum computing opens new edges of computational power, while having the potential to handle problems that are too complex for classical computers. Even if the technology is still immature, its practical use is becoming a tangible perspective.

According to our research, **23% of companies worldwide** already consider or start preparing to **embrace** the **incoming emergence** of quantum computing (Capgemini Research Institute, 2022). The use cases range from battery manufacturing optimization to new materials discovery and to risk management. To find out more about the opportunities of quantum computing across sectors, check our report *How to prepare your organization for a quantum advantage now.*

The healthcare industry is among the key sectors to benefit from quantum computing advances that would help address the extraordinarily dynamic complexity of biological systems of living organisms.



2.1 KEY CONCEPTS AND MAIN APPLICATIONS

Quantum computing is associated with unprecedent computational power.

Quantum computing is a new generation of computing leveraging quantum mechanical laws to process information (40 years of quantum computing, 2022). To understand the impact of the technology would have in the next few years, let us explore its basic principles.

The classical computing process applied in all today's computers is binary. It is based on mechanical chips containing millions of bits, each of which can have only one of two possible values: 0 or 1, on or off. Quantum computing does not rely on mechanical laws, i.e., the exact measurement of the state at a precise moment. The bits are replaced by qubits, which have properties based on quantum mechanics. A qubit can have any value between 0 and 1 at the same time, thus being not only on or off, but also in what is called the "superposition".

Let us look into an example of a 2-bit classical computer. With two bits, one can encode one of the four states: 00, 01, 10, or 11. As the number of bits grows, the number of possible states increases exponentially. Yet only one of these states can be stored at a time.

Let us now imagine a quantum computer with 2 qubits. Each of the qubits would store any proportion of 0 and 1 (with a certain probability of being 0 or being 1). Thus, all the four information points (00, 01, 10, or 11) would be stored in such a computer at the same time. As the number of qubits grows, the number of states stored simultaneously grows exponentially.

The possibility of each qubit to be in the superposition should enable quantum computers to solve problems in parallel, thus, having a large computational power.

Other properties of qubits would also promote **the speed of information processing**. For example, qubits can be **entangled**, meaning that changing the state of one would automatically change the state of the other.

For example, in 2019, with a **53-qubits** quantum computer, Google claimed to have completed in **200 seconds** a task that would have taken the world's most powerful **classical computer 10,000 years** to complete (Google, 2019). And even if we are not talking about a concrete task of commercial use, the comparison remains interesting.

Quantum algorithms could open new ways to solve complex problems better or faster.

Some of the problems that cannot be solved by classical computers (due to computational complexity, too much required time, and too much computational power) might be tackled with quantum computing. For instance, quantum computers are relevant for solving problems that require calculating many possible combinations (Microsoft, 2022). As the **scientific community** began to have a **better understanding of quantum technologies**, several cases in which quantum computing could unleash its full potential have been identified.

OPTIMIZATION

Optimization problems can be reduced to finding **the best combination of parameters** for an important number of variables. The complexity of such problems resides in the extensive number of combinations to test in order to find the best solution

The quantum computing parallelism enables testing multiple combinations simultaneously (and not sequentially, as in the case of a classical computer). Additionally, the high calculation power of quantum computers makes it possible to solve optimization problems faster.

EXAMPLE *Optimization of a supply chain network to avoid shortages.*

SIMULATION

Simulation can be thought of as an attempt to mirror real-world conditions to either predict a future instance, determine the best course of action, or validate a model.

The limitations in simulation problems are often linked to the number of elements to mimic. A traditional complex simulation would often require a high computational power, as well as a thorough choice of adequate algorithms and hypotheses to limit the number of variables to simulate.

Thanks to the parallelism and high computational power of quantum computers, new approaches to simulation are becoming possible, such as direct simulation (it consists in testing each possible combination to find the right one).

In addition, current AI models are often limited by the size and nature of the dataset they are trained on. The use of generative models is becoming common to increase datasets and create more reliable AI solutions. In this area, quantum computing can improve the quality and variety of the created data.

EXAMPLE *Molecular simulation and protein folding; generating medical imaging data.*

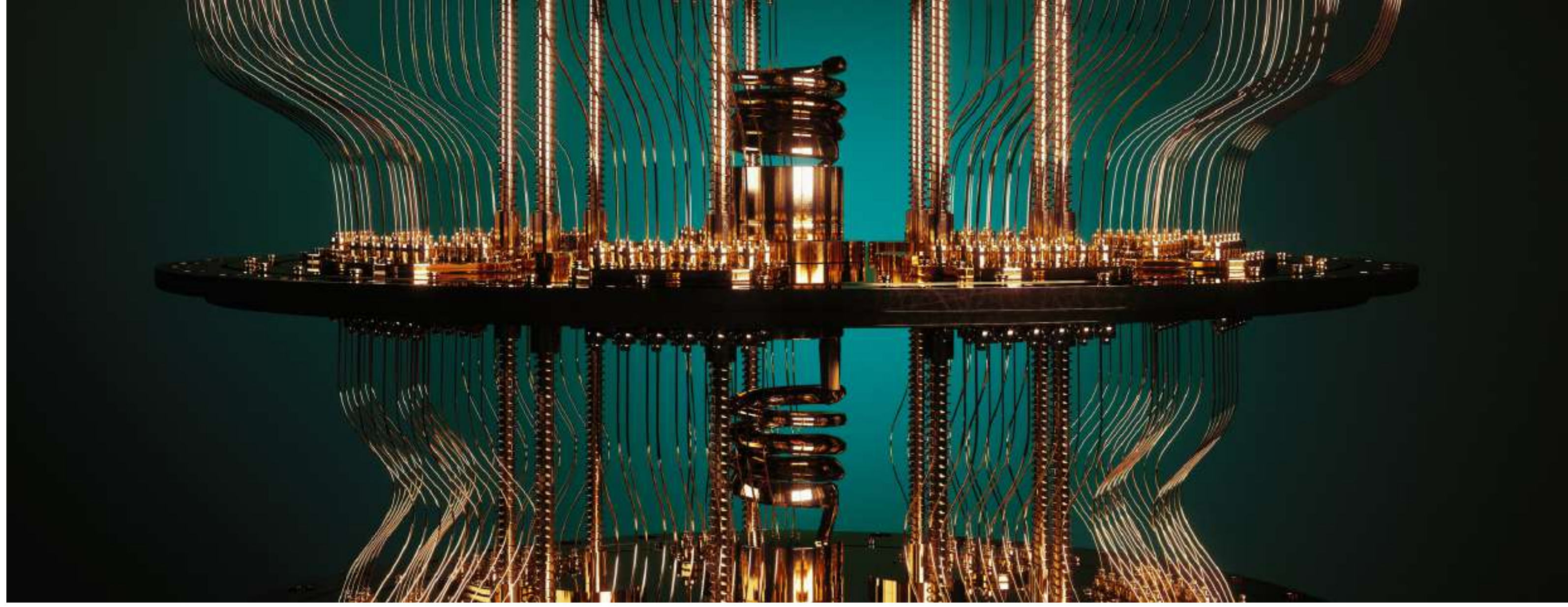
MACHINE LEARNING

Machine learning (ML) refers to a vast set of algorithms used for discovering patterns in massive amounts of data and drawing inferences from them.

