Report on High Performance and Innovative Computing (HPIC) Workshop

Place: ESA/ESRIN,

Date: October 12th, 2023

https://indico3-jsc.fz-juelich.de/event/135/

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The **Quantum Computing for Earth Observation (QC4EO) initiative**[1], spearheaded by the European Space Agency (ESA), aims to explore the potential synergies between quantum computing and Earth observation (EO). This initiative aims to identify promising use-cases, gather both communities, and prepare for the opportunities that will arise with quantum computing advancements. Quantum computing has the potential to improve performance, decrease computational costs, and solve previously intractable problems in EO by exploiting quantum phenomena.

To further explore the intersection of High-Performance Computing (HPC) and EO, the **HPC and Innovative Computing (HPIC) workshop** was organized. The workshop, held at ESRIN, the ESA center for Earth Observation in Frascati, Italy, on October 12th, 2023, brought together experts from the HPC and EO fields to discuss their interconnections, future prospects, and challenges. The event featured speakers from European HPC centers such as FZ Julich, Cineca, and CSC, as well as representatives from IQM computers, the University of Padova, and ESA. The workshop had 25 attendees in person and an additional 75 participants online.

This report provides a summary of the presentations delivered by the various speakers and the ensuing discussions.

HPC and Quantum Computing: Impact and Future Trends *(Gabriele Cavallaro / FZ Julich - DE)*

In the evolving landscape of High-Performance Computing (HPC) and Earth Observation (EO), a notable shift is occurring as these independent domains are now converging. Historically, EO and HPC operated in “isolation”, but current trends indicate a growing interdependence between the two communities.

Supercomputing, defined by its capacity to solve complex problems beyond the reach of standard computers, is experiencing intensified recognition. The integration of Artificial Intelligence (AI) with HPC is a significant driver, with major industries establishing internal HPCs specifically for AI tasks, particularly large-scale deep learning models. Distributed learning, emphasizing parallel training of deep learning models, is identified as a key concept in this evolving landscape.

Exascale computing, representing the capability to perform a quintillion operations per second, presents a series of challenges. Notably, applications must be adapted to support billions of individual threads, a task still in progress. Energy consumption and efficiency, the gap between compute performance and memory bandwidth, and the need for extensive device communication further complicate the journey to Exascale. JUPITER[2], the first European exascale supercomputer, showcases a solution through its ensemble of hardware configurations.

In response to the challenges of Exascale, the adoption of innovative computing paradigms becomes imperative. The convergence of Quantum Computing and HPC emerges as a promising avenue, offering a unified infrastructure for practical applications. While acknowledging the difficulty in achieving this integration, the recognition of Quantum Computing as a practical tool within the realm of HPC is gaining traction. This unified approach is anticipated to start a new era of computational capabilities.

Quantum Computing in Europe *(Gabriella Bettonte / Cineca – IT)*

EuroHPC[3], the European High Performance Computing Joint Undertaking, has identified six sites within the European Union to host and operate quantum computers. In Italy, CINECA is at the forefront, managing a quantum computer. Given the uncertainty about the superior technology for quantum computers, EuroHPC collaborates with other sites, particularly Spain (for quantum annealers), France (for photonic quantum

[1] https://philab.esa.int/flagship-programmes/qc4eo/
[2] https://www.fz-juelich.de/en/ias/jsc/jupiter
[3] https://eurohpc-ju.europa.eu

computers), and Poland (for trapped-ion-based quantum computers), to explore various solutions simultaneously. CINECA manages Leonardo[4], the fourth most powerful supercomputer globally, aligning with the modular supercomputer concept presented by Gabriele Cavallaro. The ambitious goal is to have 500+ digital/analog quantum computers by 2025. Looking ahead, EuroHPC anticipates deploying at least four quantum computers across Italy and numerous others throughout Europe, positioning the region as a key player in the evolving landscape of quantum computing.

