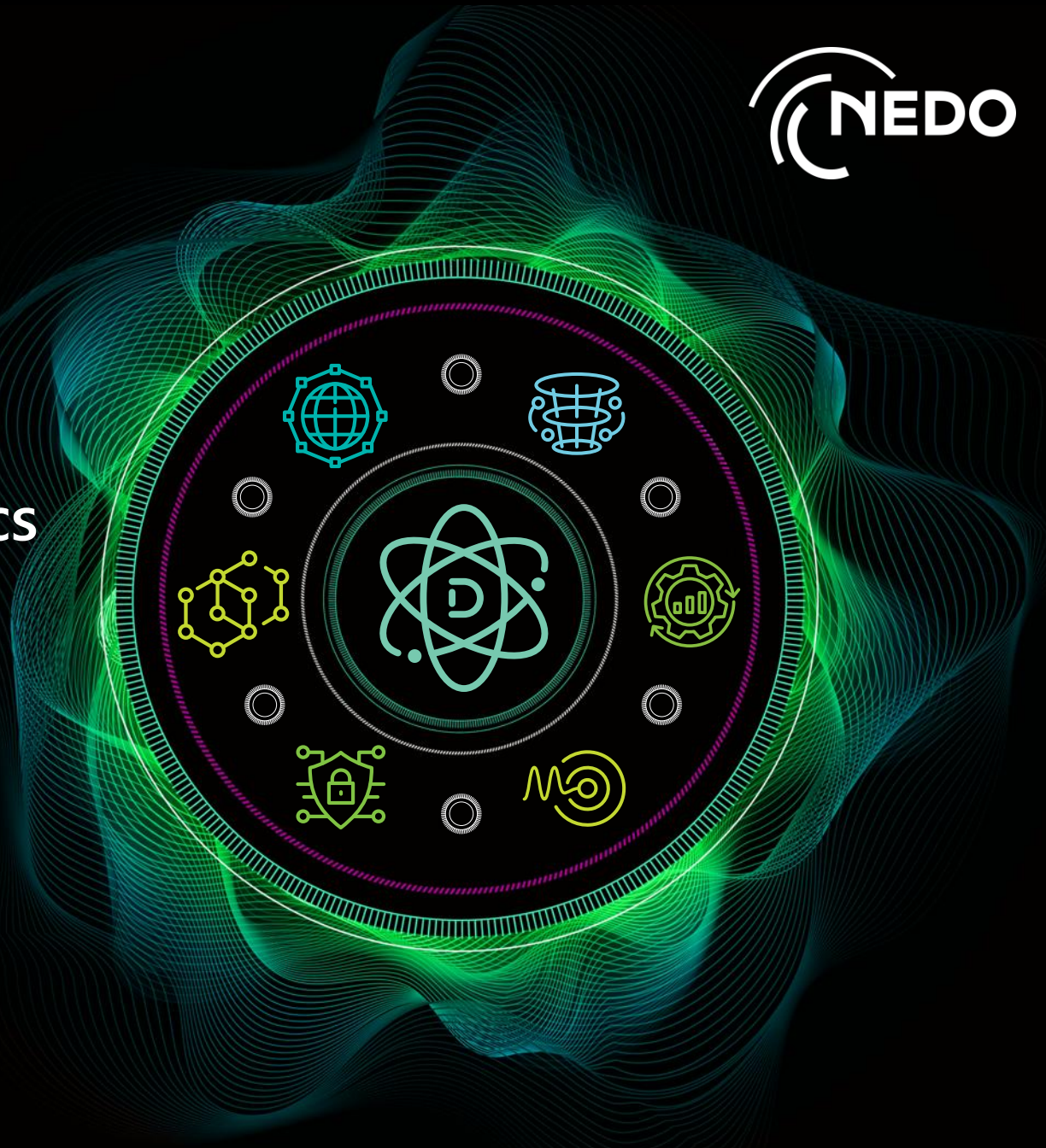
Quantum Computing Use Cases

Quantum–HPC Integration for Reaction-Center Electron Dynamics Toward DX in Drug Discovery

Kyoto University and Quantinuum



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

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

Background

- **In new drug development**, **considerable time and cost are required** from the search for candidate compounds to the verification of efficacy and safety. Improving R&D speed and confidence is therefore an important management issue
- **In the discovery process, accurate understanding of drug metabolism and enzymatic reactions is directly linked to assessing the efficacy, safety, and metabolic properties of candidate compounds, and therefore to more efficient candidate selection and experiment planning**
- To improve the probability of success in new drug development and shorten development time, **drug discovery DX platforms using AI, data analysis, molecular simulation, and HPC are being developed**. However, **the electronic states involved in drug metabolism and enzymatic reactions are extremely complex**, and conventional computational methods may not always predict them with sufficient accuracy. For this reason, the use of quantum computers, as a new computational platform capable of higher-precision analysis, was examined
- This effort was carried out **as part of the JHPC-Quantum Test User Program under NEDO's R&D project on a quantum-supercomputer linked platform for expanding computable domains**

