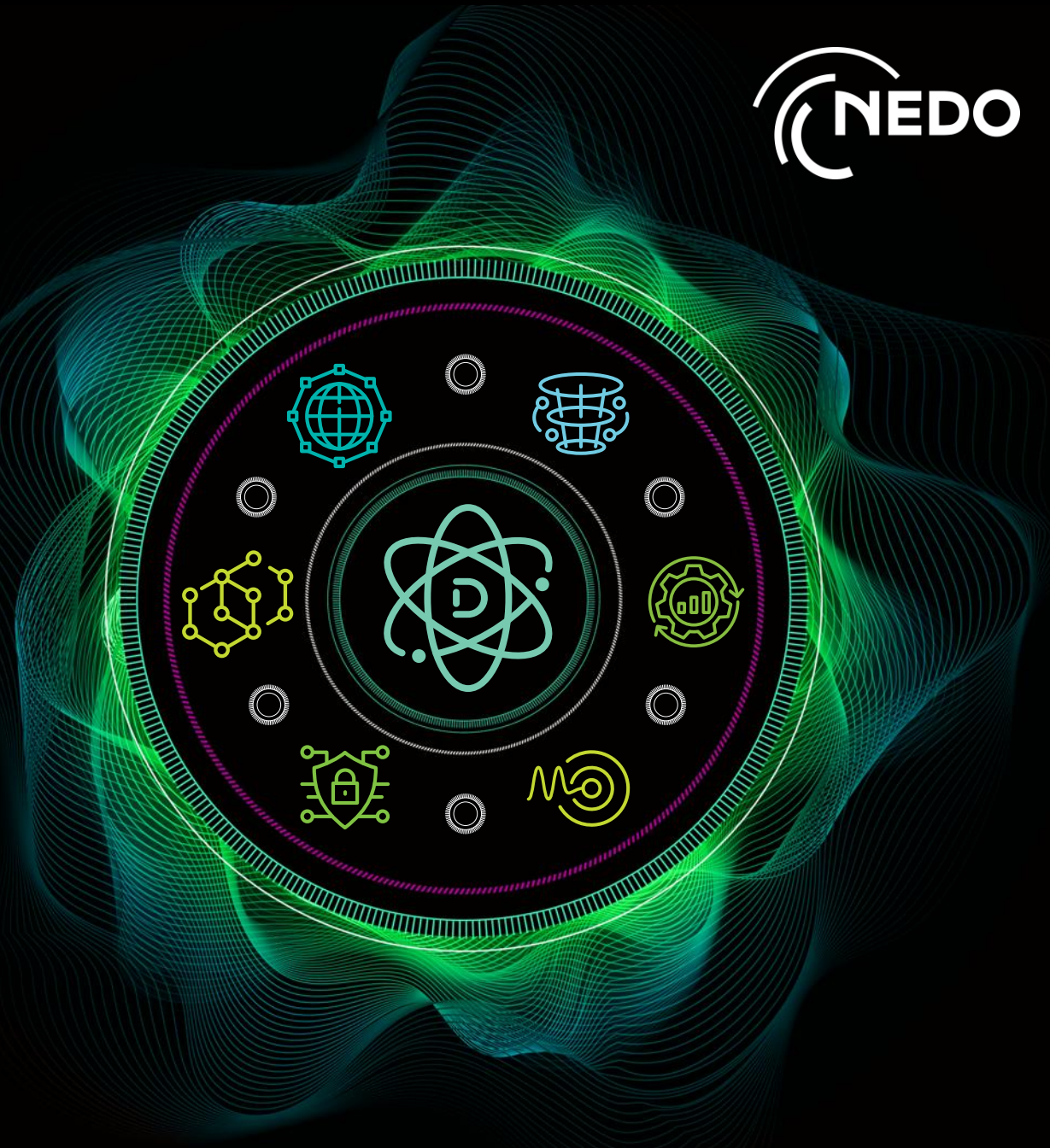
Quantum Computing Use Cases

Functional Protein Optimization Technology

Tohoku University



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

Industry	Process Manufacturing
Process	material search
Method	AI
Category	Ising*

Background

- Proteins are being explored for use not only in the pharmaceutical field but also in food, environmental, and materials applications. However, **designing proteins with the desired functions and properties is difficult, and development costs are high, which slows the pace of developing new effective drugs and enzymes**
- Against this background, an amino acid sequence optimization process has been developed that combines machine learning with experimental methods to increase the probability of discovering target proteins within sequence spaces that cannot be fully explored through experiments alone
- Furthermore, **by applying quantum annealing as well, a new amino acid sequence optimization process is being developed for even larger sequence spaces that cannot be handled by conventional machine learning methods. The goal is social implementation through both a platform business that supports partner companies in the development of functional proteins and a pipeline business that conducts in-house drug discovery and development**