Quantum Computing Platforms *(Jiri Guth Jarkovsky / IQM Computers[5] – DE)*

In modular supercomputers, classical supercomputers are paired with cutting-edge computing devices such as quantum computers. This presentation provided a comprehensive overview of the diverse architectures being investigated today to develop these innovative devices.

Prior to delving into different quantum computing platforms, it is essential to establish the criteria for a quantum computer, as outlined by the Di Vincenzo Criteria for quantum computation. These criteria include the necessity for a scalable physical system with well-characterized qubits, the capability to initialize qubit states to a simple fiducial state, long relevant decoherence times for stability, the presence of a "universal" set of quantum gates, and a qubit-specific measurement capability.

Superconducting Qubits: Superconducting qubits employ small electric circuits with states represented by |0> and |1>. Their operations, state changes, and measurements are realized through microwave/flux pulses. This technology is relatively mature, boasting good gate fidelity and fast gates. However, limitations exist in qubit connectivity due to the circuit structure, and challenges arise in packaging and wiring.

Superconducting Quantum Annealers: These devices rely on adiabatic computation without traditional gates, instead changing the Hamiltonian to solve problems. While achieving high qubit numbers (5000+), there's a tradeoff between speed and quality. They suffer from limited connectivity and are not considered universal quantum computers.

Trapped Ions: In this approach, qubits are ions trapped by an electromagnetic field. Laser-controlled operations, including entanglement, demonstrate excellent gate fidelities. Although offering better connectivity, scalability issues and slower gate operations are challenges.

Cold Atoms: Similar to trapped ions, this method involves trapping atoms with laser lights. Cold atoms exhibit good connectivity and fidelity, allowing for a potentially large number of qubits (100+). However, scalability problems and initialization errors persist.

Photonics: Photonics uses photons as qubits, with various implementations like integrated optics or optical tables. This approach facilitates easier optical network connectivity, featuring a modular architecture with minimal cooling requirements. However, it suffers from significant photon loss, and certain processes require post-selection.

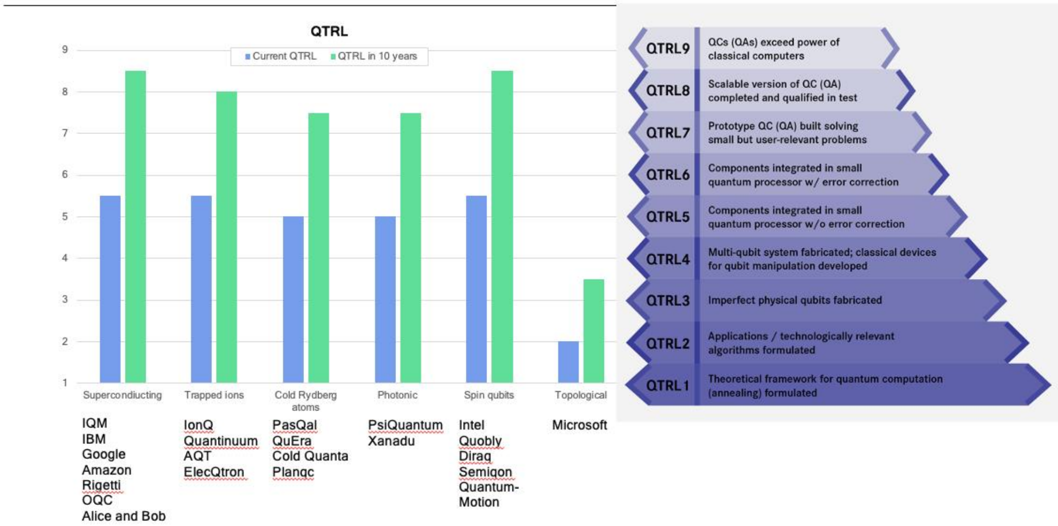
Photonic Boson Sampling: This technology encodes matrices in interferometers, demonstrating quantum supremacy. However, its practical utility requires a hybrid algorithm and is not considered universal.