Quantum computing is expected to enable the treatment of very large, unsorted data sets to uncover patterns or anomalies extremely fast. With a quantum computer's ability to manipulate multiple elements in a database simultaneously, it would be possible to identify similarities within seconds.

Quantum ML models have shown promising results in providing quantum speed-up for learning problems, including those for which solutions are easy to verify, but difficult to model with classical computers (Huang, et al., 2021). Quantum ML might also offer an advantage of providing generalizable results based on a small training dataset (Caro, et al., 2022).

EXAMPLE *Algorithm development for better and earlier diagnosis of a rare disease.*



Hardware and software challenges still need to be overcome before commercializing and scaling quantum computing use cases.

Several technologies are being explored for the physical implementation of qubits, including superconducting, trapped ions, photons, natural atoms, and more. Today, there are still numerous challenges linked to **errors** stemming from **noise, faults, and loss of quantum coherence** caused by vibrations, temperature fluctuations, electromagnetic waves, and other interactions of qubits with the outside environment, which eventually compromise the quantum nature of the computer.

To remediate these problems, quantum error- correction techniques are implemented. Thus, a single logical qubit can be created from several physical qubits with error corrections applied to mitigate errors (Takeda, Noiri, Nakajima, Kobayashi, & Tarucha, 2022; Livingston, et al., 2022).

One of the constraints of quantum computers in their current state is that they require specific conditions to run properly, such as ultra-cold temperatures. These conditions might raise questions concerning the environmental impact of quantum computing when scaled up.

Considering the existing hardware quality, speed, and scale challenges in quantum computing, a breakthrough is probably still several years away.

EXAMPLE *Two major families of quantum computers being explored are **universal gate-based quantum computers** (also called general purpose quantum computers) and **quantum annealers**. Quantum annealing is a method used for combinatorial optimization. By leveraging quantum physics phenomena, such as tunneling, it might get better or faster answers for problems with multiple possible solutions.*

It should be noted that loading information to a quantum computer requires a different **encoding process** compared to the one used for a classical computer. Creating quantum states from classical **datasets** currently requires a high number of operations, potentially limiting big data use cases. On the other hand, the **data stored in quantum state needs to be retrieved** from qubits and reconstructed in classical form. However, this process might be associated with information loss and is prone to error. Error-correction techniques are also applied to make quantum memory resilient against errors (Nakazato, et al., 2022). Researchers are looking for ways to easily interact with quantum computers, which would facilitate adoption in upcoming years.

Additionally, to take the full advantage of quantum computers new types of **applications** need to be developed with new architecture and based on new types of algorithms. The challenges with the development of these applications are linked to qubit noisiness and proneness to error, as well as to the complexity intrinsic to quantum computers. Indeed, quantum computers are exceedingly difficult to program. Provided the limited number of qubits available, most of today's implementations of quantum algorithms can be seen rather as proofs of concept.

2.2 ECOSYSTEM AND ADOPTION TIMELINE

In the recent years, quantum computing has been rapidly developing, and this tendency will likely persist. Indeed, the constant stream of investments in quantum computing is fed by both big tech players, like Google or IBM, and the funds raised by startups (Gartner, 2022). For instance, IQM Quantum Computers, a Finnish company specialized in building superconducting quantum computers for multiple use cases (including drug development), raised a record for Europe: €128 million in July 2022 (IQM, 2022).

An increasing number of actors are already positioning themselves in the race for the most reliable quantum computer technology or services. The offers range from end-to-end solutions enabling the clients to use quantum technology on cloud to software as a service platforms containing quantum and quantum-inspired algorithms for a wide range of applications (Gartner, 2022)) (AIMultiple, 2022). In addition to commercial tech players, research laboratories founded by university-industry cooperation or governments are also actively working on the topic.

EXAMPLES *of quantum computing players*

QUANTUM HARDWARE | **QUANTUM SOFTWARE**

END-TO-END SOLUTIONS PROVIDERS
– QCaaS, quantum cloud –

IBM, rigetti, IONQ, D-Wave The Quantum Computing Company, Google, amazon, Microsoft

QUANTUM HARDWARE OFFER
– Technology enablers –

qci, intel, hp

QUANTUM SOFTWARE & SERVICES
– Technology enablers –

1QBit, CLASSIQ, CQC Cambridge Quantum Computing, MULTIVERSE COMPUTING

Despite the progress in quantum technology observed over the past years, we are still in the first era of this technological breakthrough.

