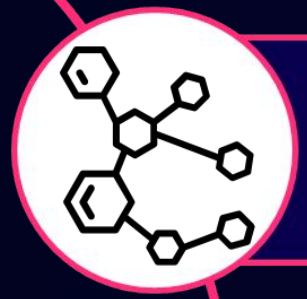
MERCK x PushQuantum

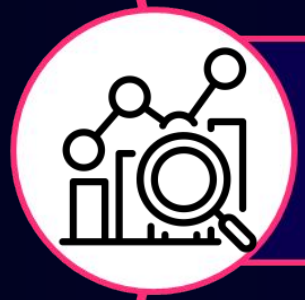
Team Merck ideation deliverable

General problem space

What goals does Merck have using Quantum?



Quantum simulation promises enormous acceleration in the calculation of various processes required for drug production

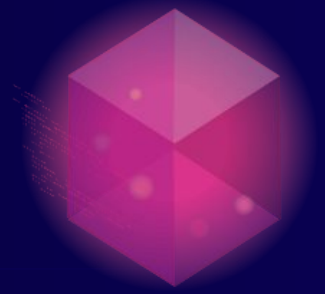


Ensuring Merck’s long-term sustainable profitability through business analytics at different points of the product life cycle

Potential of reduction in CO2-emissions through optimizations in supply chain processes

Quantum Chemistry - Protein Folding

Prediction of protein folding by means of quantum simulations



What?

The 3D-structure of novel proteins cannot be predicted by conventional methods. Quantum simulations make this possible.

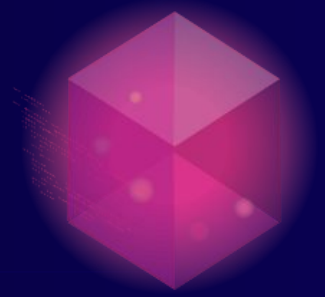
Why?

Accurate predictions of protein folding are enormously useful for tailoring the production of new drugs. Companies from the pharmaceutical industry can benefit enormously from this.

How?

Selling a software simulation service based on existing algorithms and the continuously improved hardware which predicts the 3D-structure of novel proteins.

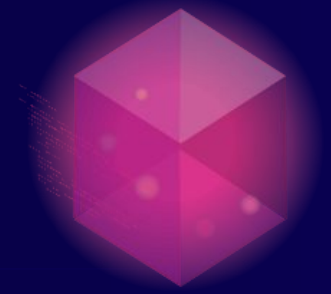
Business Analytics



What?	Current methods for pricing securities and evaluation of risk measures for risk management processes are computationally intensive	Optimizing product portfolio with both sustainability and profitability constraints
Why?	Using quantum algorithms such as Amplitude estimation (AE) to estimate unknown parameters offers a quadratic speed-up over classical algorithms like Monte Carlo.	Need to focus on r&d of products that are compatible with sustainability goals
How?	Development of a software aided by QC to determine VaR and CVaR of a portfolio that yield a better performance than current techniques and provide it at a cost for pharmaceutical companies	Formulating product portfolio creation as a knapsack problem and solving it and selling the software to companies

Supply Chain optimization

Maximizing a sustainability coefficient within SCM with max CO2 footprint constraint.



What?	Current factory placement is not well coupled with production needs and modes of transportation	Traditional transportation assets in drug production have high carbon emissions and routing optimization process is out-of-date on low-emission transportation mode alternatives
Why?	A more efficient factory placement that benefits from Quantum Annealing and QAOA can lead to sustainable profitability and low CO2 emissions.	Efficient routing schemes benefit from Quantum Annealing and QAOA with costs and emissions as constraints
How?	Providing companies with a software for factory placement optimization based on a QAOA/quantum annealing prototype	Providing companies with a platform for transportation optimization based on a QAOA/quantum annealing prototype