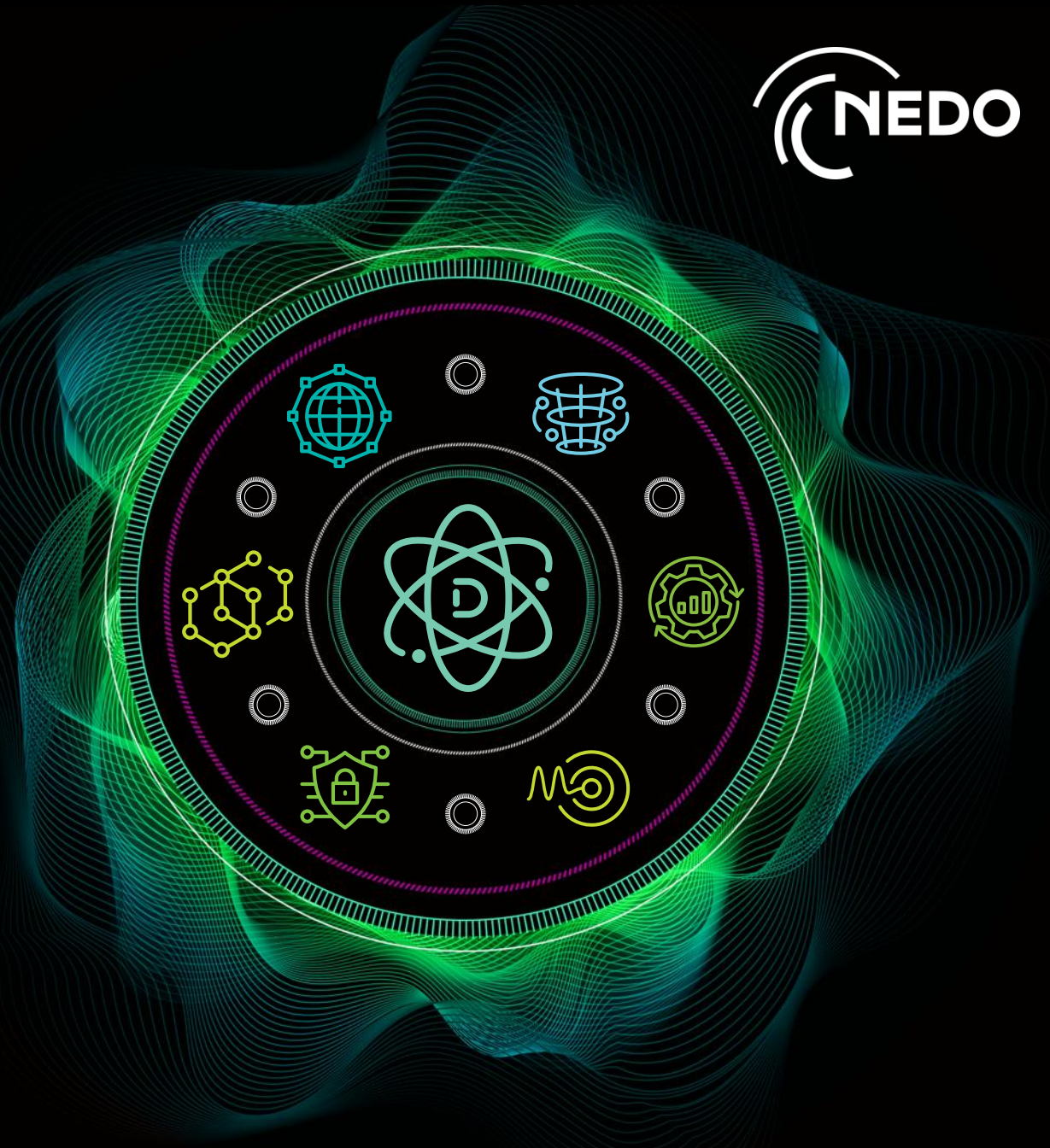
Quantum Computing Use Cases

Development of a Biomolecular Reaction Analysis Platform Integrating FMO and Quantum Computers

