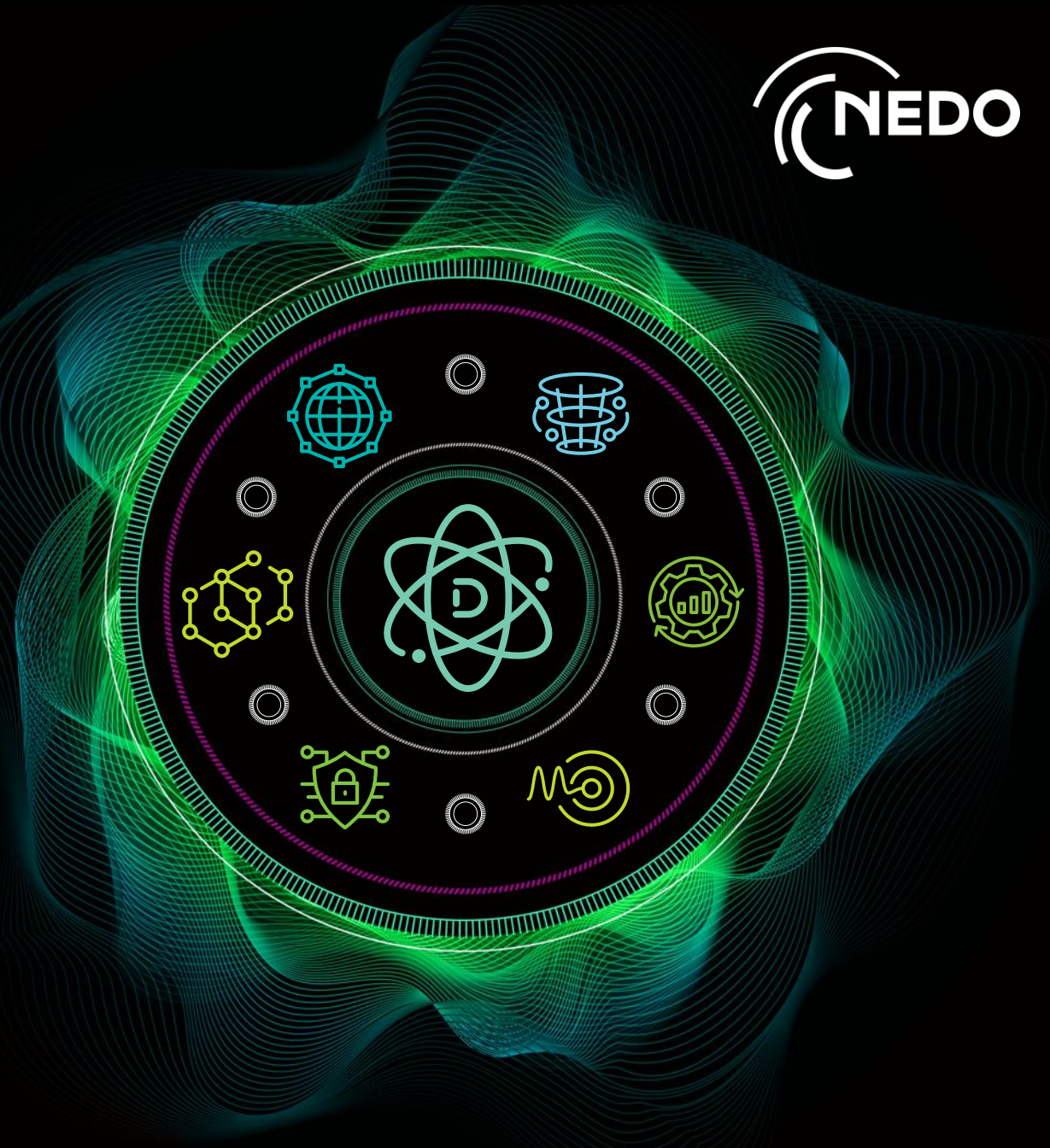
Quantum Computing Use Cases

Nitrogen Fixation Reaction Simulation for Efficient Ammonia Synthesis

ETH Zurich, Microsoft Research



New Energy and Industrial Technology Development Organization (NEDO)

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Concept

Industry	Energy
Process	fuel synthesis
Method	Simulation
Category	Gate*

Background

- Ammonia is attracting **attention as a clean fuel alternative to fossil fuels** in global efforts to combat climate change
  - ✓ Contributing to decarbonization by not emitting CO2 during combustion
- On the other hand, **the way ammonia is made consumes a lot of energy and emits CO2.**
  - ✓ The **Haberbosch process,** which is currently the mainstream manufacturing method, is a synthesis method under high-temperature and high-pressure conditions (high temperature of 400~600°C and high pressure of 100~300 atm).
  - ✓ **It uses 1~2% of the energy consumed by the entire earth, and the amount of CO2 emitted during manufacturing also accounts for 1~3% of human emissions.**
- There is a need for an alternative, environmentally friendly, low energy consumption, low CO2 emission, ammonia production method to replace the "Haberbosch process"

Issues and motivation to be solved

- In the Haberbosch process, **most of the energy is consumed in the process of fixing nitrogen in the air,** but in nature, in particular, **in biological systems, nitrogen-fixing enzymes (nitrogenase) present in the roots of leguminous plants stimulate ammonia synthesis at normal temperature and pressure.**
  - ✓ The mechanism involves **a cofactor called FeMoco,** * and
    *Chemicals other than proteins necessary for the catalytic activity of enzymes
- **The chemical reactions involving FeMoco are complex and quantum, making them difficult to simulate on a classical computer (supercomputer),** he said.
  - ✓ **The FeMoco cofactor in the nitrogenase enzyme is involved in ammonia synthesis as a transition metal catalyst,** but **the electron-electron interaction is strong,** and **the Hartree-Fock and DFT approximations do not capture the exact chemical reactions** that are commonly used in classical computers.
- Molecular simulations using quantum acceleration algorithms for quantum chemical calculations are currently being studied on quantum computers.

