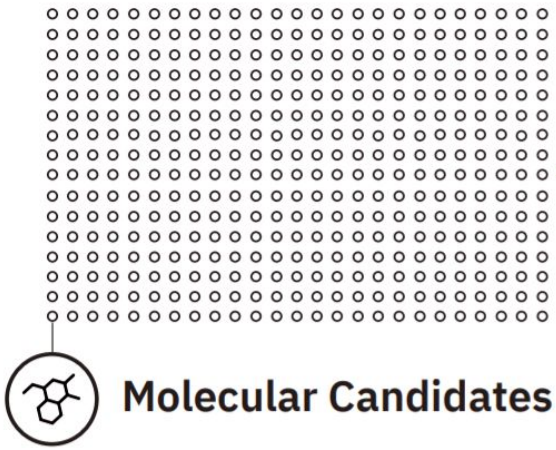
Molecular
Quantum
Solutions

Molecular Quantum Solutions

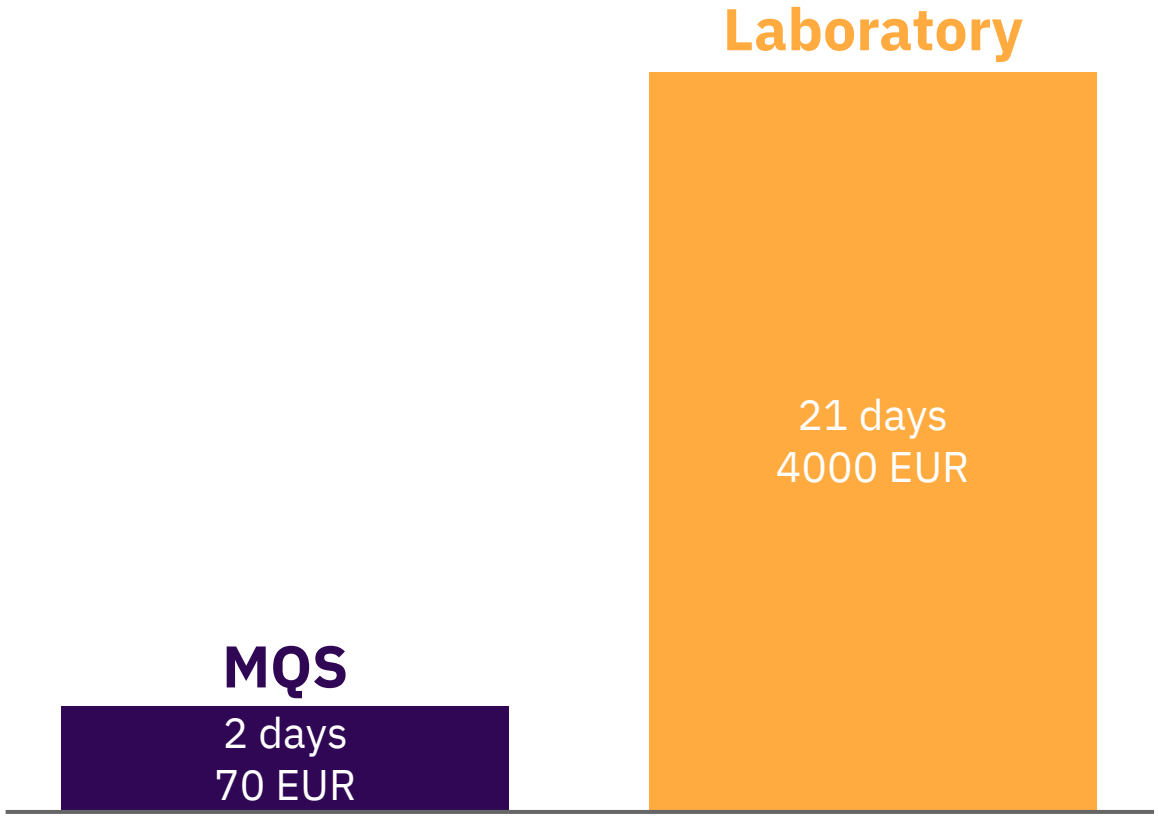

Molecular Candidates
Quantum Chemistry Simulations
Ranked Candidates

Actual case with a pharma company

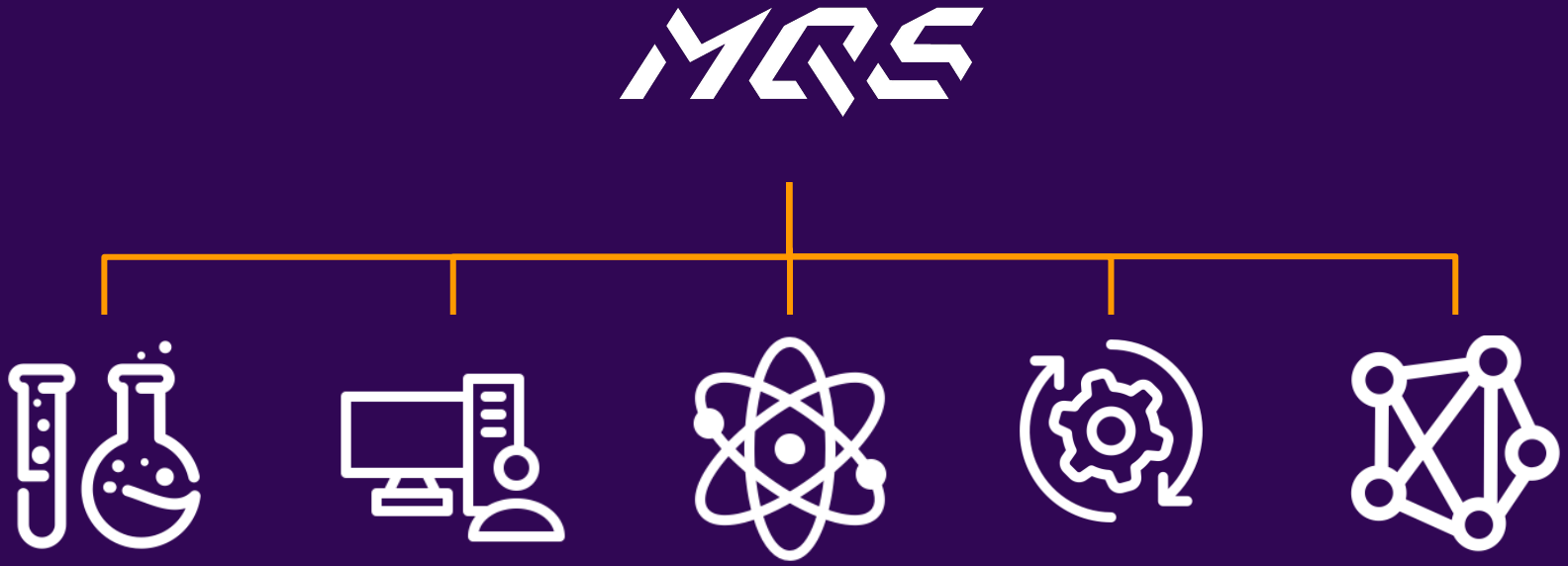
90%

reduction in time and cost

for an experimental study with a complex mixture of 5 compounds



