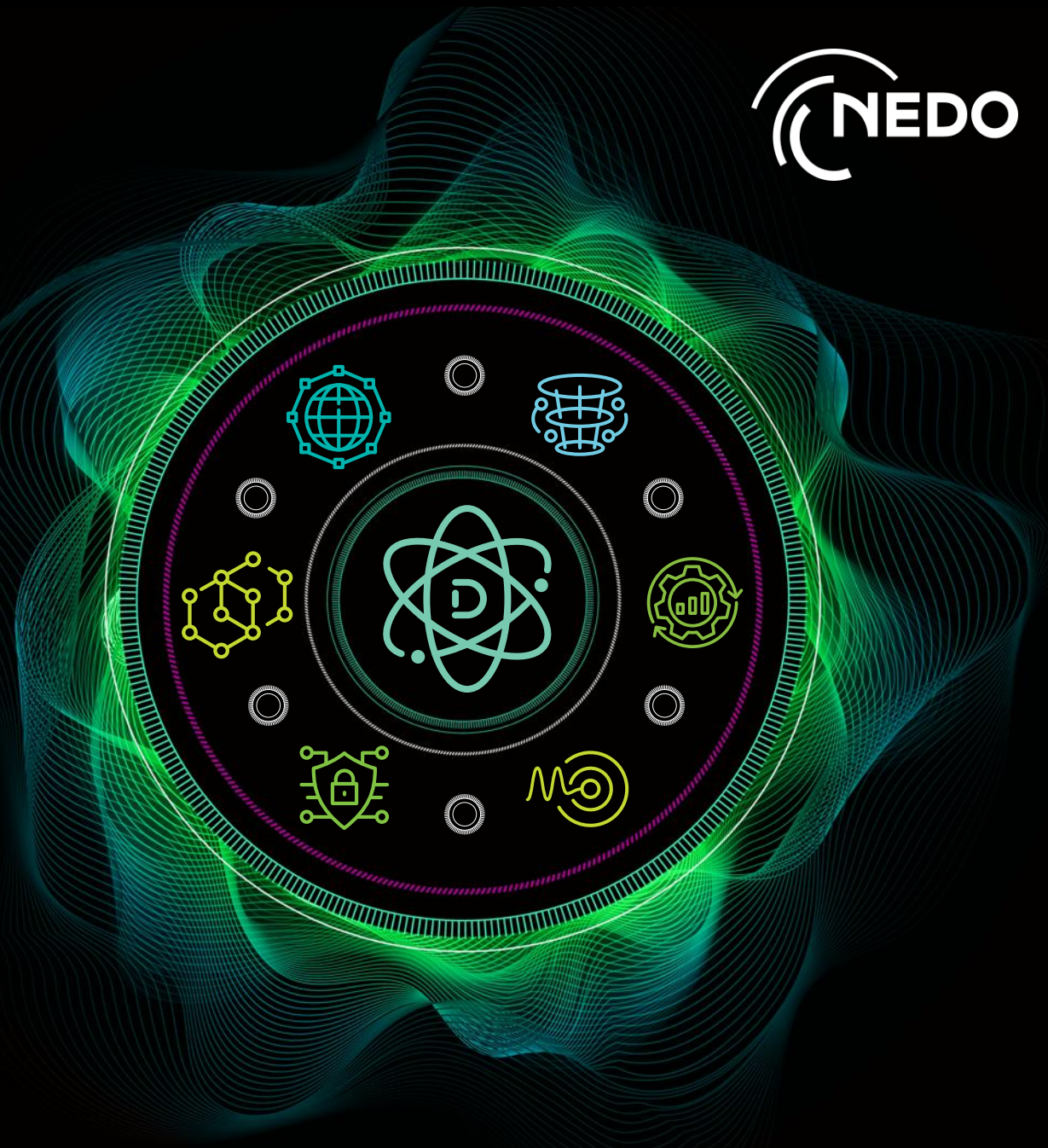
Quantum Computing Use Cases

Development of anticancer drug candidates using quantum AI

Zapata AI



New Energy and Industrial Technology Development Organization (NEDO)

Zapata AI:
Development of anticancer drug candidates using quantum AI [2024/2] 1/2