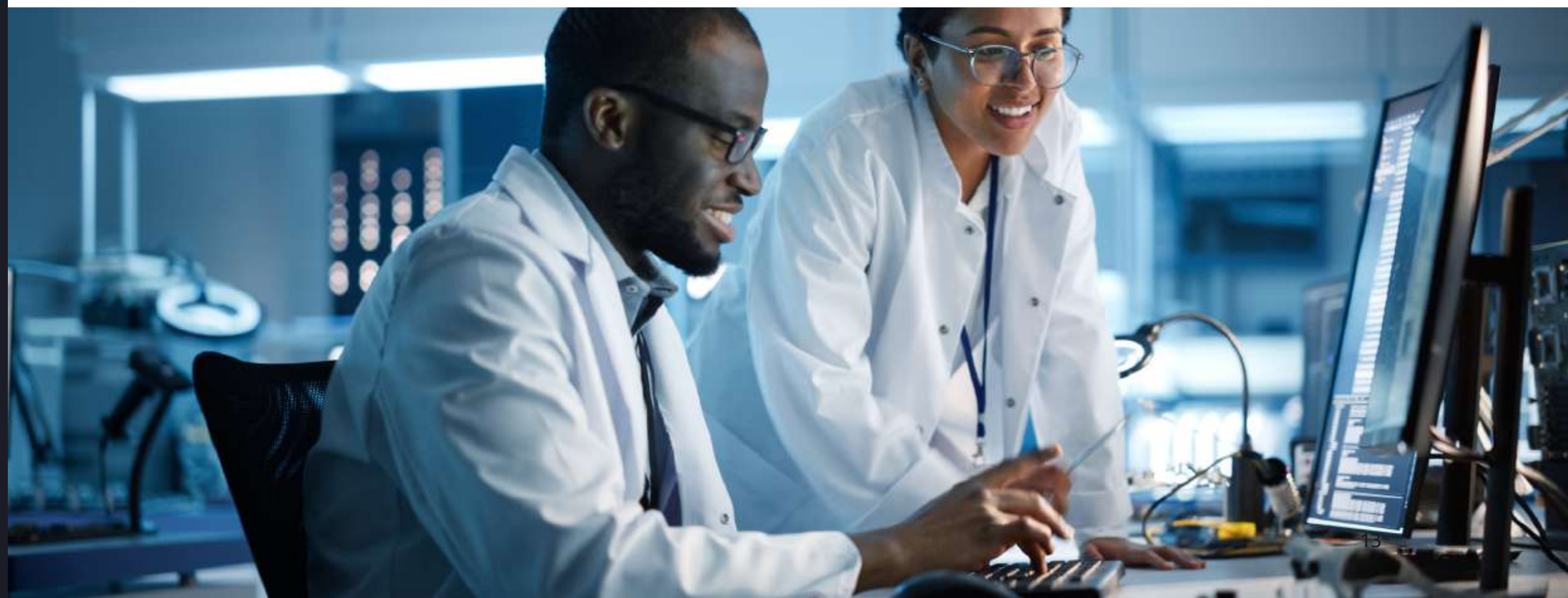
While the promise of **quantum** computing was first introduced in the eighties, the size of quantum computers **available on the market** has grown considerably in **recent years**. At the end of 2022, IBM presented a 433-qubits processor and was expecting to issue another one with over 1,000 qubits in 2023 (IBM, IBM Unveils 400 Qubit-Plus Quantum Processor and Next-Generation IBM Quantum System Two, 2022).

However, commercial adoption thus far remains out of reach, as an **important number of limitations** regarding qubit number, quality, and speed persist. A more accurate quantum technology is necessary, with the goal being full-scale fault-tolerant quantum computing. If the evolution of quantum hardware and applications continues its momentum, we should witness the emergence of the first commercial applications in the next 3 to 5 years, with significant advances over 5 to 10 years.

ACTUAL STATE OF QUANTUM TECHNOLOGIES	INCOMING IN THE NEXT 3 TO 10 YEARS	INCOMING IN THE NEXT 10+ YEARS
NOISY INTERMEDIATE SCALE QUANTUM (NSIQ)	**BROAD QUANTUM ADVANTAGE**	**FULL SCALE FAULT TOLERANCE**
The technological ecosystem is still working on a more stable qubit to move towards a more reliable quantum computer. Most companies are still seeking to understand how quantum could be leveraged.	A more stable quantum hardware is available on premises or via cloud. The first applications are commercialized and early adopters are harvesting the benefits.	Quantum computers are fully integrated in tech stack. Stabilized qubits allow the implementation of a full range of applications across industries. Companies gain maturity in leveraging quantum computing.

Even if the commercial use of quantum computing will not be immediate, it is important to prepare for its arrival now.

According to the Capgemini Research Institute, 10% of organizations expect quantum technology to become available for use in at least one major commercial application in 1 to 3 years (Capgemini Research Institute, 2022). Indeed, even for the companies already working on quantum computing or planning to do so, the commercialization is not planned in the short term. Yet, as with all the breakthrough technologies, it is important to prepare the launch pad for adoption as early as possible.



3 QUANTUM COMPUTING FOR PHARMA R&D

Quantum computing can be leveraged by pharmaceutical companies to optimize and speed up R&D in order to reduce the drug time to market and thus deliver relevant therapeutic solutions to patients faster.

3.1 DISCOVER BEST-IN-CLASS DRUG CANDIDATES FASTER

The drug discovery process is associated with a high level of biological and chemical complexity.

The research of a **druggable biological target** implies decoding disease pathophysiology and discovering the underlying and hidden mechanisms. This is achieved with the use of "omics" technologies, transcriptomic and proteomic profiling across cells and tissues, or genetic interaction and genomic methods. Due to the complexity of such analysis, it is often difficult to determine the optimal drug target. Several diseases remain incompletely understood, such as Alzheimer's disease, multiple sclerosis, and Sjögren's syndrome to name only a few.

Once the target is identified, **selecting the right molecule** to bind to it becomes the main challenge. Indeed, the chemical space contains no less than 10^{60} organic molecules with mass under 500 Da which can potentially be a drug candidate (Jean-Louis Reymond, 2010). We have recently observed increased interest in **phenotypic drug discovery**, which is agnostic to a specific drug target or a hypothesis about its role in disease. Yet, this approach involves complex analyses to identify the effects of a potential drug candidate on the phenotype.

Thus, understanding the physiochemical properties of **small molecules and biologics** (from therapeutic proteins, such as peptides and antibodies, to nucleic acid-based therapies or cellular and tissue therapies) is on the critical path to increasing the efficiency of drug discovery.

Artificial intelligence-powered solutions, which have a great potential of accelerating drug discovery, could be completed by quantum technologies.

Artificial intelligence (AI) has recently been more and more extensively used in drug development, e.g., through **virtual screening, target protein structure prediction, or computer-aided drug design**. Thus, the number of strategic partnerships between pharmaceutical companies and AI players, such as BenevolentAI, Exscientia, and Insilico Medicine, in the sphere of drug discovery skyrocketed from 10 in 2015 to 105 in 2021 (Taylor, 2022).

Because of the size and complexity of the biochemical systems that need to be understood to discover drug candidates, it makes sense to treat them using **quantum theory**, which can in turn be facilitated by running algorithms on quantum computers (Cheng, Deumens, Freericks, Li, & Sanders, 2020). How to simulate the behavior and interactions of molecules in chemical reactions? How does a protein's amino acid sequence dictate its 3-D structure? These and many other questions might be efficiently answered by leveraging quantum technologies.

