Quantum Computing for Climate Change Detection, Climate Modeling, and Climate Digital Twin

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Abstract

This study explores the potential of quantum machine learning and quantum computing for climate change detection, climate modeling, and climate digital twin. We additionally consider the time and energy consumption of quantum machines and classical computers. Moreover, we identified several use-case instances for climate change detection, climate modeling, and climate digital twin that are challenging for conventional computers but can be tackled efficiently with quantum machines or by integrating them with classical computers. We also evaluated the efficacy of quantum annealers, quantum simulators, and universal quantum computers, each designed to solve specific types and kinds of computational problems that are otherwise difficult.

Keywords: quantum machine learning, quantum computer, high-performance computing, quantum resource estimation, climate change detection, climate modeling, climate digital twin, Earth observation, remote sensing, hyperspectral images, image analysis.

1 Introduction

Quantum computing is a novel computing paradigm that processes digital information based on quantum mechanical principles in contrast to conventional classical computing. Quantum machines using primitives of quantum computing, in principle, promise to generate better and faster solutions to some inherently hard computational problems [1]; the hardness of computational problems refers to time and memory-space measures in computational complexity theories/conjectures required for finding their solutions. Some quantum machines are even known to utilize less electrical power compared to conventional supercomputers. For example, a D-Wave quantum annealer consumes 25 KW of power, whereas the Summit supercomputer consumes 13 MW [2]. Based on the time and memory-space measures, computational problems are classified according to their hardness (see Fig. 1). Intractable computational problems are ubiquitous in space and the aerospace industry. Examples include resource allocation, planning, object scheduling, and artificial intelligence (AI) model training while considering time, memory space, and electrical consumption. Hence, there already exist some quantum approaches for real-world intractable computational problems in the aerospace industry, e.g., a flight-gate assignment [3], satellite mission planning for Earth observation [4], numerical weather modeling and climate simulation involving partial differential equations (PDEs) [5], energy optimization and a renewable energy sector [6, 7], and quantum AI for climate change detection [8, 9]. However, there still needs to be demonstrated a quantum advantage for tackling practical problems over conventional classical techniques. In particular, quantum machines are in their fancy, and it needs to be well known which practical problem will inherently profit from quantum machines or which quantum machine will meet dead-end. There is an ongoing effort to identify hard computational problems in the space and aerospace industry that can be tackled more efficiently using quantum machines than supercomputers or how to profit from both quantum machines and supercomputers [8]. Therefore, we



Fig. 1 Computational complexity for computational problems. In the provided diagram, the orange star indicates a class of computational problems that are considered to be hard for a classical computer but relatively easy for a quantum computer. This is because a polynomial-depth quantum algorithm exists for these particular problems. In the diagram, **NP** stands for non-deterministic polynomial time problems, **P** stands for polynomial time problems, and **BQP** stands for bounded-error quantum polynomial problems. The diagram has been taken from Fig. 1 of the article [8].

assess different quantum machines and provide their performance-related parameters while considering their time and electric power consumption. We also identify some climate-related use-cases that are inherently hard for supercomputing systems but can be tackled using quantum machines or by integrating them with supercomputers.

2 The assessment of quantum technology

The development of quantum computing encompasses a wide range of technologies, from hardware systems to software tools depicted in Fig. 2. The quantum computing industry is still in its infancy and, like the early days of classical computing, without well-defined interfaces between the various parts of the quantum computer. The quality of a quantum algorithm is affected not only by the quality of the individual constituent components (qubits, gates, measurements) but also by the interplay of global device and algorithmic properties such as device topology, multi-qubit noise correlations, and circuit structures. Also, the quantum compilers and middleware affect the algorithm performance to be run on specific hardware. Typically, the machine instructions are optimized for execution on all hardware platforms. After the execution, additional postprocessing may also be employed to improve readout efficiency. These optimizations typically include:

- 1. depth reduction and logical transpilation: A sequence of compiler passes is used to mathematically reduce the gate depth (e.g., T-gate count) of the quantum circuit and the logical operations in the circuit are mapped to the native gates available on the hardware.
- 2. error-aware hardware mapping: Error-aware compilation is used to best select the appropriate subset and logical assignment of qubits on a device.



Fig. 2 Quantum stack by European Quantum Industry Consortium (QuIC) showing the software, middleware, and hardware layers that have direct impact on the use cases and their prospects [11].

- 3. elimination of circuit crosstalk: Dynamical decoupling sequences are incorporated to mitigate various idling errors, including dephasing and ZZ crosstalk at the algorithmic level.
- 4. optimized gate replacement: The process involves automated parsing of the device topology to ensure parallel gate optimizations do not share qubits and relevant single and or multi-qubit gates are optimized.

QC's usefulness heavily depends upon the achievable fidelities and the number of qubits of the quantum processing unit (QPU). Scaling the quality and number of qubits will require advanced 3D architectures and assembly techniques. Some estimates say that achieving practical quantum advantage requires running millions of parallel high-fidelity gates at high speed and reading out millions of qubits in parallel. With current error-correction overheads, practical quantum advantage will be achieved, albeit only for algorithms with small I/O requirements and super quadratic (ideally exponential or quartic) speed-ups over their classical counterparts [10].

In the current noisy intermediate-scale quantum (NISQ) era, the computation results are limited mainly by errors in single- and two-qubit quantum gates. To succeed roughly half the time in a 100-qubit circuit of depth five, one needs at least 99.9% gate fidelity. In practice, the number of qubits and especially the gate depth required for practical NISQ advantage is likely higher, leading to a fidelity target of 99.99% for all quantum gates, not yet demonstrated. Producing commercially viable QCs requires technologies that facilitate scalable manufacturing, requiring manufacturing process efficiency, reliability, integration, and packaging. Due to manufacturing variability, some qubits may not be functional and available for use; the exact number of qubits yielded will vary with each specific processor manufacturer. The enabling hardware that connects to the QPUs, such as cryogenic coolers, electronic systems, and cabling, must also be matured. The widely accepted approach to remedy the effects of noise and decoherence in quantum computers is using quantum error correction (QEC) [12]. While the hardware requirements to implement fault-tolerant (FT) quantum algorithms have not been met yet, the steady progress in the development of quantum hardware has initiated the introduction of a set of techniques that we refer to broadly as quantum error mitigation. These techniques immediately translate advances in qubit coherence, gate fidelities, readout precision, and speed to measurable advantage in computation. Quantum error mitigation offers the continuous path

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that will take us from today's quantum hardware to tomorrow's FT quantum computers. They might even be applicable to enable near-term practical quantum advantage without using QEC for certain use cases. A major use case for near- to medium-term quantum computers is accelerating existing HPC workflows. For this, tight integration between HPC and QC, beyond cloud access or the operation of separate computing systems, is critical to avoid idle time due to resource allocation or communications latency. The following three current trends can be identified:

- 1. Stay at "small" scales (below 100 qubits) and try to solve coherence problems and create useful applications before scaling up.
- 2. Go for large scales (over 1,000 qubits) and try to implement quantum error correction for quantum advantage or superiority while scaling up.
- 3. Scale up and solve large-scale hardware (HW) and software (SW) integration at systems levels.

