Frontiers of near-term quantum computing – Program

	Tue August 29	Wed August 30	Thu August 31	Fri, September 1
8:00 - 8:50	Registration and Coffee			
8:50 - 9:00	Opening remarks			
9:00 - 9:50	H.-Y. Huang	I. Tavernelli	A. Montanaro	D. Muñoz-Ramo
9:50 - 10:40	A. Natajaran	S. Economou	S. Gharibian	S. Knecht
10:40 - 11:10	Coffee break			
11:10 - 12:00	R. García-Patrón	F. Tacchino	C. Nirkhe	P. Ollitrault
12:00 - 13:30	Lunch break			Final remarks
13:30 - 14:20	P. Barkoutsos	M. Coudron	S. Endo	
14:20 - 15:10	Z. Holmes	T. Metger	C. Gogolin	
15:10 - 15:30	Coffee break			
15:30 - 16:20	A. Izmaylov	J. Bermejo-Vega	X. Yuan	
16:20 - 17:10	J. Kottmann	B. Brown	B. Koczor	
17:15 -	Lab visit		Poster session	
18:30		Conference dinner for invited speakers		

Titles and Abstracts

Tuesday - 29th of August, 2023

Hsin-Yuan (Robert) Huang, California Institute of Technology **09:00 - 9:50**

Title: The Complexity of NISQ

Abstract:

The recent proliferation of NISQ devices has made it imperative to understand their computational power. In this work, we define and study the complexity class NISQ, which is intended to encapsulate problems that can be efficiently solved by a classical computer with access to a NISQ device. To model existing devices, we assume the device can (1) noisily initialize all qubits, (2) apply many noisy quantum gates, and (3) perform a noisy measurement on all qubits. We first give evidence that BPP $\subsetneq$ NISQ $\subsetneq$ BQP, by demonstrating super-polynomial oracle separations among the three classes, based on modifications of Simon's problem. We then consider the power of NISQ for three well-studied problems. For unstructured search, we prove that NISQ cannot achieve a Grover-like quadratic speedup over BPP. For the Bernstein-Vazirani problem, we show that NISQ only needs a number of queries logarithmic in what is required for BPP. Finally, for a quantum state learning problem, we prove that NISQ is exponentially weaker than classical computation with access to noiseless constant-depth quantum circuits.

Anand Natarajan, Massachusetts Institute of Technology **09:50-10:40**

Title: Compiled nonlocal games: from CHSH to BQP verification

Abstract:

We present a step towards the goal of producing a general cryptographic 'compilation' procedure which can translate any entangled nonlocal game into a single-prover interactive protocol while preserving quantum completeness and soundness, using cryptography to simulate the separation between the provers. A candidate for such a procedure was introduced by Kalai et al. (STOC '23), who defined a black-box cryptographic compilation procedure that applies to any nonlocal game and showed that it preserves classical value. In this work, we make progress towards a full understanding of the quantum value of the single-prover protocols that result from applying the Kalai et al. compilation procedure to entangled games. For the special case of CHSH, we prove that the Tsirelson bound holds under the compilation procedure introduced by Kalai et al., and we also recover a strong version of the 'rigidity' property that makes CHSH so useful. As an application, we give a single-prover cryptographically sound classical verification protocol for BQP, and we prove its soundness using our CHSH rigidity analysis. Our protocol replicates the functionality of Mahadev's protocol (FOCS '18) but with two advantages: (1) the protocol is conceptually intuitive and requires fewer bespoke ingredients, and the soundness analysis is simpler and directly follows the analysis of the nonlocal case, and (2) the soundness analysis does not explicitly use the assumption of a TCF or an adaptive hardcore bit, and only requires QFHE as a black box (though currently the only known constructions of QFHE use TCFs). Joint work with Tina Zhang (MIT)

Raúl García-Patrón, University of Edinburgh **11:10 - 12:00**

Title: Benchmarking Quantum Advantage

Abstract:

Whether current and next generation quantum computers solve relevant problems that are unachievable to our traditional devices remains an open problem. A central question is whether the imperfections present in quantum computers can be overcome or they fundamentally restrict quantum computers. In this talk I will present a way of comparing classical algorithms to quantum ones running on near-term quantum devices for a large family of problems that consist of minimizing a cost function, classical or quantum. We will then discuss the capability of current and next-generations quantum computer to solve relevant optimization problems.