Some of the companies seeking to improve drug discovery are **already focusing on the use of quantum technologies**. Such start-ups are mainly headquartered in Europe (e.g., Aquemia and Qubit Pharmaceuticals in France, HQS Quantum Simulations and CreativeQuantum in Germany, Cambridge Quantum Computing in the UK, Molecular Quantum Solutions in Denmark) or in the North America (e.g., Netramark in Canada, ODE, Polarisqb, QSimulate, and Zapata in the US) (The Quantum Insider, 2021).

As of today, these companies are extensively leveraging artificial intelligence to optimize the identification of drug candidates. For example, Qubit Pharmaceuticals, which raised 16 million in June 2022, is leveraging advanced simulation software and AI-powered medicinal chemistry to perform the drug discovery process in less than two years, from target optimization through hit screening and validation to lead optimization (Qubit Pharmaceuticals, 2020).

The applicability of quantum computing for molecular modeling can be leveraged in pharmaceutical research, from compound identification and optimization to biological target identification.

The nature of quantum computing, based on the laws of quantum mechanics, makes it possible to accurately model the molecular structure and behavior, as well as interactions between molecules (Leontica, Tennie, & Farrow, 2021).

Firstly, modeling the biological or pharmacological activity of small molecules with quantum computers can help **identify potential drugs** and optimize their design.

In what concerns **small molecules drug discovery**, one of the main limitations in the existing approaches is the amount of available experimental data, or the time needed to generate it.

Thus, **quantum chemistry simulation of molecules or their fragments** can be of great value for accelerating drug discovery. Furthermore, absorption, distribution, metabolism, excretion, and toxicity properties can be modelled, facilitating a more accurate **lead compound** selection. Indeed, quantum optimization could help to short-list candidate molecules from large combinational spaces.

Quantum computing could also be leveraged to **understand a protein's 3D structure**. Over a longer time horizon, it can also be used in the assessment of protein-target bond by simulation.

PROTEIN STRUCTURE PREDICTION WITH QUANTUM COMPUTING

One of the major themes of interest in drug discovery today is the determination of a protein's three-dimensional shape from its amino-acid sequence.

The most classical way to determine the protein structure is by trying each sequence of candidates one by one. This method might take a few years before finding the right protein structure for a given sequence of amino acids. Machine learning is being progressively adopted, notably with the release of AlphaFold, a deep learning algorithm developed by Google's DeepMind to predict protein structures (John Jumper, 2021), and with the recent advances of Meta's teams, which lead to obtaining results faster but with lower accuracy (Zeming Lin, 2022). However, the use of machine learning for protein structure exploration is restricted by the limits of computational power.

Quantum computing can be leveraged for speeding up protein structure prediction and making it more accurate. The first experiments were conducted to showcase the feasibility of developing such algorithms (Wong & Chang, 2021).

Thus, quantum computing can help to quickly understand protein structure in order to speed up or eliminate the drug candidate screening phase and decrease the drug discovery cost while improving the accuracy. This is thanks to being able to obtain the real behavior and structure of a given protein.

Finally, quantum computing might be used to identify proteins and nucleic acids, which are **druggable biologic targets.** Modeling the potential target can help assess its role in a disease pathophysiology. It can also lead to a better understanding of its 3D structure. Additionally, quantum machine learning, including new flexible models for classification and regression, could be leveraged to identify the causes of pathologies.

The computational power advantage brought by quantum computing could also help leverage multiple data sources. Indeed, while new approaches are being explored to apply systems biology to understand disease etiology and drug interactions by integrating omics data, computational load might be a limiting factor for the usage (Yue & Dutta, 2022). Quantum computing might provide a solution. For instance, Allosteric Biosicence and Polarisqb, two young companies specialized in quantum computing, partner to research protein targets for dealing with aging, longevity, and aging-related diseases. They do this by incorporating the knowledge from genetics, genomics, system biology, epigenetics, and proteomics (PolarisQb, 2022).

Quantum computing is also well suited for simultaneously testing and assessing the performance of different drugs on different targets in silico. The simulation of protein configuration with quantum computing, using a high-resolution physics model, could help to screen a drug on to multiple targets and assess the bond probability. The ultimate vision would be to perform extensive pre-clinical experimentation in silico to launch clinical trials only for the drugs with the highest **probability of success.**

The first actors specialized in quantum-enabled drug discovery are emerging in the market and starting collaborations with pharmaceutical companies. For example, a French start-up Aquemia specialized in leveraging quantum-inspired physics and machine learning for drug discovery, which raised €30 million in October 2022, had collaborated with Sanofi, Janssen, and Servier (BusinessWire, 2022).

The application of quantum computing for drug discovery appears the first future application of the technology in pharma sector.

POTENTIAL GAINS (Capgemini estimate)

UP TO **€200 - 400 M**
PER MOLECULE, THANKS TO:

- **Faster drug** candidate identification
- **Higher probability of success** for the selected drug candidates

EXPECTED TIMEFRAME

FIRST
APPLICATIONS
IN **3-5** YEARS

WHAT WILL BE THE IMPLICATIONS OF USING QUANTUM COMPUTING FOR DRUG DISCOVERY?

PORTFOLIO MANAGEMENT

Discovering drug candidates faster would mean that pharmaceutical companies can have a vaster choice of promising candidates. This would imply a change in the strategical and operational decision making around portfolio management. Indeed, the risk mitigation would be less associated with the choice of the disease to target and more with the capacity to accelerate clinical development.

Moreover, expanding the portfolio to include treatments for rare and neglected diseases would become more accessible.

POTENTIAL RESEARCH RE-INTERNALIZATION

Over the past decade, many pharmaceutical companies have moved to the research model based on outsourcing research activity or licensing in the molecules developed by biotech start-ups. Leveraging quantum computing might promote the reverse trend, as testing and discovering drugs would become quicker and less risky.

The adoption of quantum computing would also mean an expanding role for computational chemists and biologists in the research process. Consequently, it is important to build up the ecosystem for a fruitful collaboration and expertise sharing between the chemists and biologists and the data scientists within pharmaceutical companies and across the pharma ecosystem.

HOW CAN THE EXISTING TECHNOLOGIES BE LEVERAGED PRIOR TO QUANTUM COMPUTING ADOPTION?

AI IS ALREADY BEING LEVERAGED TO SPEED UP DRUG DISCOVERY.

For instance, machine learning algorithms already help to assess hit likelihood in high throughput screening, to predict protein structure, or identify genetic targets.