We mentioned in the abstract that QC hardware could be characterized by the kinds of computation they can run into three categories:

- 1. Annealers. Quantum annealers are a kind of analog quantum simulator relying on the adiabatic theorem and mimicking an Ising Hamiltonian to solve quadratic unconstrained binary optimization (QUBO) problems such as satisfiability and combinatorial search problems. QUBO problems are solved by finding their global minimum over a given set of candidate solutions (candidate states) using quantum fluctuations. In adiabatic computing, noise- and error-tolerance are higher, and it is hard to create entangled states, the primary resource for quantum computational advantage over a conventional classical computer.
- 2. Analog Quantum Simulators. Analog quantum simulators are special-purpose devices designed to study quantum systems programmatically. They exploit superposition and entanglement to provide insight into specific physics problems mimicking the Hamiltonian evolution of the system. Analog quantum simulators are especially suited for simulating quantum physical systems; also, more general optimization is possible. As the quantum interactions between quantum particles are a built-in feature of quantum simulators, near-term quantum advantage is expected for the specific class of problems they can describe.
- 3. Digital or Fault-Tolerant Universal Quantum Computers. The most powerful class of quantum machines that directly exploit superposition, entanglement, and wave-function interference and run quantum algorithms in a step-by-step procedure. In principle, a digital universal quantum computer can solve some computable problems, with the additional advantage of up to exponential speed-up over classical computers. Digital quantum computers operate using quantum gates, logical operations on the fundamental quantum information primitives. These units are usually two-state quantum bits (qubits), but continuous-variable (CV) approaches are under development. Qubits can be implemented using several different technologies, e.g., superconducting, trapped ions, neutral atoms, or photonics, which all come with their unique strengths and weaknesses. There are some differences in algorithms between discrete and continuous quantum states, with CV approaches especially suited for, e.g., sampling and regression tasks.

3 The qubit implementation techniques

Many approaches exist to develop scalable qubits with acceptable coherence time and error rate. Some approaches are on a shallow TRL level, and estimating their potential is difficult. This chapter describes the six most promising approaches based on published information [13]. The connectivity of a quantum gate processor impacts the depth of actual quantum circuits. During transpilation, an input quantum circuit is compiled into a sequence of native gates or universal gate set such that all operations agree with a specific quantum processor's qubit topology and noise properties. The signal-to-noise ratio impacts the number of shots required to get a correct answer by recovering the signal. By increasing the gate fidelity a little, the number of shots and runtime of a given algorithm may decrease drastically. Even a minor improvement of 0.16 percent in accuracy could reduce the processing time by half [14, 15]. Building large circuits requires long coherent times of the qubit, strong interqubit interaction for fast and high-fidelity two-qubit gates, and small to zero coupling between qubits when no interaction is needed. Transmon qubits allow for various coupling concepts with various pros and cons. Two of the most promising technologies are superconductors and ion traps. At the time of writing, at most 433 and 20 qubits are available for superconducting and ion trap devices, respectively, that is, the IBM Osprey processor, USA, and the AQT PINE processor, Austria. And at most 5627 qubits for quantum annealing devices, i.e., D-Wave Advantage. According to the roadmap in 2023, the Advantage 2^{TM} quantum the system will incorporate a new qubit design that enables 20-way connectivity in a new topology containing 7000 + qubits and making use of the latest improvements in quantum coherence in a multi-layer fabrication stack (see Fig. **3**).

1. Superconducting circuits. Physical implementations of superconducting qubits reside on the chip at fixed locations and are connected via a well-defined pattern, the so-called connectivity structure. Structures are designed to minimize the possibility of frequency collisions and optimize the hardware performances. The larger the number of neighbors of a qubit, the more frequencies are required to realize twoqubit gates using cross-resonance interaction. Current technology can turn off the coupling of transmon qubits with close frequencies, but this is prone to crosstalk errors. A more efficient pulse shape could be optimized with tunable couplers to achieve a CZ gate with higher fidelity and lower unwanted leakage. Fixed couplers with constant coupling strength have been the mainstay devices until recently. However, there is now a growing interest in tunable couplers, which are considered to offer the necessary adjustable coupling strength to enhance performance [16, 17]. Roadmaps aim for increased coherence, yield, and reproducibility, enabling higher gate fidelity and, consequently, larger circuit depth on an equal footing with increased qubit number. Three-dimensional multi-chips allow massive scaling of QPUs. It is also necessary to reduce variation of all critical parameters and tolerances for all steps of chip fabrication and 3D integration. Chip engineering needs to consider signal routing, the electromagnetic environment, quantum coherence, and robustness against variations in device parameters. The advanced state of the art in quantum-processor performance requires the development of novel components

for fast and highly selective multiplexed readout, elements for mid-circuit leakage detection, coupling schemes to accelerate parity measurements, conditional and unconditional reset capabilities, and highly parallelizable two-qubit gates. Ramp-up and operating large-scale QPU also requires advancing the room-temperature electronic (RTE) systems with sufficient control and readout channels and capability for real-time quantum error correction [18].

