<NE|AS|QC>

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About NEASQC

NEASQC stands for NExt ApplicationS of Quantum Computing. This research project brings together academic experts and industrial end-users to investigate and develop a new breed of Quantum-enabled applications that can take advantage of NISQ systems in the near future.

NEASQC is use-case driven, and this brochure introduces the 9 practical problems we are addressing.

Machine Learning and Optimisation

These four use cases address a wide variety of industries, such as energy, oil & gas and finance. They have one thing in common: they can benefit from Quantum-enhanced machine learning and optimization methods

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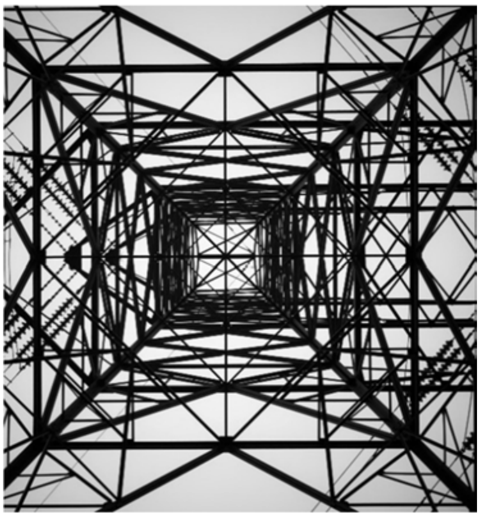

Symbolic AI and graph algorithmics

These use cases provided by a wide variety of sectors (linguistics, oncology, energy) all aim to develop methods and implementations in the areas of artificial intelligence and graph algorithmics.

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Chemistry

This group of use cases aims to bridge the gap between the recent proof-of-concept quantum chemical computations on NISQ processors and actual, industrial-scale quantum chemistry problems.

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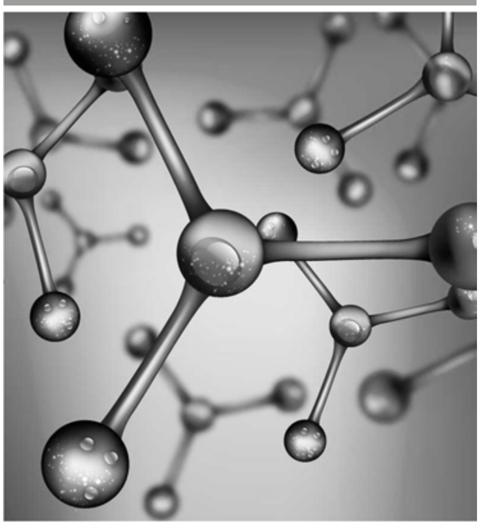
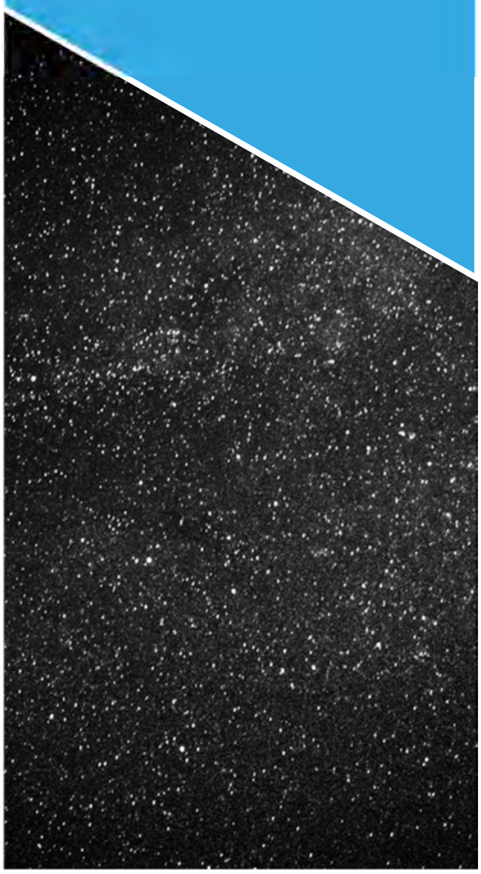




Machine Learning and Optimisation

Hard optimisation problems for smart-charging of e-vehicles

Smart-charging is a mandatory condition to allow electric mobility expansion. The high level of power required to load electrical vehicles, especially on fast load stations, require optimal modulation of this load demand in time. Further, the use of vehicle batteries as energy storage devices and power sources (“Vehicle to Grid” or “V2G”) could significantly improve the flexibility of the electrical system, reduce high-peak of electricity demand and generate significant energy savings. We are investigating the pertinence of quantum computing on real instances of smart-charging optimisation problems.

