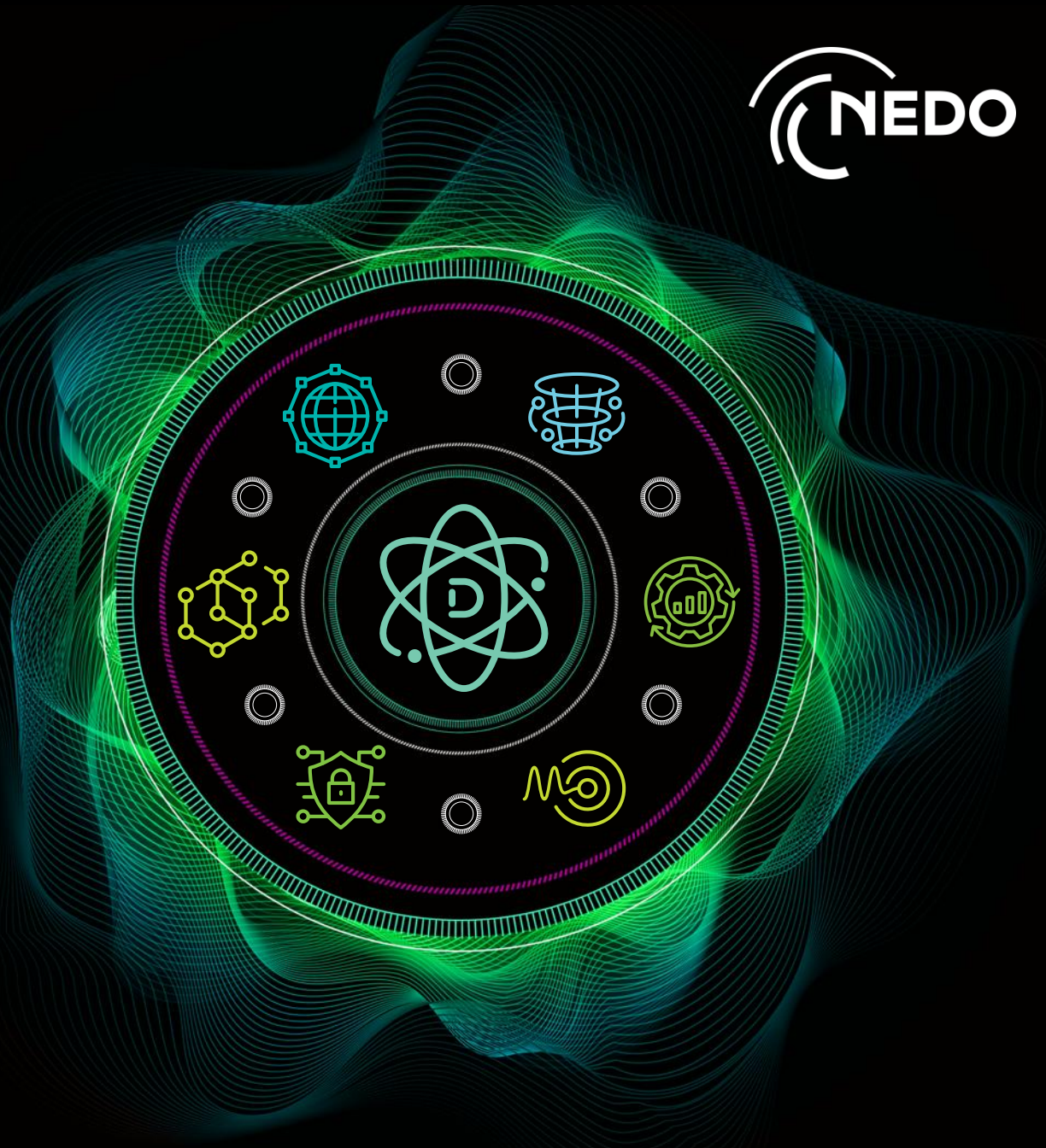
Quantum Computing Use Cases

A Quantum–Classical Hybrid Molecular Dynamics Simulation Framework for Materials Development and Drug Discovery