- 2. Trapped ions. Ions traps rely on single-charged atoms or ions as qubits to store and process information. The ions are confined using electric fields, with the electronic state of the ions encoding the information. Customized laser pulses actively modify the state of the ions. Ion-trap quantum computers offer high-fidelity local operations and optical interfaces. By physically moving ions across micro-scale segmented ion traps, multiple ion-trapping potentials can be deterministically connected, thus creating an architecture for a scalable quantum information processor [19]. Realizing trapped-ion qubits requires the orchestrating of several devices, including the ion source, dedicated lasers, several optical components and sensors, a vacuum, cooling mechanisms, and control and measurement electronics. The respective systems routinely operate with about 20-30 qubits but can be pushed (at reduced levels of control) up to 50 qubits. The devices hold fully connected quantum registers, which facilitate the implementation of quantum algorithms. For trapped ion qubits, the main noise is not relaxation with time T_1 but instead dephasing with time T_2 induced by fluctuation of magnetic fields. Also, the state-detection efficiency decreases with the motional heating of the ion without laser cooling.
- 3. Photonic. Qubits are realized by processing states of different light modes through both linear and nonlinear elements. The fundamental building blocks include deterministic single-photon sources, integrated photonic circuits, and efficient single-photon detectors. Photonic systems have the unique property that they can operate at room temperature and allow for easy transfer of quantum information. The main disadvantage of photonic systems is that performing a precise interaction between photons takes much work. In recent years, some programmable and scalable architectures for photonic quantum computing were introduced, and specific quantum algorithms such as Gaussian boson sampling, molecular vibronic spectra, and graph similarity were executed in laboratories. Due to photons' properties, photonic circuits have different features from qubit-based systems from the point of view of computing and operations [20].
- 4. Neutral atoms. Qubits are realized by internal states of neutral atoms trapped in an optical lattice. Like ion-trap systems, qubits can be programmed using the energy levels of the atoms. Light, or electromagnetic radiation, can be used to trap and manipulate the quantum states of uncharged (neutral) atoms [21]. When multiple qubits are placed close to each other, they can be made to interact using two-qubit gates. This allows for new and unique quantum-computing circuit topologies. Using neutral atom platforms for quantum processing could lead to highly scalable systems with a larger quantum register. The amount of trapping laser power and the performance of the optical system that generates the optical tweezers limit the size of the quantum register.



Fig. 3 Reproduction of Fig. 2 from [24] presenting a selection of quantum computing hardware. (CC-BY 4.0)

- 5. Silicon spin. QPU integrates both qubits and control electronics and operates at a liquid helium temperature (4K), which is higher than the usual millikelvin temperatures of superconducting qubit systems. The higher operating temperatures result in lower quality qubits but extensive and efficient control electronics [22].
- 6. **NV diamond.** Nitrogen-vacancy (NV) centers in diamonds are used to realize qubits. These centers are created by replacing a carbon atom with a nitrogen atom in an artificial diamond structure near a carbon atom gap. Microwaves, a magnetic field, and an electric field are used to implement qubit gates, while qubit readout is achieved through the use of a laser and fluorescence detection [23].

3.1 QPU performance consideration

Implementing a functional quantum computer requires an integrated system consisting of a quantum processor, its fabrication, packaging and wiring, room temperature electronics, enabling software, system integration, application development, and testing system. Improving QPU performance requires concurrent and individual optimization of all subsystems and subcomponents while maintaining system harmony [14, 15]. Here, we focus on the Quantum Processing Unit, QPU. There has yet to be a standard to assess the performance levels of the processor. Some approaches include benchmarking metrics such as Quantum volume, Algorithmic volume, and Randomised benchmarking. To keep the qubit error rates below a certain threshold for faulttolerant computation, extending the coherence time of qubits is crucial. Here, we list some critical areas in Qubit implementation, Qubit control, Qubit calibration, and Code running. Currently, only trapped ions and superconducting qubits satisfy the five required criteria for quantum computing defined by DiVincenzo [25]:

- 1. A scalable physical system with well-characterized qubits;
- 2. The ability to initialize the state of the qubits to a simple fiducial state;
- 3. Long relevant decoherence times;
- 4. A "universal" set of quantum gates;
- 5. A qubit-specific measurement capability.

Typical physical indicators of quantum computers include T_1, T_2 , single-qubit gate fidelity, two-qubit gate fidelity, and readout fidelity. The aggregated benchmarks can help the user determine the performance of a quantum processor with only one or several parameters. The aggregated metrics can be calculated with randomly generated quantum circuits or estimated based on the basic physical properties of a quantum processor. Typical aggregated benchmarks include quantum volume (QV) and algorithmic qubits (AQ). Different quantum machines have specific attributes that make them better suited for certain tasks than others. However, this doesn't mean that one machine is superior to the others in absolute terms. Instead, the choice of a particular QPU for QC4Climate and QC4EO use-case instances should be based on the problem it needs to solve rather than an arbitrary rating system. For instance, ion trap devices offer better connectivity, compensating for their slower operation speeds. On the other hand, superconducting systems have much faster operation times, making them competitive despite having sparser connectivities. Additionally, trapped ion qubits have longer coherence times, making them more resilient to mid-circuit measurement, a crucial requirement for error-correction [26]. However, superconducting systems with 1000x faster gate speeds are better suited for variational benchmarks like QAOA, which require millions of sequential iterations [13]. We presented example quantum machines in Table 1.

3.2 Sizing QPUs

Modern classical central processing units (CPUs) operate at around 3GHz clock cycle speed or around 0.30ns clock cycle time. Nowadays, intractable computational problems are even tackled on several hundreds of parallel CPUs and general processing

Table 1Some dominating quantum machines in the global market are offered by large organizations. SeeFig. 4 for the projection of the roadmap of some quantum machines and Table 2 for parameters of quantum machines [27] [speculation].

Organizations	Locations	Technology	Current qubits	Projected qubits (3-5 years)
IBM	USA	superconducting	433	4,158
Google	USA	superconducting	73	100
IQM	FI	superconducting	20	54
USTC	CN	superconducting	66	100
AQT	AT	trapped ions	20	200
IONQ	USA	trapped ions	29	256
Xanadu	CA	photonic	216	216
USTC	CN	photonic	113	300
D-Wave	CA	superconducting-annealing	5,000	10,000
QuEra	USA	neutral atoms	256	1,000

Table 2 Sizing quantum machines: SC-superconducting QCs [18], T.ions-trapped ions QCs [28], N.atoms-neutral atoms QCs [21], Photonic-photonic QCs [20], S.spin-silicon spin QCs [22], NV-nitrogen vacancy in diamond QCs [13], CPUs- conventional central processing units [approximate values, potential to change]. See also the Table 1.

