CIFRE PhD Topic
Molecular Chemistry, Variational Quantum Algorithms, and Applications to the Study of Molecular Vibrations

1 Context

This CIFRE PhD project is part of the development of the LabCom (Joint Laboratory) TeleMAQ (Testing the Limits of Quantum Machines and Algorithms), established between the start-up ColibrITD (https://www.colibritd.com/) and the DiTeQ team (Dijon Quantum Technology, https://icb.cnrs.fr/diteq/) of the Laboratory Interdisciplinary Carnot of Burgundy (ICB, UMR 6303).

ColibrITD is a start-up specialized in the development of quantum algorithms for multiphysics simulation, with a particular focus on industrial use cases. In particular, the company is developing a quantum solver for differential equations (ODEs/PDEs), currently accessible through IBM's quantum platform [1, 2, 3]. Its R&D team consists of around ten permanent researchers specializing in variational quantum algorithms and their implementation on simulators and quantum machines.

The DiTeQ team at ICB is a theoretical physics group specializing in quantum control. In recent years, its activities have expanded toward quantum technologies, in particular through the integration of experimental devices such as online-accessible quantum computers and NV-center experimental platforms. The recent arrival of specialists in quantum chemistry strengthens the team's ability to support ColibrITD in the development of quantum algorithms dedicated to the simulation of molecular systems.

2 Description of the Research Project

The quantum computers currently accessible through the cloud belong to the class of NISQ machines (Noisy Intermediate-Scale Quantum). Their limited size and intrinsic noise prevent the efficient implementation of the asymptotically advantageous quantum algorithms developed in the 1990s, such as those of Grover, Shor, or HHL.

In this context, variational quantum algorithms [4] represent a promising approach for exploiting current quantum machines and reaching an initial form of *quantum utility*. Among them, the Variational Quantum Eigensolver (VQE) is particularly well suited to problems in quantum chemistry.

The principle of VQE is based on the preparation of a parameterized quantum state $|\psi(\theta)\rangle$, whose parameters are optimized through a classical loop in order to minimize the average energy :

$$\langle\psi(\theta)|H|\psi(\theta)\rangle.$$

This approach makes it possible to approximate the ground state of a given molecular Hamiltonian.

Software libraries such as Qiskit [5] now provide tools that make it possible to encode Hamiltonians and variational ansätze efficiently, thereby facilitating experimentation on simulators and quantum processors. However, as the size of molecular systems increases, several bottlenecks arise : the explosion of the search space, *barren plateau* phenomena, sensitivity to noise, and the lack of guaranteed convergence.

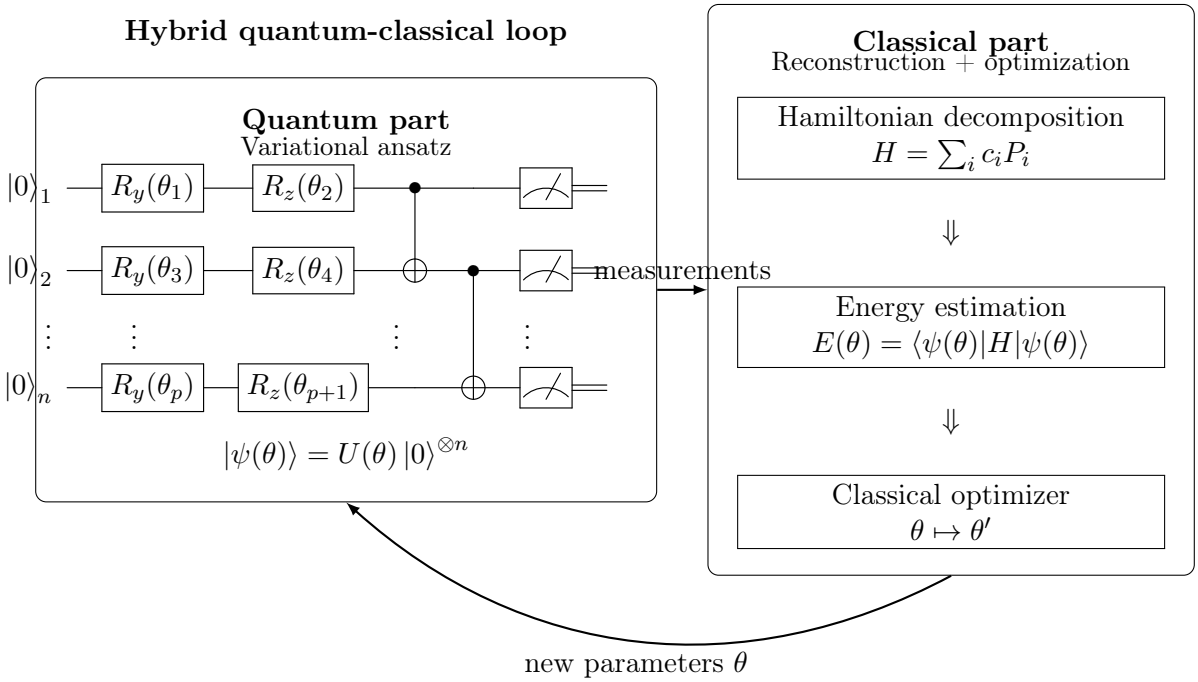

FIGURE 1 – Schematic representation of the *Variational Quantum Eigensolver* (VQE). A parameterized quantum circuit prepares a state $|\psi(\theta)\rangle$, which is measured in order to estimate the energy associated with the molecular Hamiltonian. A classical optimizer then updates the circuit parameters, forming a hybrid loop until convergence.