All-in-one combined expertise in one software tool



Laboratory technology

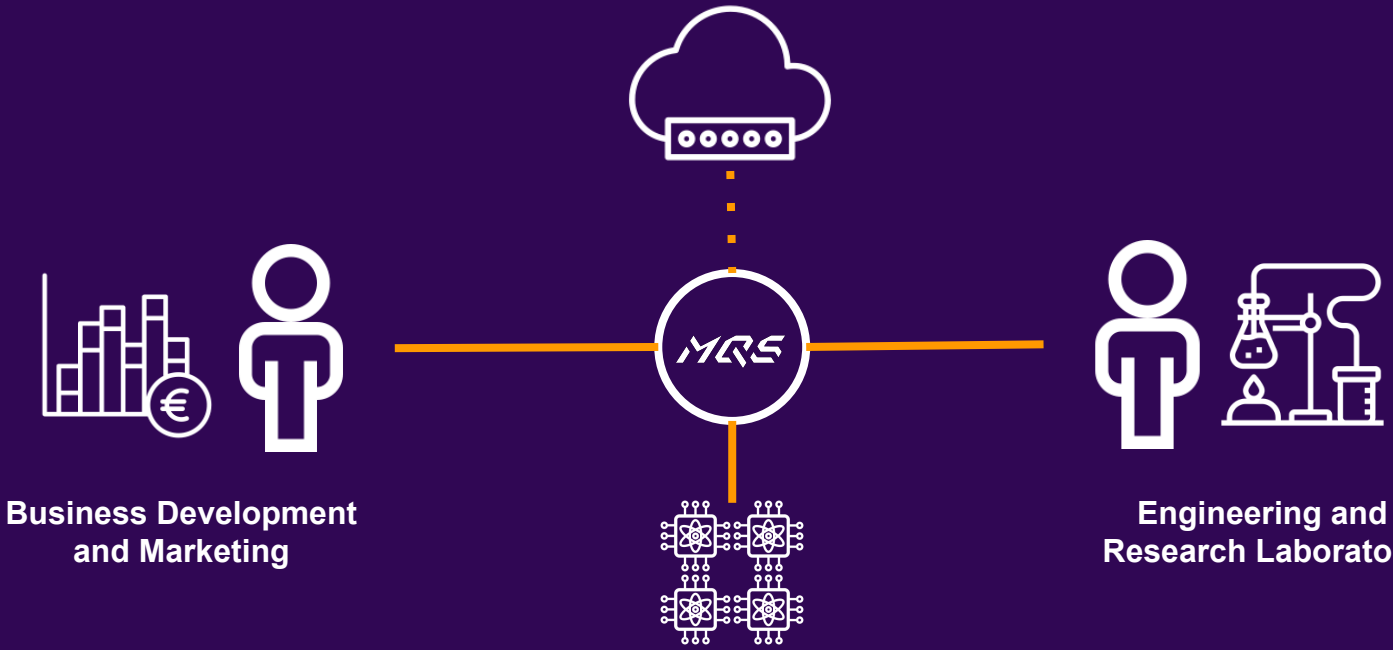
IT and systems operation (DevOps)

Quantum chemistry via CPUs, GPUs & quantum computing

Product, process and material design

Data analysis/ machine learning

Enable an efficient workflow for distributed lab facilities & teams



Partition coefficients for chromatographic separations