Parameters	\mathbf{SC}	T.ions	Photonic	N.atoms	S.spin	NV	CPUs
Clock cycle	1MHz	1KHz	10 Hz	1MHz	$0.76\mathrm{MHz}$	1MHz	$3 \mathrm{GHz}$
Measurement	660ns	$300 \mu s$	х	200ms	$1.3 \mu s$	х	x
2-qubit gate	34ns	$200 \mu s$	х	$< 100 \mu s$	х	700ns	x
1-qubit gate	25ns	$15 \mu s$	х	х	х	9ns	x
Readout fidelity	99.4%	97.3%	50.0%	99.1%	99%	98%	x
1Q fidelity	99.99%	99.99%	99.84%	99.83%	99.99%	99.99%	x
2Q fidelity	99.97%	99.9%	99.69%	99.4%	99.5%	99.2%	x

units (GPUs). The fastest QPU is currently a superconducting-based QPU (see below tables) in terms of the qubit and quantum gate operation time or clock cycle time. However, the I/O speed is 10,000 slower in the QPU compared to the CPU. Logical qubit/magic state distillation (creating more accurate quantum states from multiple noisy ones) is another restriction, and another restriction is high-bandwidth, low-noise classical electronics. Hence, to beat CPUs, there is a need to improve the speed of the I/O system in QPUs from register preparation to readout. More than exponential speed-up is also required in the quantum algorithm [10]. Only some of the problems are meaningful to compare depending on their parallelizability on CPUs and GPUs (see Table 2 and Fig. 4). Regardless of the qubit technology, there is the persisting challenge to scale logical error-free qubits due to the quantum state generation having a high fidelity and classical electronics controls, to name a few [13].

3.3 Error mitigation and correction

Various interactions, whether they are electromagnetic or mechanical, and occur between qubits and their immediate environment generate errors that are associated with the phenomenon of quantum decoherence. While progress is being made in error removal, it is barely managing to gain one or two orders of magnitude in error reduction. In an ideal world, however, we would require improvements of ten orders of magnitude [23]. It is possible to correct errors, even by using noisy gates, provided that the noise level remains below a certain threshold. The drawback is that it requires a massive overhead of physical qubits and classical information processing (see Fig. 5) [12]. There is an optimal "code size", i.e., a number of physical qubits per logical qubit, that maximizes the performance metric - and beyond which more error correction degrades the computation accuracy rates. Also, less noise mandates a more significant code and more physical qubits, but more physical qubits give rise to more heat generation, hence more noise. To execute a quantum application successfully, QEC is necessary for creating logical qubits that can store and process quantum information more effectively than physical qubits. This QEC capability is central to scalable quantum computers. However, the costs are formidable, often multiplying the number of qubits needed by a factor of thousands and runtimes by a factor of hundreds. One of the trends for improving the error correction rate characteristics is employing AI models for this process [29]. This would, in turn, allow us to reduce the number of quantum computation instances needed before obtaining a reliable result or decrease the number of physical qubits in QC systems. In Europe, there exists a start-up that develops a toolkit for providing this form of QC improvement [30]. An important metric for a QEC approach is its threshold, which specifies the maximum error rate that it can tolerate. Physical error rates on Clifford operations below 0.1% (including qubit preparations, measurements, and gates) are typically required to avoid prohibitive QEC overheads. These values are possible only in the setting where operations can be applied in parallel, which may pose a significant hardware challenge for some platforms, such as trapped ions. In many QEC schemes, the non-Clifford gates (typically T gate) are pretty costly when requiring fault tolerance [31]. The required low error rate T states are produced using a T state distillation factory involving a sequence of rounds of distillation, where each round takes in many noisy T states encoded in a smaller distance code, processes them using a distillation unit, and outputs fewer less noisy T states encoded in a larger distance code, with the number of rounds, distillation units, and distances all being parameters which can be varied. This procedure is iterated, where the output T states of one round are fed into the next round as inputs. T factories incur significant physical overheads, requiring several thousand physical qubits and only producing new T states once every 10 to 15 logical time steps [32].

Microsoft (MS) has evaluated three use cases, concluding that to achieve practical quantum advantage, quantum machines need to be able to control millions of parallel operations with low error rates and to read out those millions of qubits in parallel to enable decoding of the errors at speed, all while ensuring the overarching logical clock time is fast enough to complete the computation within a month runtime or less [33]. MS concluded that logical gate times under $10\mu s$, requiring physical gate times around 100ns, would be needed to complete the quantum chemistry algorithm



Fig. 4 Quantum machines roadmap of some organizations which provide the open-data for their quantum development projection [speculation].

within a month, using a few million physical qubits. In order to measure syndromes on these qubits and decode them, a large quantum-classical bandwidth and processing power are required. The exact estimates of bandwidth requirements depend on the choice of QEC code, system size, and physical operation times. However, roughly, with a few million qubits, the estimation is that several terabytes per second of bandwidth will be required between the quantum and classical planes. Furthermore, processing these measurements at a rate sufficient to correct errors effectively requires petascale classical computing resources tightly integrated with the quantum machine.

4 Investment in quantum computing

Across Europe and the World, quantum computing is gathering investment from states and organizations, as well as private investors. In 2022, the investment in quantum technology was globally around 30 billion euros; in 2023, the investment amounts to 36 billion euros. By 2028, the overall investment in quantum technology is projected to reach 53.2 billion euros globally, and quantum computing investment alone is estimated to be around 17.6 billion euros [34]. Several major players are [35]:

- 1. **European Union** The EU Chips Act, with a total budget of around 43 billion euros, has a quantum component included, and the European Quantum Flagship program invests around one billion euros in quantum computing, excluding other quantum technologies like quantum sensing.
- 2. **USA** The USA Chips Act, with a total budget of around 50 billion euros, has a quantum component included, and the US National Quantum initiative invests around 3.75 billion euros in quantum computing alone.



Fig. 5 [Top Left] the trend line for scaling superconducting-based error-prone qubits, or physical qubits, [Top Right] their corresponding logical qubits, when we assume that a single logical qubit is represented by 75 physical qubits based on the error-correction [12], [Bottom] the gate fidelity over the years [projection, speculation].

3. China - One of the leading players in quantum computing alongside the USA, China's quantum initiative invests around 15 billion euros in quantum computing.