Quemix × DENSO



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

Industry	Process Manufacturing
Process	material search
Method	Simulation
Category	Gate*

Background

- Molecular dynamics (MD), which computationally captures behavior at the atomic and molecular level, **is important in materials development and drug discovery**, and is used across a wide range of fields including batteries, polymer materials, drug discovery, and chemical process design
  - ✓ MD is a computational technology that tracks the motion of atoms and molecules and evaluates material properties and chemical reactions
- At the same time, **conventional MD tends to involve a large computational burden as higher accuracy is pursued**, because it requires long-time tracking of many-particle systems and statistical processing, which can easily impose constraints on target scale and computation time
- Against this background, Quemix and **DENSO worked to establish a quantum–classical hybrid molecular dynamics simulation framework in order to assess the applicability of quantum computing to MD calculations**

Issues and motivation to be solved

- Conventional MD **had limitations in handling time evolution and coordinate-space scales close to real-world environments** with high accuracy, making it a challenge to balance accuracy and computational cost
  - In particular, obtaining physical properties such as diffusion coefficients **requires tracking a large number of trajectories over long periods and then performing statistical processing**
- Although the potential use of quantum computers had long been discussed, **the key challenges in building a practical framework for MD calculations were the representation of distribution functions, the handling of temperature and heat baths, and the readout of physical properties**
- In this project, a computational framework for molecular dynamics using a quantum computer was developed, and **its applicability to chemical-state prediction was examined**

Reference: [Press Release] Extending Molecular Dynamics Computation Supporting Materials Development and Drug Discovery to a Quantum Computing Framework（https://www.quemix.com/post/20260601-denso）
*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

- Classical molecular dynamics (MD) was **reformulated into the Koopman–von Neumann (KvN) framework, in which the distribution function is represented as a quantum state and time-evolved, and was defined as a problem to be handled within a quantum–classical hybrid MD framework**
  - ✓ Specifically, by describing **MD in the Koopman–von Neumann (KvN) formalism**, the distribution function—which had conventionally been evaluated through trajectory tracking and statistical averaging—was made amenable to direct representation and manipulation as a quantum state
- In addition, **temperature control required to reproduce real-world conditions was reformulated into a wavefunction representation so that it could be handled on quantum circuits**
  - In addition, for constant-temperature (NVT) conditions required to reproduce real-world environments, methods for handling Nosé–Hoover and Langevin heat baths on quantum circuits were considered, and Quemix's PITE® was applied to the Langevin-type approach
- Furthermore, **methods were developed to extract the diffusion coefficient and vibrational density of states (VDOS)** from the time-evolved distribution function
  - ✓ For readout, the framework was configured to **use quantum phase estimation (QPE) or quantum amplitude estimation (QAE)**, depending on the application
- The framework was then applied to a proof of concept for simplified chemical-state prediction targeting H_2 dissociation under high-temperature conditions, demonstrating the feasibility of the developed framework