Based on joint work with Daniel Stilck Franca: `https://www.nature.com/articles/s41567-021-01356-3`

Panagiotis Barkoutsos, PASQAL **13:30-14:20**

Title: Quantum Scientific Machine Learning as pathway towards practical quantum advantage.

Abstract:

The natural and socioeconomic world is fundamentally governed by conservation laws and rates of change; these systems are mostly modelled by differential equations (DEs). Solving intricate DEs can be computationally challenging due to their scale and complexity. As such, recently novel methodological approaches and computational paradigms have been explored to target them efficiently and accurately. In our work, we combine the efforts made by the classical machine learning community towards Scientific Machine Learning (SciML), i.e. using machine learning to solve and optimize systems governed by DEs, and the recent developments in the field of Quantum Machine Learning (QML), to form Quantum Scientific Machine Learning (QSciML). In the talk we will focus specifically on the advancements of variational quantum algorithms in this direction, including the Differentiable Quantum Circuits paradigm, and present results of their applications in various types of physics and engineering problems towards industrial-scale relevant applications that can become demonstrative examples for practical quantum advantage applications.

Zoë Holmes, EPFL **14:20-15:10**

Title: Hybrid Variational Classical-Quantum Computing: Ingredients to make it work

Abstract:

Parameterized quantum circuits serve as ansätze for solving variational problems and provide a flexible paradigm for programming near-term quantum computers. Here we discuss three fundamental criteria for this paradigm to be effective: expressibility, trainability and generalisability. We will introduce these concepts and present recent analytic progress quantifying to what extent these criteria can be achieved. While more generally applicable, the discussion will be framed around the example of trying to variationally learn an unknown quantum process. We will end with some more open-ended dreaming about the applications of these ideas for experimental quantum physics and quantum compilation.

Artur Izmaylov, University of Toronto **15:30-16:20**

Title: Accelerating quantum measurements in variational quantum algorithms for quantum chemistry

Abstract:

Obtaining the expectation value of an observable on a quantum computer is a crucial step in the variational quantum algorithms. For complicated observables such as molecular electronic Hamiltonians, a common strategy is to present the observable as a linear combination of measurable fragments. The main problem of this approach is a large number of measurements required for accurate estimation of the observable's expectation value. We consider several partitioning schemes based on grouping of commuting multi-qubit Pauli products and fermionic fragments diagonalizable by orbital rotations. Several optimization techniques minimizing the number of measurements will be discussed and connections with techniques of shadow tomography will be established.

Jakob Kottmann, Augsburg University **16:20-17:10**

Title: Molecular Quantum Circuit Design

Abstract:

We propose a novel approach that leverages unitary coupled-cluster (UCC) principles tailored for quantum computers. In conventional methods like CCSD or UCCSD, the exponential form with a single generator prevents that there is a time-ordering between the independent excitations. However, on quantum processors, operations are applied sequentially, so costly decomposition schemes have to be applied in order to implement standard UCC methods.

Instead of trying to implement the fixed UCC approaches, flexible bottom-up constructions that assemble primitive operations (fermionic excitations) represent a more promising approach on quantum processors. In this work we develop the design principles for such bottom-up approaches, allowing exploration of multiple orbital bases and cost-effective introduction of correlations.

Unlike traditional coupled-clusters, our method allows operations in multiple orbital bases. A key guiding heuristics into the grouping and initialization of the orbital bases is provided by chemical graphs – or valence bond resonance structures. We explicitly demonstrate initial methodologies on several benchmark systems highlighting the advantages compared to standard UCC approaches and local bottom-up approaches like the ADAPT protocol.

