QUANDELA

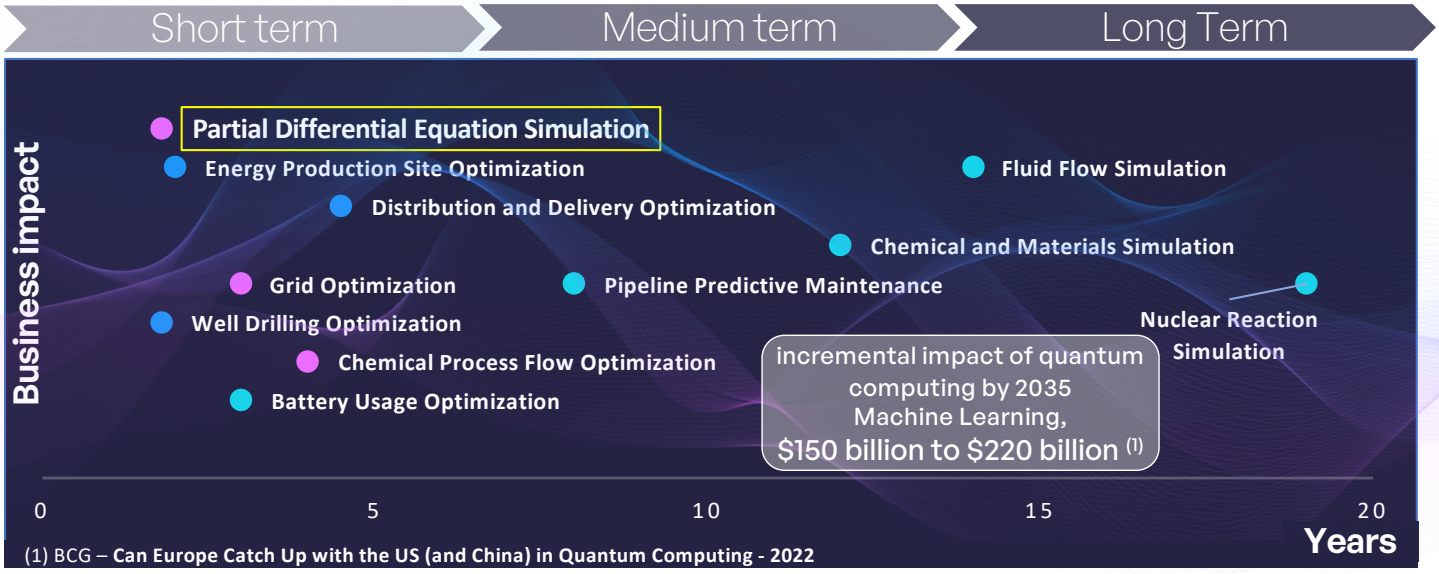
2023- Case story

Energy

EDF improves safety & durability of its industrial infrastructures with Quantum optimization

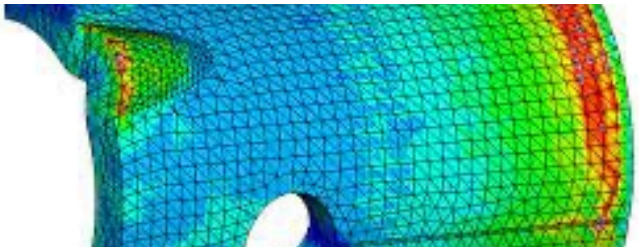
Use-cases for Energy

Quantum Machine Learning	**Partial Differential Equation Simulation**, Chemical Process Flow Optimization, Grid Optimization Prediction
Quantum Simulation	Chemical and Materials Simulation, Nuclear Reaction Simulation, Fluid Flow Simulation, Pipeline Predictive Maintenance, Battery Usage Optimization
Quantum Optimization	Structural Optimization, Energy Production Site Optimization, Well Drilling Optimization, Distribution and Delivery Optimization



(1) BCG – **Can Europe Catch Up with the US (and China) in Quantum Computing - 2022**

Challenge : handling a huge number of parameters with better precision and less computation consumption



EDF, French national electricity provider, needs to deal with **safety and reliability** for its dams and nuclear plants. In particular, it must prevent the occurrence of cracks from a large variety of factors, including environmental factors, aging, or even human errors. Impacts of these cracks can be catastrophic, leading to structural failure, casualties, and significant economic damage.