Reinforcement learning

In geoscience, inventory management and process optimization, optimal results depend on ideal sequences of decision. They require adaptive strategies, involving many correlated parameters. Quantum -enabled reinforcement learning could make it possible to tackle more complex correlations better and faster.

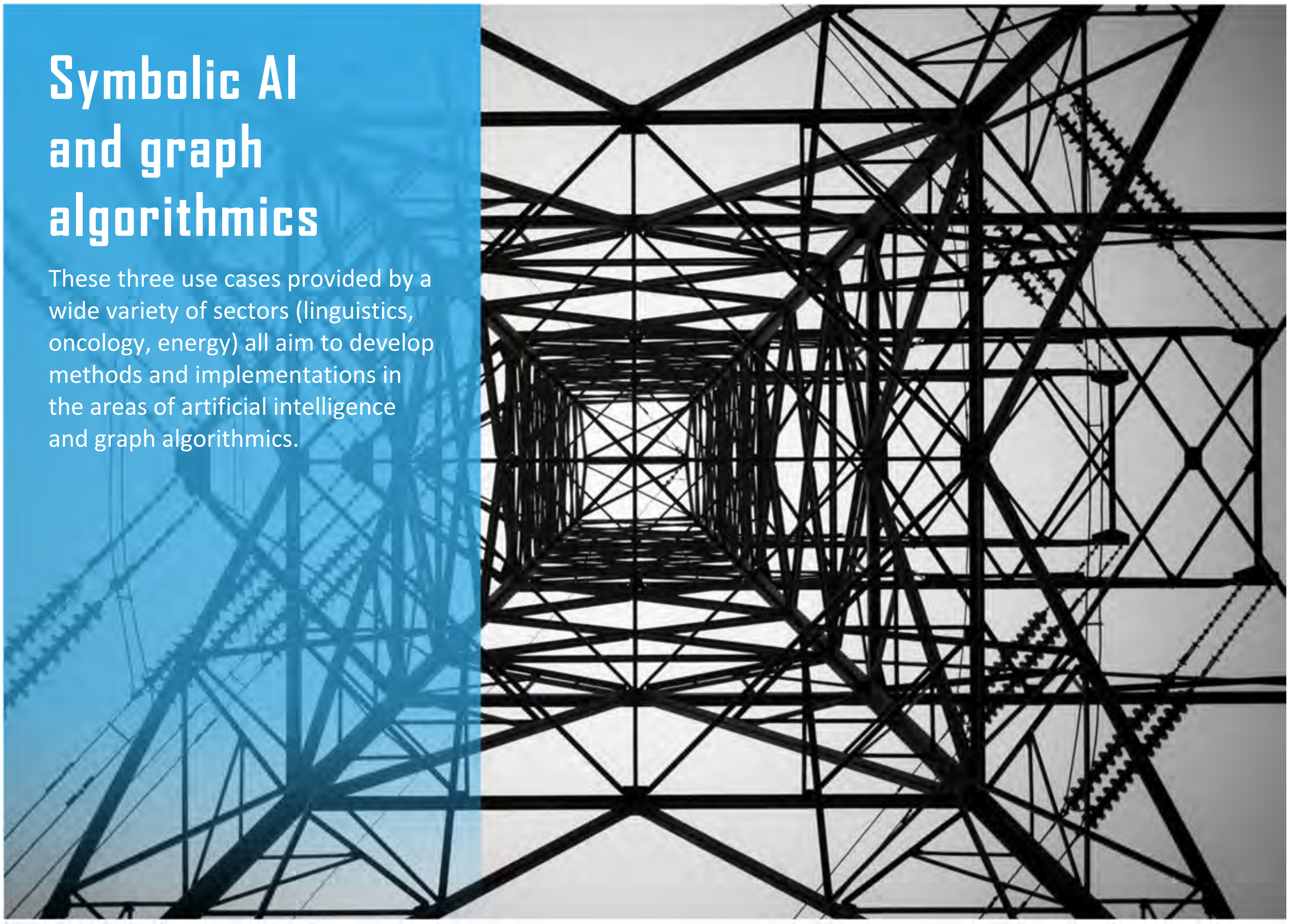
Financial applications

The aim of this use case is to develop efficient algorithms that could either substitute or redefine Monte Carlo (MC) techniques in NISQ computers. These new algorithms could be used to significantly increase the efficiency of:

- derivative pricing,
- risk management models,
- hybrid discrete-continuous optimization problems and
- exploring quantum implementation of Principal Component Analysis.

