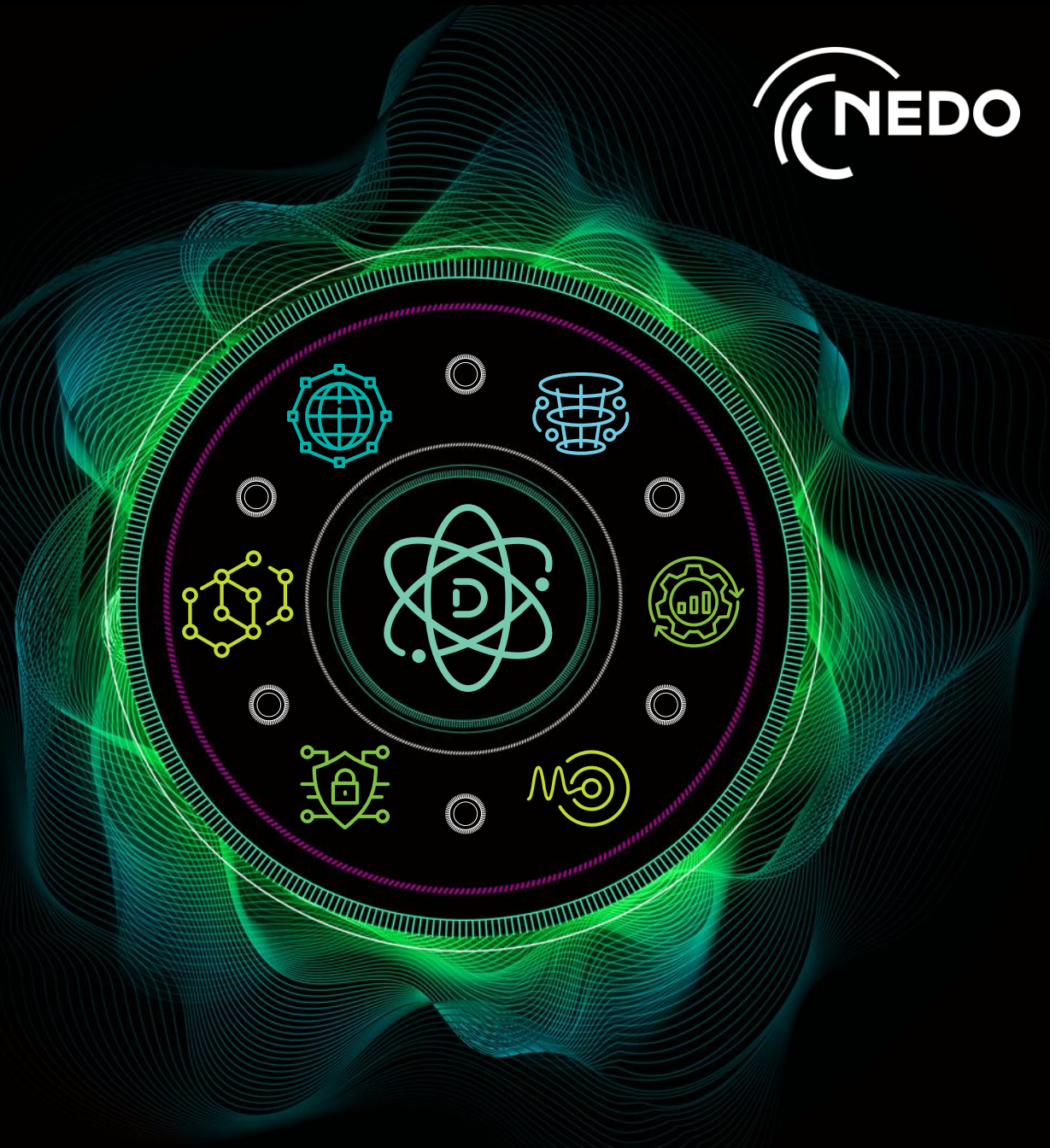
Quantum Computing Use Cases

Proof of Concept of Quantum AI Drug Discovery Process

JT



New Energy and Industrial Technology Development Organization (NEDO)

JT: Proof of Concept of Quantum AI Drug Discovery Process [2024/10] 1/2

Concept

Industry	Drug Discovery and Healthcare
Process	research and development
Method	AI
Category	Ising*

Background

- Generative AI has rapidly spread due to the large amount of data that can be learned on the Web. On the other hand, **human data is necessary for drug discovery, and the need to generate massive amounts of data to train AI is a barrier to development.**
  - ✓ Build drug discovery AI by running simulations and letting AI learn the data obtained
- **JT (Japan Tobacco Inc.) is currently focusing on the compound creation process,** but AI technology **has the potential to bring about innovative changes in all drug discovery processes, including translational research.**
- As it advances AI drug discovery, JT is **focusing on the innovation of quantum computers, both in terms of speed and the quality of the data they produce.**
  - ✓ **Strategic Partnership for Small Molecule Drug Discovery** with Qsimulate, a world leader in quantum simulation technology
- JT and D-Wave jointly announced **this initiative aimed at the development of innovative drug discovery technologies using AI and quantum computers**

Issues and motivation to be solved

- **Pharmaceutical companies need to remain competitive while dealing with the challenges of difficulty, uncertainty, and time in drug development**
- **Accelerate the process of discovering first-in-class small molecules** and create **quality improvements in various processes of drug discovery**

Problem setting as a quantum computer

- JT is currently in the implementation stage of developing its own advanced AI drug discovery technology. **Especially, the technology development in which physical simulation based on the basic principle and AI are interlocked and synchronized organically and closely is emphasized.**
- This initiative aims to **expand the development and application of AI for drug discovery in terms of speed, quality, and scope** by utilizing **D-Wave annealing type quantum computer** with JT's original AI technology

Reference: D-WAVE"Japan Tobacco and D-Wave announce joint project to develop innovative drug discovery technology using AI and quantum computers" (https://dwavejapan.com/%E6%97%A5%E6%9C%AC%E3%81%9F%E3%81%B0%E3%81%93%E7%94%A3%E6%A5%AD%E3%81%A8-d-wave%E3%80%81ai%E3%81%A8%E9%87%8F%E5%AD%90%E3%82%B3%E3%83%B3%E3%83%94%E3%83%A5%E3%83%BC%E3%82%BF%E3%82%92%E6%B4%BB%E7%94%A8/)

*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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Expected business benefits

- Using quantum AI, **we aim to establish new advanced technologies to expand the quality and horizon of the search space for small molecules**.
- After the proof-of-concept project, JT's pharmaceutical division plans to **advance the creation of 'quantum AI drug discovery' technology and move to the stage where quantum computers can be used to design real molecules.**

Reference: D-WAVE"Japan Tobacco and D-Wave announce joint project to develop innovative drug discovery technology using AI and quantum computers" (https://dwavejapan.com/%E6%97%A5%E6%9C%AC%E3%81%9F%E3%81%B0%E3%81%93%E7%94%A3%E6%A5%AD%E3%81%A8-d-wave%E3%80%81ai%E3%81%A8%E9%87%8F%E5%AD%90%E3%82%B3%E3%83%B3%E3%83%94%E3%83%A5%E3%83%BC%E3%82%BF%E3%82%92%E6%B4%BB%E7%94%A8/)

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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

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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".