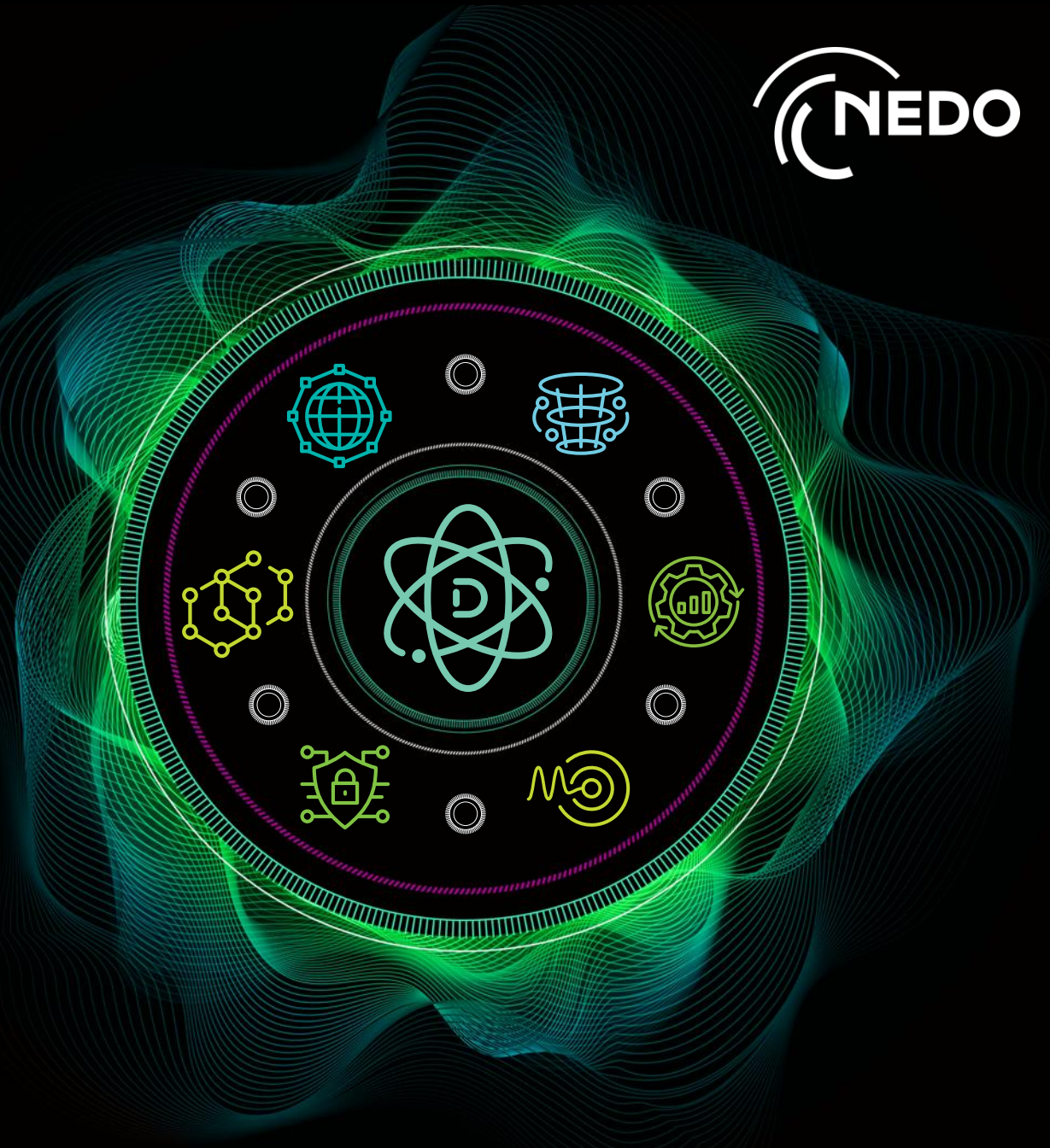
Quantum Computing Use Cases

Development of DMFT Computational Technology for Higher Accuracy and Faster Materials Simulation

Quemix × MITSUI KINZOKU



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

Industry	Process Manufacturing
Process	material search
Method	Simulation
Category	Gate*

Background

- In materials development, the search for high-performance new materials requires extensive trial and error, **making both experiments and computations time- and cost-intensive**
- While the use of computer simulation is important for efficiently narrowing down promising material candidates, it has **not been easy to achieve both higher analytical accuracy and shorter computation time**
  - ✓ There is a **trade-off in that improving accuracy tends to increase computational load, while reducing computation time makes it difficult to secure the required level of accuracy**
- Against this background, Mitsui Kinzoku and Quemix conducted joint research on **a new technology for materials computation using quantum computers**