Oita University and Quantinuum



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

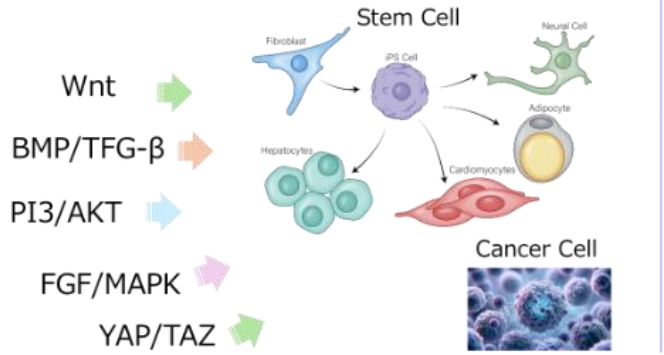
Industry	Drug Discovery and Healthcare
Process	drug target selection
Method	Simulation
Category	Gate*

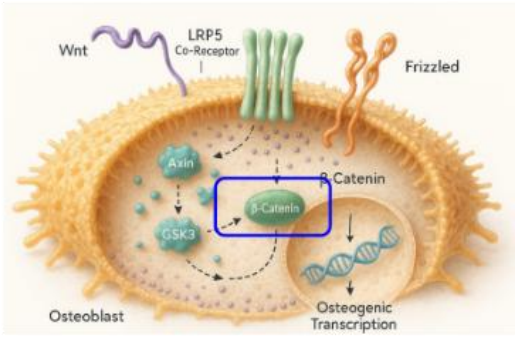
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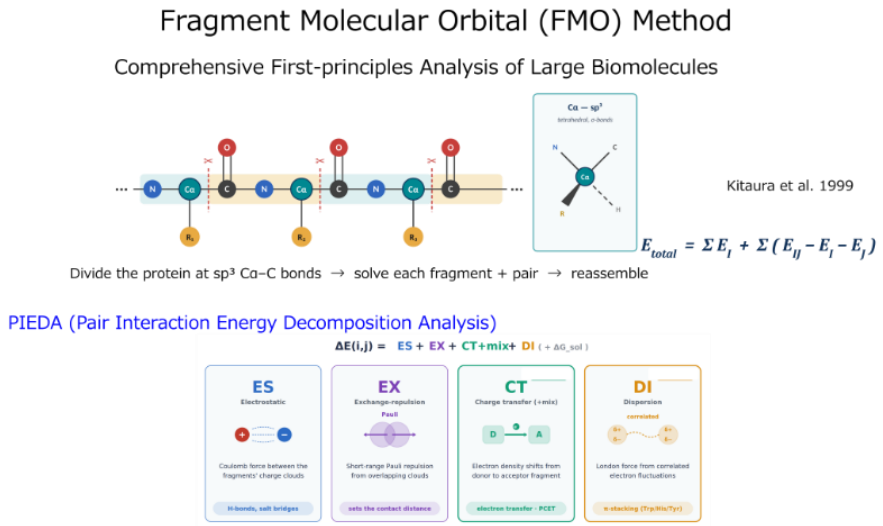
- In research on cancer and other diseases, **it is important to understand the function and stability of disease-related proteins at the molecular level**
- As one example, this use case focused on β-catenin, a protein important for regulating cell proliferation and differentiation
- Abnormality of β-catenin or its excessive accumulation in cells is closely related to cancer development
- **Understanding the molecular mechanisms that support the function of β-catenin is therefore an important issue for elucidating disease mechanisms and for future drug discovery research**

