

HYBRID QUANTUM-CLASSICAL WORKFLOWS IN MODULAR SUPERCOMPUTING ARCHITECTURES WITH THE JÜLICH UNIFIED INFRASTRUCTURE FOR QUANTUM COMPUTING

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ABSTRACT

The implementation of scalable processing workflows is essential to improve the access to and analysis of the vast amount of high-resolution and multi-source Remote Sensing (RS) data and to provide decision-makers with timely and valuable information. The Modular Supercomputing Architecture (MSA) systems that are operated by the Jülich Supercomputing Centre (JSC) are a concrete solution for data-intensive RS applications that rely on big data storage and processing capabilities. To meet the requirements of applications with more complex computational tasks, JSC plans to connect the High Performance Computing (HPC) systems of its MSA environment to different quantum computers via the Jülich UNified Infrastructure for Quantum computing (JUNIQ). The paper describes this unique computing environment and highlights its potential to address real RS application scenarios through high-performance and hybrid quantum-classical processing workflows.

Index Terms— Quantum computing, hybrid quantum-classical computing, quantum annealing, modular supercomputing architecture, high performance computing, remote sensing.

1. INTRODUCTION

There is an increasing number of applications that can benefit and advance from the improved availability of data acquired by heterogeneous RS sensors. Nonetheless, planetary-scale applications, space-based observations and deep space missions are further increasing the complexity of RS data and its processing [1], thus requiring high computational power and data storage capabilities. Therefore, it is paramount to develop processing workflows based on parallel algorithms that

can scale on heterogeneous and HPC technologies. These are requirements that make necessary the use of innovative computational approaches, from HPC platforms such as clusters or clouds to hardware accelerators such as Graphics Processing Units (GPUs) or Field-Programmable Gate Arrays (FPGAs) or novel Quantum Processing Units (QPUs) solutions, among others.

In the context of Quantum Computing (QC), there is a growing interest in using Quantum Machine Learning (QML) to improve upon classical Machine Learning (ML) algorithms [2]. QC was already leveraged to enhance Support Vector Machines (SVMs) for handwriting recognition [3], to speed up the prediction performance of fully connected Boltzmann machines [4], to classify data obtained from biology experiments [5], to enhance the compression and generation of images with Quantum Variational AutoEncoders (QVAE) [6] and to develop a quantum version of a Convolutional Neural Network (CNN) for image recognition [7].

In the field of RS there are particular applications of QC that were developed recently. For example in [8, 9, 10, 11, 12] QML algorithms such as the SVM and neural networks were applied for classifying multispectral and hyperspectral images. In [13], the authors proposed quantum-assisted ML approaches to register MODIS images and in [14] a quantum-based approach for compressive sensing was proposed. In the context of Synthetic-Aperture Radar (SAR) processing, in [15] an alternative QML classifier was presented and in [16] a quantum approach for phase-unwrapping was implemented.

One disadvantage that is shared among all these methods is that they are still limited to small-scale applications. The main reason is that the current state of quantum processors have limited qubit capacity. QC devices cannot, yet, process large datasets and deliver the computational speedups associated with fully fledged universal quantum computers (i.e., today's devices are known as noisy intermediate-scale quantum computers (NISQ)[17]). Nevertheless, existing quantum algorithms are usually implemented within cloud computing

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services that offer very limited storage and processing capabilities (e.g., D-Wave Leap, IBM Quantum Experience, etc.). These hybrid classical-quantum environments do not leverage the HPC capabilities of conventional hardware accelerators (e.g., GPUs) or state-of-the-art HPC systems.

The MSA systems of the JSC represent a concrete solution that can tackle the challenges posed by large-scale RS applications. The MSA is a system that can fulfill the requirements of both simulation and data analytics applications, enabling additionally large dense memory extension modules close to the processors, as well as novel QC technologies via the JUNIQ¹.

This paper offers insights into this unique computing environment, which is based on the synergy between MSA and JUNIQ. While the classical HPC systems of the MSA can satisfy the demands of data-intensive RS applications (e.g., based on Deep Learning (DL) algorithms), quantum computers can be used as accelerators for carrying out selected computing tasks. The combination of MSA and JUNIQ provides fertile ground for the development of high-performance and hybrid quantum-classical processing workflows that can exploit the flexibility of the MSA system by selecting the right mix of computing resources and assigning each processing task to be run on an exactly matching computing platform.

