# Marco Polo Scientific Report - Simone Gasperini

Application of Quantum Computing technology to High-Energy Physics: Quantum Annealing for Distributions Unfolding at the Large Hadron Collider (CERN)

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Quantum Computing is emerging as a promising technology that High-Energy Physics (HEP) experiments could adopt to possibly achieve better performance in some specific types of tasks (e.g. sampling, searching, tracking, optimization problems, Machine/Deep Learning) [1]. The first generation of real Noisy Intermediate-Scale Quantum (NISQ) computers is already available on the market for research purposes, raising the interest of HEP communities. The quantum hardware capable of hosting large-scale applications is expected in the next few years and it will gradually achieve the stability to run quantum algorithms effectively, overcoming problems lying for instance in the computational complexity of traditional classical algorithms.

CERN Openlab started in 2020 the so-called Quantum Technology Initiative (QTI) program, opening many discussions about this new research front with representatives of the CERN Member States, the Worldwide LHC Computing Grid, the HEP Software Foundation, and many external industrial partners such as IBM Quantum and, more recently, IonQ [2, 3, 4].

In this context, my research activity at CERN was based on the investigation of the actual potential of these new quantum technologies, from the identification of possible HEP use-cases to the design of quantum or hybrid quantum-classical algorithms. In particular, thanks to my applied physics background and the skills developed in the scientific computing domain, I have been working on the mathematical formulation and the practical implementation of a quantum-based approach to tackle the so-called *distributions unfolding* problem in HEP [5].

## 1 From classical to quantum unfolding

In HEP experiments, each measurement apparatus exhibit a unique signature in terms of detection efficiency, resolution, and geometric acceptance. The overall effect is that the distribution of each observable measured in a given physical process could be smeared and biased. Unfolding is the statistical technique employed to correct for this distortion and restore the original distribution. This process is essential to make effective comparisons between the outcomes obtained from different experiments (e.g. detectors operating at the LHC) and the theoretical predictions (e.g. Standard Model theory). Several classical methods have been proposed to solve the unfolding problem: the most common algorithms practically used within the HEP community are the Iterative Bayesian Unfolding (IBU) and the Singular Values Decomposition (SVD) unfolding [6, 7]. However, a new method based on Quantum Computing could represent an enticing opportunity to enhance the unfolding performance and potentially yield more accurate results. The quantum approach originates from the idea of reformulating the unfolding problem in a combinatorial optimization setting: in particular, starting from the regularized log-likelihood minimization formulation of the unfolding, it's possible to translate it into a Quantum Unconstrained Binary Optimization (QUBO) problem, known to be addressable by quantum algorithms.

## 2 D-Wave Quantum Annealing

Quantum annealing is a computational technique that leverages principles from quantum mechanics to naturally solve optimization problems written in the QUBO form. In general, optimization problems involve finding the best solution in a large set of possible variables configurations: in classical computing, these problems can become unattainable as their size increases. Quantum annealing aims to address this challenge by exploiting quantum superposition to efficiently explore the exponentially-large space of possible solutions. During the annealing process, the system starts in a simple, well known quantum state, and external parameters are gradually varied, guiding the system towards the lowest-energy configuration corresponding to the optimal solution of the QUBO problem. Quantum tunneling effects also play a role in allowing the system to overcome energy barriers that may impede classical optimization methods.

Together with few colleagues from the University of Bologna and INFN based at CERN, I worked on the design, implementation, and validation of *QUnfold*, an open-source Python project based on following workflow [8]:

1. take a regularized unfolding problem instance as input (measured histogram, detector response matrix, regularization parameter);

2. mathematically reformulate the input instance as a QUBO problem (defining the Hamiltonian energy function to be minimized);

3. implement user-friendly features to run the algorithm by heuristic classical solvers as well as physical quantum annealing devices;

4. post-process the result and provide the user with some simple tools to visualize the final unfolded histogram and make comparisons with the classical unfolding methods.

This approach has been validated on a simulated sample of particles collisions data generated combining the Madgraph Monte Carlo event generator and the Delphes simulation software to model the detector response. A variety of fundamental kinematic distributions are unfolded and the results are compared with conventional unfolding algorithms commonly adopted in precision measurements at the LHC, such as the aforementioned IBU and SVD.

The implementation of the QUBO unfolding model relies on the D-Wave Ocean software, which provides all the needed functionalities to run the algorithm by heuristic classical solvers as well as the physical D-Wave Advantage quantum annealer [9, 10].

## 3 IonQ multi-angle QAOA

The Quantum Approximate Optimization Algorithm (QAOA) is a hybrid quantum-classical algorithm designed to solve combinatorial optimization problems by running a variational ansatz circuit on a gate-based quantum device [11]. As in the case of quantum annealing, the basic idea behind QAOA is to use a quantum computer to prepare a quantum state that encodes a potential solution to the QUBO problem. The algorithm then evolves this state through a series of parameterized layers in the circuit, adjusting the parameters to maximize the probability

of obtaining the optimal solution. This process is based on a classical optimization procedure and it is repeated iteratively to enhance the algorithm's performance. In theory, the quality of the output approximate solution improves increasing the number of layers but noise and circuit complexity undermine the performance in practice.

Multi-angle ansatz for QAOA reduces the circuit depth and improves the approximation ratio by increasing the number of classical parameters. Even though the number of parameters to optimize is larger, good parameters values can be found in polynomial time. Moreover, for practical applications, the multi-angle QAOA has been shown to require a shallower circuit than the standard QAOA, making it more viable for NISQ devices available nowadays [12].

CERN just started a research collaboration with the IonQ company, specialized in trapped-ions quantum computing and providing an optimization platform to run the multi-angle QAOA for any given QUBO problem. Under the supervision of the QTI group during my period at CERN, I had the possibility to present the unfolding problem to the IonQ team and we started collaborating to solve some test-case unfolding problem instances running the multi-angle QAOA on their simulator. More work is in progress to analyze the first results and possibly run the algorithm on their real trapped-ions quantum computers as well.

The following step would be to compare this QAOA-oriented approach, tailored for a gate-based quantum architecture, with the quantum annealing solver, starting from the same QUBO formulation of the unfolding problem.

## References


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