To benefit from the progress of AI for drug discovery, pharmaceutical companies can adopt a strategy based on partnerships with specialized start-ups and large tech players or develop internal expertise in computational chemistry and biology.

ADDITIONALLY, QUANTUM-INSPIRED SOLUTIONS MIGHT BE USED IN DRUG DISCOVERY.

Quantum-inspired solutions are based on using classical computers for simulating quantum effects. For example, this method was tested for the research of novel pharmacologic inhibitors (Jimenez-Guardeño, et al., 2022). Even though quantum-inspired solutions are not fully harnessing the quantum advantage that could be reached with quantum computers, they might be leveraged efficiently starting today. To find out more about quantum-inspired solutions, see our insights on the topic.

3.2 DE-RISK PHASE 3 CLINICAL TRIALS

Today, one third of molecules entering long and costly phase 3 trials fail.

Even though the chances of success for a drug increase throughout the development cycle, 38% of molecules entering phase 3 clinical trials fail (Dowden & Munro, 2019).

When phase 3 is planned, the data on the medication's efficacy and safety in only several dozens to several hundred patients is available, following phase 2 trials. Thus, optimizing phase 3 clinical trials is not a trivial task, requiring the enrollment of several hundred to several thousand patients and last for 1 to 4 years (FDA, 2018). Indeed, the passage to scale from a small and often relatively homogeneous population to a larger and heterogeneous one amplifies the risk of compromised efficacy or adverse events. It appears that most phase 3 clinical trial failures are due to inadequate efficacy, which might be linked to multiple factors, including suboptimal study design (Fogel D. B., 2018).

At the same time, the scale and duration of phase 3 trials, as well as the cumulative past investment, make its failure very costly. And the longer the trials last (for instance, due to delays in patients' recruitment), the higher the cost at stake.

Biological, clinical, and epidemiological complexity create limitations for predicting the probability of clinical trial success with the existing analytical tools.

Indeed, to successfully model the outcome of a clinical trial, one would need to comply with the following three requirements.

Accurately **model the biologic phenomena** based on the existing theoretical knowledge and the results of experiments

For example, to conduct an in-silico experiment in oncology, one would need to parametrize the elementary biological mechanisms8 (such as the rates and results of cell division or the interactions between antigen and antigen presenting cells), as well as biologic, anatomic, and chemical processes (e.g., the dynamic of tumor growth).

Consider the impact of multiple **factors describing and individual patients and corresponding medical history**

While the universal chemical and biological laws exist, in order to predict the safety and efficacy of a treatment in a concrete individual, one would need to consider this individual's genomics (DNA), transcriptomic (RNA), proteins, and metabolism, as well as the age, the environmental factors, and even the behavioral characteristics.

Factor in the **characteristics of the overall patient population**

Indeed, the combination of patient characteristics create a multitude of possible individual patients. The existing computational power limitations make it difficult to perform epidemiological analyses and scenario simulations with a very high number of parameters.

The advances in computational biology, machine learning applied to medical literature, real-world and clinical data, and other advanced analytics combined with ever growing corpus of medical data have already opened exciting opportunities for intelligent clinical trials.

Yet, several limitations remain.

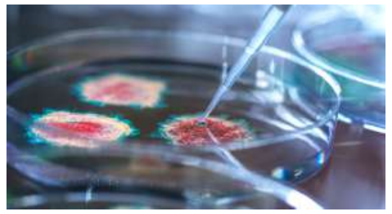
1 The complex phenomena cannot be modelled fully	**2** The number of generated and assessed scenarios is limited by the constraints of computational power	**3** The data might be missing and would need to be generated

Modelling disease and treatment effect at gene, cell, tissue, organ, patient, or population level can be leveraged to optimize clinical development.

Quantum computing offers the possibility to model complex phenomena that cannot be modelled with existing tools, while also harnessing a much superior computational power. Therefore, it provides two necessary ingredients to model the disease and treatment, as well as to generate and assess a multitude of scenarios to choose the best one.

Quantum computing enablers could be beneficial to decode the complexity and assess the effects of the experimental therapy at three levels:

BIOLOGICAL



- Modelling anatomic, histological, and biochemical metrics; the structure and behavior of organs, biological pathways, etc.

CLINICAL

- Modeling and simulation of patient profiles based on the data on demographics, clinical data, pathology, medical imaging, genomics, transcriptomics, proteomics, metabolomics, etc.
- Prediction of metrics and endpoints for these profiles.

EPIDEMIOLOGICAL

- Accounting for trends and characteristics at the population level to factor in the probability of different scenarios.
- Predicting the future pharmacovigilance trends.

Phase 3 clinical trials can be de-risked by enhancing clinical trial design or reducing patient cohort size.

To enhance clinical trial design, quantum-computing-based modelling using available data would help to:

- formulate the research question, including the target disease phenotype or stage, treatment paradigm (e.g., drug alone or in combination), and the key endpoints,
- define eligibility criteria determining the target population,
- take the patient-centric considerations into account (e.g., ensure the inclusiveness of the clinical trial cohort and adapt the protocol to the patients' needs).

Preparing the clinical trials by **modelling** the treatment effect and then optimizing the design could increase the probability of success. For example, developing a digital twin of human cells and organs and assessing the effect of the investigational drug in silico might help identify the phenotypes that would be the best responders.

Similarly, leveraging quantum computing on a large corpus of data from the medical literature and from the pre-clinical or first clinical phases can help identify the profiles at risk of severe adverse events. It should be noted that the coherence and relevance of clinical trial design should be ensured to make both the protocol and the results acceptable by the healthcare authorities. Thus, leveraging the information on past studies and the corpus of medical literature is especially important.

These findings can in turn help adjust the target population and the clinical trial eligibility criteria to **increase the probability of clinical trial success**.

To **reduce patient cohort size while ensuring generalizable results**, quantum computing would help to partially of fully virtualize the trial population. It is noteworthy that the virtualization of clinical trials would help address ethical issues linked to, for example, assigning patients to the control arm. It can also serve as enabler for trials in the context of patient scarcity (e.g., in rare diseases).

Additionally, **to speed-up patient recruitment**, quantum computing might accelerate the data-driven mapping of medical and disease communities to streamline the identification of relevant site, HCPs, and patients (use cases that are already addressable with AI-powered solutions today).