HPC mesh segmentation

Creating numerical meshes for realistic simulations is a computationally challenging task. We will employ bleeding-edge quantum algorithms for graph-based problems to improve the performance and quality of solutions. This could lead to significant benefits: faster and higher-quality mesh segmentation would considerably improve the pre-processing stage in classic numerical simulation problems such as seismic depth imaging and reservoir simulations.



Symbolic AI and graph algorithmics

These three use cases provided by a wide variety of sectors (linguistics, oncology, energy) all aim to develop methods and implementations in the areas of artificial intelligence and graph algorithmics.

Quantum natural language processing

Natural Language Processing (NLP) is often used to perform tasks such as machine translation, sentiment analysis, relationship extraction, word sense disambiguation and automatic summary generation.
However standard NLP methods scale poorly with performance and accuracy with increased problem complexity. Methods based on Distributional Compositional techniques offer potential for better accuracy with increased complexity. They are classically resource intensive but are compatible and better scalable on quantum computers.
This use-case will use a hybrid classical-quantum workflow to implement and demonstrate **sentence similarity algorithms** applied to parallel data extraction applications (such as machine translation) and intent detection applications (such as chat bots).

Quantum probabilistic safety assessment

Probabilistic safety assessment is a mainstream method to assess the safety and reliability of various safety-critical systems, such as nuclear plants, airplanes, railways, etc. However, when these systems are very large, the time spent on analysis is no more compatible with the industrial use of these models to support decision making.
The objective of this use-case is to apply novel Quantum Computing methods (algorithms for approximation, divide & quantum, Markov chains) to enhance the Probabilistic Safety Assessment methods in **Risk informed decision making**, and use relevant methods and approaches which are now beyond the capacity of classical computers but may be possible in the “big spaces” provided by quantum computing.

Quantum rule-based systems for breast cancer detection.

This use-case focuses on a specific type of AI program, the so-called rule-based system (RBS).
An inherent problem with RBS is their great sensitivity to the number of hypotheses, data and rules of the system itself. More specifically, selecting which rules are applicable at each moment can greatly slow down the inferential process. This process, called pattern matching, is an unresolved issue in AI. It is precisely here that quantum computing, by its intrinsically parallel nature, will be useful for AI in general, and for RBS in particular. The algorithms and their implementation will be used to build a quantum rule-based system that solves a specific problem: **diagnosing and treating a specific type of breast cancer** known as Invasive Ductal Carcinoma (IDC).

Chemistry

The goal of this group of two use cases is to bridge the gap between the recent proof-of-concept quantum chemical computations on NISQ processors and actual, industrial-scale quantum chemistry problems. To this aim, we will create software tools to integrate classical quantum chemical codes with quantum computing (QC) modules.

Drug discovery

This use case addresses the calculation of the ground-state energy of a large number of molecular conformations.

For simulations in pharmaceutical research, in particular for discovering new drugs, it is often quite important to sample the energy landscape of the conformations of large molecules, e.g., proteins, at room temperature. This is usually achieved by moving the atoms to different positions and solving the electronic structure problem for each of these atomic conformations. However, with 1000 atoms and more this approach becomes quite time-consuming, and even if the solver of the electronic structure problem is extremely fast, sampling all relevant atomic positions can be computationally prohibitively expensive. The sampling problem can be massively accelerated by solving the electron structure problem, while also considering the atomic positions as quantum mechanical degrees of freedom.

CO_2 recapture

As a representative use case for industrial-grade quantum chemical problem, we will study the capture of CO_2 by so-called Metal-Organic Frameworks (MOFs) and graphene-like systems.

Finding efficient ways to compute interactions between CO_2 and an adsorptive system is one of the key global challenges today. A first step towards solving the problem on a quantum computer does not only bring immediate value to TOTAL's CO_2 capture efforts but allows the global community to build up on the open-source code, finally contributing to a carbon-emission-free world.

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