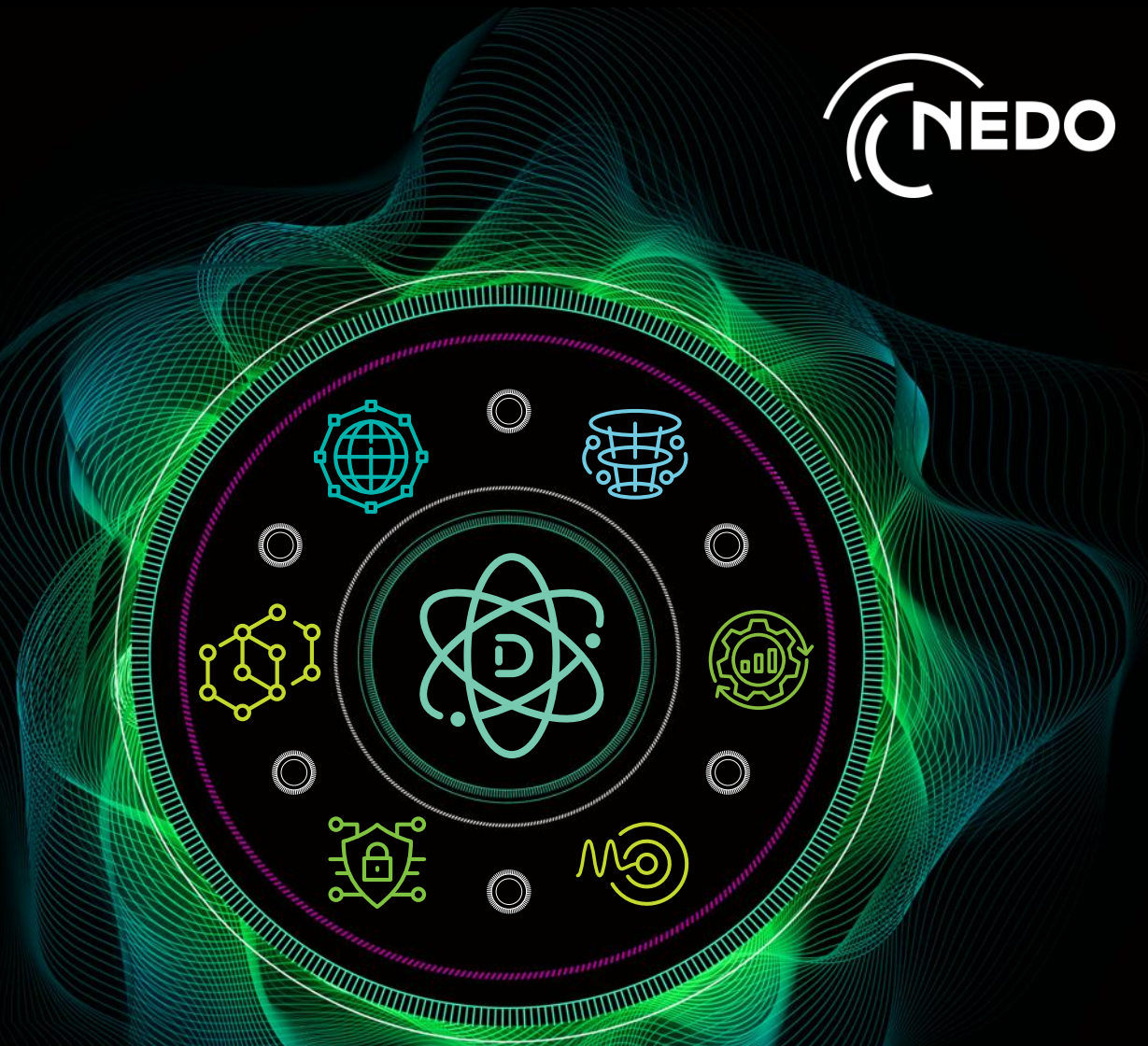
Quantum Computing Use Cases

Lead compound against Alzheimer's disease-causing enzyme BASE1

Roche, Quantinuum



New Energy and Industrial Technology Development Organization (NEDO)