Our methodologies come in two forms: one aligns with a variational quantum eigensolver, rotating through various orbital bases and introducing correlations before returning to the initial basis. The second mirrors valence bond theory, efficiently computing interactionsbetween resonance structures on the quantum processor, bypassing complex classical computations.

Wednesday - 30th of August, 2023

Ivano Tavernelli, IBM Research Zurich **09:00-09:50**

Title: Quantum algorithms for quantum chemistry and quantum dynamics: a path towards quantum advantage

Abstract:

Quantum computing is emerging as a new paradigm for the solution of a wide class of problems that are not accessible by conventional classical computers. This is particularly true in the domain of many-body physics, and more specifically in quantum chemistry, where quantum computers can contribute to the solution of problems, which are exponentially hard classically. Thanks to the recent developments in quantum technologies, we expect significant contributions to these fields already with the next generation of near-term, noisy quantum computers. To achieve this goal, noise-resilient quantum algorithms together with error mitigation schemes have been proposed and implemented in hybrid quantum-classical workflows. In this talk, we will discuss recent quantum algorithms developments in many-body physics and quantum chemistry aiming at optimizing the quantum resources (number of qubits and circuit depth), focusing in particular on the transcorrelated approach. After a short description of the main algorithmic error mitigation schemes available in Qiskit, we will then present embedding techniques for combining quantum electronic structure algorithms with density functional theory, which enable an efficient partitioning of the problem while preserving a good level of accuracy. The methods will be demonstrated in a series of case studies focusing on the calculation of ground and excited states properties in molecules and solids, as well as on quantum dynamics. Finally, we will assess the quality of the recent hardware calculations on IBM quantum computers and comment on the future of quantum computing for quantum chemistry applications.

Sophia Economou, Virginia Tech **09:50-10:40**

Title: Adaptive quantum simulation algorithms

Abstract:

Variational quantum eigensolvers (VQEs) constitute a class of hybrid quantum-classical simulation algorithms that are envisioned as possibly appropriate for noisy intermediate scale quantum processors. For VQEs to be useful, it is important to reduce the size of the ansatz and the number of required measurements. I will present our work addressing these issues with an ADAPT-VQE, adaptive, problem tailored approach to ansatz construction. I will also discuss recent work showing how the overhead can be lowered in ADAPT-VQE.

Francesco Tacchino, IBM Research Zurich **11:10-12:00**

Title: Qantum machine learning and the natural sciences: technology and applications

Abstract:

Over the last few decades, quantum information processing has emerged as a gateway towards new, powerful approaches to scientific computing. Quantum technologies are nowadays experiencing a rapid development and could lead to effective solutions in different domains including physics, chemistry, and artificial intelligence. In this talk, I will review the state-of-the-art and recent progress in the field, with a focus on quantum machine learning and its applications to problems in the domain of natural sciences. More specifically, I will discuss the use of advanced parametrised quantum circuit models for the generation of molecular force fields and for the analysis of quantum data in high-energy physics. I will also consider the practical implementation of paradigmatic quantum machine learning algorithms on superconducting quantum processors and present dedicated error suppression strategies based on pulse-efficient gate transpilation.

Matthew Coudron, University of Maryland & NIST **13:30-14:20**

Title: Quasi-polynomial time approximation of output probabilities of geometrically-local, shallow quantum circuits.