2. MODULAR SUPERCOMPUTING ARCHITECTURE

A MSA is a computing environment that integrates heterogeneous HPC systems, which can include different types of accelerators (GPUs, FPGAs) and cutting-edge computing technologies (e.g., quantum and neuromorphic computing) and that is “modularized” by its software stack. The MSA achieves global heterogeneity by interlinking the different modules, allowing for a dynamic allocation of calculation resources from different modules for a given program or workflow [18]. It was pioneered through the series of EU-funded DEEP projects² coordinated by the JSC. As Fig. 1 shows, the MSA is based on a modular design that connects different computing modules with distinct hardware and performance characteristics. While each module is a parallel clustered system (of potentially large sizes), a high-performance federated network connects the module-specific interconnects. This creates a single high-performance heterogeneous system seamlessly integrating a multi-tier storage system.

With the MSA, users can take advantage of the HPC systems that best suit their needs [19]. Users with low/medium-scalable codes can benefit from a general purpose cluster mainly consisting of CPUs (i.e., cluster module). Other users with highly scalable codes (e.g., training of DL models) and

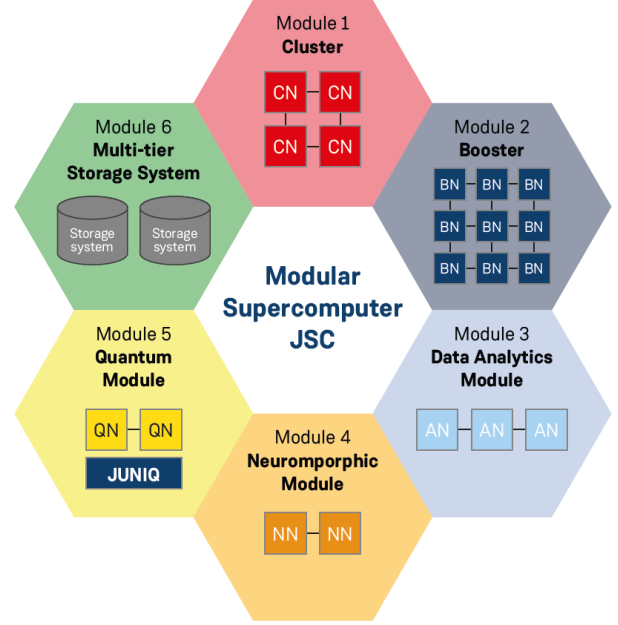


Fig. 1: The MSA connects compute modules with different hardware and performance characteristics to create a single high-performance heterogeneous system.

more regular communication patterns can profit from a massively parallel and scalable HPC system consisting of mainly GPUs (i.e., booster module). Furthermore, users with more complex processing workflows can benefit from some characteristics of both of these two architecture elements. They can take advantage of the above mentioned classical architectures (i.e., general purpose cluster vs. highly scalable booster) in combination with innovative computing architectures such as those specifically designed for data analytics (i.e., with large memory), quantum computing, or neuromorphic computing.

JSC has already implemented the MSA in its large-scale production systems, such as the JURECA [20] and JUWELS [21] systems. According to the November 2021 Top500 list³, JUWELS is currently the fastest supercomputer in Europe and 8th fastest worldwide, and has two modules: cluster and booster. The cluster module provides general purpose computational resources with more than 2300 compute nodes. The booster is the highly scalable module of the system, leveraging GPUs to provide computing performance. Both modules are combined through their network fabric and file system, and can be used at the same time by heterogeneous computing tasks through a tight integration via the workload manager.

3. JUNIQ

JSC is researching advanced computing architectures such as quantum computers, quantum simulators, quantum annealers,

¹JUNIQ - Jülich UNified Infrastructure for Quantum computing, https://www.fz-juelich.de/ias/jsc/EN/Expertise/JUNIQ/_node.html

²<https://www.deep-projects.eu/>

³<https://www.top500.org/>

digital annealers and neuromorphic computers. JSC is currently focusing on the integration of quantum computing systems into its MSA environment through JUNIQ (see Fig. 2).

JUNIQ is a manufacturer-independent quantum computing user facility, which provides European users from academia and industry access and support to various types of quantum computer emulators and quantum computing technologies with different levels of technological maturity.