Validation

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

Background

- Zapata AI started out as a quantum algorithm development software company as a spinout of Harvard, **before moving to focus on generative AI.**
  - ✓ Collaborates with quantum processor provider IonQ to **forge strategic partnership on quantum-generated AI technologies**
  - ✓ However, Zapata AI has since gone bankrupt (October 12, 2024).
- Zapata AI is working on industry-specific generative AI, trying to **apply quantum-generated AI to time-consuming and costly pharmaceutical research and development**

Issues and motivation to be solved

- **Drug R & D takes time and money**
- **demonstrate that quantum-generated AI effectively solves real-world problems**

Expected business benefits

- Quantum GANs using VQC **successfully produced molecules with physicochemical properties and performance that outperformed previous benchmarks**
- In addition, the small number of parameters **allowed us to observe quantum superiority in expressivity.**
- This study showed **the practical possibility of supporting drug discovery by quantum computer**.

Reference: QKAI"Zapata AI (ZPTA) goes public on NASDAQ. Completed management integration with Andretti Acquisition Corporation as a generative AI company that pivoted from the quantum field. Trading begins on April 1, 2024" (https://www.qcrjp.com/post/zapata-ai-zpta-nasdaq-go-public), QKAI "Interpretation of the Bankruptcy of Zapata AI in Japanese Market and Its Impact " (https://www.qcrjp.com/post/zapata-ai-form8k?utm_source=twitter&utm_medium=blog.post-promoter&utm_campaign=efa0e2ed-a78a-4f84-aa0a-ac0e2b9dae5c), ACS"Exploring the Advantages of Quantum Generative Adversarial Networks in Generative Chemistry" (https://pubs.acs.org/doi/full/10.1021/acs.jcim.3c00562)
*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.

Zapata AI:
Development of anticancer drug candidates using quantum AI [2024/2] 2/2

Validation

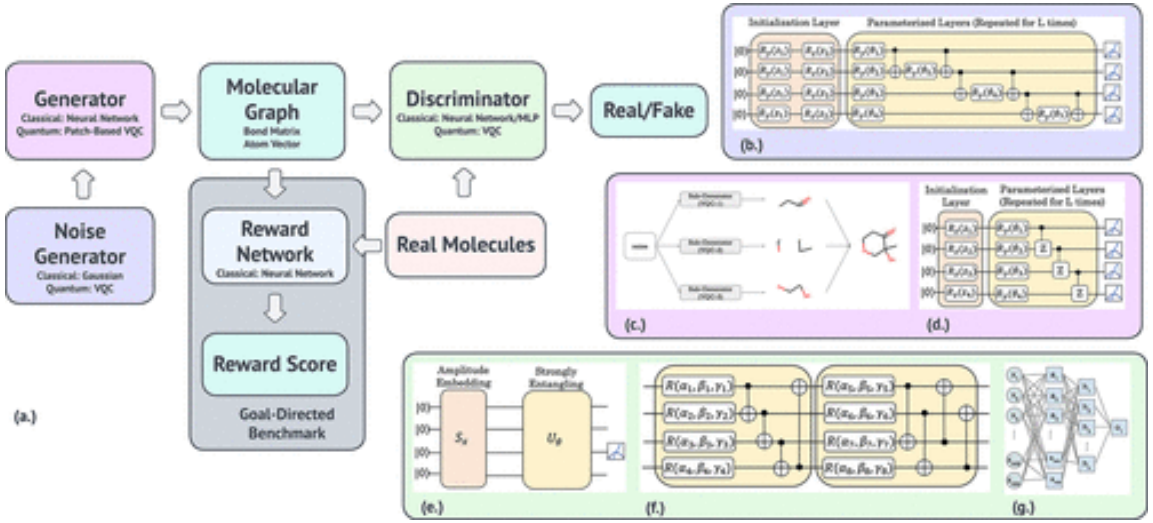
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Problem setting as a quantum computer

- Utilizing the Quantum-Classical Hybrid GAN *1 for the Discovery of Low-Molecule Compounds
- **Replaced each element of GAN with variational quantum circuits (VQC),** *2 and demonstrated the advantages of quantum in drug discovery
- This project utilizes a 16 qubit IBM quantum computer

*1: A GAN is a network that alternately competes with a Discriminator and a Generator to generate real data.

*2: VQC refers to quantum circuits that implement quantum-classical hybrid computing



Overview of this initiative

Reference: ACS"Exploring the Advantages of Quantum Generative Adversarial Networks in Generative Chemistry" (https://pubs.acs.org/doi/full/10.1021/acs.jcim.3c00562)
*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".