Annual Report (PhD Student)

University of Genoa, Italy

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Training Activities:

Course / Topic	Instructor	Institute	Dated
Italian Language and Culture	Prof. Silvano Tosi	Dep of Physics, UniGe	Mar 2025 ~ June 2025
Imprecise Probabilistic Machine Learning (IPML)	Prof. Krikamol Muandet	CISPA Helmholtz Center for Information Security, Germany	Nov 2025 ~ Jan 2026
Research Project			
Practical Hands-on Related Software including python			
Practical Hands-on Related Software including Latex/Overleaf			

Other Training Activities:

Course / Topic	Role/ Participation	Institute/By/Tool	From-to
50th Intl. Nathiagali Summer College on Physics and Contemporary Needs	Speaker/Participant	National Centre for Physics, Islamabad, Pakistan	June 2025-June 2025
IBM–UNITO Innovation Lab on Future Computing Technologies	Participant	Department of Computer Science, UniTo, Italy	October 2025-October 2025

Publications

Title	Journal/Publisher	Year
Resource reduction for variational quantum algorithms by non-demolition measurements arXiv:2503.24090	The European Physical Journal D (EPJ D)/Springer Nature	2025

Research Project

1. Introduction- Hybrid Quantum-Classical Optimization and the Role of QNDM

Complex physical system simulations and huge linear algebra calculations that are beyond the capabilities of classical computers can be solved with the aid of quantum computers. Although today's quantum devices are noisy and limited in size, hybrid quantum-classical algorithms like QAOA and VQE make quantum observations practical by combining them with classical optimization. These techniques involve a quantum circuit evaluating a cost function and a classical processor updating the circuit parameters in response to the results of the measurements. However, this procedure becomes costly due to the need for numerous circuit evaluations to compute gradients accurately, due to noisy hardware and restricted qubit counts. Many significant applications, including drug design, molecular simulation, and material discovery, rely on solving such optimization problems, which aim to determine the minimum of a cost function. The typical Direct Measurement (DM) approach calculates gradients by assessing the circuit at two close parameter values for each parameter, which is slow and resource-intensive. The process is further complicated by the lack of a single preferred measuring approach because derivatives cannot be associated with a simple Hermitian operator. The Quantum Non-Demolition Measurement (QNDM) approach, which connects a quantum detector to the system so that the detector phase contains information about the observable and its gradient, is one way to overcome these constraints. As a result, the gradient can be taken from a single measurement instead of several measurements. Both theoretical and numerical results demonstrate that QNDM offers significant resource savings even for moderately complex systems when DM and QNDM are compared in terms of statistical error, circuit repetitions, and total computational cost. Even greater benefits are anticipated for realistic problems of intermediate size where resource efficiency is crucial.

2. Comparison of Direct Measurement (DM) and Quantum Non-Demolition Measurement (QNDM) Approaches

This work compares two methods to determine a quantum system's lowest energy state: Direct Measurement **(DM)** and Quantum Non-Demolition Measurement **(QNDM)**. In variational quantum algorithms, both methods are used to improve molecular simulations, such as those for lithium-hydrogen (Li-H), Hydrogen (H_2), and lithium-lithium (Li_2) molecules. While **DM** has been a widely studied algorithm in the quantum optimization literature, **QNDM** provides a new computing strategy that leverages higher derivatives in a single run of a quantum circuit to reduce the computing resources required.

DM computes the cost function and its gradient by querying specific elements of the Hamiltonian. Quantum circuits are executed in **DM** to obtain the expectation values and the parameter shifts, after which the parameter-shift rule is used to compute the gradient. It requires different measurements for each parameter, leading to a more computationally hefty approach as the circuit grows more complex, especially in highly qubit-limited systems or where high-accuracy results are desired.

The unique feature of Quantum Non-Demolition Measurement **(QNDM)** is that the quantum detector is coupled to the system; thus, you can obtain information about the phase derivative of the observable, and it will be performed during the measurements.

This approach provides access to both the gradient and all higher-order derivatives directly from a single run of a single circuit, thereby reducing the number of repetitions we need to perform.

QNDM is helpful in optimization algorithms, like gradient descent, because it speeds up convergence by skipping the need for extra measurements for each gradient calculation.

3. Methodology

The **QNDM** method connects a quantum system with a quantum detector, which gathers information about the observable gradient in its phase during a system-detector interaction. This happens through a few key steps:

1. **System-Detector Coupling:** The quantum system evolves under a unitary operator based on Hamiltonian parameters. While they interact, the system state is "frozen," allowing the detector's phase to store information about the desired derivative of the observable.
2. **Detector Measurement:** The quasi-characteristics function, which shows the accumulated phase of the detector, gives us the gradient of the cost function with less computational demands.
3. **Implementation with Qiskit for Molecule Optimization:** For practical use, the **QNDM** method was tested on molecular systems, including Lithium-Hydrogen (Li-H), Hydrogen (H_2), and Lithium-Lithium (Li_2), through **Qiskit**. The process includes:
    i. **Constructing the Hamiltonian:** The Hamiltonian becomes a sparse Pauli operator, prepared for the quantum states of Li-H, H_2, and Li_2 molecules.
    ii. **Quantum Circuit Setup:** Layered parameterized quantum circuits are built using rotation and entangling gates, optimized by **QNDM**.
    iii. **Gradient Calculation and Optimization: QNDM** calculates gradients effectively to iteratively lower the Hamiltonian energy, the molecule's ground-state energy.

This approach was compared with the Direct Measurement **(DM)** technique, showing that **QNDM** can reach similar accuracy but needs less circuit depth and fewer measurements, highlighting its practical implementation in optimizing quantum tasks.

4. Accuracy and Statistical Behavior Across All Molecules

Both the DM and QNDM approaches reached the same minimum energy for each of the three molecules (H_2, Li-H, and Li_2), demonstrating their similar accuracy in calculating ground-state energies. Both approaches performed comparably in the simplest system, H_2, but as the circuit size grew, QNDM already demonstrated less uncertainty and smoother convergence. For the more complex Li-H, QNDM demonstrated more steady convergence across various starting parameters and used roughly 79% fewer resources while maintaining the same level of accuracy as DM. In the largest system, Li_2, QNDM demonstrated less statistical fluctuations and used about 71% fewer logical operations while still matching the final energy determined by DM. Overall, the results from all three molecules demonstrate that QNDM offers faster, smoother, and more resource-efficient convergence while maintaining accuracy, particularly as molecular complexity increases.

5. The Large Hamiltonian

To evaluate the behavior of the DM and QNDM approaches on larger and more complex systems, we tested them on Hamiltonians with a high number of Pauli terms ($J = 750$) and ($J = 1000$), while keeping the system size fixed at ($n = 10$) qubits. With this configuration, we could raise the Hamiltonian complexity without adding more qubits, which made it simpler to examine the scaling of both approaches. The two approaches achieved comparable minimum energies in both situations, demonstrating that they are still accurate even for huge Hamiltonians. In contrast to DM, QNDM required far fewer logical operations and converged more smoothly. These findings demonstrate that QNDM scales more effectively than DM and maintains its efficacy even at very large Hamiltonian sizes.

Dated: 27/11/2025