FUJITSU Project

Title Mathematical and data-driven approaches to materials sciences

Industrial Partner FUJITSU LIMITED

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Background and challenges

In the fields of materials sciences, advancements in both experimental techniques and simulation techniques have significantly enhanced the quality of data, resulting in an era of unprecedented data richness. NanoTerasu Synchrotron Light Source, which began operation at Tohoku University in 2024, enables the measurement of molecular, atomic, and electronic states with nanometer-level high spatial resolution (Fig. 1) [1,2].
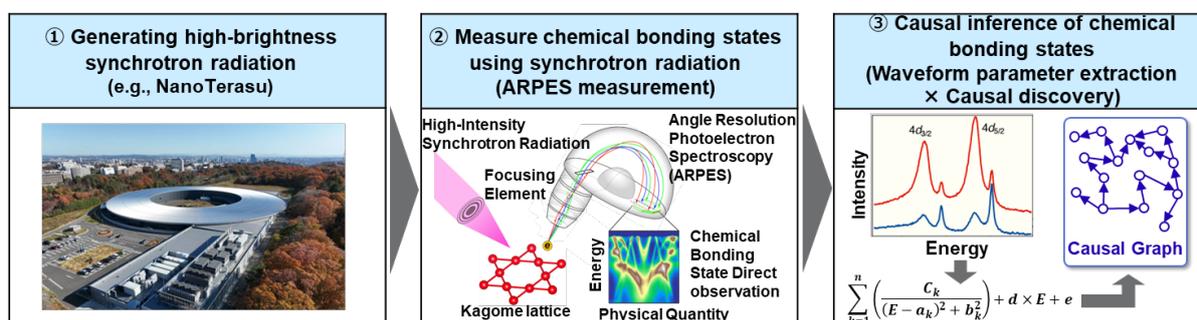

Fig. 1 Causal discovery from NanoTerasu ARPES experimental data [2]

AI-assisted molecular dynamics simulation has successfully reproduced high-precision motions and chemical reactions of large-scale systems exceeding 100,000 atoms (Fig. 2) [3,4].
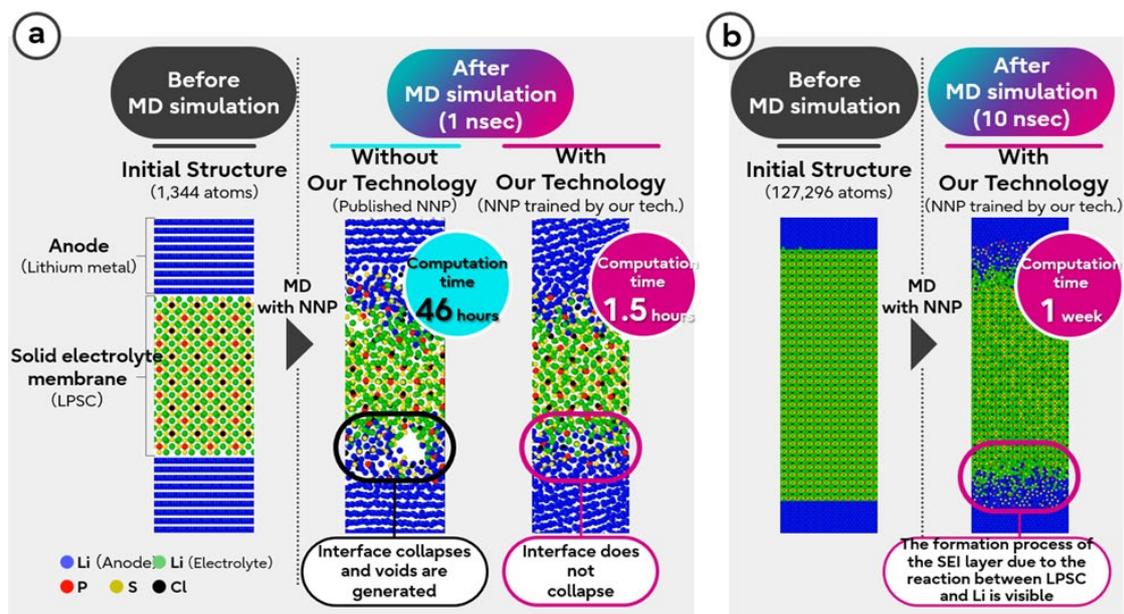
Fig. 2. AI-assisted molecular dynamics simulation [3]

As experiment and simulation performances improve drastically, the amount of data created increases accordingly. One big challenge here is to exhaustively extract useful and exciting information from such a huge amount of experimental and simulation data without the bias of human experiences or intuitions in order to finally lead to new discoveries [1,2]. While computing power and AI have been playing an important role to solve the issue, the power of mathematics to clarify the essence of things is now essential.

The purpose of materials sciences is to develop new functional materials to drive innovation and contribute to resolving societal issues, including environmental challenges. Considering the purpose, another practically important challenge is to connect new insights into micro-level chemical reaction mechanisms to the performance of macro-level devices and products. This requires bridging the gap among different levels of physics and the gap between experiment and simulation. The power of mathematics to model relationships and structures among different things or systems will help to solve the issue.

Project overview

In this project, you will develop methods for analysis of data in the field of materials sciences assisted by mathematics. You can use Fujitsu Causal AI [5] as a fundamental analysis method. The analysis may include simulation and explanation features. For purposes of development, you should consider several aspects such as those

presented below.

1. Convincingness: Analysis results must be convincing and accepted by users. "Simple" and "logical" are important factors for convincingness.
2. Comprehensiveness: Analysis should exhaustively extract useful and exciting information from data without the bias of human experiences or intuitions.
3. Discoverability: When analysis results are not convincing to users, this does not always imply that they are not correct. It might be a new finding that users have not noticed before. Therefore, it is also important to remind them that it may be a new discovery even when it is not convincing.

Expectations

We look forward to welcoming students who are interested in AI, statistics, simulation and chemistry. In addition, students who are interested in answers to the following questions are welcome.

- ✓ What is data-driven approaches to materials sciences?
- ✓ What is AI-assisted molecular dynamics simulation?
- ✓ What is causal AI?
- ✓ What is the gap among different levels of physics?
- ✓ What is the gap between experiment and simulation?

Requirements

Programming skills in Python.

References

[1] K. Fujita and K. Nakayama et al., "Extracting causality from spectroscopy," Sci Rep 15, 43291 (2025).
   https://doi.org/10.1038/s41598-025-29687-8
[2] Fujitsu Press Release, "Tohoku University and Fujitsu utilize Causal AI to discover superconductivity mechanism of promising new functional material"
   https://global.fujitsu/en-global/pr/news/2025/12/23-01
[3] Fujitsu Press Release, "Fujitsu achieves high-precision, long-duration molecular dynamics simulation for all-solid-state battery interphases with over 100,000 atoms"
   https://global.fujitsu/en-global/pr/news/2025/12/01-01

[4] N. Matsumura et al., "Generation of Neural Network Potential for Molecular Dynamics: Constructing Robust and Accurate Potentials with Active Learning for Nanosecond-Scale Simulations," J. Chem. Theory Comput. 2025, 21, 8, 3832-3846.
https://doi.org/10.1021/acs.jctc.4c01613

[5] G-RIPS Sendai 2025 Fujitsu Group Final Report.
https://www.mccs.tohoku.ac.jp/g-rips/report/2025/pdf/fujitsu_final_report.pdf