Molecular Quantum Solutions

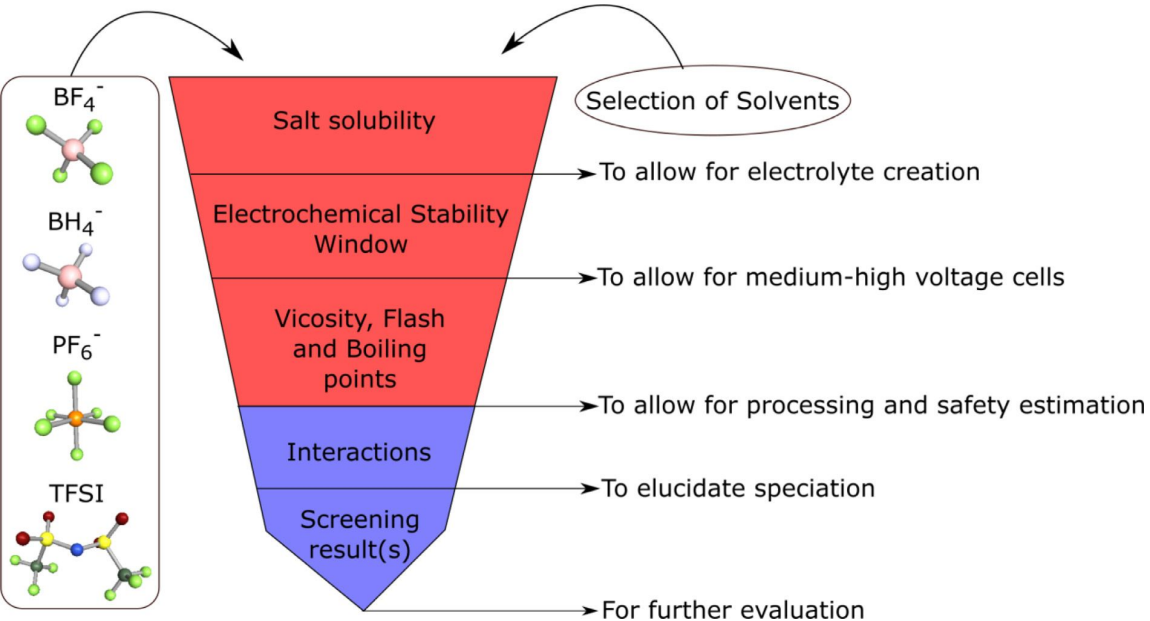
Organic raw materials

Process design for chromatography

Natural oils / health products

TEMP °C	SOLUTE	PHASE 1	PHASE 2	VALUE
25	Not disclosable	Octanol	Water	Not disclosable
25	Not disclosable	Heptane	menthol/levulinic acid	Not disclosable
35	Not disclosable	Octanol	Water	Not disclosable