Moreover, the clinical trial process can be enhanced by **portfolio management optimization and life-cycle management anticipation**. In fact, quantum computing can be leveraged to prioritize the indications to target a certain molecule.

EXAMPLES *of quantum computing applications to de-risk phase 3 clinical trials*

	ENHANCE CLINICAL TRIALS DESIGN (I.E., REFINE INCLUSION AND EXCLUSION CRITERIA)	FACILITATE THE IMPLEMENTATION OF THE SYNTHETIC CONTROL ARM
QUANTUM OPTIMIZATION	Selection of the optimal set of eligibility criteria to enhance efficacy and safety	
QUANTUM MACHINE LEARNING	New flexible models for classification & clustering to identify sub-groups of best responders or to develop the synthetic control arm	
QUANTUM SIMULATION	Using quantum-based models to simulate the study outcome based on the combinations of eligibility criteria	Using a quantum-based synthetic control arm

The application of quantum computing for clinical development optimization might be leveraged by the pharma sector in the next decade.

POTENTIAL GAINS (Capgemini estimate)	EXPECTED TIMEFRAME
UP TO €300 - 500 M PER MOLECULE, THANKS TO: • De-risking the clinical trials and thus diminishing the costs associated with trial failures • **Faster clinical developwment** process	**FIRST** APPLICATIONS IN **5-7** YEARS

The first demonstrations of the quantum computing capacity to enhance the analysis of patient data and perform the modelling of complex biological systems are being made.

Researchers are currently working on the approaches to simulate with quantum computing biochemical systems, which are intractable with classical algorithms on classical computers, such as studying histone demethylases (enzymes involved in the transcription of genetic information contained in DNA) or understanding some specific cases of molecular recognition (Cheng, Deumens, Freericks, Li, & Sanders, 2020).

Another direction of research is linked to the shift from traditional machine learning to quantum-based models applied to medicine. For example, the accurate classification of the subtypes of non-small-cell lung cancer was performed by leveraging quantum computer technologies was performed by Canadian startup, Netramark (Jain, Ziauddin, Leonchyk, Yenkanchi, & Geraci, 2020).

There is also an ongoing effort to leverage quantum computing to model the patients at cellular, tissue, organ, and even behavioral level. Thus, quantum algorithms might be used to study human brain based on the data gathered by genetics, genomics, neuroimaging, and deep behavioral phenotyping (Emani, et al., 2022).

Some of the first applications of quantum computing for patient modelling are being considered. For instance, according to IBM, quantum machine learning could be used to improve the prediction of the sensitivity of cancer cells to drugs based on the genomic and chemical data (IBM Institute for Business Value, 2020).

QUANTUM COMPUTING AND DIGITAL TWINS

With the advent of quantum computing, one of the key tools for de-risking phase 3 clinical trials might be quantum digital twins.

In general, a digital twin is a virtual representation of a system or a process based on the data points generated by it. The digital twin can be used for solving optimization problem, simulating possible scenarios, and early default detection.

In addition to the optimization of clinical trials, digital twins might be considered at two levels.

- **Digital twins of patients, organs, tissues, or cells** could be used to model the disease, treatment mode of action, and patients' response to the treatment. Such "biological" digital twins would be helpful for better understanding the efficacy and safety of the investigational drug. Indeed, by leveraging quantum computing, it might be possible to leverage the medical literature, the real-world data, and the data from previous clinical trials to develop digital twins of real-world patients and use them to model the control and potentially the active arm, thus virtualizing clinical trials. Partial or complete virtualization of clinical trials would mean not putting real patients under risk associated with receiving an investigational drug, while speeding up the clinical development.
- **Digital twin of a clinical trial and its ecosystem** could help to better analyze the actual patients and their response to drugs, as well as to mitigate the risk of trial discontinuation or failure. This implies developing and analyzing digital twins of the clinical trial stakeholders (including patients, healthcare professionals, sites, sponsors) and interactions between them. The analysis of such digital twins can make it possible to decipher risks quickly and to build up data for the optimization of future trials. For example, if problems of hypersensitivity to the drug are detected, their root causes can be analyzed quickly, thus ensuring participants' safety and securing the trial success.

Today, there is a growing interest in developing digital twins in a clinical context. For example, digital twins of patients with cardiovascular diseases can be developed based on data from electronic health records, biological, clinical, genetic, molecular, and imaging data, as well as from mobile data sensors and wearable devices (Coorey, et al., 2022). Digital twins of patients could be used, for example, to predict complications (Thiong'o & Rutka, 2022)

Some of the challenges on the way to a wider use of digital twins are linked to the data ecosystem. For a digital twin of a patient to function, multi-modal clinical, demographic, and even behavioral data would need to be collected and analyzed in an exhaustive and continuous manner. This raises questions around the availability of tools for data collection and ensuring the quality of collected data (e.g., how many laboratory tests and medical images could be performed, whether wearables should be used for continuous data collection, whether patients' questionnaires can be trusted to collect behavioral data). Moreover, the questions linked to data security and privacy would need to be resolved.

Yet, the volume of the available clinical data is constantly growing and one of the key limitations to the use of digital twins is in mastering the treatment of the multimodal data and modelling complex phenomena by taking all this data into account. And that is where quantum computing technologies could be leveraged to remediate the limitations of the existing algorithms and existing computers.

By leveraging the power of quantum computing we might be able, for example, to simultaneously analyze physical patients participating in a clinical trial and their corresponding digital twin models to improve the quality of trial results. For example, in a multi-center clinical trial, centralized digital twins of patients could help mitigate judgmental errors by analyzing the center-level specificities.

Patient data augmentation (which can be based on quantum simulation) could support the avoidance of justifiable geo-political or ethical constraints that can limit the number of patients enrolled into clinical trials, such as pediatric patients (Subramanian, 2020). Quantum machine learning algorithms trained on multimodal patient data could help discover new patterns in drug effects and identify good responders or patients at risk of adverse events.

WHAT WILL BE THE IMPLICATIONS OF USING QUANTUM COMPUTING FOR DE-RISKING PHASE 3 CLINICAL TRIALS?

DRUG POSITIONING AND SHIFT TOWARDS PERSONALIZED MEDICINE

De-risking phase 3 clinical trials with the help of quantum optimization, machine learning, and simulation would often imply the identification of sub-populations of patients who are the best responders to a drug or who have the lowest risk of the adverse effects. Such insights would put a pharmaceutical company in front of a dilemma: decreasing the targeted population and securing the trial or taking a risk in order to target a larger indication. Thus, the decision-making concerning drug positioning might need to evolve.