[4] https://leonardo-supercomputer.cineca.eu/
[5] https://www.meetiqm.com/

Spin Qubits: Spin qubits leverage spins in semiconductor-based quantum dots or NV centers in diamond. With exchange-based gates and a scalable architecture compatible with CMOS, this approach is underdeveloped, featuring low fidelities and qubit numbers.

Topological Qubits: Topological qubits use Majorana zero modes on a topological superconductor. Gates are formed by "braiding" qubits' wordlines, theoretically ensuring stability. However, no acceptable demonstrations have been achieved.

When it comes to evaluating the different technologies in the field, the question arises of how to assess them effectively. This assessment involves considering both hardware and algorithm-oriented metrics. Hardware metrics encompass factors such as the number of qubits, cycle/gate time, gate fidelity, connectivity, scalability, T1/T2 times, and the native gate set. On the other hand, algorithm-oriented metrics focus on logical qubit numbers, logical gate fidelities, quantum volume, CLOPS, Q-score, algorithmic qubits, and the QTRL rating, which draws inspiration from TRL (Technology Readiness Level) for quantum technologies. These metrics provide a comprehensive evaluation across various dimensions, facilitating the comparison and selection of quantum computing platforms.



Quantum devices status and expectation according to Quantum Technology Readiness Level

Climate Digital Twin + Quantum? *(Mikael Johansson / CSC – FI)*

The following presentation tackled a potential application of quantum computing highly relevant for EO: climate modelling.

In the realm of Quantum Computing (QC), it's essential to grasp its distinct nature, not merely as a faster version of classical computing. The future lies in a hybrid fusion of High-Performance Computing (HPC) and Quantum Computing. Climate Digital Twin[6] (ClimateDT), an integral part of the Destination Earth program, aids climate adaptation and decision-making. Crafted by 13 European organizations, it creates precise climate models, incorporating diverse parameters.

ClimateDT, a data-intensive climate information system, explores high-resolution simulations and impact modeling. Its intricate calculations, especially in fluid dynamics, may benefit from quantum computing, enhancing

[6] https://stories.ecmwf.int/destination-earth/index.html#group-section-Digital-Twins-sAJHunyh2a

precision. Observing current ClimateDT workflows reveals the challenge of vast data, hindering direct quantum adoption. Two main hurdles surface: the "big data" issue and the need for rapid, complex problem-solving.

1. "Big Data" Problem: Quantum excels with moderate input and output, requiring a complex equation relationship for efficient quantum algorithm solutions.

2. Time-to-Solution Challenge: Quantum advantage demands solving complex algorithms within on a time-scale of at least seconds, a challenge considering current ClimateDT time-steps.

Taking a broader perspective, quantum acceleration requires innovative approaches. In the medium term, advantages lie in exploring unique quantum features. In the long term, integration of fault-tolerant Quantum Processing Units (QPUs) with classical processing may offer significant advancements.

Machine Learning (ML) and Artificial Intelligence (AI) in climate modeling find a new dimension with Quantum Machine Learning (QML). While classical ML is potent, QML introduces a distinctive approach, potentially achieving more with less training data. Addressing the omission of certain processes due to computational constraints, quantum computing holds promise in reducing complexity, offering a solution for accurate modeling in atmospheric chemistry.

In summary, current digital twins of the climate pose a challenge for quantum acceleration. However, the potential lies in intelligent algorithm use, enhanced machine learning, and introducing missing physics. Preparing workflows for quantum readiness requires a multidisciplinary approach, combining expertise in mathematics, quantum physics, computer science, and the application field. Collaboration between High-Performance Computing and quantum technologies is crucial for identifying bottleneck problems and accelerating classical HPC.