Electrochemistry and energy storage



- Selection of solvents using quantum chemistry-supported methods
- Novel electrolytes for supercapacitors based on green solvents (ionic liquids, DES)
- Screening for new battery materials (calcium and magnesium-based)
- Novel quantum-aided screening strategy is efficient and a useful stepping-stone to reduce the overall effort

ACS Sustainable Chem. Eng. 2020, 8, 1, 372–381
https://doi.org/10.1016/j.ensm.2021.04.015

Evolution of computing

Molecular Quantum Solutions

Applications

Expert systems

Neural networks

Credit scoring

Image analysis

Marketing analysis

Portfolio optimisation

Network load analysis

NLP

Image classification

Predictive maintenance

Supply chain analysis and optimisation

Self-performing, automated systems

High-throughput analysis and advanced materials design

1950 1980 1990 2000 2020 Time [Year]

Mainframes

Workstations

Servers & PCs

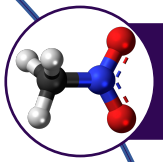
GPUs & ASICs

Quantum Computers

MQS' Quantum Computing Methodology

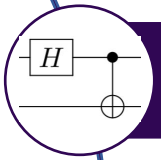
Molecular Quantum Solutions

Problem formulation



Choose a problem well suited for quantum simulation

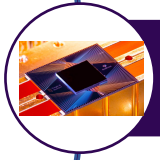
Quantum algorithm design



Considerations for hardware
- ❏ connectivity
- ❏ size
- ❏ available operations

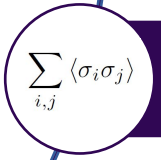
Design principles
- ❏ fewer qubits
- ❏ shorter circuits
- ❏ fewer multi-qubit gates

Quantum computation



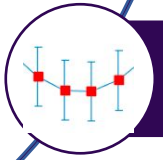
Reduce cost of this as much as possible

Calculation



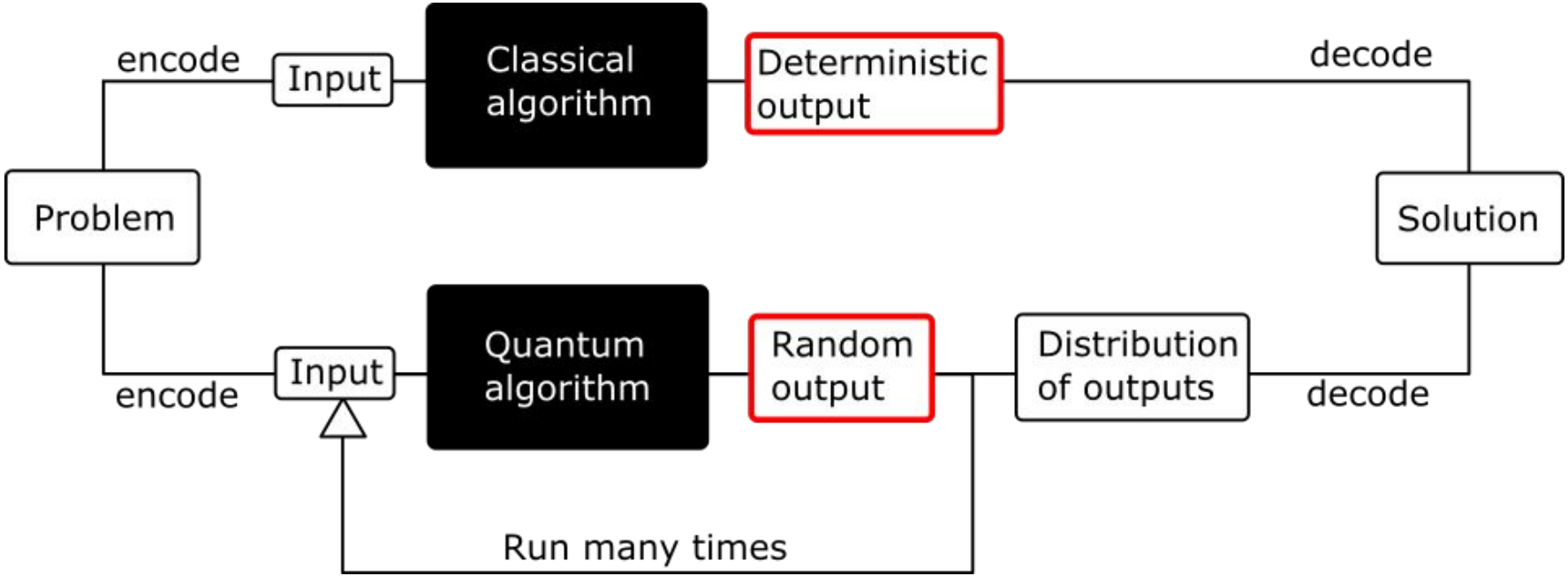
- ❏ Group calculations that can be performed simultaneously
- ❏ Classical pre and post-processing methods for higher precision