Issues and motivation to be solved

- Focusing on the DMFT method, which **enables high-precision calculations but had the challenge of long computation time in this case**
- In particular, in DMFT calculations, quantum phase estimation (QPE), a key component, **had been a factor hindering the achievement of both high speed and high precision, because increasing energy resolution led to increases in the number of gate operations and computational cost**
- The goal was to **establish a new computational workflow for efficiently executing DMFT on a quantum computer, while improving the performance of quantum phase estimation (QPE),** which plays an important role in the computational process
  - ✓ Rather than simply replacing existing computations with quantum computing, they aimed to improve computational efficiency with a view to applying the technology to practical materials simulations

Reference: Mitsui Kinzoku and Quemix Develop a New Technology for Materials Calculations on Quantum Computers Accelerating the Practical Use of Materials Simulation（https://www.mitsui-kinzoku.com/LinkClick.aspx?fileticket=QhyijuGgx%2fY%3d&tabid=100&mid=826）

*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 setting as a quantum computer

- DMFT was targeted for application to quantum computation, and a new computational workflow was developed for its efficient execution on a quantum computer
- In addition, **a new technology, QAVG (QPE Averaged over Variable Grids), was developed to improve quantum phase estimation (QPE), a key component of the computational process**
  - ✓ QAVG is a technique that improves the accuracy and speed of computation while suppressing the increase in gate operations and computational cost that conventionally accompanies higher energy resolution in QPE
- Furthermore, **simulations assuming catalytic materials were carried out on Quantinuum's quantum computer hardware, confirming the effectiveness of QAVG as an important component of the DMFT computational workflow**
- As a result, **an important element of the DMFT workflow was validated in a hardware environment**, demonstrating the feasibility of materials computation using a quantum computer

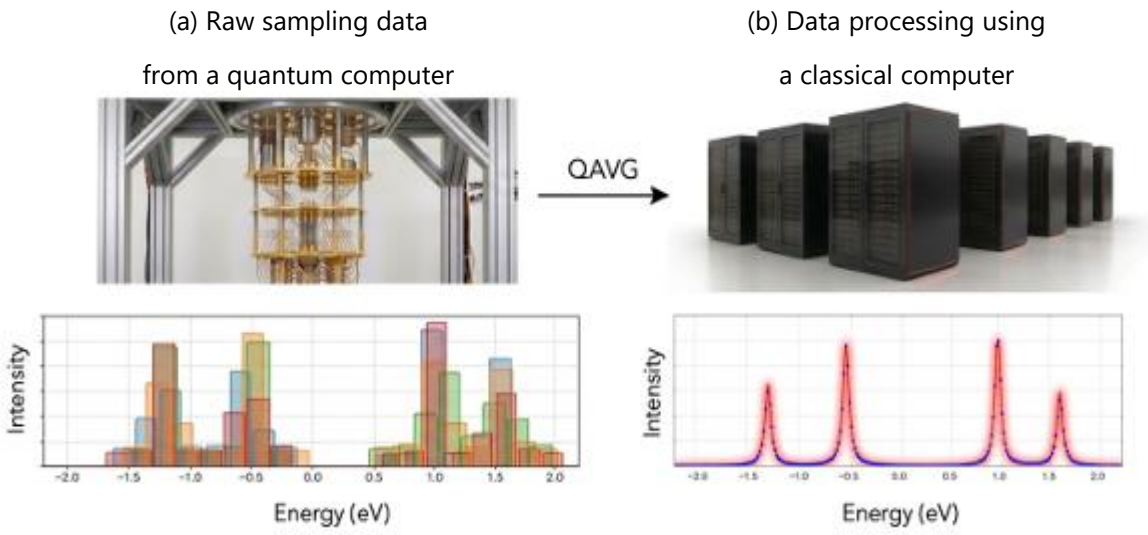


Figure: Conceptual illustration of QAVG
Bottom-left: Four types of data obtained by executing QPE on a quantum computer (distinguished by four different colors)
Bottom-right: Continuous spectrum obtained by executing QAVG based on the four types of data obtained from the quantum computer (the blue dots represent the actual QAVG results, and the red line represents the exact solution)

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Expected business benefits

- **QAVG is expected to enable higher-precision and faster DMFT calculations on quantum computers while suppressing the increase in computational cost**, thereby bringing practical materials simulations closer to reality
- In hardware validation, it **achieved on current machines a level of computational accuracy that would normally be expected only after about two more years of hardware progress**, raising expectations for the early practical use of quantum-computer-based DMFT calculations
- In addition, because **quantum phase estimation (QPE) is widely used in the field of materials computation, QAVG is expected to have applications and spillover effects beyond DMFT calculations and into other materials computation**
- As a result, it may **promote the use of high-precision simulations in materials development themes, including catalytic materials, thereby improving the efficiency of promising-material discovery and shortening development timelines**

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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”.