5 When can we expect quantum advantage in climate change detection, climate modeling, and climate digital twin?

The United States is perceived as the leading player in quantum technology, even though Europe has made the most public investments in the industry. In the United States, big technology enterprises such as Microsoft, Google, Intel, and IBM have driven commercial development efforts. In Europe, development has been slowed down by fragmentation. Currently, there are about 140 projects, less than half commercial. Many groups listed are universities, government labs, or departments within larger tech companies. Here, we can make a distinction between two approaches:

- components provided addressing parts of the HW stack, which then may be integrated using so-called open architecture,
- a system integrator capable of bringing together and coordinating all the needed competencies and components to make up a commercially viable quantum computer.

Superconducting qubit-based approaches are the most researched (and have received the most development resources). Almost all the startups in this space are based on technology from university labs. Manufacture a stable QC requires more than an exploratory chip. As of early 2023, there have been around a dozen successful attempts to build quantum computers worldwide. Some specialized companies are developing middleware for the calibration, management, and optimization of quantum computers to overcome some of the problems caused by errors. Predicting the timeline for developing scalable and useful quantum computers is a challenging task. The opinions of experts in the field of quantum computing range from optimistic to pessimistic, with a significant disparity. According to their 2020 roadmaps, leading tech giants such as Google, IBM, and Amazon anticipate achieving true quantum supremacy in the near future and developing a quantum computer with 100 logical qubits within a decade [23]. On the other end, some pessimistic views are saying that there is no hope of reaching quantum speed-up ever. There is not any strong scientific obstacle preventing the creation of reliable quantum computers. In the scientific community, there is a belief that the uncertainty is primarily a technological and engineering one, and the pace of quantum usability is accelerating. However, there is pessimism about fixing qubit noise, regardless of type. A quantum speed-up provided by quantum computers may vanish when large amounts of classical data need to be loaded [36]. Generally, quantum computers are considered practical for "big compute" problems on small data or classical datasets, which inherit the "specificity" of qubits, not big data problems [37]. There is a growing number of informative end-to-end resource analyses, but typically, these single out very specific algorithms and hardware and make very different assumptions across the stack. Different choices can result in different resource requirements. One can, for example, trade-off more qubits against shorter run times or trade-off faster qubit gate operations against lower fidelities. It is obvious that the number of physical qubits and the duration of a logical time step reduce as physical error rates improve. Entanglement has long been considered to play an essential role in quantum computing and promise for exponential speed-up of various quantum algorithms that require asymptotically fewer operations than their classical counterpart. Specific examples where this is the case are quantum problems in chemistry and materials science. Entanglement can be seen as the key feature that sets quantum computing apart from classically simulable processes. Thus, the key metrics to follow the development should include the number and quality of entangling gates provided. The GHZ states provide the strongest non-local correlations for an n-particle entangled state. These GHZ states are very fragile, as the loss of a single particle completely destroys the entanglement. Also, because all particles contribute to phase evolution, the dephasing time decreases with the particle number. Such states are challenging to create, requiring either many particles to interact with each other or a series of two-particle interactions performed in sequence. Some of the recent approaches to improving the SC qubit fidelities include

- redesigning the qubit geometries,
- use of new low-loss materials and
- optimizing the control pulse that drives the quantum system.

Based on the expert estimation, starting in 2025, we believe that we will see some relevant quantum advantages with actual data and useful algorithms running on NISQ hardware in climate change detection, climate modeling, and climate digital twin domain. A quantum advantage can come from the computing time, system energetic footprint, and/or the precision of the outcome (metrics: time to solution, energy consumed to reach the solution, and precision of the solution). We estimate that the threshold of 150-ish high-quality qubits, with a low error rate and long coherence time, is necessary to achieve any real quantum advantage. With these qubits, it may be possible to form about ten logical qubits. However, entangled qubits are required for exponential speed-up and significant quantum advantage. We estimate that the number of maximally entangled logical qubits will start growing exponentially around 2030 with advancements in qubit engineering. We summarise this development in three phases.

- 1. Late NISQ era: (100 200+ physical qubits; 99.99%+ fidelities, especially 2Q gate fidelity; high qubit connectivity) (3 5 years from now).
- 2. Early Fault Tolerant QC era delivering significant advantage (< 10 maximally entangled logical qubits) (5 10 years from now).
- Fault Tolerant QC era delivering exponential advantage (> 50 maximally entangled logical qubits) (10 − 20 years from now).

6 Quantum for climate change detection

Earth observation satellites capture changes on Earth's surface, and the captured signals are in a very narrow spectral band. For example, an Environmental Mapping (EnMAP) satellite detects spectral wavelengths in ranges of 420 nm to 1000 nm and from 900 nm to 2450 nm. Its main task is to collect hyperspectral imaging data in order to provide vital information for climate change detection and environmental monitoring, such as climate change impact and land cover changes [38]. However, current DL techniques and conventional numerical methods for climate change detection and environmental monitoring are costly in terms of computational time and electric power consumption. There are three possible quantum approaches to tackle this problem:

1. The first one is Variational Quantum Algorithms (VQAs): VQAs are a class of Quantum Machine Learning (QML) models aimed at the application in the NISQ era. These algorithms employ jointly parameterized quantum Circuits (PQCs) and classical optimization techniques for finding optimal quantum circuits that have desirable properties from the point of a given application. From the perspective of computational time required and electrical power consumed, VQAs require less training datasets compared to conventional DL models [39] - it implies faster training time than its counterpart classical technique, whereas quantum machines also consume less electric power than supercomputers at the same time [2] (e.g., a D-Wave quantum annealer operates at around 25 kW power, whereas the Summit supercomputer consumes around 13 MW power). VQAs are already applied to, for example, change detection [40, 41], chlorophyll concentration estimation in water

Table 3 Summary of the identified feature selection methods for hyperspectral imagerydata: RFE-Recursive Feature Elimination, QSVM-Quantum Support Vector Machine,and VQAs-Variational Quantum Algorithms.

Method	RFE for QSVM	RFE for VQAs	Quantum optimization
	[55]	[56]	[48]
Resources	high	moderate	low/moderate
	$\gtrsim 10^5$ logical qubits	$\sim 10^2$ logical qubits	$\sim 10^2$ logical qubits
Time horizon	> 15 years	3-5 years	now/3-5 years
Architecture	gate-based	gate-based	annealing/gate-based
	quantum	hybrid	hybrid
speed-up	exponential	polynomial	polynomial/exponential

[42], detecting clouds [43], and phase unwrapping for synthetic aperture radar datasets [44, 45].