JUNIQ hosts and operates a D-Wave AdvantageTM quantum system with more than 5000 qubits. By the end of next year it will host also a quantum simulator with more than 100 qubits and this in the context of the recently funded EuroHPC Joint Undertaking project HPCQS⁴. In addition to these two quantum computers, JUNIQ will provide cloud access to various other quantum computers with different levels of technological maturity (i.e., experimental quantum computing devices from university laboratories and startup companies). The access is portal-based in the form of a Quantum Computer Platform as a Service (QC-PaaS), which uses the modern JupyterHub technology. The latter helps to lower entry barriers for new users and facilitates the re-use of simulation results in line with the European policy of open science and open computing.

JUNIQ will provide a unique, manufacturer-independent variety of quantum computing and hybrid quantum HPC capabilities to researchers across Europe via the cloud on a non-commercial basis and is embedded in JSC's unique service, support, and education infrastructure.

With its mission to provide a manufacturer-independent, comprehensive user infrastructure, JUNIQ develops software tools, algorithms, and prototype applications. With the access to the innovative hardware technologies, computing resources and infrastructures of the JSC, different communities will be able to advance in their research fields.

4. CONCLUSIONS AND OUTLOOK

To efficiently extract interpretable information and knowledge from large amounts of complex and multi-source RS data it is necessary to leverage innovative HPC technologies and create novel software and tools for enhancing the processing and addressing data storage challenges. The MSA environment of the JSC brings substantial benefits for heterogeneous workloads since each processing step can be run on an exactly matching system, improving time to solution and energy use. The MSA is a successful approach to heterogeneous computing that enables the most efficient use of computing resources while providing application developers with all necessary tools to take the step from Petascale to emerging Exascale computing.

In this context, the strategy of JSC is not to replace classical HPC systems but rather augment them (i.e., like

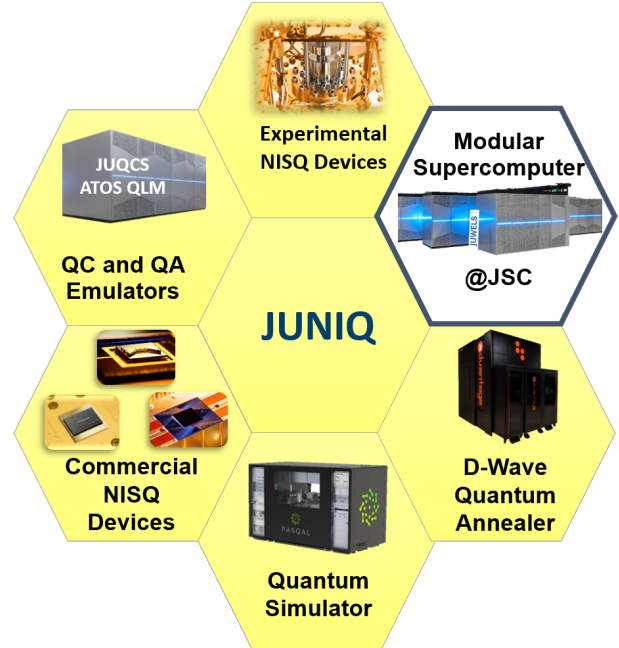


Fig. 2: JUNIQ: Unified portal for cloud access to quantum computer emulators and to different types of quantum computers with different levels of technological maturity.

GPU accelerators did with CPUs) with innovative computing paradigms for speeding up selected optimization problems. The deep integration of quantum computers in conventional HPC systems is currently the most feasible way to address real RS applications.

5. REFERENCES

- [1] M. Reichstein, G. Camps-Valls, B. Stevens, M. Jung, J. Denzler, N. Carvalhais, and Prabhat, "Deep Learning and Process Understanding for Data-Driven Earth System Science," *Nature*, vol. 566, no. 7743, pp. 195–204, 2019.
- [2] J. Biamonte, P. Wittek, N. Pancotti, P. Rebentrost, N. Wiebe, and S. Lloyd, "Quantum Machine Learning," *Nature*, vol. 549, no. 7671, pp. 195–202, 2017.
- [3] P. Rebentrost, M. Mohseni, and S. Lloyd, "Quantum Support Vector Machine for Big Data Classification," *Physical Review Letters*, vol. 113, no. 13, 2014.
- [4] M. Henderson, J. Novak, and T. Cook, "Leveraging Quantum Annealing for Election Forecasting," *Journal of the Physical Society of Japan*, vol. 88, no. 6, 2019.
- [5] D. Willsch, M. Willsch, H. De Raedt, and K. Michielsen, "Support Vector Machines on the D-Wave Quantum Annealer," *Computer Physics Communications*, vol. 248, pp. 107006, 2020.

