（別紙様式５）

変革を駆動する先端物理・数学プログラム（FoPM）

国外連携機関長期研修　報告書

氏　　名	ハフィド　アユーブ・Ayoub Hafid
所属部局	数理科学研究科　　数理科学専攻
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I have had the opportunity to participate in a long-term internship at the quantum computing start-up Qunasys Inc. since 2023. There, thanks to guidance through weekly meetings, I have been conducting research on quantum advantage, namely the fact that quantum computers are expected to be more powerful than classical computers for certain computational tasks. I have been focusing on proving that certain computational tasks related to quantum chemistry are intractable for classical computers. This provides evidence toward the superiority of some quantum algorithms with potential real-world applications, such as drug discovery.
This area of research is fascinating in that it combines computer science with insights from physics and mathematics. As it differs from my main research topic, it gave me the opportunity to learn about new fields such as computational complexity theory (at least on the quantum side). Through the internship, as well as workshops and conferences, I was able to interact with researchers in the quantum chemistry industry and in the field of quantum information and computing. As a result, I am willing to continue research projects in this direction.

Motivation and background of the research

One of the main expected applications of quantum computing is the simulation of quantum phenomena, since problems exhibiting quantum behavior are expected to be more tractable for quantum computers than for classical computers. In this direction, one practical application is estimating ground states and ground-state energies of molecules, a task tightly tied to the properties of the materials these molecules form. Several optimization algorithms bridging quantum and classical computers (hybrid approaches) have been devised to approximate molecular ground states.
A natural question that would provide evidence in favor of such approaches is whether classical computers can simulate these algorithms. The claim that quantum computers or quantum algorithms cannot be efficiently simulated by classical computers is called *simulation hardness*. This question has been investigated for several more or less restricted models of quantum computation (for instance Boson Sampling), but the literature on simulation hardness for practical algorithms is still relatively young.
The company I worked with devised an algorithm for the molecular ground-state and energy estimation problem, called Quantum-Selected Configuration Interaction (QSCI). This algorithm relies on first fixing an ansatz (a guess) for the form of the ground state, and then repeatedly sampling states using the quantum circuit representing this ansatz in order to optimize its parameters. In this setting, and given the quantum advantage problem described above, we ask the following question: Given a quantum circuit representing an ansatz, is the task of sampling from its output classically hard to simulate?
To begin to answer this question, one needs to fix a type of ansatz. In quantum chemistry, one popular choice is the Unitary Coupled Cluster (UCC) ansatz, which is a unitarized version of coupled-cluster operators made from balanced products of creation and annihilation operators. It takes the form

$$U_{\mathrm{UCC}} = e^{T-T^{\dagger}},$$

where

$$T = T_1 + T_2 + \cdots + T_n, T_k = \sum_{\substack{i_1,\ldots,i_k \\ a_1,\ldots,a_k}} t_{i_1\ldots i_k}^{a_1\ldots a_k}\ a_{a_1}^{\dagger}\cdots a_{a_k}^{\dagger} a_{i_k}\cdots a_{i_1}.$$

Here, i_j label occupied orbitals, a_j label virtual orbitals, $a^{\dagger}$ and a are fermionic creation and annihilation operators, and $t_{i_1\ldots i_k}^{a_1\ldots a_k}$ are the parameters of the ansatz.
A further simplification of this ansatz, which has the advantage of being more practical to implement, is the Unitary Cluster Jastrow (UCJ) ansatz. The k-UCJ unitary is

$$U_{k\text{-UCJ}} = \prod_{\ell=1}^{k} \exp\ \left(K^{(\ell)}\right)\exp\ \left(iJ^{(\ell)}\right)\exp\left(-K^{(\ell)}\right),$$

where

$$K^{(\ell)} = \sum_{p,q} \kappa_{pq}^{(\ell)}\ a_p^{\dagger} a_q, \kappa^{(\ell)} = -\left(\kappa^{(\ell)}\right)^{\dagger},$$

and

$$J^{(\ell)} = \sum_{p} \theta_p^{(\ell)}\ n_p + \sum_{p<q} \theta_{pq}^{(\ell)}\ n_p n_q,$$