Abstract:

We present a classical algorithm that, for any geometrically-local, constant-depth quantum circuit C, and any bit string $x \in \{0,1\}^n$, can compute the quantity $|\langle 0^n|C|x\rangle|^2$ to within any inverse-polynomial additive error in quasi-polynomial time. It is known that it is #P-hard to compute this same quantity to within 2^{-n^2} additive error [Mov20, KMM21]. The previous best known algorithm for this problem used $O\left(2^{n^{1/3}}\text{poly}(1/\epsilon)\right)$ time to compute probabilities to within additive error ϵ [BGM20]. Notably, the [BGM20] paper included an elegant polynomial time algorithm for the same estimation task with 2D circuits, which makes a novel use of 1D Matrix Product States carefully tailored to the 2D geometry of the circuit in question. Surprisingly, it is not clear that it is possible to extend this use of MPS to address the case of 3D circuits in polynomial time. This raises a natural question as to whether the computational complexity of the 3D problem might be drastically higher than that of the 2D problem. In this work we address this question by exhibiting a quasi-polynomial time algorithm for the 3D case. In order to surpass the technical barriers encountered by previously known techniques we are forced to pursue a novel approach: Constructing a recursive sub-division of the given 3D circuit using carefully designed block-encodings.

Our algorithm has a Divide-and-Conquer structure, demonstrating how to approximate the desired quantity via several instantiations of the same problem type, each involving 3D-local circuits on at most half the number of qubits as the original. This division step is then applied recursively, expressing the original quantity as a weighted sum of smaller and smaller 3D-local quantum circuits. A central technical challenge is to control correlations arising from the entanglement that may exist between the different circuit "pieces" produced this way. We believe that the division step, which makes a novel use of block-encodings, together with an Inclusion-Exclusion style argument to reduce error, may be of interest for future research on constant-depth quantum circuits. Our algorithm for 3D circuits can be extended to constant depth quantum circuits which are geometrically local in K-dimensions for any fixed constant K.

Tony Metger, ETH Zurich **14:20-15:10**

Title: Concentration bounds for quantum states and limitations on the QAOA from polynomial approximations

Abstract:

We prove concentration bounds for the following classes of quantum states:

1. output states of shallow quantum circuits;
2. injective matrix product states;
3. output states of dense Hamiltonian evolution, i.e. states of the form $e^{iH^{(p)}}...e^{iH^{(1)}}|\psi_0\rangle$ for any n-qubit product state $|\psi_0\rangle$, where each $H^{(i)}$ can be any local commuting Hamiltonian satisfying a norm constraint, including dense Hamiltonians with interactions between any qubits.

Our proofs use polynomial approximations to show that these states are close to local operators. This implies that the distribution of the Hamming weight of a computational basis measurement (and of other related observables) concentrates. An example of (iii) are the states produced by the quantum approximate optimisation algorithm (QAOA). Using our concentration results for these states, we show that for a random spin model, the QAOA can only succeed with negligible probability even at super-constant level $p = o(\log \log n)$, assuming a strengthened version of the so-called overlap gap property. This gives the first limitations on the QAOA on dense instances at super-constant level.

Full version: arXiv:2209.02715, joint work with Anurag Anshu.

Juani Bermejo-Vega, University of Granada **15:30-16:20**

Title: Quantum advantages from quantum simulation

Abstract:

Demonstrating quantum advantages in near term quantum devices is a notoriously difficult task. Ongoing efforts try to overcome different limitations of quantum devices without fault-tolerance, such as their limited system size or obstacles towards verification of the outcome of the computation. Proposals that exhibit more reliable quantum advantages for classically hard-to-simulate verifiable problems lack, at the same time, practical applicability. In this talk we will review different approaches to demonstrate quantum advantages inspired from many-body quantum physics. The first of them use entangled quantum resources such as cluster states, which are useful to demonstrate verifiable quantum advantages based on sampling problems. The second probe measurement of many-body quantities such as dynamical structure factors in quantum simulation setups.