Tensor Network applications to quantum computing *(Ilaria Siloi / University of Padova – IT)*

Ilaria is a staff researcher in the Quantum group led by Prof. Simone Montangero at the University of Padua. The group's effort is mainly dedicated to advancing the field of tensor network simulations as applied to condensed matter problems, quantum computing, and lattice gauge theories. Their flagship project is Quantum Tea[7] a tensor network framework spanning multiple tensor network simulations. This well-established software development initiative has been led by Prof. Montangero's group for over 15 years and it is now available under an open license.

Quantum Tea unfolds into two significant branches: Quantum Green Tea and Quantum Matcha Tea. Quantum Green Tea focuses on the exploration of ground state search and time evolution in many-body quantum systems. On the other hand, Quantum Matcha Tea represents a quantum circuit emulator, and it has been developed in collaboration with CINECA and made accessible to the public. The driving force behind the development of Quantum Matcha Tea lies in the recognized intrinsic difficulties in quantum simulation methods. The team addresses the challenges by developing tensor network (TN) methods relying both on Matrix Product States and Tree Tensor network ansatzes. TNs serve to simulate a large number of qubits while imposing constraints on the order of entanglement. Drawing an analogy to image compression techniques like Singular Value Decomposition (SVD), the tensor network enables the compression of quantum information within the wave function. By controlling the level of entanglement truncation (bond dimension), they achieve a controllable approximation of the quantum wave function. This approach ensures that the simulation of quantum systems is not hindered by an exponential scale based on the number of qubits, but rather progresses polynomially in the bond dimension.

[7] https://www.quantumtea.it/

The efficacy of TN methods is underscored by practical demonstrations where the team successfully simulated circuits comprising over >60 qubits and >10 layers without compromising fidelity. This achievement attests to the scalability and efficiency of their Quantum Matcha Tea approach.

Beyond the realm of quantum computing, the team utilizes Quantum Green Tea to create a digital twin of a Quantum Processing Unit (QPU). This digital twin serves a dual purpose: providing invaluable insights into quantum hardware for QPU development and supporting large-scale simulations that contribute to the evolution of quantum hardware in the coming decades.

The impact of their work extends beyond the quantum realm, as tensor network techniques find application in many different fields such as the solution of optimization problems related to Earth Observation mission planning. This diversification underscores the versatility of their simulations and the potential for broad-ranging contributions across different domains.

Destination Earth – The potential of high-performance computing *(Luca Girardo / ESA)*

Destination Earth[8] (DestinE) is a program leveraging high-performance computing, machine learning, and satellite data to create digital twins offering accurate representations of past, present, and future global changes. Aligned with the European Union's Green Deal and Digital Strategy, DestinE supports informed decision-making for policymakers and users.

The program's objectives include contributing to policy-making by monitoring Earth's system, anticipating environmental disasters, and evaluating sustainable development scenarios. It also aims to assist researchers by providing access to diverse Earth-related data and establishing a science development ecosystem with modern tools, especially machine learning. Additionally, DestinE seeks to engage the general public by facilitating access to Earth-related information to raise awareness about sustainability and environmental crises.

Implementation involves three main branches: Core Service Platform (DESP) by ESA, offering user access; Data Lake (DEDL) by EUMETSAT, managing datasets, including Copernicus data; and Digital Twin Engine (DTE and DTs) by ECMWF, handling complex simulations at high resolution.

The digital twins within DestinE require running intricate simulations, utilizing comprehensive toolkits, accessing diverse data, and managing data at an extreme scale.

Several key questions remain unanswered, such as identifying the need for open access to High-Performance Computing (HPC) for rapid analyses, assessing the strategic advantages of HPC versus cloud implementation, addressing technical and organizational challenges associated with HPC resource access, and exploring the feasibility of implementing 'HPC as a Service' for the public via the cloud.

Roundtable:

High-Performance and Innovative Computing for EO, needs, opportunities and challenges *(All speakers + Claudio Iacopino and Bertrand Le Saux / ESA)*

[8] https://digital-strategy.ec.europa.eu/en/policies/destination-earth

The round table discussion opened with a brief introduction to the panel, highlighting its diversity with representatives from various sectors, including ESA, Science Applications, Climate Department, University of Padova, and supercomputing centers.

