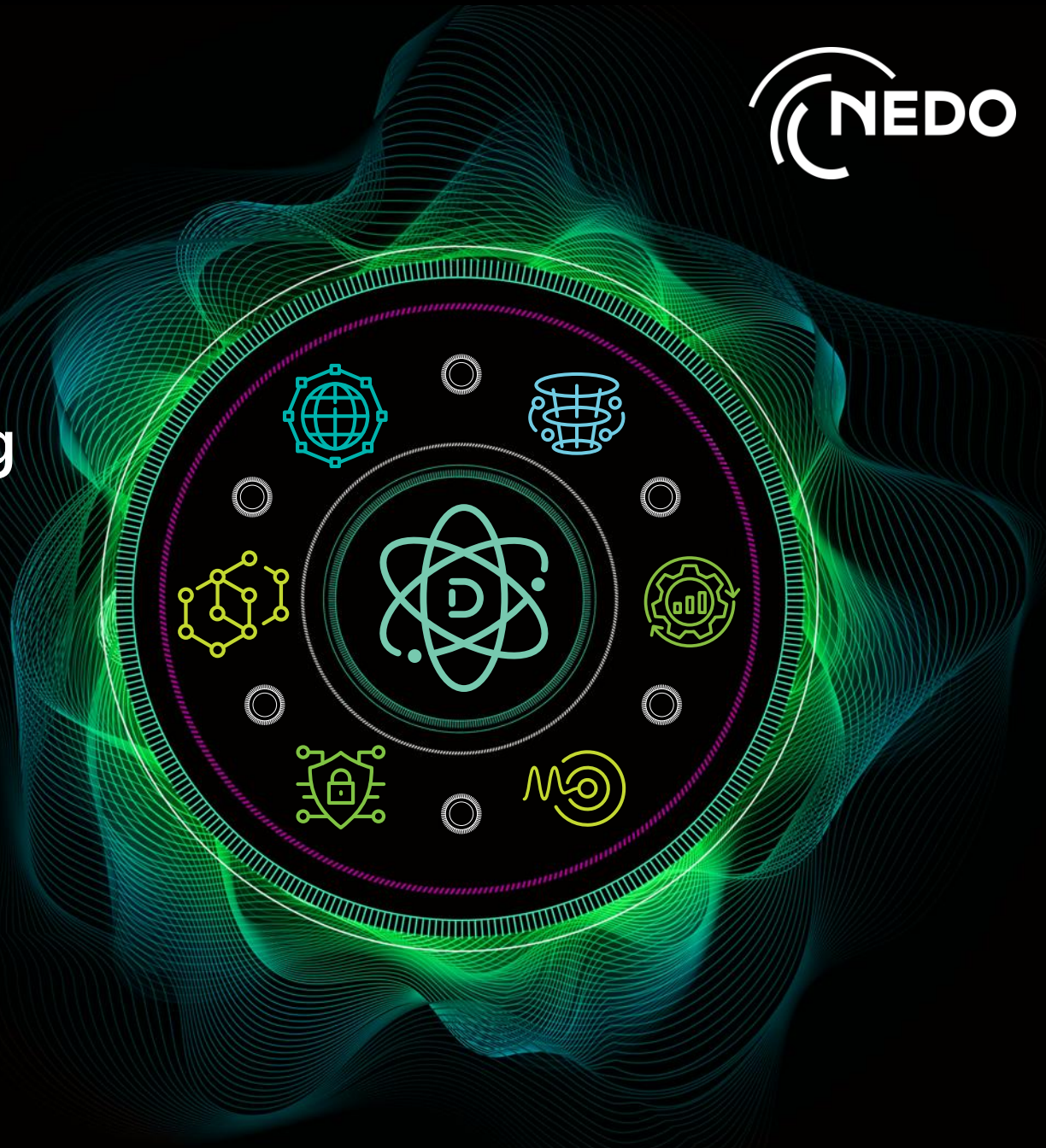
Quantum Computing Use Cases

Material property prediction using existing material data x machine learning

SEKISUI CHEMICAL and Hitachi



New Energy and Industrial Technology Development Organization (NEDO)

SEKISUI CHEMICAL and Hitachi: Material property prediction using existing material data × machine learning [2022/12] 1/2

Validation

Industry	Process Manufacturing
Process	research and development
Method	Simulation
Category	Ising*