Roche, Quantinuum:
Lead compound against Alzheimer's disease-causing enzyme BASE1 [2021/10] 1/2

Validation

Industry	Drug Discovery and Healthcare
Process	research and development
Method	Simulation
Category	Gate*

Background

- Simulating complex and strongly correlated chemical systems is widely believed to be one of the areas that will benefit most from advances in quantum computing because standard methods are inaccurate or expensive.
  - ✓ In fact, over the past half century, there has been an explosion of research on quantum algorithms for materials simulation, and research has been conducted in a variety of fields
- The synthesis of new drug candidates requires considerable medicinal chemistry effort. The need for synthesis can be limited by **screening candidate molecules using a variety of approaches to prioritize the most promising compounds in CADD (computer-aided drug design).**
  - ✓ At CADD, **quantum technology is expected to be utilized.**

Issues and motivation to be solved

- Development of low-scaling quantum mechanical methods that can simulate proteins using DFT (density functional) and CC (coupling cluster) approaches is underway, but there is a need for **accurate Methods for large-scale simulations.**
- **A team of Roche and Quantinuum (formerly Cambridge Quantum Computing) worked on protein-ligand binding energy calculations using a real quantum computer,** the team said.

Reference: arXiv"Quantum Computational Quantification of Protein-Ligand Interactions" (https://arxiv.org/pdf/2110.08163)
*Gate（gate-based）: A computing approach in which operations are applied sequentially to qubits to perform calculations. Similar in concept to logic circuits in classical computers, it can address a wide range of problems.

Roche, Quantinuum:
Lead compound against Alzheimer's disease-causing enzyme BASE1 [2021/10] 2/2

Validation

Industry	Drug Discovery and Healthcare
Process	research and development
Method	Simulation
Category	Gate*

Problem setting as a quantum computer

- We used quantum techniques to calculate the protein-ligand binding energy **for the BACE1 enzyme, which has been linked to Alzheimer's disease pathogenesis.**
- In order to perform energy calculations, we combine a numerical method density matrix embedding theory (DMET) embedding method for solving strongly correlated electronic structure problems with a variational quantum eigenvalue solver (VQE) approach for finding electronic ground states of molecules.
- The machine used the following two
  - ✓ **IBM superconducting quantum computer**
  - ✓ **Quantinuum (formerly Honeywell Quantum Solutions) ion trap quantum computer (NISQ)**

Expected business benefits

- The previous method used a quantum emulator, but this verification was able to **calculate protein-ligand binding energy for the first time using an actual quantum computer**
  - ✓ **NISQ's quantum computer** showed that we could calculate the binding energy of a protein **- ligand.**

Reference: arXiv"Quantum Computational Quantification of Protein-Ligand Interactions" (https://arxiv.org/pdf/2110.08163)
*Gate（gate-based）: A computing approach in which operations are applied sequentially to qubits to perform calculations. Similar in concept to logic circuits in classical computers, it can address a wide range of problems.

More use cases are available on our website. We invite you to explore them.
https://www.quantum-computing-use-cases.nedo.go.jp/english/

More Use Cases

New Energy and Industrial Technology Development Organization (NEDO)
AI and Robotics Department (e-mail: quantum_ai@ml.nedo.go.jp)

This collection of use cases was obtained as a result of the work commissioned by the New Energy and Industrial Technology Development Organization (NEDO) "Cyber-Physical Development Business of Quantum/Classical Hybrid Technology/Study of Use Case of Quantum Technology" and the "Post-5G Information and Communications System Infrastructure Reinforcement R & D Project (Quantum Industrialization)/Comprehensive Study for Promoting the Industrialization of Quantum Computers".