Issues and motivation to be solved

- Obtain enzyme variants with more than double the catalytic activity of natural proteins and more than double the stability
- Obtain antibodies that exhibit antigen-binding performance at the nanomolar (nM) level in dissociation equilibrium constant, and a thermal denaturation midpoint of 60°C or higher
- **Obtain lead molecules whose antigen-binding performance is more than 10 times higher than lead molecules identified through experiments alone, while also showing improved physical properties such as stability**

Reference: AI and Robot Department, New Energy and Industrial Technology Development Organization (NEDO), "Cyber-Physical Development Project for Quantum-Classical Hybrid Technologies" (https://www.nedo.go.jp/content/800030349.pdf)
*Ising: A computing approach, mainly associated with quantum annealers and simulators specialized for the Ising model, in which a problem is first formulated as an Ising model and then solved computationally. It is particularly well suited to problems that involve finding the optimal combination from a vast number of possibilities.

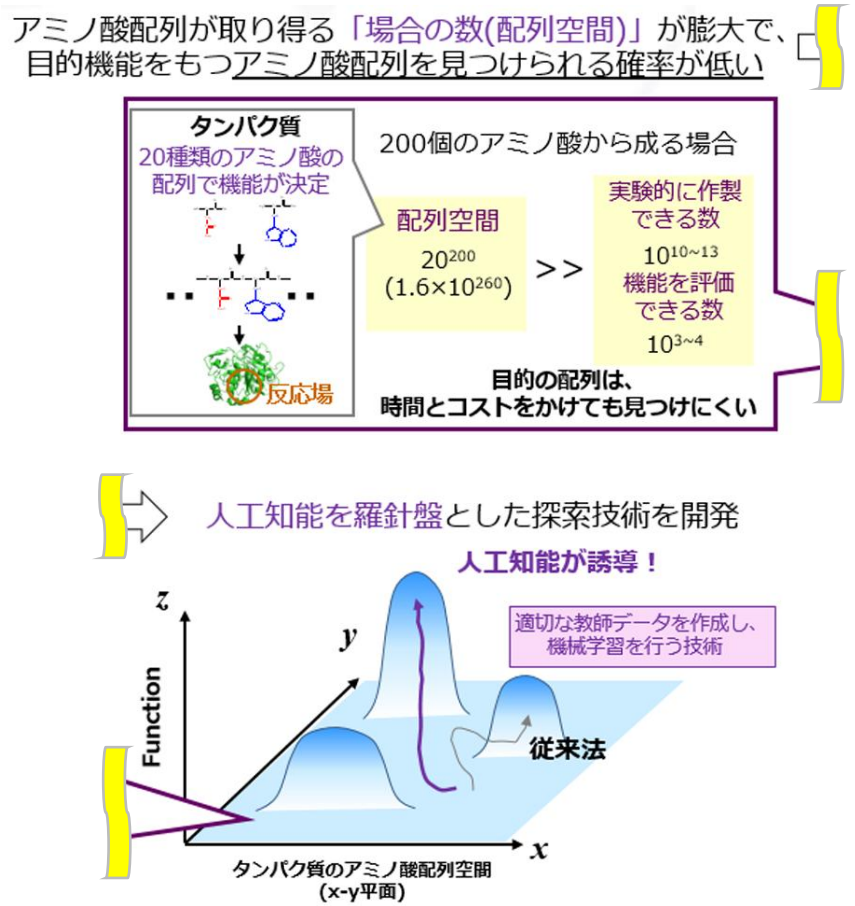
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Problem formulation for quantum computer

- Protein amino acid sequence design incorporating machine learning is being pursued worldwide. However, **there are limits to the number of amino acid sequence combinations that can be explored—that is, the scale of the sequence space—so the proteins and properties (functions and physicochemical characteristics) that can be targeted tend to depend on the accuracy of the sequence space design**
- **By using quantum annealing,** the aim is to extend this limit and build a technology that can address a wide range of proteins and properties without depending on the precision of sequence space design



Expected business benefits

- Through the startup company already established (RevolKa), the company will operate both a platform business that supports partner companies in creating desired functional proteins and a pipeline business for in-house drug discovery and development

Reference: AI and Robot Department, New Energy and Industrial Technology Development Organization (NEDO), "Cyber-Physical Development Project for Quantum-Classical Hybrid Technologies" (https://www.nedo.go.jp/content/800030349.pdf); AI and Robot Department, New Energy and Industrial Technology Development Organization (NEDO), "Cyber-Physical Development Project for Quantum-Classical Hybrid Technologies" (https://www.nedo.go.jp/content/800030348.pdf)
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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)
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”.