- 2. The second approach is feature reduction and selection: Feature selection and feature extraction are common methods for reducing the number of features in large, high-dimensional data sets. A basic distinction between these methods is that the first involves transforming the original features, while the second preserves the features. The procedures have profound practical consequences, allowing for less electric power consumption and more effective data storage. The hyperspectral data satellite data, with even hundreds of narrow spectral bands, provide an example of the area in which utilization of the methods seems virtually unavoidable. The rich spectral information may simply surpass the needs of certain applications. On the other hand, since the number of possible selections (subsets) grows exponentially with the number of features, the application of the selection methods involves hard optimization tasks (see Tables 3 and 4). Another approach is to select the core of a dataset ("coreset") that is representative of an original dataset [46, 47]. There are already some first attempts for selecting informative features [48] and assembling the coreset from satellite datasets [46, 49]. By either selecting an informative subset feature, reducing the dimensionality, or assembling the coreset of highdimensional datasets via a quantum approach, the training time and the electric power consumption of both QML and DL models can be reduced substantially.
- 3. The third approach is to integrate physics laws and models with practical datasets and QML models when a physical model for an event is known, and data is scarce in nature. Here, Quantum Physics-Informed Neural Networks (QPINNs) proposed by the authors of the articles [50, 51] can be applied to, e.g., a rainfall-runoff model that is used for the prediction of flooding and drought analysis [52]. Here, PINNs are ML and DL models imposed by physics laws and PDEs [53, 54], and QPINNs refer to PINNs whose conventional NNs are replaced by QML models. Using QPINNs, we can tackle climate-related challenges and generate better prediction and projection probabilities for about-to-fold as well as already unfolded events than conventional PINNs, when data is too small in quantity for data-driven methods and decisionmaking time is a critical factor for human-centered decisions [39].

Table 4Summary of the identified feature extraction methods for hyperspectral imagerydata:QPCA-Quantum Principal Component Analysis, and QAutoencoders-QuantumAutoencoders.

Method	QPCA	variational QPCA	QAutoencoders
	[57]	[58]	[59]
Resources	high	moderate	low/moderate
	$\gtrsim 10^3$ logical qubits	$\sim 10^2$ logical qubits	$\sim 10^1 - 10^2$ logical qubits
Time horizon	15 years	3-5 years	3-5 years
Architecture	gate-based	gate-based	gate-based
	quantum	hybrid	hybrid
speed-up	polynomial	polynomial	polynomial

7 Quantum for climate modeling

Climate modeling refers to modeling the behavior of the climate system for predicting and projecting the Earth's climate [60]. The prediction and projection of climate models depend on the so-called grid cells, each of which represents the point on/in the Earth. The grid cells are characterized by the spatial resolution and their evolution governed by a climate model is defined by the temporal resolution. We note that the amount of data in a climate model is large. With a typical spatial resolution of 10 km, the total number of grid cells representing the atmosphere is in the hundreds of millions. Each grid cell has several variables associated with it, such as air density, temperature, wind speed, humidity, etc. The total parameter space is thus counted in the billions. The finer the spatial and temporal resolution, the more computationally expensive the climate model; climate models governed by PDEs generate better outputs than pure data-driven approaches but are computationally expensive as the spatial and temporal resolution get finer [61]. Doubling the model's resolution typically requires halving the time steps, following the Courant-Friedrichs-Lewy condition [62]. Thus, doubling the resolution, e.g., going from 10 km to 5 km increases the computational cost roughly by a factor of 8. To tackle computationally expensive climate DL and climate PDEs using quantum algorithms, we could utilize the following approaches:

- 1. VQAs can be used to test and solve climate PDEs [5] since they have more expressive power than their classical counterparts [63],
- 2. Due to the limitation of the memory capacity of computing devices and large-scale climate datasets, we need to train conventional DL models on a small subset of climate datasets, and however, they do not generalize well on small-scale datasets compared to large-scale ones [64]. To overcome the small dataset challenge, QPINNs can be utilized for predicting and projecting some climate states [50, 51, 61].
- 3. Another promising approach is to decrease the spatial resolution of grid cells without losing accuracy by using climate QML models for interpolation identical to a conventional classical method [65],
- 4. Quantum machines can be used to simulate atmospheric chemistry [66]. Having fast, highly accurate methods for simulating atmospheric chemistry is crucial, as the number of possible reaction pathways also grows rapidly with the size of



Fig. 6 Digital twins of the Earth attempt to replicate the behavior of certain aspects of the planet based on Earth Observation data and physical models.

the molecules involved in the reactions. Here, quantum chemistry algorithms and quantum machines can play a decisive role.

In addition to quantum approaches for the computational time and electrical power consumption reduction, quantum-inspired algorithms like quantum tensor networkbased methods may also help decrease the time and computational cost for tackling climate change detection tasks and climate models [67]. Another advantage of quantum tensor network-based methods is that we can deploy them on an HPC system and quantum machines and utilize them to benchmark the performance of quantum machines with respect to an HPC system [68, 69]. We can also utilize quantum tensor networks for compressing climate Deep Neural Networks (DNNs) and climate PINNs to decrease their computational time and electrical power consumption [67, 70]. The impact of quantum machines will be, therefore, enormous for processing satellite-based datasets and computational methods for climate change detection and climate modeling for making high stake decisions (safety-critical and human-centered decisions) when we have an access to reasonable noisy intermediate-scale and fault-tolerant QCs integrated with an HPC system: HPC+QCs for intractable computational problems of practical significance.