⁴www.hpcqs.eu

- [6] J. Sleeman, J. Dorband, and M. Halem, "A Hybrid Quantum Enabled RBM Advantage: Convolutional Autoencoders for Quantum Image Compression and Generative Learning," in *SPIE*, 2020, vol. 11391, pp. 23–38.
- [7] M. Henderson, S. Shakya, S. Pradhan, and T. Cook, "Quantum Neural Networks: Powering Image Recognition with Quantum Circuits," *Quantum Machine Intelligence*, vol. 2, pp. 1–9, 02 2020.
- [8] P. Gawron and S. Lewiński, "Multi-Spectral Image Classification with Quantum Neural Network," in *IEEE IGARSS*, 2020, pp. 3513–3516.
- [9] A. Delilbasic, G. Cavallaro, M. Willsch, F. Melgani, M. Riedel, and K. Michielsen, "Quantum Support Vector Machine Algorithms for Remote Sensing Data Classification," in *IEEE IGARSS*, 2021, pp. 2608–2611.
- [10] S. Otgonbaatar and M. Datcu, "Classification of Remote Sensing Images with Parameterized Quantum Gates," *IEEE GRSL*, 2021.
- [11] S. Otgonbaatar and M. Datcu, "A Quantum Annealer for Subset Feature Selection and the Classification of Hyperspectral Images," *IEEE JSTARS*, vol. 14, pp. 7057–7065, 2021.
- [12] A. Sebastianelli, D. A. Zaidenberg, D. Spiller, B. Le Saux, and S. L. Ullo, "On Circuit-based Hybrid Quantum Neural Networks for Remote Sensing Imagery Classification," *IEEE JSTARS*, pp. 1–1, 2021.
- [13] C. Pelissier, T. Ames, and J. Le Moigne, "Quantum Assisted Image Registration," in *IEEE IGARSS*, 2020, pp. 3696–3699.
- [14] R. Ayanzadeh, M. Halem, and T. Finin, "An Ensemble Approach for Compressive Sensing with Quantum Annealers," in *IEEE IGARSS*, 2020, pp. 3517–3520.
- [15] S. Otgonbaatar and M. Datcu, "Natural Embedding of the Stokes Parameters of Polarimetric Synthetic Aperture Radar Images in a Gate-Based Quantum Computer," *IEEE TGRS*, 2021.
- [16] K. A. H. Kelany, N. Dimopoulos, C. P. J. Adolphs, B. Barabadi, and A. Baniasadi, "Quantum Annealing Approaches to the Phase-Unwrapping Problem in Synthetic-Aperture Radar Imaging," in *IEEE QCE*, 2020, pp. 120–129.
- [17] J. Preskill, "Quantum computing in the NISQ era and beyond," *Quantum*, vol. 2, pp. 79, 2018.
- [18] E. Suarez, N. Eicker, and T. Lippert, *Modular Supercomputing Architecture: from Idea to Production*, vol. 3, pp. 223–251, CRC Press, 2019.
- [19] E. Erlingsson, G. Cavallaro, H. Neukirchen, and M. Riedel, "Scalable Workflows for Remote Sensing Data Processing with the Deep-Est Modular Supercomputing Architecture," in *IEEE IGARSS*, 2019, pp. 5905–5908.
- [20] Jülich Supercomputing Centre, "JURECA: Data Centric and Booster Modules implementing the Modular Supercomputing Architecture at Juelich Supercomputing Centre," *Journal of large-scale research facilities*, vol. 7, no. A132, 2021.
- [21] Jülich Supercomputing Centre, "JUWELS Cluster and Booster: Exascale Pathfinder with Modular Supercomputing Architecture at Juelich Supercomputing Centre," *Journal of large-scale research facilities*, vol. 7, no. A138, 2021.