Issues and motivation to be solved

- To understand the function of biomolecules, **it is necessary to analyze intermolecular interactions and chemical reactions with high accuracy**
- **The fragment molecular orbital (FMO) method is a powerful approach that divides large biomolecules into fragments, performs quantum chemical calculations, and analyzes the types of interactions between fragments**
- On the other hand, to understand with even higher accuracy the electronic states involved in reactions that play important roles in biomolecules, more advanced analysis may be required
- In this use case, **the aim was to further enhance biomolecular reaction analysis by using FMO analysis results and connecting them to electronic-state analysis with a quantum computer**







RIKEN Center for Computational Science (R-CCS), "Oita University Develops a New Drug Discovery Platform Using the Quantum Computer 'Reimei' and 'Fugaku' — Selected for the JHPC-quantum Test User Program" (https://www.r-ccs.riken.jp/outreach/topics/20251027-1/)

*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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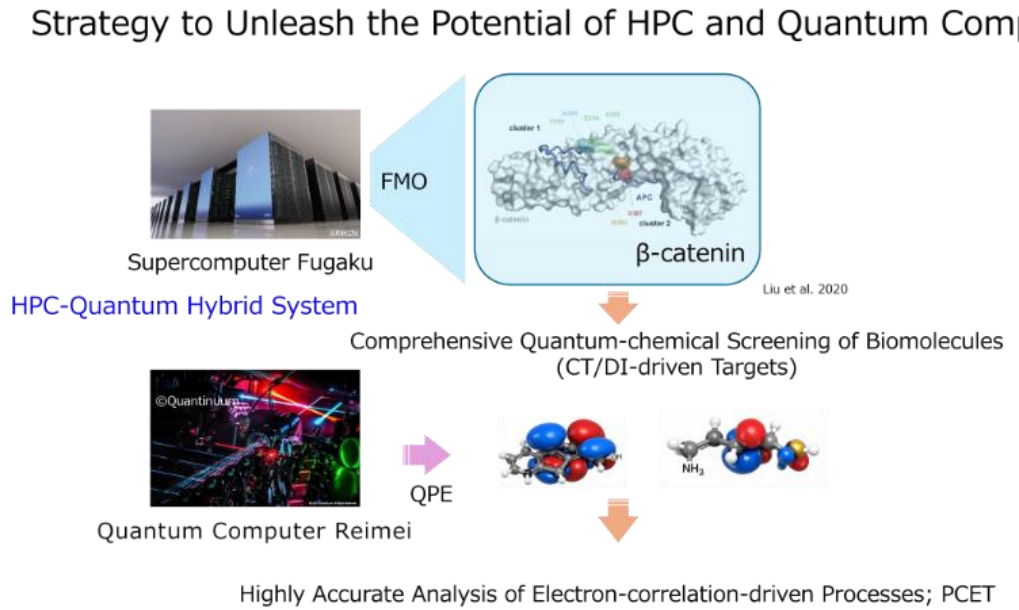
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Problem formulation for quantum computer

- First, large-scale FMO calculations are performed on HPC using biomolecular information obtained from sources such as the Protein Data Bank, and the breakdown of interactions between fragments is analyzed to narrow down the region where the target chemical reaction occurs. Based on this result, a model system to be handled by the quantum computer is constructed
- With future acquisition of chemical reaction pathways in mind, highly accurate energy calculations are required at each point on the potential energy surface. However, there are points where electron correlation is strong and computational cost becomes high for a classical computer alone, so a quantum computer is used for such electronic-state calculations
- As the quantum algorithm for energy calculation, **the quantum phase estimation (QPE) algorithm was adopted in view of the medium- to long-term development of quantum computer hardware, and a quantum error-correcting code that takes advantage of the all-to-all connectivity of an ion-trap quantum computer was used**

Expected business benefits

- **The analysis technology developed in this use case can be applied not only to β-catenin but also to a wide range of biomolecules**. As a foundation for next-generation simulation technology in life science and drug discovery, it is expected to contribute to business through:
  - ✓ **improved accuracy in candidate compound selection**
  - ✓ **shorter R&D periods**
  - ✓ **reduced experiment and validation costs**



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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”.