8 Quantum for climate digital twin

8.1 Climate digital twin

The Climate Adaptation Digital Twin (ClimateDT) is a project issued by the European Centre for Medium-Range Weather Forecasts (ECMWF) in the Destination Earth initiative, where the goal is to develop a highly accurate digital model of the Earth (see Fig. 6). The aim is to develop an accurate model of the Earth in order to monitor and simulate the interactions between the natural environment and human activities with as high precision as possible. Through this, the effects of various natural phenomena and human actions on the climate can be studied. The underlying goal is to move from plausibility assessments of local and regional climate to fully developed



Fig. 7 Operational version of the ClimateDT workflow that will be developed during 2023.

risk assessments. The Climate Digital Twin (ClimateDT) workflow is presented in Fig. 7. The workflow begins with the typical initialization and preparatory steps required by a climate or Earth System Model (ESM). In the Climate DT project, the ESMs in use are ICON and IFS. In the workflow, the current model state, illustrated as a Model State Vector (MSV), is propagated forward in time to produce a new state and, simultaneously, the model output or Output State Vector (OSV). This output is streamed (not saved) through a processing pipeline – that introduces additional diagnostic variables and handles interpolation, meta-data conversion, and simple operations on the fields – to generate a Generic State Vector (GSV). The GSV is saved directly to Fields DataBase, which is a domain-specific object store developed at the ECMWF, another streaming approach, is also being developed using Maestro (https://www.maestrodata.eu/). The GSV is then forwarded to the applications and quality assessment and uncertainty quantification (AQUA), all of which can also utilize external data sources, e.g., observations, climatologies, and reanalysis. Indeed, the most resource-heavy and time-consuming part of this workflow, i.e., the bottleneck, is the climate model itself. Fig. 8 shows the relation between different processes in the ICON-Sapphire Earth system model [71]. What can be seen is that different processes are updated at different intervals, that is, with different Δt . This is partly due to the varying computational complexity for propagating specific processes in time in the Earth and climate models. The shortest time steps are those of the dynamical core computations that solve the fluid dynamics equations of atmospheric motions, while the radiative transfer computations have the longest time steps. There is roughly a 1:30 ratio between the shortest and longest time steps. In the latest climate models within ClimateDT, with a resolution of 10 km, the time steps for dynamics and radiation are typically 60 s and 30 min, respectively. Presently, the wall time for computing the individual time steps ranges from the subsecond regime to around 10 s on the LUMI supercomputer.



Fig. 8 Time stepping in the ICON-Sapphire Earth system model. ICON-A: atmosphere component; ICON-L: land component; YAC: atmosphere-ocean coupler; ICON-O: ocean component. Reproduced from [71] under the Creative Commons Attribution 4.0 license.

8.2 Missing physics in the climate models

Cloud feedback and cloud-aerosol interactions are likely contributors to the high values and increased range of equilibrium climate sensitivity in CMIP6 [72]. In the past, clouds have been poorly represented in Earth System Models (ESMs) due to the complex cloud formation process and because the models could not be run on the scales at which clouds form. Additionally, numerical cloud modeling has relied on the Eulerian continuous medium approach for all cloud thermodynamic variables. However, recently, modeling has shifted towards Lagrangian particle-based probabilistic approaches in small and cloud-scale simulations. Clouds are being taken seriously the World Climate Research Programme has launched a Grand Challenge on Clouds, Circulation and Climate Sensitivity, and NASA has a Grand Challenge, "Uncertainty Project," [73] tackling cloud physics knowledge on ESMs. Clouds are also a focus point for the DYnamics of the Atmospheric general circulation Modeled On Non-hydrostatic Domains (DYAMOND) initiative, where a relatively recent review [74] proposed a protocol for the first intercomparison project of global storm-resolving models. The review presents 40-day global model simulations (these include ICON and IFS) with a grid resolution uniformly lower than 5km and addresses both scientific aspects and computational performance analysis. The authors note that fully resolving shallow cloud systems, which may only be a few kilometers in scale, requires substantially smaller

grid distances. Despite this, the outlook is optimistic. This ties in with machine learning efforts for cloud cover modeling [75] and, consequently, with quantum machine learning efforts discussed above. We expect cloud representation to improve in all ESMs, including ICON and IFS. In the first phase, we will likely use purely classical supercomputing and, subsequently, quantum-accelerated HPC.

8.3 Quantum approaches for ClimateDT

From the previous section, we can identify two main challenges that hamper the direct adoption of quantum computing to climate modeling problems within ClimateDT:

- 1. "big data" problem, and
- 2. "short wall-time" for individual calculations.

First, the climate models work on a large amount of data, both as input and output. However, these "Big data" problems are unsuitable for quantum computers. The strength of quantum computers lies in being able to solve problems with a moderate amount of both input and output variables, where the relation between input and output variables is a highly complex equation that can be solved efficiently by some quantum algorithm, exploiting quantum parallelism [76]. In other words, quantum computing typically requires problems with a large potential solution space but only a small set or even a single solution, with the additional provision that the input parameters must be of the same order of magnitude as the number of qubits in the system. Second, for quantum computers to show a wall-time advantage over classical computers, they need to solve sufficiently complex algorithms. This means that the algorithms have to be sufficiently deep; that is, the number of basic operations has to be high. In practice, single useful quantum computing calculations will take at least seconds to complete [77]. Individual variational circuits can and do take a shorter time, but the wall time to solution is, of course, much longer, as several iterations need to be performed. On the other hand, now, the shortest individual time-steps in the climate digital twins take less than a second, and even the longest is around 10 seconds. Further, the ClimateDT initiative aims to speed up the individual time steps significantly, with up to a factor of one hundred. This would push *all* of the individual propagation calculations into the sub-second regime. Thus, quantum computers cannot speed up these calculations further, as they already are faster than the fastest useful quantum computer calculations. Climate models would thus, at first glance, seem to be rather unsuitable for quantum acceleration. To gain some quantum advantage, we need to consider the problem at hand from a broader perspective. Simply taking present classical algorithms and the approximations they include and rely on and transforming these to quantum versions of the same will not work. Instead, the quantum advantage will be found by approaching the problem from different, new angles, utilizing the unique features of quantum machines. A large part of the calculations in the current ClimateDT workflows are, in effect, Computational Fluid Dynamics (CFD or PDEs). Here, we have a direct connection to solving linear systems of equations. The HHL quantum algorithm for linear systems of equations, named after its authors Harrow, Hassidim, and Lloyd [78], and variations thereof, thus have the potential to speed up CFD simulations. As noted by Lapworth [79], classical algorithms running on supercomputers

are highly efficient at solving matrix equations by, for example, side-stepping the need for matrix inversions. Quantum algorithms do not need to, even *should* not rely on the exact approximations as classical algorithms, however. Quantum algorithms like HHL and the Quantum Singular Value Transformation (QSVT) [80] can efficiently perform direct matrix inversions and should, therefore, be utilized for quantum advantage. The approach presented by Lapworth [79] relies on fault-tolerant quantum computers, but hybrid classical/quantum algorithms for the NISQ era have been proposed and discussed [81].