The conversation kicks off with an emphasis on exploring the synergy between high-performance computing, supercomputing, and innovative computing within the context of Earth observation needs.

Challenges highlighted by the participants include the scattered nature of data, the complexity of bringing data together for computation, and the ongoing need for optimization in computations. The importance of enhancing production chains and leveraging digital twins for efficient data utilization is stressed.

In addition, meeting usages and expectations of end-users is important. In scientific missions, dedicated communities use Space and EO data for analysis, and leverage their own resources. On the operational side, such as the Copernicus program, the process of consolidating data from various sources is crucial for extracting valuable insights and generating relevant data products. However, the challenge lies in effectively distributing both the data and the computational tasks. This distribution can be approached in two ways: either by centralizing the data and computations in a single location (monolithic approach) or by adopting a federated processing model that allows for distributed processing across diverse locations.

The concept of modular HPC was explained, highlighting a system where specialized modules are interconnected to create a highly efficient supercomputer. Modules mean that at least two HPC systems are connected to each other in a very specialized way, not only at the hardware level but also at the software management level. In the future, a typical HPC workflow will automatically determine which module is used for each task. The potential integration of classical and quantum algorithms is mentioned, with an ongoing emphasis on research in this area.

Then, the discussion shifted towards the accessibility of high-performance computing (HPC), with a call to make it more practical and understandable for a broader audience. Indeed, HPC technology may not yet be accessible to a broader public (e.g., the scientific community), and the software stack needs further development to make the transition smoother. This includes addressing issues like AI, data modeling, and forecasting that remain untapped due to limited access. Various challenges in data management and processing were discussed, emphasizing the need for practical solutions and better education on HPC usage.

The role of the industry and end-users in the new technology scenario was discussed, emphasizing collaboration to understand specific needs and tailor technology solutions for optimization. Participants stress the win-win situation of co-design, where expertise in supercomputing can benefit industries, and industry and expert domain knowledge can enhance technology development. This is how a supercomputer institute works, bringing people from various backgrounds together, and this is also very similar to the kind of open environment ESA creates with EO experts and application scientists. Efforts for education and training are pivotal in supporting these developments.

The participants also shared perspectives on how to favorize the uptake of HPC by Earth observation stakeholders, stressing the need for collaborative efforts to develop solutions beneficial to both science and industry. There's a focus on making HPC more accessible to a wider audience of service providers, including scientific, industrial, and policymaker communities. This is important to ensure technological transfer to the industry of solutions developed by scientists that can be also exploited in a commercial way. A first set of solution examples will be useful for commercial and policy-maker communities to understand how to use the tools and adopt them.

In conclusion, the round table discussion highlighted the potential of synergy between high-performance computing, supercomputing, and innovative computing to address the complex challenges in Earth observation. On the technical side, the panel emphasized the importance of distributed data processing and computing, and the integration of classical and quantum algorithms in a modular HPC environment. On the implementation side, the participants stressed the importance of collaboration between industry, academia, and end-users to develop practical solutions and of co-design approaches to tailor technology solutions to specific needs. The discussion also mentioned the need for better education and training to make HPC technology more accessible to a broader audience, and to favor the uptake of HPC by Earth observation stakeholders.

Acknowledgements

Gabriele Cavallaro and Bertrand Le Saux chaired the workshop.

Sabrina Ricci, Peter Naylor, and Amer Delilbasic helped in the organisation of the workshop.

Gabriele Cavallaro, Gabriella Bettonte, Jiri Guth Jarkovsky, Mikael Johansson, Ilaria Siloi, Luca Girardo presented in the workshop, and participated to the roundtable along with Claudio Iacopino and Bertrand Le Saux.

Amer Delilbasic, Alessandro Sebastianelli, and Bertrand Le Saux prepared this report with the help of all authors.

Group photo of the workshop participants