TARGETED RECRUITMENT FOR CLINICAL TRIALS

In order to recruit patients with specific disease phenotypes quickly, pharmaceutical companies might need to adopt new practices of HCP and patient engagement.

HOW CAN THE EXISTING TECHNOLOGIES BE LEVERAGED PRIOR TO QUANTUM COMPUTING ADOPTION?

Today, AI-powered solutions can be leveraged to partially address the stakes linked to de-risking phase 3 clinical trials. This means advanced analytics applied to real-world data and trials data, as well as to the medical literature can be leveraged to optimize the design of phase 3 trials. Even though practical applications of quantum computing for patient modelling appear rather remote, it is important to consider how the AI models developed today might be enhanced by the quantum advantage in the future.

4 STEPS TO TAKE TODAY TO GAIN THE COMPETITIVE EDGE WITH QUANTUM TOMORROW

To prepare for the quantum advantage, pharmaceutical companies should start to act as soon as possible.

We propose 4 actions to take in our recent Point of view: *The Future of Quantum in Life Sciences*.

1 CALIBRATE THE R&D INVESTMENT	2 DEVELOP A QUANTUM ROADMAP	3 BUILD QUANTUM SKILLS AND EXPERTISE	4 DEVELOP A PARTNER ECOSYSTEM

First, let us discuss **calibrating the R&D investment in quantum computing.**

Pharma industry has already started its journey towards investing in quantum computing for R&D through partnerships with tech giants, startups, and research institutions.

As of today, the pharmaceutical industry has not yet internalized quantum computing expertise. Yet, the first collaborations on quantum computing emerged in the past two years.

Some pharmaceutical companies chose to team up with the **tech giants**, thus betting on the innovation capacity of the latter. For instance, in January 2021, Boehring Ingelheim launched a collaboration with Google Quantum AI, with a specific focus on molecular dynamics simulation (Boehringer Ingelheim, 2021). Bayer is also planning on leveraging Google Cloud's high-speed processors for large quantum chemistry calculation to accelerate drug discovery (Bayer, 2023).

Others opt for collaborations with **startups specialized in the development of quantum computing software**. Since January 2021, Roche has been collaborating with UK-based Cambridge Quantum on quantum computing applied to early-stage drug discovery and development (Cambridge Quantum, 2021). Pfizer is also seeking to optimize its drug discovery process by collaborating with XtalPi, a quantum physics-based, AI-powered pharmatech platform operating in the US and China (Pfizer, 2018).

Finally, some pharma players are investing in **long-term collaboration with research institutions** to foster quantum computing innovation. In September 2022, Novo Nordisk launched a Quantum Computing Program with the University of Copenhagen. Novo Nordisk's grant of approximately €200 million (DKK 1.5 billion) in a program that will last for 12 years shows the company's conviction in the technology's potential (Novo Nordisk Foundation, 2022)

In the years to come, it will be important for pharma companies to foresee the investments in quantum computing, and to gradually adjust their size and structure, depending on the conjuncture of the quantum technology development.

In the following pages, we zoom in on several pragmatic aspects, notably the operating model to adopt and the software to invest in.

4.1 OPERATIONAL MODEL: MAKING TODAY'S USE CASES QUANTUM-COMPATIBLE IN THE FUTURE

Let us focus on **building quantum skills and expertise** and **developing a partner ecosystem**. To do so, we can draw a parallel with the adoption of artificial intelligence (AI) by the pharmaceutical sector.

The adoption of Big Data, Big Data analytics, and AI by pharma companies was slowed down by regulatory constraints, the absence of in-house expertise, and a disconnect between data and AI and business teams.

Pharmaceutical companies have long been used to operating data, notably the results of clinical trials, which serve as the basis for market access authorization. Yet, several technologies have entered the scene and needed to be adopted by the sector, notably Big Data and advanced analytics, including AI. The adoption of these technologies across the pharma industry was hindered by a mistrust in the robustness of AI-based solutions and their limited interpretability. Indeed, the pharmaceutical industry is highly regulated and no "black box" technologies could be adopted for the analyses, which would be further used to support drug submission or used in medical practice. Additionally, the adoption of Big Data and AI technologies was slowed down by the absence of in-house expertise and potentially mistrust in the robustness of AI-based solutions. Many pharmaceutical companies filled this gap by partnering with tech giants, investing in specialized startups, and launching in-house data labs and data squads.

Traditionally, digital initiatives have been managed by IT and digital departments. So naturally AI and data teams were first created within these departments. The launch of the first proofs of concept was performed successfully by small, isolated teams. Yet, for AI initiatives to be successful they need to account for clinical and biological context, while being anchored in business stakes. Moreover, the robustification and industrialization of use cases with real business impact required new governance between IT and business teams, notably the launch of cross-functional initiatives.

Today, the adoption of AI and the move towards data strategy is orchestrated within pharmaceutical companies by dedicated departments. The construction of data lakes and control towers is also among the key trends aimed at establishing solid foundations for the implementation of AI use cases with a tangible ROI.

The timeline of quantum computing adoption will likely be similar to that of AI adoption: going from first proofs of concept run by small dedicated teams to use case industrialization and the formation of dispersed teams.

To prepare for the quantum advantage, pharma companies could build small teams of experts in quantum computing and or dedicate resources to scanning the progress within the ecosystem.

As pharma companies move towards industrialization of AI use cases, we recommend starting to adopt the quantum computing expertise via one of two ways:

- Build small teams of quantum experts who would act as single point of contact for data and AI, IT, and business teams. The advantage of internalizing the expertise is in the possibility to maximally adjust it to the needs of the company and its business priorities.
- Create a small quantum innovation team to orchestrate the collaboration with software and service companies or research labs specialized in quantum computing. It appears important to perform regular scans of the progress in quantum computing applied to the healthcare sector in order to identify opportunities early.

For more thoughts on the choices to make when building the quantum computing team within a pharmaceutical company, please also check out *the perspective of one of our quantum experts.*

It is necessary to set up the process for ensuring AI-based use cases implemented today can be enhanced with quantum tomorrow.

Most of the use cases that can be tackled with quantum computing are already partially addressable with AI. With this in mind, to prepare the adoption of the newest technology and to successfully leverage both approaches in parallel in the future, it is important to bear in mind the potential of the quantum advantage when building data and AI strategy and governance.

