Data Profiling and Benchmarking of Hybrid Quantum-Classical Computational Workflows

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2 Context and Overview

The evolution of application requirements in modern computing is pushing the need to integrate a diverse portfolio of services for high-performance computing (HPC), artificial intelligence (AI), cloud computing and other large-scale computing environments and their associated data [BDF+20, MDM+21]. Looking ahead, key players in cutting-edge technologies are making strong investments and long-term strategic decisions about how the future landscape of distributed computing and supercomputing infrastructures might look like [Des22]. In the European environment, quantum computing (QC) is receiving major funding support through the EU Quantum Flagship project [Qua24] to produce computational technologies that could be integrated into HPC environments once they reach sufficient maturity. To that end, the EuroHPC Joint Undertaking [Eur24a] is working towards integrating quantum systems into European supercomputers like Joliot-Curie at GENCI (France) [Eur24b]. These developments are the first steps towards a pan-European quantum-HPC infrastructure to integrate extreme scale computing and data driven technologies with emerging computing paradigms.

The successful interoperability between classical and quantum systems will depend on middleware able to interact with heterogeneous hardware technologies (e.g., CPU, GPU, TPU, FPGA, QPU) and their associated software stacks and data management methods. Furthermore, immediate approaches towards leveraging quantum computing are hybrid and involve interaction with classical systems [BBB+24]. This leads to complex open challenges on how to combine multiple programming models in a single application with workflow steps combining quantum and classical processing in a domain-agnostic manner. Current works on the integration of QC into classical computing ecosystems focus on the interoperability and performance of the algorithms without considering data-oriented optimizations (e.g., data encoding, arrangement, locality, or mapping to high-level data abstractions), and workflow-specific challenges like task-resource mapping are rarely explored [WBLV22].

3 Research Objectives and Envisioned Approach

This project has the overarching goal of paving the way towards researching novel data interfaces for hybrid quantum-classical workflows able to reconcile quantum and classical data representations.

Specifically, we will build on our active collaboration with the Technical University of Vienna (TUW) to study the data structures and patterns in existing software tools for interacting with quantum devices.

We will focus on the most realistically feasible approach to near-term hybrid systems: loosely-coupled integration of the classical and quantum devices through classical computing networks. Cloud access platforms like Orquestra [Zap24] and Covalent on IBM Quantum [Agn24]) are examples of programming frameworks for these loosely-coupled hybrid systems. Although these solutions provide the possibility to offload computation to quantum systems, they do not have data models suitable for high-level hybrid programming. First, we will study their low-level data structures. Then, we will profile and characterise their data access and transfer patterns in small scenarios of variational quantum algorithms [CAB+21], starting from a use case in molecular dynamics workflows. Finally, we will explore the formalisation of a data-oriented benchmark for hybrid quantum-classical workflows covering aspects of data encoding, arrangement, locality, and mapping to high-level data abstractions with the goal of facilitating the assessment of the diverse data representations, volumes and processing rates in existing software.

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