Reference: The University of Tokyo "World's First Synthesis of Ammonia from Nitrogen Gas and Water — World's Highest Catalytic Activity at Normal Temperature and Pressure, Toward a Sustainable Society —" (https://www.t.u-tokyo.ac.jp/hubfs/shared-old/press/data/setnws_20190425105724638383038O_077019.pdf) and National Institute of Science and Technology Policy "Interview with Mr. Keisuke Fujii, Professor, Department of Electronics and Optical Science, Graduate School of Basic Engineering, The University of Osaka: Leading the field of quantum information science in research and development of quantum software to realize universal quantum computer" (https://www.nistep.go.jp/activities/sti-horizon%E8%AA%8C/vol-07no-04/stih00273)
*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.

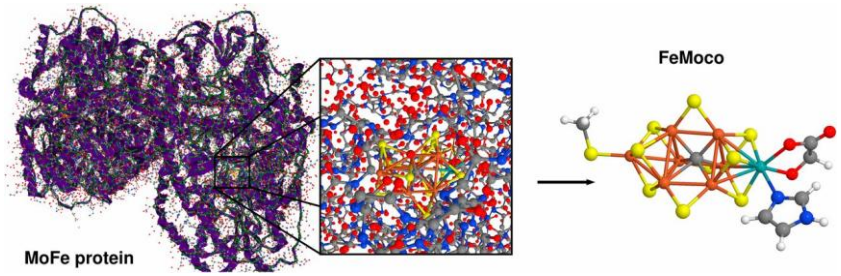
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Problem setting as a quantum computer

- **Taking into account the electron correlation**, combining the density matrix renormalization group and the CASSCF (multi-configuration self-consistent field) method, which allows calculations involving a larger number of orbitals, **performing quantum computer calculations using quantum phase estimation**, performed.
- **As a quantum computer, it calculates under two conditions.**
  - ✓ **FTQC computable error rate achievable in the short to medium term, 10-3, Gate speed 100 ns**
  - ✓ **Future achievable FTQC computable error rates, 10-6, Gate speed 10 ns**



The iron-molybdenum cofactor (FeMoco) at the active center of the nitrogenase enzyme (left panel) causes the conversion of nitrogen gas to ammonia (right panel).

Reference: PNAS"Elucidating Reaction Mechanisms on Quantum Computers"(https://www.pnas.org/doi/10.1073/pnas. 1619152114)
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Expected business benefits

- **Due to the complexity and strong quantum nature of the chemical reactions involved in FeMoco, which are difficult to calculate with a classical computer, we** calculated **the computational resources and time required to simulate two conditions with a quantum computer.**
  - ✓ In order to keep the tolerance within 0.1 mHartree *1 of the exact solution, it takes more than 3 years with 111 logical qubits for both Structure1 and Structure 2 in Serial (single thread).
  - ✓ On the other hand, in PAR (multi-threaded), both are executed in 1.5 to 3 months at around 2000 logical qubits.
- showed that **quantum computers can be used to understand reaction mechanisms in complex chemical systems, taking as an example the unsolved problem of biological nitrogen fixation in nitrogen genase**

Table 1. Simulation time estimates

Structure	T gates	Cl. gates	Δt (10 ns)	Δt (100 ns)	Qubits
Quantitatively accurate simulation (0.1 mHa)					
Structure 1					
Serial	1.1×10^{15}	1.7×10^{15}	130 d	3.6 y	111
Nesting	3.5×10^{15}	5.7×10^{15}	15 d	4.9 mo	135
PAR	3.1×10^{16}	3.1×10^{16}	110 h	1.5 mo	1,982
Structure 2					
Serial	2.0×10^{15}	3.1×10^{15}	240 d	6.6 y	117
Nesting	6.5×10^{15}	1.0×10^{16}	27 d	8.9 mo	142
PAR	6.0×10^{16}	6.0×10^{16}	210 h	2.9 mo	2,024
Qualitatively accurate simulation (1 mHa)					
Structure 1					
Serial	1.0×10^{14}	1.6×10^{14}	12 d	3.9 mo	111
Nesting	3.3×10^{14}	5.6×10^{14}	1.4 d	14 d	135
PAR	3.0×10^{15}	3.0×10^{15}	11 h	4.6 d	1,982
Structure 2					
Serial	1.9×10^{14}	3.0×10^{14}	22 d	7.2 mo	117
Nesting	6.0×10^{14}	9.9×10^{14}	2.5 d	25 d	142
PAR	5.5×10^{15}	5.5×10^{15}	20 h	8.3 d	2,024

Listed are the number of Clifford and T-gate operations, the estimate of the run time (Δt), and the number of logical qubits required to obtain energies within 0.1 mHa or 1 mHa for two different structures of FeMoco on a quantum computer. Structure 1 is for spin state $S = 0$ and charge $+3$ elementary charges with 54 electrons in 54 spatial orbitals. Structure 2 is for spin state $S = 1/2$ and charge 0 with 65 electrons in 57 spatial orbitals (see *SI Appendix* for further details). These run times and gate counts are likely to be pessimistic.

Reference: PNAS"Elucidating Reaction Mechanisms on Quantum Computers"(https://www.pnas.org/doi/10.1073/pnas. 1619152114)
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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)
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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".