Benjamin Brown, IBM Quantum **16:20-17:10**

Title: Encoding a magic state with beyond break-even fidelity

Abstract:

We distill magic states to complete a universal set of fault-tolerant logic gates that is needed for large-scale quantum computing. By encoding better quality input states for our distillation procedure, we can reduce the considerable resource cost of producing magic states. We demonstrate an error-suppressed encoding scheme for a two-qubit input magic state, that we call the CZ state, on an array of superconducting qubits. Using a complete set of projective logical Pauli measurements, that are also tolerant to a single circuit error, we propose a circuit that demonstrates a magic state prepared with infidelity $1.87 \cdot 10^{-2}$. Additionally, the yield of our scheme increases with the use of adaptive circuit elements that are conditioned in real time on mid-circuit measurement outcomes. We find our results are consistent with variations of the experiment, including where we use only post-selection in place of adaptive circuits, and where we interrogate our output state using quantum state tomography on the data qubits of the code. Remarkably, the error-suppressed preparation experiment demonstrates a fidelity exceeding that of the preparation of the same unencoded magic-state on any single pair of physical qubits on the same device.

Thursday - 31st of August, 2023

Ashley Montanaro, University of Bristol/Phasecraft **09:00-09:50**

Title: Accelerating variational quantum Monte Carlo using the variational quantum eigensolver

Abstract:

Variational Monte Carlo (VMC) methods are used to sample classically from distributions corresponding to quantum states which have an efficient classical description. VMC methods are based on performing a number of steps of a Markov chain starting with samples from a simple initial distribution. In this talk I will discuss recent work where we propose replacing this initial distribution with samples produced using a quantum computer, for example using the variational quantum eigensolver (VQE).

We show that, based on the use of initial distributions generated by numerical simulations and by experiments on quantum hardware, convergence to the target distribution can be accelerated compared with classical samples; the energy can be reduced compared with the energy of the state produced by VQE; and VQE states produced by small quantum computers can be used to accelerate large instances of VMC. Quantum-enhanced VMC makes minimal requirements of the quantum computer and offers the prospect of accelerating classical methods using noisy samples from near-term quantum computers which are not yet able to accurately represent ground states of complex quantum systems.

This talk is based on the paper arXiv:2307.07719, which is joint work with Stasja Stanisic.

Sevag Gharibian, Paderborn University **09:50-10:40**

Title: The optimal depth of variational quantum algorithms is QCMA-hard to approximate

Abstract:

Variational Quantum Algorithms (VQAs), such as the Quantum Approximate Optimization Algorithm (QAOA) of [Farhi, Goldstone, Gutmann, 2014], have seen intense study towards near-term applications on quantum hardware. A crucial parameter for VQAs is the depth of the variational "ansatz" used - the smaller the depth, the more amenable the ansatz is to near-term quantum hardware in that it gives the circuit a chance to be fully executed before the system decoheres. In this work, we show that approximating the optimal depth for a given VQA ansatz is intractable. Formally, we show that for any constant $\epsilon > 0$, it is QCMA-hard to approximate the optimal depth of a VQA ansatz within multiplicative factor $N^{(1-\epsilon)}$, for N denoting the encoding size of the VQA instance. (Here, Quantum Classical Merlin-Arthur (QCMA) is a quantum generalization of NP.) We then show that this hardness persists in the even "simpler" QAOA-type settings. To our knowledge, this yields the first natural QCMA-hard-to-approximate problems.

Joint work with Lennart Bittel (HHU Dusseldorf → FU Berlin) and Martin Kliesch (HHU Dusseldorf → Hamburg University of Technology).

Chinmay Nirkhe – IBM Research **11:10-12:00**

Title: Making the leap to Quantum PCPs

Abstract:

Last year, Anshu, Breuckmann, and I published a proof of the NLTS conjecture based on recent developments in quantum error-correcting codes. That result demonstrates the existence of robust entanglement even at low temperatures. Our motivation for studying NLTS was that it is a necessary precursor for the quantum PCP conjecture.

In this talk, I'll speak about why our first construction of NLTS is based on codes and what I believe are the appropriate next questions to tackle for the quantum PCP conjecture. I'll discuss the connections of these questions to other interesting problems in quantum complexity theory.

This talk will be math-light and intuition-heavy with a particular emphasis on identifying key challenges.