For instance, drug effect modelling is already partially accessible with AI. In the future, when relevant, it might be performed more accurately or faster with quantum computing, while leveraging more data points. In order to prepare to embrace the quantum advantage, it is important to ensure, starting today, that as much data as possible is collected from real-world and digital clinical trials.

Pharma companies need to consider the risk of digital native players challenging traditional operational models.

If digitally native players like GAFAM enter the scene of quantum computing-powered drug discovery and clinical trials, the operational model of pharma companies might need to be changed drastically. For example, for a long time, the bottle neck in the protein folding simulation was the lack of algorithmic solutions and limited computational power, obstacles which have since been overcome by players like Google with its AlphaFold. Note that the OpenFold project, which uses AlphaFold, to date has no representatives of the pharma industry and is comprised of companies that have large computational capabilities.

Similarly, if tech players monopolize the use of quantum computing for life science applications, pharma companies will be faced with some tough choices, such as licensing in the molecules discovered by tech players.

Large tech players are at the forefront of quantum computing. However, the traditional business model of pharma is being challenged by newcomers from the tech sector.

Digitally native players, including GAFAM: Google (Alphabet), Apple, Facebook (Meta), Amazon, and Microsoft, are apt to conquer the health sector. These players are multiplying the investments in healthcare. For instance, Alphabet made over 90 investments in the healthcare sector over the past two years, with one of its ventures, Verily, raising $1 billion in September 2022 (CBInsights, 2022). GAFAM are collaborating with pharmaceutical companies, but also with the healthcare providers, with most of the projects focused on leveraging AI, (e.g., to develop cancer vaccines, analyze pathology, automate administrative tasks, or support medical decisions) (The Medical Futurist, 2022). Tech giants are also directly investing in the health sector. For instance, Amazon cashed out almost $4 billion to acquire One Medical, a US primary care company, in July 2022 (Amazon, 2022). GAFAM's expansion to primary care sector, as well as their active role in accompanying citizens in their daily health routines open a highway for becoming a trusted health partner for patients, thereby generating valuable health data. As such, digital players are progressively establishing their presence in the healthcare sector, with the aim to re-think and change it.

4.2 HARDWARE: DEVELOPING IT INFRASTRUCTURE WITH THE FUTURE QUANTUM ADVANTAGE IN MIND

Let us now have a look at the hardware part of the quantum roadmap.

The choice of hardware platform implies an important investment and might easily become a hurdle to updating the IT paradigm in the future. Enriching the IT infrastructure with new types of computers and ensuring compatibility with already existing assets is investment heavy. Moreover, work that is undertaken to update elements that are not yet obsolete can have an unnecessary negative ecological impact, generating pollution that could easily be avoided. Thus, to what extent should you invest in **classical, high-performance, and quantum computers**?

High-performance computers, including supercomputers, perform calculations faster than classical computers.

High-performance computing (HPC) is the practice of using parallel data processing to improve computing performance and make complex calculations. HPC achieves these goals by aggregating computing power, so even advanced applications can run efficiently, reliably, and quickly as per user needs and expectations. A **supercomputer**, one of the best-known examples of HPC, is made up of many computers and processors working together to achieve parallel processing and high performance. Consequently, it delivers much higher power and better performance than a traditional computer. Supercomputers are used by scientists and engineers to address challenging computational tasks.

However, some problems are too difficult even for supercomputers, especially if the problem at hand is characterized by a high degree of complexity. Thus, **problems with multiple variables interacting in intricate ways are frequently unsolvable for supercomputers**. For instance, modeling the behavior of individual atoms in a molecule is a challenging task. Supercomputers can be well adapted to tasks like sorting through a large database of protein sequences, but quantum computers might be needed to identify subtle patterns in data in order to understand these proteins' behavior (IBM, 2022). Noteworthy, many HPC centers plan to invest in quantum computing to expand their hardware offerings in the foreseeable future.

Consider a hybrid approach with the possibility to progressively adopt quantum computing.

Today, classical computing remains the mainstream, while high performance computers are used more and more often for computationally heavy, data-intensive tasks. As for quantum computers – according to most predictions, they will reach maturity in the following decade. Another technological trend to follow is **quantum cloud computing**, which might be of use for those pharmaceutical companies that choose not to invest in owning quantum computing capabilities but to rather access them via cloud tech.

Future technological developments will probably depend on a **hybrid approach** to computing, where companies take advantage of the flexibility of HPC in the cloud and the powerful, specific nature of quantum technology hardware. Many believe that too much emphasis is placed on comparing classical and quantum computing and speculating over which hardware will dominate the future of computing. **The future is likely to be more complex, with both technologies being used to support big data projects and AI and ML applications**. Quantum computers will likely not replace all other computers. For some use case, quantum computers will not be needed, and for other use case, the hybrid version should be enough.

CONCLUSION

Pharmaceutical research and development are likely to benefit from quantum computing in multiple ways, including those going beyond time and cost savings.

The promise of quantum computing for pharmaceutical R&D resides in its relevance for analyzing and simulating complex chemical and biological phenomena. Essentially, it can mean a shift towards more in-silico experimentations, meaning less risk for the participants of clinical trials.

Additionally, factoring in multiple data sources would facilitate finding the right molecule for each patient, based on their genotype, endotype, or even socio-economic background and behavioral characteristics. The enhanced computational power and the potential of performing more complex calculations offered by quantum computers can help promote personalized medicine. It is worth noting the availability of high-quality data on patients (such as patient registries) would be needed to leverage quantum computing capacities to their fullest.

In the longer term, quantum computing can be leveraged by pharmaceutical companies beyond R&D, optimized supply chains and bioproduction being noteworthy examples.

From plant scheduling to chemical and biologic process optimization to predictive maintenance and quality control, quantum computing is applicable when optimizing pharmaceutical production.

Moreover, modelling complex supply chains can help ensuring the stability of components flow, to both avoid shortages and facilitate a more flexible production.

Even though quantum technology must still evolve, pharmaceutical companies need to start considering the potential of quantum computing in their operational and tactical decisions today.

Quantum computing is still an emergent technology that has not reached its commercial potential. As the stability and quality of qubits improves and the technology becomes more refined, quantum computing might play a major role across the pharma value chain, in both the mid- and long-term perspective. Early adoption of quantum computing in addition to traditional and high-performance computing used for statistical and advanced analysis can be essential for remaining competitive.

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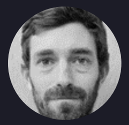

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