As such, **it is essential to understand and assess the behavior of cracks in these structures.** In order to improve the predictions from its computational simulations, EDF uses an increasing number of parameters. Therefore, its models lead to an exponential need for computation.

Besides the computing techniques is the sheer scale of the simulations involved. To accurately model the behavior of these structures, simulations must be run on a massive scale, often involving millions or even billions of data points. This **requires powerful computational resources, including high-performance computing clusters and specialized software tools.**

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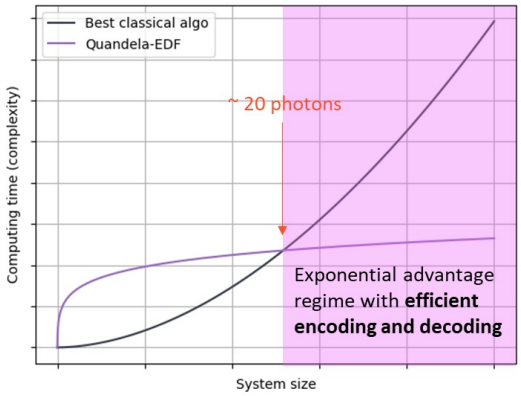
Energy

"We have developed Quantum algorithms for mechanical simulation and are testing them on Quandela computers. We are extremely positive with both the perspectives of Quandela Quantum technology to address some of our hardest industrial challenges such as the simulation of hydroelectric dams, and the scientific excellence of the team."

Joseph Mikael - Head of Quantum Computation & Quantum Information project at EDF

Solution : gain an exponential speed-up on the short-term for the simulation of mechanical structures



Quandela and EDF developed a method that brings value to EDF on the short-term (NISQ era). The method is based on a **variational quantum algorithm** and aims at solving a specific set of partial differential equations. A set of differential equations is first converted into a linear system of equations, whose solution is represented by the minimum energy of a quantum observable.

Use of Quantum Computing may lead to an exponential speed-up. Indeed, computing the energy of this system only requires a number of qubits. Besides, only few measurements are needed to have useful information of the system (key point as many methods requires exponential amount of measurement which kills any quantum advantage).

Use of Photonic Quantum Computer scale gives an exponential advantage. **Crossing point between the classical and the quantum curve is system size that can be reached with 20 photons.**

A general framework that can be applied to many other use-cases :

This framework is generic: from an energetic formulation of the problem, candidate **to be encoded efficiently on a Quantum Computer, only a few measurements are necessary to retrieve useful information.**

Therefore, if another use-case fulfills this powerful framework, it can be simply solved and deliver value for the end-users even with the actual Quantum Computing capabilities.

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Identification of computational problems where Quantum will bring you the most value

Consultation with Quantum scientists to explore the best approaches

Test and benchmark these approaches on state-of-the-art Quantum Processors (QPU)