with $n_p = a_p^{\dagger} a_p$ the number operators. The parameters $\kappa_{pq}^{(\ell)}$, $\theta_p^{(\ell)}$, and $\theta_{pq}^{(\ell)}$ define the ansatz.
In quantum chemistry, such an ansatz is applied to a reference state $|\Phi_0\rangle$ representing molecular orbitals filled sequentially. One then seeks parameters for which $U_{k\text{-UCJ}}|\Phi_0\rangle$ is close to the ground state. Then QSCI uses repeated sampling from $U_{k\text{-UCJ}}|\Phi_0\rangle$ and thus the simulation-hardness problem naturally specializes in this setting.

Result

By exploiting previous work showing that certain restricted classes of quantum circuits are hard to simulate, we were able to show that sampling from the UCJ ansatz is classically hard for some carefully chosen parameters $\kappa_{pq}^{(\ell)}$, $\theta_p^{(\ell)}$, and $\theta_{pq}^{(\ell)}$. This hardness already holds with a single layer, that is, for ansatze of the form

$$\exp(K)\exp(iJ)\exp(-K).$$

In other words, 1-UCJ is classically hard to simulate in the worst case.

Experience conducting research in industry

During this internship, the research methodology was similar to that of academia: studying existing literature and holding meetings to discuss results and ideas. The main difference (especially with pure math) was that the motivation was more practically oriented and grounded in real-world problems.

Experience attending workshops and presenting at an international conference

In relation to this research project, I had two international academic experiences.
First, I attended a research school at the Centre International de Rencontres Mathématiques (CIRM) in Marseille, France in summer 2024, entitled *Random Quantum Channels: Entanglement and Entropies*. While I had additional motivation for attending this workshop related to other research projects, one motivation was directly connected to this work. The result presented above concerns only worst-case hardness, meaning that only specific (possibly atypical) parameters are shown to lead to hard instances. A natural next step is to establish simulation hardness for more generic parameters, or at least for a non-negligible fraction of circuits (average-case hardness). One approach used in related contexts involves estimating expectations of functions of random matrices specified by the randomly sampled parameters. One way to estimate these quantities in certain

settings relevant to UCJ is via Weingarten calculus, which was one of the topics of the school. Second, I presented the above result as a poster at the Conference on Quantum Information Processing (QIP 2025) in winter 2025. This is one of the main annual events in quantum information and computing, and it gave me the opportunity to interact with researchers in the field and to learn about current problems and results. I was particularly interested in talks on quantum complexity, approximations to random circuits (quantum t-designs), and connections with my main field of research in mathematics, operator algebras.

Outlook

The result described above is only a first step toward providing evidence for the superiority of practical quantum circuits. Important open questions include noise tolerance and the fraction of hard instances (average-case hardness as opposed to worst-case hardness). These questions are especially interesting from a mathematical point of view, as they involve estimates of quantities depending on random matrices, as well as techniques from interpolation and numerical analysis. I plan to continue working on this direction, and it is fascinating since it may connect to techniques in random matrix theory and representation theory.

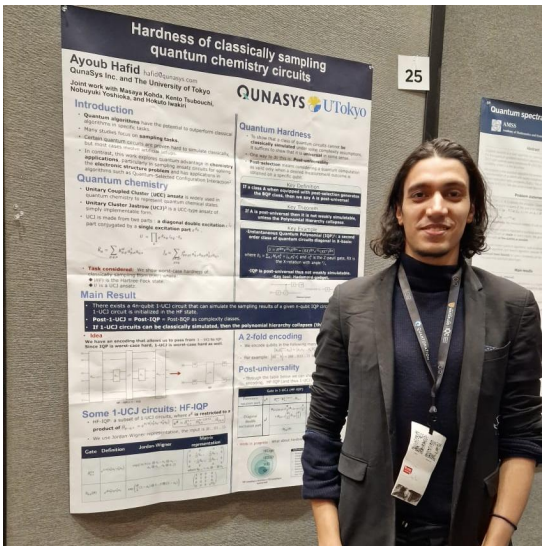


Figure 1 Poster presentation (QIP 2025)



Figure 2: The reception building of CIRM (2024)