Suguru Endo, NTT Japan **13:30-14:20**

Title: Quantum error mitigation for fault-tolerant quantum computing

Abstract:

Quantum error mitigation (QEM) is a class of hardware-friendly error suppression techniques for improving computation accuracy in quantum computing. While QEM has been proposed mainly for NISQ computing, the benefits for fault-tolerant quantum computing (FTQC) have been recently pointed out. In this talk, we report that applying QEM for FTQC can dramatically reduce the resource overhead, e.g., the code distances. Also, we show the general method for performing quantum error detection "virtually" through a QEM manner, which can be performed with significantly lower overheads. We also discuss the applications for bosonic codes.

Christian Gogolin, Covestro **14:20-15:10**

Title: Preserving quantum numbers and reducing measurement counts in simulations of chemistry

Abstract:

In this talk I will give an overview of quantum computing research activities at Covestro and then discuss two contributions in more detail. The first is a proposal for how to construct variational state preparation circuits by applying a small set of physically motivated gate elements in a repeating pattern that has low connectivity requirements such that the chemically relevant quantum numbers under the Jordan Wigner mapping are preserved. In the second I will discuss how a doble factorization technique leveraging the 8-fold symmetry and sparsity of the two electron integrals entering electronic structure Hamiltonians can be used to drastically reduce the measurement count needed in VQE type experiments when compared to Pauli grouping based approaches (at the expense of an only linear overhead in circuit depth) as well as reduce the runtime of fault tolerant qubitization schemes.

Xiao Yuan, CFCS, Peking University **15:30-16:20**

Title: Quantum algorithms for near-term quantum hardware

Abstract:

Quantum computer could solve classically intractable problems. While since realizing a universal quantum computer is challenging with current technology, a more practical question before having a fully-fledged quantum computer is what we can do with current and near-term quantum hardware. Focusing on the noisy-intermediate-scaled-quantum regime, we introduce variational quantum algorithms for solving static and dynamic problems of many-body physics. Considering the limitations on the qubits number and circuit depth, we introduce the hybrid tensor network and perturbative quantum simulation methods that allow us to solve practical large problems. With the rapid development of quantum hardware, variational quantum algorithms may finally enable genuine quantum advantage demonstration in the noisy-intermediate-scaled quantum era.

Bálint Koczor, University of Oxford **16:20-17:10**

Title: Will (near-term) quantum computers deliver real advantage?

Abstract:

Quantum computers are becoming a reality and current generations of machines are already well beyond the 50-qubit frontier. However, hardware imperfections still overwhelm these devices and it is generally believed the fault-tolerant, error-corrected systems will not be within reach in the near term: a single logical qubit needs to be encoded into potentially thousands of physical qubits which is prohibitive.

Due to limited resources, in the near term, we need to resort to quantum error mitigation techniques. I will explain the basic concepts and then discuss breakthrough results on exponentially effective error mitigation [PRX 11, 031057 (2021)], including an architecture of multiple quantum processors that perform the same quantum computation in parallel [PR Applied 18, 044064 (2022)]; using their outputs to verify each other results in an exponential suppression of errors.

I will then explain that hybrid quantum-classical protocols are the most promising candidates for achieving early quantum advantage. These have the potential to solve real-world problems—including optimisation or ground-state search—but they suffer from a large number of circuit repetitions required to extract information from the quantum state. I will explain recent breakthroughs as hybrid quantum algorithms that exploit extremely powerful classical shadows in order to extract and post-process a large amount of information from the quantum computer [PRX 12, 041022 (2022)] and [arXiv:2212.11036]. I will finally identify the most likely areas where quantum computers may deliver a true advantage in the near term.

Friday - 1st of September, 2023

David Muñoz Ramo, Quantinuum **09:00-09:50**

Title: Quantum chemistry simulations on ion trap quantum computers: experiments with Green's functions and bayesian quantum phase estimation

Abstract:

Enabling the use of quantum computers for quantum chemistry simulations is a hard task that requires developments both in hardware capabilities and new algorithms, in order to tackle a variety of issues still preventing the widespread use of this technology. In this talk, I present some advances in quantum algorithms for chemistry problems developed in my group this year and their implementation on Quantinuum's H1-1 ion trap quantum computer.