Result



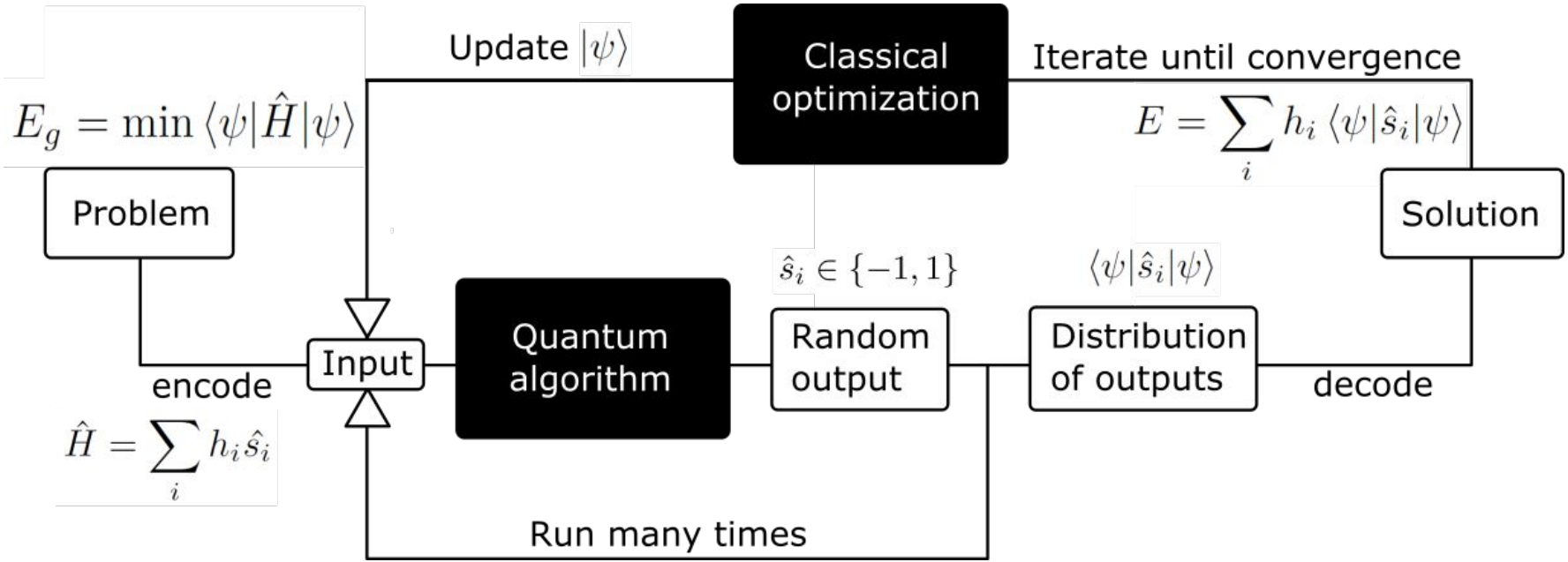
Validation and benchmarking of quantum algorithms against each other and against classical methods.