Issues and motivation to be solved

- To predict drug metabolism and enzymatic reactions on a computer, a model that appropriately represents the electronic states at the reaction center is required. However, **in complex reactions involving multiple electronic states, it is not easy to evaluate the validity of that model**
- In particular in regions where multiple electronic states have similar energies and interact with one another, static energy comparison alone may not be sufficient to judge the validity of the reaction model or the reliability of the prediction results. A new method is therefore **needed to analyze the behavior of electronic states in greater detail and improve the reliability of models and predictions**
- In this effort, **attention was given to quantum computers, which are highly compatible with time-evolution simulation of quantum states**, and **an ion-trap quantum computer characterized by high gate fidelity and flexible qubit connectivity was used**. By performing time-evolution analysis of electronic states with a quantum computer on reaction models constructed with HPC, the study examined a new evaluation method for diagnosing characteristics of state mixing that are difficult to capture with conventional methods, with **the aim of improving the reliability of reaction models**

Reference: Drug Discovery DX Platform (https://3dxpf.med.kyoto-u.ac.jp)
arXiv, "A Quantum-HPC Hybrid Workflow for Reaction-Center Electronic Dynamics: Application to a Cytochrome P450-Inspired Iron-Complex Model" (https://arxiv.org/abs/2607.05786)
*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 formulation for quantum computer

- **Input data:**

  Reaction-coordinate-dependent effective Hamiltonian calculated using HPC

- **Objective:**

  Analyze electronic-state mixing and population transfer through time evolution of the effective Hamiltonian

- **Evaluation metric:**

  Fraction of the population transferred from the reactant state to the product-state group

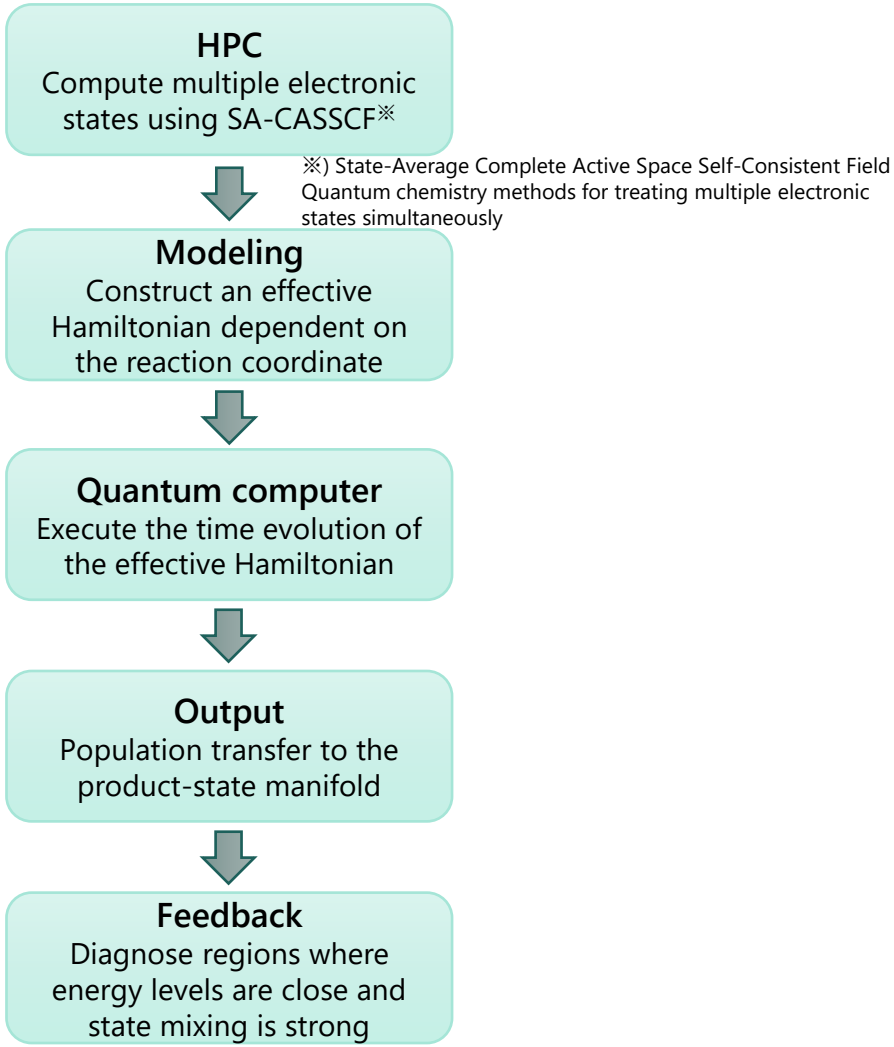
- **Why classical methods are difficult:**

  In systems involving many electronic states, computational cost increases rapidly as the number of target states grows

- **Expected role of quantum computing:**

  Application to time evolution of the effective Hamiltonian and dynamic model diagnosis

Quantum–HPC hybrid workflow



Expected business benefits

- **The quantum-HPC hybrid workflow showed the potential to dynamically analyze changes in electronic states that are difficult to capture with conventional methods, and to use this to improve the reliability of computational models for predicting drug metabolism reactions**. In the future, it is expected to support more efficient candidate compound selection and experiment planning, contributing to higher R&D productivity, shorter development time, and lower costs in new drug development

Reference: arXiv, "A Quantum-HPC Hybrid Workflow for Reaction-Center Electronic Dynamics: Application to a Cytochrome P450-Inspired Iron-Complex Model" (https://arxiv.org/abs/2607.05786)
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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”.