In this context, adaptive variants of VQE [6], as well as so-called *hardware-efficient* or *problem-inspired* approaches [7, 8], appear necessary in order to dynamically construct ansätze that are better adapted to the structure of the problem and to hardware constraints.

The PhD project will be structured around the following two main research questions :

— What are the practical limits of VQE-type approaches in terms of the size of molecular systems and the spectroscopic accuracy achievable on NISQ machines ?

— What improvements, inspired by classical quantum chemistry methods such as basis selection, electronic correlation methods, and initialization strategies, can be integrated into VQE algorithms, particularly at the level of ansatz construction and Hamiltonian representation ?

3 Methodology

The PhD project will combine theoretical developments, numerical implementation, and experiments on quantum hardware.

Several methodological directions will be explored :

— **Benchmarking molecular systems** : selection of test molecules, including small systems and molecules of industrial interest, and comparison with classical reference methods such as Hartree-Fock and CCSD.

— **Design of efficient ansätze** : study and development of adaptive ansätze, such as ADAPT-VQE, *hardware-efficient* ansätze, and ansätze inspired by quantum chemistry, such as UCCSD and truncated variants, while taking circuit-depth constraints into account.

— **Optimization strategies** : analysis of classical optimization algorithms, including gradient-based and gradient-free methods, as well as the study of cost landscapes and *barren plateau* phenomena.

— **Noise reduction** : integration of *error mitigation* techniques, including zero-noise extrapolation, probabilistic error cancellation, and measurement error mitigation.

— **Hardware implementation** : execution of the algorithms on quantum processors accessible through the cloud, including IBM machines and industrial partners, together with an analysis of real-world performance.

4 Objectives and Expected Outcomes

The objective of the PhD project is to identify relevant use cases in molecular simulation for which current quantum computers can offer a practical advantage or complementarity with classical approaches.

The expected outcomes include :

— a better understanding of the limitations of VQE approaches on NISQ machines ;

— the development of new algorithmic strategies adapted to hardware constraints ;

— experimental validation on quantum hardware.

At the end of the PhD project, one of the expected deliverables is the development of a software module dedicated to quantum chemistry within ColibrITD's QUICK platform (Quantum Innovative Computing Kit).

5 Profile

The candidate should hold a Master's degree with a specialization in quantum information, quantum algorithms, and/or quantum chemistry. Strong skills in scientific programming, especially Python, are expected.

The recruited candidate will join ColibrITD's R&D team. They will carry out research work including a literature review, algorithmic development, implementation, and experimental validation. The results will be regularly presented to the team and will contribute to guiding the company's developments.

6 Joining ColibriTD

— **Innovation first :** Work on cutting-edge quantum algorithms with immediate real-world applications.

— **Dynamic team :** Collaborate with a diverse group of quantum experts, software engineers, and innovators at Le Village by CA, Paris.

— **Impactful projects :** Drive quantum-powered breakthroughs in industries that shape our future.

— **Culture of growth :** Enjoy a collaborative and inclusive environment that values creativity and supports your professional development.

— **Competitive package :** Attractive salary, benefits, and opportunities for career growth.

— **Collaboration at its best :** Work in a supportive, inspiring, and inclusive team environment.

— **Flexible setup :** Benefit from hybrid work options and a balance between autonomy and teamwork.

The PhD student will be based in Paris, at ColibrITD's premises in Le Village by CA. Regular travel to Dijon should also be expected in order to interact with the academic supervisors.

Send your CV and cover letter to `jobs@colibritd.com` with the subject : *CIFRE PhD Thesis – TeleMAQ Project.*

Feel free to include links to your publications, GitHub repositories, or any relevant projects.

Take the leap and join ColibriTD in shaping the quantum future — apply now !

We strongly encourage applications from women and other underrepresented groups in STEM. Our team is committed to diversity and inclusion.

Useful links :

- Website : https://colibritd.com
- Preprint : https://arxiv.org/abs/2410.01130
- MPQP Launch Video : https://youtu.be/IVd10kmSNA0
- GitHub : https://github.com/ColibrITD-SAS/mpqp
- LinkedIn : https://www.linkedin.com/company/colibritd/
- Discord : https://discord.gg/c8dqkWBb
- YouTube : https://www.youtube.com/@ColibriTDQuantumInnovations
- Medium : https://medium.com/@colibrITD

Références

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[4] Marco Cerezo, Andrew Arrasmith, Ryan Babbush, Simon C Benjamin, Suguru Endo, Keisuke Fujii, Jarrod R McClean, Kosuke Mitarai, Xiao Yuan, Lukasz Cincio, et al. Variational quantum algorithms. *Nature Reviews Physics*, 3(9) :625–644, 2021.

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