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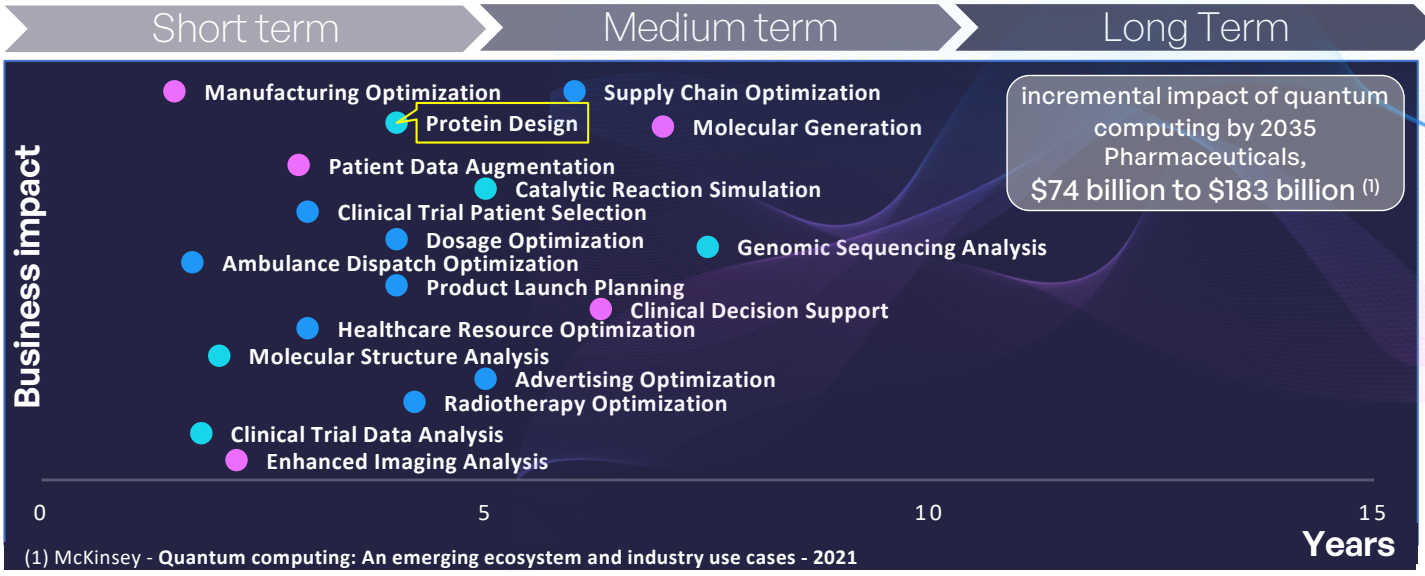
2023- Case story

Healthcare & Life Sciences

Biopharma drug discovery boosted by Quantum Simulation

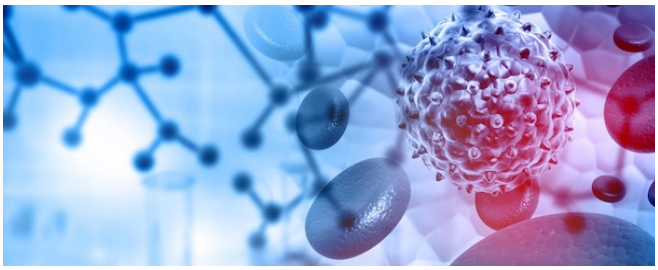
Use-cases for Healthcare & Life Sciences

Quantum Machine Learning	Molecular Generation, Genomic Sequencing Analysis, Enhanced Imaging Analysis, Patient Data Augmentation, Clinical Decision Support
Quantum Simulation	**Protein Design**, Molecular Structure Analysis, Catalytic Reaction Simulation, Clinical Trial Data Analysis, Supply Chain Optimization
Quantum Optimization	Clinical Trial Patient Selection, Dosage Optimization, Radiotherapy Optimization, Product Launch Planning, Manufacturing Optimization, Healthcare Resource Optimization, Advertising Optimization, Ambulance Dispatch Optimization



(1) McKinsey - **Quantum computing: An emerging ecosystem and industry use cases - 2021**

Challenge for Biopharma : increasing the R&D efficiency



The biopharma R&D process—from drug discovery to development—is a **costly (~ $180 billion/year)**[1], lengthy, and risky endeavor. A new drug typically takes **10 to 15 years to progress from discovery to launch**, and the capitalized costs exceed $2 billion[1] for a single new drug. The success rate is less than 10% from entry into clinical development to launch.

In 2022, **Bio Artificial Intelligence market was estimated at $1.200 millions**[1]. High-performance computing is already key for drug discovery and development = modeling of molecular structures, mapping of the interactions between a drug and its target, simulations of the drug's metabolism, distribution, and interactions in the wider human system.

Next technical revolution should be **computational chemistry algorithms** aim to predict how a potential drug molecule will bind to specific target proteins, by modeling the binding energy of interaction.

(1) Source McKinsey

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Healthcare & Life Sciences

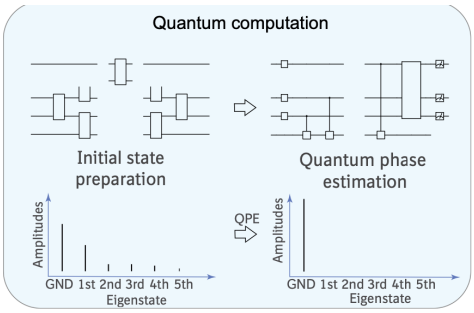
"Quantum computing is likely to have a profound impact on biopharma R&D, potentially changing the competitive set and dynamics of drug discovery."

