

# NEASQC project

Next ApplicationS of Quantum Computing

<NE|AS|QC>

## Boosting practical applications of quantum computing on the early quantum computers – the NISQ (Noise Intermediate-Scale Quantum) systems

### About us

- A multidisciplinary consortium of 12 companies and research labs
- A 4-year project started 1st September 2020
- Funded by the European Commission's Horizon 2020 programme as part of the Quantum Technology Flagship

### Our 4 objectives

- 1 Develop **industrial Use Cases** for NISQ machines
- 2 Develop **open-source application libraries** for the myQLM free programming platform
- 3 Build a strong **community** dedicated to industrial NISQ applications
- 4 Develop SW stacks and benchmarks for the **QT Flagship HW platforms**

### Our results

Libraries on GitHub

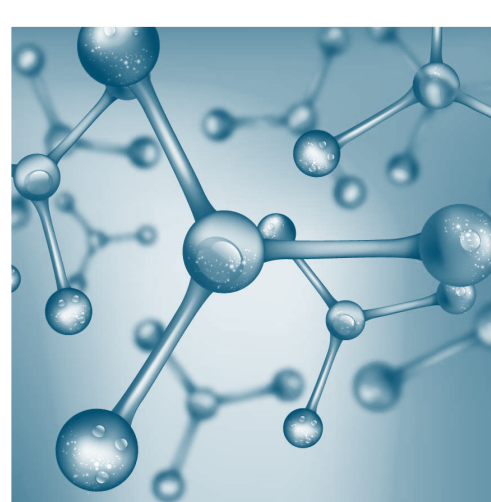


Publications



## Our 9 NISQ-compatible use cases

Each use case is endorsed by an industrial partner and investigated by an integrated team of industrial and academic partners. Each use case has published open source beta software and/or publications, visit their web page to access those documents.



### Chemistry

Bridging the gap between recent proof-of-concept quantum chemical computations on NISQ processors and actual, industrial-scale quantum chemistry problems

#### 1 CO<sub>2</sub> recapture

We investigated two methods for improving the measurement results of a quantum computation, one based on enhanced sampling using Bayesian statistics and one based on projecting the result to fulfill so-called n-representability constraints which may be violated in a noisy quantum computation. We also investigated the use of quantum computing to analyze the formation of a benzene-CO<sub>2</sub> dimer.

[github.com/NEASQC/D4.2](https://github.com/NEASQC/D4.2)

#### 2 Drug discovery

Our repository collects Python scripts and Jupyter notebooks that allow the user to test different variational algorithms. It contains custom functions developed by NEASQC, such as Variational Hamiltonian Ansatz and PBO (Pre-Born-Oppenheimer) Hamiltonian.

[github.com/NEASQC/Variationals\\_algorithms](https://github.com/NEASQC/Variationals_algorithms)  
We also released the Krachem package, a beta-version Python library designed for working with chemical molecules, fragmentation, based on chemical files input and mathematical tools from graph theory. It can be used for Intermolecular Fragmentation and Intramolecular Fragmentation

[github.com/NEASQC/qfrag](https://github.com/NEASQC/qfrag)



### Machine Learning & Optimisation

Quantum-enhanced machine learning & optimization methods for:

3 Quantum reinforcement learning for optimal **inventory management**  
[zenodo/D5.5 Implementation of a QRL algorithm on real architecture](https://zenodo.org/record/5158025)

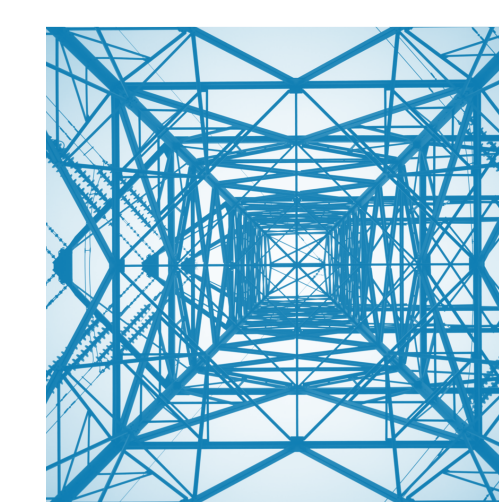
4 QAOA\*-type algorithms for **mesh segmentation problems**

5 QAOA\*-type algorithms for **smart-charging of electrical vehicles** and Vehicle2Grid optimization.

We are developing a hybrid quantum/ classical architecture for tackling large instances of these problems, as well as a ZX-Diagrams based approach to optimize QAOA circuits  
[zenodo/D5.8 Specification and implementation of coloring-based QAOA algorithm for minimizing charging station numbers](https://zenodo.org/record/5158025)

6 Applications of QML optimisation and quantum Monte-Carlo methods in **finance**, such as Option pricing or Value-at-Risk estimation  
Our Quantum Quantitative Finance Library assembles different quantum algorithms and techniques for use in the financial industry  
[github.com/NEASQC/FinancialApplications](https://github.com/NEASQC/FinancialApplications)

\* QAOA = Quantum Approximate Optimisation Algorithm



### Symbolic AI and graph algorithmics

Developing methodologies and implementations in the areas of AI and graph algorithms for:

7 Quantum **natural language processing**

Our alpha SW prototypes explore a) the DisCoCat-based model using parameterised quantum circuits to encode a pre-defined dataset of sentences and b) Dressed Quantum Circuits in which pre-trained classical models are used as pre-processing layers in a transfer learning fashion  
[github.com/NEASQC/WP6\\_QNLP](https://github.com/NEASQC/WP6_QNLP)

8 Quantum **probabilistic safety assessment** for large infrastructure installations. Our open source code helps implement fault trees

[github.com/NEASQC/ft-2-quantum-sat](https://github.com/NEASQC/ft-2-quantum-sat)

9 Quantum rule-based systems for **diagnosis and treatment**

of Breast Invasive Ductal Carcinoma  
Main efforts have been done in a) implementation of inferential networks in a quantum environment, and b) definition of a quantum model for dealing with inaccurate knowledge  
[github.com/NEASQC/qrbis](https://github.com/NEASQC/qrbis)



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