MERIT Domestic Internship Report

EEIS, Graduate School of Engineering

D3 student, Iwamoto Lab. and MERIT 7th

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1. Internship overview
    - Working period
    September 13, 2021 to October 14, 2021 (for one month)
    - Hosting company
    Quantum Computing Research Center, Fujitsu Research, Fujitsu Limited
    - Research subject
    A Study on Quantum Chemical Calculations of Molecules Using a VQE Simulator

2. Research background and issue

Since quantum computers can handle a variety of states as qubits, they have the potential to perform complex calculations faster than conventional classical computers. Currently, research efforts are focused on the practical application of error-prone Noisy Intermediate-Scale Quantum (NISQ) devices, and one of their applications is quantum chemical calculations to derive the energy of atoms and molecules[1]. Variational Quantum Eigensolver (VQE) is a typical quantum chemical calculation algorithm running on NISQ devices, but as the number of qubits required for the calculation increases with the size of the molecule, further investigation is required to improve the calculation time and accuracy.

In this internship, we first performed quantum chemical calculations of H_2 molecules using the Python-based VQE simulator to study the influence of different calculation conditions on the calculation time and accuracy. Based on the knowledge obtained from the H_2 molecule, I also worked on the quantum chemical calculation of the more complicated CH_4 molecule, searching for the optimal calculation conditions and improving the calculation algorithm.

[1] Sam McArdle, Suguru Endo, Alán Aspuru-Guzik, Simon C. Benjamin, and Xiao Yuan, "Quantum computational chemistry," Rev. Mod. Phys. **92**, 015003 (2020).

3. Internship procedures

This internship was conducted through Microsoft Teams meeting and exchanges via email. During the internship, we discussed the previous day's progress for about 30 minutes to an hour every morning from 9:00 a.m. In the morning, we mainly discussed the validity of my calculation results and confirmed the tasks to be done on the day. After the progress report I started my work and worked on it for about eight hours every day. In the afternoon, I had a coffee break meeting (about 30 minutes) to check the progress of the day, ask questions, and chat. On October 4, we held a technical exchange

meeting with researchers from Quantum Computing Research Center of Fujistu Research and I had an opportunity to introduce my research in the graduate school. On the last day of the internship, I presented my findings at the final report meeting in the center.

4. Impressions about the internship

My knowledge of quantum computers was limited to a rough understanding through general lectures, including the MERIT special lecture by Yoshiaki Shimada-san (Japan Science and Technology Agency), but this internship gave me a first-hand experience of the advantages and disadvantages of quantum computers by actually working on quantum chemical calculations, which is one of the expected applications. As a student majoring in a field close to physics, quantum chemistry was a new field of research for me, and I was a bit anxious before starting the internship. However, by understanding the connection with quantum mechanics, I was able to understand it smoothly.

During the internship, I had several stumbling blocks in coding and calculations, but I was able to find solutions with the help and kind guidance of the mentors. In this research, I implemented simulators using Python, which I have many opportunities to use in my own research, and I was also able to learn several things that I can use in the future. Although my internship period was limited, there were a huge number of issues to be dealt with. As a result, I succeeded in undertaking all the issues we had planned in advance, although some of them ended up a little half-finished.

Unfortunately, this internship was conducted completely online, but we had discussions every day as if we were actually meeting face-to-face. I think I was able to spend a fulfilling internship period because they accepted me in a friendly manner. Especially since I have always been interested in research laboratories within companies, it was a great opportunity for me to experience their atmosphere and environment.

5. Acknowledgements

I would like to express my gratitude to Fujitsu Research for accepting me for this internship under the global pandemic of COVID-19. I would also like to deeply appreciate Hirotaka Oshima-san, Norihiko Takahashi-san, and Shintaro Sato-san, who belong to the Quantum Computing Research Center of the institute, for their valuable time and instructions on this research. In addition, I would like to thank the people from the Human Resources Department of the Research Management Center of the institute for their help in the orientation for the internship held on the first day. During the internship period, I also had the opportunity to deepen our discussions with people from the Quantum Computing Research Center at the technical exchange meetings and final report meeting. Although the internship period was only one month, I would like to thank everyone involved.

Finally, I gratefully thank my supervisor, Prof. Satoshi Iwamoto, my MERIT associate supervisor, Prof. Masao Ogata, the MERIT program of the University of Tokyo, and its secretariat for kindly agreeing to participate in this internship.