Background

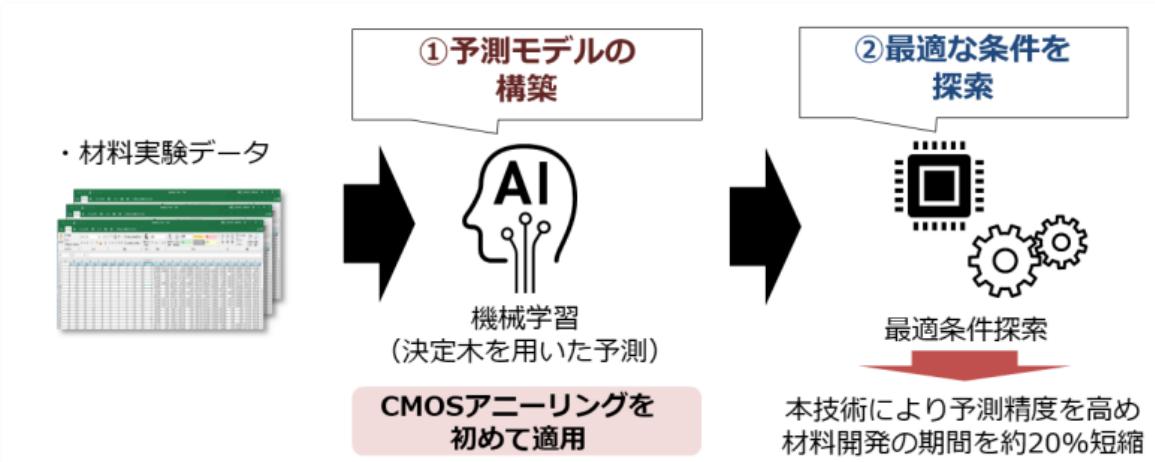
- Until now, material development has **depended on the experience and intuition of researchers, and took a long time and cost to commercialize**
- On the other hand, in the market, demands for material development are becoming more diverse and sophisticated due to shorter product life cycles and resource constraints, and **MI (Material Informatics) efforts are in full swing** to meet these demands.
- Hitachi has continued to develop technologies to realize a data management and analytics platform that uses data to streamline the material development process. **We have responded to the needs of customers in the materials industry by providing materials development solutions that apply MI.**

Issues and motivation to be solved

- In conventional materials development, various conditions related to material creation were selected based on the experience and intuition of researchers, and prediction models were constructed to predict the properties of materials. However, there was a **limitation in improving accuracy because the conditions were not examined comprehensively**
- In this demonstration, SEKISUI CHEMICAL and Hitachi jointly developed a new machine learning model to accelerate material development and verified the possibility of shortening the material development period.

Problem setting as a quantum computer

- **We have developed a new method to improve prediction accuracy** by using quantum technology and comprehensively considering the conditions involved in the creation of materials.
- The developed prediction accuracy model was **applied to the problem of predicting the properties of existing organic materials from their molecular structures, and the accuracy was compared with the conventional method**.
- The machine uses **CMOS annealing, Hitachi's pseudo quantum computer technology**



Conceptual diagram of the developed machine learning model

Reference: Hitachi, Ltd. "Demonstration that the use of pseudo quanta can further shorten the material development time by 20% using conventional MI" (https://www.hitachi.co.jp/New/cnews/month/2022/12/1216.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.

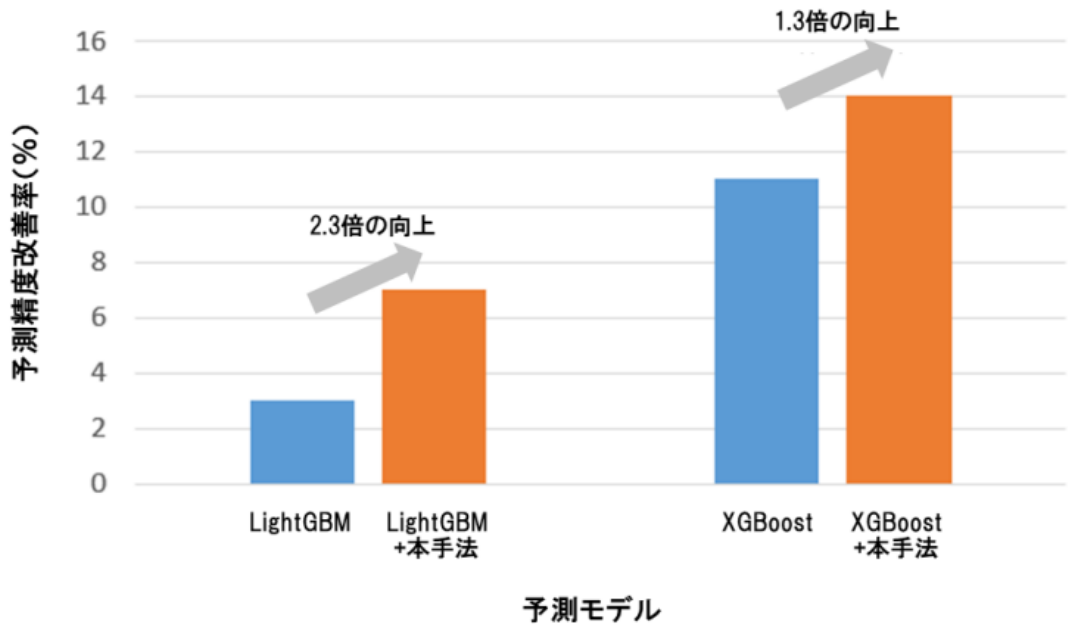
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Expected business benefits

- In terms of prediction accuracy by machine learning, we compared the conventional machine learning algorithm (LightGBM, XGBoost) alone and the method applied to the conventional machine learning algorithm. As a result, we were able to **achieve better prediction accuracy than the conventional machine learning algorithm alone.**
- In the case of material development using this technology, **the time required for material development can be reduced by about 20%** compared with the conventional method using MI.



Results of improved prediction accuracy when applying the developed method to the conventional technology

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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".