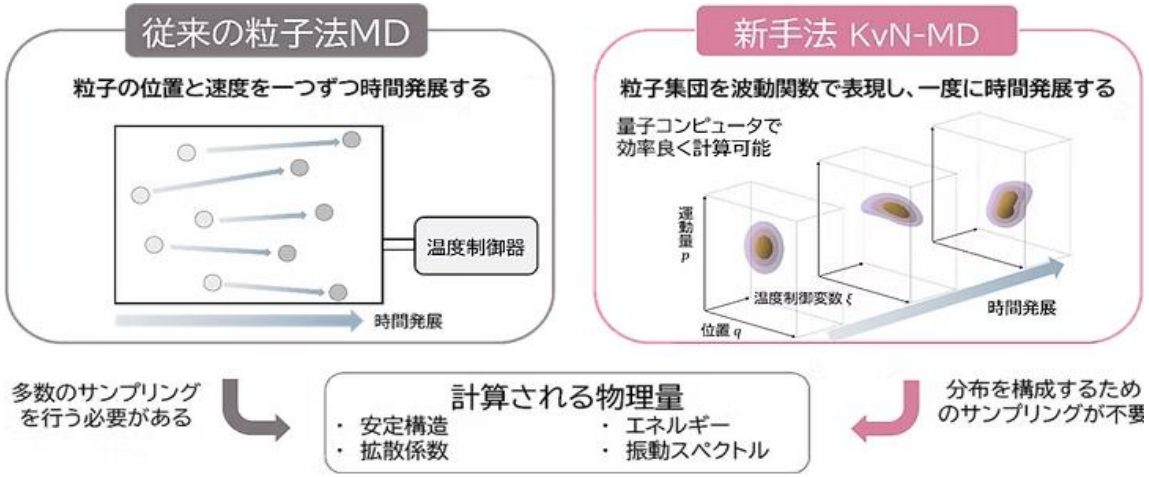


Figure: Conceptual illustration showing the difference between the particle method and the KvN method in molecular dynamics simulation

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Expected business benefits

- **Simulation capabilities in materials development and drug discovery are expected to become more advanced and faster**, with the potential to enable more direct and efficient calculation of physical properties such as diffusion coefficients
- This is expected to **improve the efficiency of candidate exploration, shorten research and development timelines, and reduce the number of trial-and-error iterations**
- In particular, applications **are envisioned in fields that require precise atomic-level analysis and performance prediction**, such as next-generation battery materials, polymer materials, catalysts, and drug discovery
- In addition, while this work is **a proof of concept focused on hydrogen molecules and currently represents only a minimal framework**, it is **expected to serve as a foundational technology for future extension to more complex systems**

(a) Distribution function obtained by the conventional method

(b) Distribution function obtained by the new method

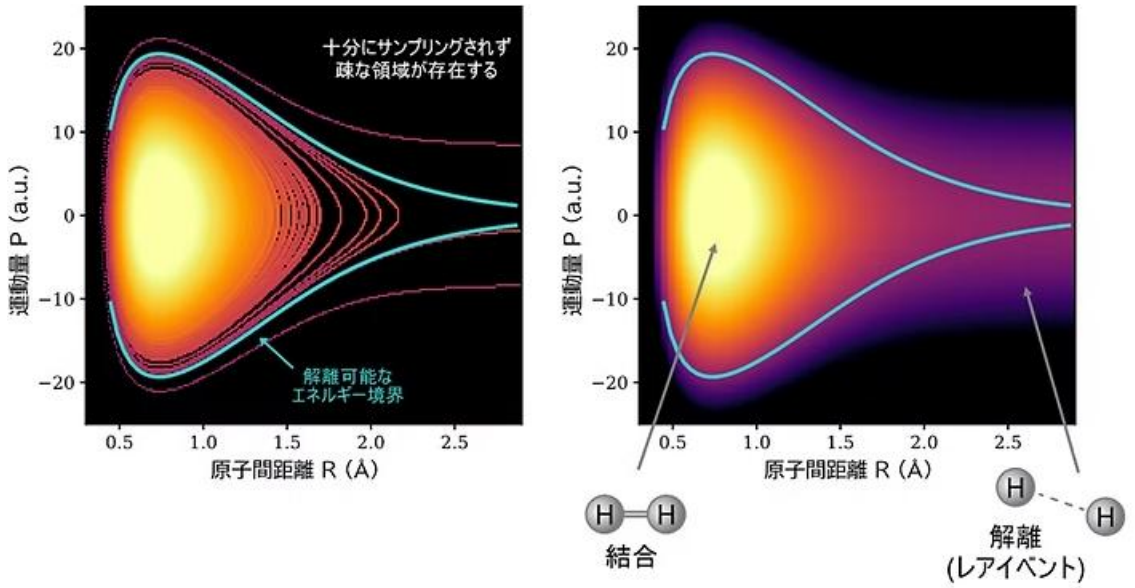


Figure: Comparison of the conventional method and the new method (KvN). Rare-event sampling of H2 → H + H dissociation at T = 5000 K
The new method (KvN) demonstrated the potential for low-computational-cost, high-accuracy prediction of chemical states by directly handling the distribution function as a quantum state

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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”.