BCG - Will Quantum Computing Transform Biopharma R&D?

"Quantum Computing's biggest impact on pharma will be in the discovery phases."

McKinsey - Pharma's digital Rx: Quantum computing in drug R&D

Solution : leverage Computer Assisted Drug Discovery (CADD)



Quantum Computing could make current CADD tools more effective by helping to **predict molecular properties with high accuracy.** That can affect the development process in several ways, such as modeling how proteins fold and how drug candidates interact with biologically relevant proteins. Here, QC may allow researchers to screen computational libraries against multiple possible structures of the target in parallel. Current approaches usually restrict the structural flexibility of the target molecule due to a lack of computational power and a limited amount of time. These restrictions may reduce the chances of identifying the best drug candidates.

In the longer term, Quantum Computing may improve generation and validation of hypotheses by using Machine Learning algorithms to uncover new structure-property relationships. Once it has reached sufficient maturity, QC technology may be able to create new types of drug-candidate libraries that are no longer restricted to small molecules but also include peptides and antibodies. It could also enable a more automated approach to drug discovery, in which a large structural library of biologically relevant targets is automatically screened against drug-like molecules via high-throughput approaches.

One could even envision QC triggering a paradigm shift in pharmaceutical R&D, moving beyond today's digitally enabled R&D toward simulation-based or in silico drug discoveries—**a trend that has been seen in other industries as well.**

Quantun Computing use cases apply to multiple aspects of drug discovery and will emerge at different points over an extended timeline. All of them, however, may enable more accurate and efficient development of targeted compounds.

To go further, read Raffaele Santagati et al., Drug design on quantum computers, https://arxiv.org/abs/2301.04114

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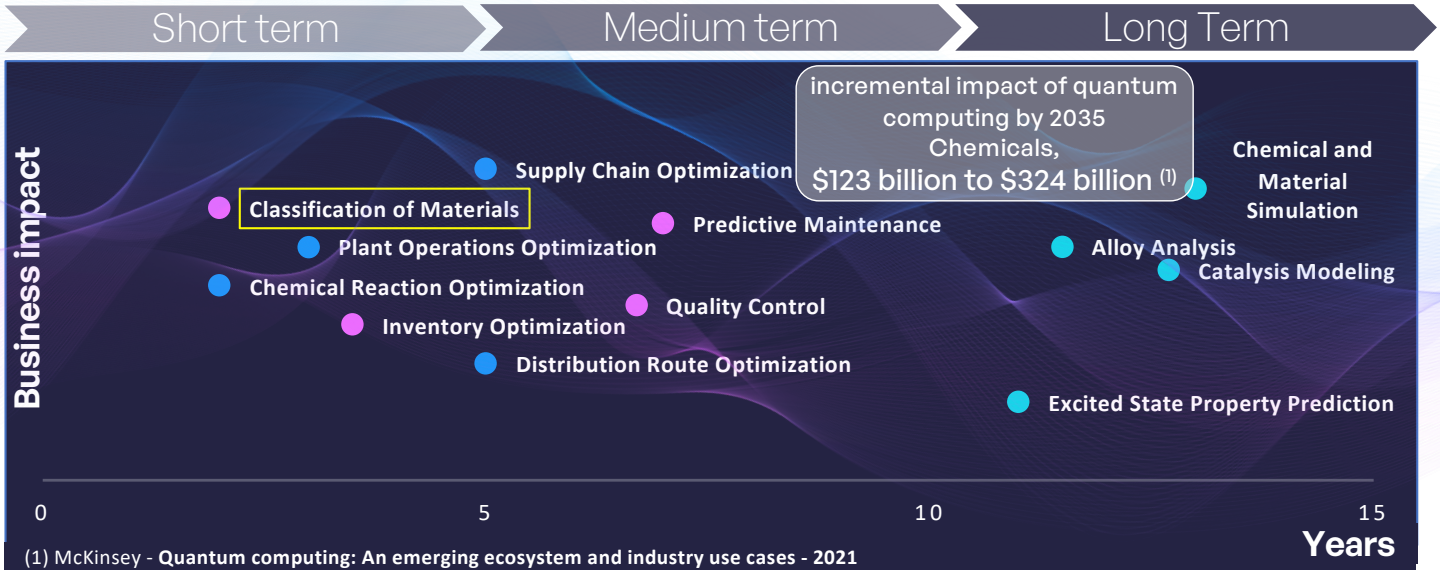
2023- Case story