Classical vs quantum computing

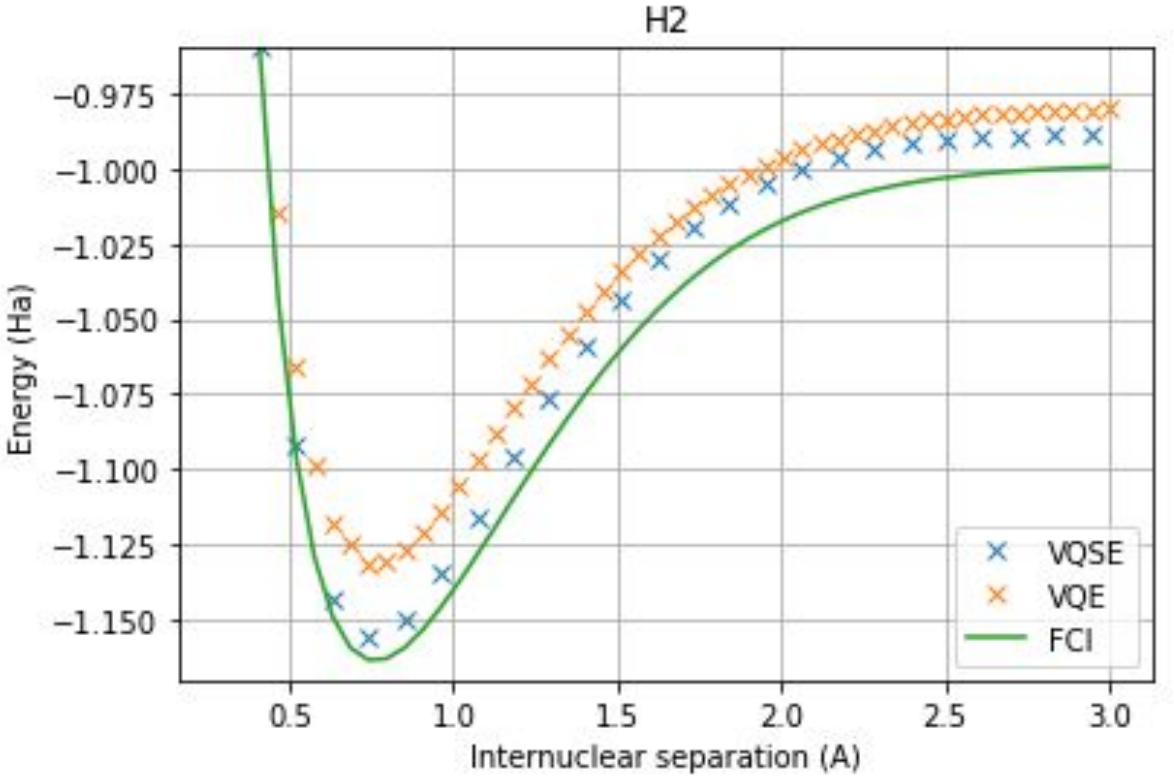


Variational Quantum Eigensolver (VQE)

- Hybrid algorithm that uses both classical and quantum computing
- Classical optimization algorithm is used to update the answer until it converges



Simplest example: energy of hydrogen molecule



- Orange data points obtained from quantum simulation
- Blue data points include corrections from classical post-processing
- Green curve is classically computed (exact for a system of this size)
- Calculation performed on 4 qubits, but could be done on as few as 2 qubits.

Software as a Service (SaaS) - Product Portfolio

	Dashboard	**API (Application Programming Interface)**	**Compiled packages for different applications**	**Services (DevOps, Workshops, Consulting)**
Sales Model	Subscription	Subscription	One time payment	Service Contract
Marketplace	Cloud Provider MQS Webpage	Cloud Provider MQS Webpage	MQS Webpage	MQS Webpage
Current state	alpha testing	beta test release in Q4 2021	currently being tested with companies	DevOps contracts Quantum computing workshop available

Molecular Quantum Solutions

Founders

Mark Jones (CEO), Postdoc Chemical Engineering

Lukasz Ruszczynski (CSO), PhD Chemical Engineering

Current team

Molecular
Quantum
Solutions

https://MQS.dk

contact@mqs.dk