First, I'll present a new quantum computational method to calculate the many-body Green's function matrix in a spin orbital basis. Our approach involves a cumulant expansion of the Lanczos method, using Hamiltonian moments as measurable expectation values. This bypasses the need for a large overhead in the number of measurements due to repeated applications of the variational quantum eigensolver (VQE), as seen in other implementations. We apply our approach to finite-sized fermionic Hubbard models and related impurity models within Dynamical Mean Field Theory, and demonstrate the calculation of Green's functions on the H1-1 device. Next, I'll show our results at implementing the Quantum Phase Estimation (QPE) algorithm on the H1-1 device. We employ a Bayesian approach to QPE and introduce a routine for efficient parameter selection, which we combine with the [[n+2, n, 2]] quantum error detection code carefully tailored to the capabilities of our hardware. We demonstrate this protocol with the calculation of the ground state energy of a 2-qubit model of the hydrogen molecule. For this experiment, we run quantum circuits containing as many as 920 two-qubit gates to estimate the hydrogen ground state energy within 0.006(7) Hartree of the exact value.

Stefan Knecht, Algorithmiq and ETH Zurich **09:50-10:40**

Title: Ground and excited states: pushing forward a frontier of computational chemistry on quantum computers

Abstract:

In the past years, the capability of near-term quantum computers to address the electronic structure problem for chemical systems has been successfully demonstrated for toy-model systems such as, for example, N_2, H_2O, and hydrogen chains $H_n (n \leq 12)$.Hence, surpassing the limited availability, reliability and capacity of current quantum hardware still poses a major challenge to date and calls for the development of efficiently scaling (embedded) quantum algorithms to treat systems of real chemical relevance, both in their electronic ground and excited states.To this end, we present in this contribution the Variational Quantum Eigensolver (VQE)combined with the self-consistent field (SCF) approach to orbital optimization[1]. Moreover, the chemistry of excited states is often governed by electron-electron correlations which necessitate to consider not only static but also dynamical correlation contributions. We address these challenges by making use of a distinct framework for VQE-SCF that can be classified as diagonalise-then-perturb.[2] Finally, fermion-to-qubitmappings are used to represent fermionic modes on quantum computers, an essential first step in many quantum algorithms for electronic structure calculations. We present formalism to design flexible fermion-to-qubit mappings from ternary trees and intuitively discuss the connection between the structure of the generating trees and certain properties of the resulting mapping, such as the Pauli weight and the delocalization of mode occupation.[3]

[1] A. Fitzpatrick, A. Nykänen, N. W. Talarico, A. Lunghi, S. Maniscalco, G. García-Pérez,and S. Knecht, arXiv:2212.11405, 2022.

[2] W. Talarico, A. Fitzpatrick, R. di Remigio Eikås, G. García-Pérez, and S. Knecht,manuscript in preparation, 2023.

[3] A. Miller, Z. Zimborás, S. Knecht, S. Maniscalco, and G. García-Pérez, PRX Quantum,4, 030314 (2023).

Pauline Ollitrault, QC Ware Paris **11:10-12:00**

Title: Quantum computing study of P450nor catalyzed NO reduction

Abstract:

In this talk I will present our very recent work on the NO reduction reaction mechanism catalyzed by the enzyme P450 nitric oxide reductase. This reaction is an important step of the denitrification process in which secondary sphere effects were shown to play an important part. We present an end-to-end scheme to calculate electrostatic interactions in several key states of the reaction mechanism. Our implementation relies on the quantum computing version of the SAPT algorithm and includes fast geometry optimization with Promethium as well as the preparation of the strongly correlated monomer's wavefunction on an AQT ion-trap quantum computer.