Chemicals & Materials

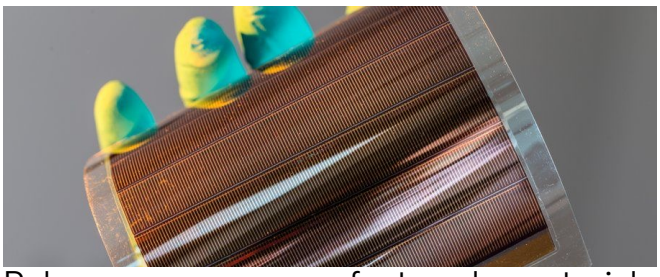
Alysophil accelerates the discovery of new polymers with Quantum Machine Leaning

Use-cases for Chemicals & Materials

Quantum Machine Learning	Classification of materials, Predictive Maintenance, Quality Control, Inventory Optimization,
Quantum Simulation	Chemical and Materials Simulation, Catalysis Modeling, Chemical Dynamics Simulation
Quantum Optimization	Chemical Reaction Optimization, Plant Operations Optimization, Distribution Route Optimization, Supply Chain Optimization, Alloy Analysis, Excited State Property Prediction



Challenge for manufacturers : designing new polymer materials with specific properties



Polymers are manufactured materials **ubiquitous in the industry**= electronics, cosmetics, drug design, carbon capture, aerospace, automotives, clothing, communication, 3D printing, organic photovoltaic, etc. To target specific needs, industrial manufacturers try to synthesis polymers with given properties, mostly from a process of trial and error, but this is costly and time-consuming.

A designing process has emerged with high-performance computation, using Deep Learning. But this sophisticated models are hard to develop and to run on classical computers due to the **gigantic chemical space of polymers** and to the complexity to search for an optimum.

A new approach should be explored. Quandela and Alysophil focused on the opto-electronic properties of polymers. To be more specific, the goal is to classify whether a polymer belongs to the near-infrared or the visual class. This **work paves the way towards designing new organics photovoltaic materials,** useful for recycling solar panels, a big challenge in the solar panel industry.

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QUANDELA

2023- Case story

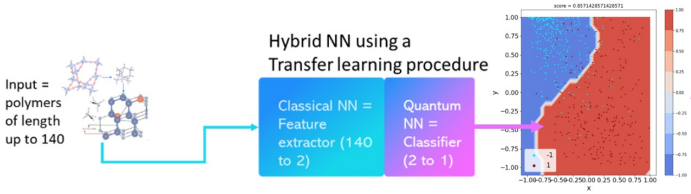
Chemicals & Materials

"With Quandela we implemented state of the art methods that outperform today's standard in production.

By joining forces, Quandela and Alysophil developed today and tomorrow best solutions."

Philippe Robin, Founder & President Alysophil, leader in AI methods for continuous-flow chemistry

Solution : develop a hybrid algorithm mixing Machine Learning with Quantum



The chosen solution is a **hybrid algorithm**. The **classical part** takes as an input a numerical representation of polymers and provides a representation in lower dimension of this dataset. The output dimension must be sufficiently small such that the **Quantum Computer** can then classify those data. In scheme above, the method is described = an embedding step, a training step and the classification in the visual (blue) or near-infrared class (red).

The results are already conclusive. This algorithm is converging, and the accuracy for the classification is comparable to what the state-of-the-art classical method obtains. This is a demonstration of a treatment of **real chemical data using a hybrid approach for classification.**

Targeted extensions to other polymers properties

In the coming years, as the size of the Quantum Computer will increase, the classical pre-processing part can be reduced, until the capability is reached to run fully the algorithm on a Quantum computer. For this reason, this hybrid approach yields best of both world and paves the way for even more success.

It must be underlined that this hybrid approach is generic. Thus, many variations might be explored to classify and to predict other polymers properties but also different chemicals and materials.

To go further, read Stoyanova et al., Photonic Quantum Computing For Polymer Classification, https://arxiv.org/abs/2211.12207

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