9 Uncertainty quantification for climate change detection, climate modeling, and climate digital twin

Quantum solutions mentioned above, such as climate QML models and climate PDEs, provide meaningful information with some uncertainty for predicting and projecting climate change detection, climate modeling, and ClimateDT (AQUA in the ClimateDT workflow shown in Fig. 7) [82]. One approach to quantify the uncertainty of quantum models and to decrease the uncertainty of classical approaches is to integrate Bayesian analysis with quantum models. Quantum models integrated with Bayesian analysis promise to tackle efficiently some hard computational problems on quantum computers [83, 84]. Moreover, quantum models promise to generate solutions to a class of computational problems much faster than conventional computing resources, resulting in less time and less electric power usage. Classical Bayesian analysis is a natural, dataefficient, and inherently interpretable model that generates probability distributions of predictions and weights, thanks to its respective uncertainties in its predictions and weights [85, 86]. In contrast, conventional DL models and numerical models involving PDEs considered uninterpretable black-box models require big labeled datasets, and they even need to be trained and tested on sub-datasets, including training, test, and validation sets, while one does not need to divide datasets into training, test, and validation sets for Bayesian analysis. For limited labeled datasets, this dataset division raises a challenge for DL and PDEs but not for Bayesian analysis [87]. Moreover, DL and PDEs also yield point estimates of predictions with point weights lacking their uncertainty or explainability due to the uninterpretable black-box paradigm [88]. DL and PDEs combined with Bayesian analysis are called Probabilistic Numerics (PN) [89]. PN quantifies uncertainties in its predictions and weights by better utilizing the available dataset, be it small or big. Namely, PN models analyze data-driven approaches using Bayesian analysis while their weights and predictions follow certain probability distributions [90]. To design PN models for climate change detection and climate modeling via a quantum approach, we first assume a model $F_{\theta} = F_{\theta}(\cdot)$ (a climate QML model or a climate PDE) for a given dataset $S = \{y_i, \mathbf{x}_i\}_{i=1}^N$. Secondly, in order to proceed, it is necessary to define the weights and predictions according to

some prior $p(\boldsymbol{\theta})$ and likelihood $p(\mathcal{S}|F_{\boldsymbol{\theta}})$ distributions:

$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta}) = \mathcal{N}(0, \sigma^2 \mathbf{I}),$$

$$p(\mathcal{S}|F_{\boldsymbol{\theta}}) = p(\mathcal{S}_y|\mathcal{S}_x, F_{\boldsymbol{\theta}}) = \mathcal{N}(\mathcal{S}_y; F_{\boldsymbol{\theta}}(\mathcal{S}_x), \sigma^2 \mathbf{I});$$
(1)

where weights $\boldsymbol{\theta}$ are sampled from a normal distribution $\mathcal{N}(0, \sigma^2)$ with zero mean and known uncertainty σ^2 . S_y and S_x denote labels $\{y_i\}_{i=1}^N$ and input data points $\{\mathbf{x}_i\}_{i=1}^N$ e.g., $F_{\boldsymbol{\theta}}(S_x)$. We note that one can represent a prior and likelihood by any probability distribution function instead of a normal distribution. For simplicity, we utilized a normal distribution $\mathcal{N}(\cdot)$. PN utilizes Bayes' theorem to quantify uncertainties in predictions and weights:

$$p(F_{\boldsymbol{\theta}}|\mathcal{S}) = \frac{p(\mathcal{S}|F_{\boldsymbol{\theta}})p(\boldsymbol{\theta})}{p(\mathcal{S})} \quad \longleftrightarrow \quad p(\boldsymbol{\theta}|\mathcal{S}) = \frac{p(\mathcal{S}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{S})}, \quad given \quad p(\mathcal{S}) = \int_{\Omega_{\boldsymbol{\theta}}} p(\mathcal{S}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$$
(2)

here $p(\boldsymbol{\theta}|\mathcal{S})$ is the posterior, and $p(\mathcal{S})$ is the evidence integrating over parameter space Ω_{θ} . Finally, after computing the posterior distribution, expressed by Eq. (2), we can calculate a probability to predict a label \hat{y} given a test data point $\hat{\mathbf{x}}$ and dataset \mathcal{S} , that is, a predictive posterior:

$$p(\hat{y}|\hat{\mathbf{x}}, \mathcal{S}) = \int_{\Omega_{\boldsymbol{\theta}}} p(\hat{y}|\hat{\mathbf{x}}, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{S}) d\boldsymbol{\theta}.$$
 (3)

The posterior $p(\boldsymbol{\theta}|\mathcal{S})$ gives uncertainties in weights –. This uncertainty is called an epistemic uncertainty, while the predictive likelihood $p(\hat{y}|\hat{\mathbf{x}}, \boldsymbol{\theta})$ yields uncertainties in predictions – this uncertainty is called an aleatoric uncertainty. Therefore, the predictive posterior $p(\hat{y}|\hat{\mathbf{x}}, \mathcal{S})$ generates total uncertainties in predictions by leveraging both epistemic and aleatoric uncertainties [91, 92]. By convention, increasing the size of a dataset can reduce epistemic uncertainty related to random noise (randomness) in data. In contrast, the aleatoric uncertainty associated with a lack of knowledge in a model $\boldsymbol{\theta}$ is irreducible even by increasing the dataset size. The parameter space $\Omega_{\boldsymbol{\theta}}$ of a given model includes several thousand to millions of tuneable weights θ . This high dimensional space of weights raises a challenge to integrate the evidence $p(\mathcal{S})$ as well as predictive posterior $p(\hat{y}|\hat{\mathbf{x}}, \mathcal{S})$ over Ω_{θ} ; computing the evidence and predictive posterior is an intractable problem [1]. Hence, the posterior $p(\boldsymbol{\theta}|\boldsymbol{S})$ is a hard-to-compute function on conventional computers due to the intractable evidence. In order to tackle these intractability challenges for climate change detection, climate modeling, and climate digital twin, there exist some quantum approaches such as quantum Monte Carlo Markov Chain (MCMC) and quantum variational inference (VI) [83, 93]. In contrast to the conventional classical MCMC and VI, their quantum approaches help generate faster and better results for climate QML models and climate PDEs. More importantly, quantum approaches for classical MCMC and VI promise to reduce the uncertainties in conventional climate models due to their better approximation property of a distribution function. Thus, it is crucial to design and use quantum VI and

the quantum MCMC to make them better on approximate samples - reduce the uncertainties in classical change detection methods and climate models - to predict climate change detection and project (simulate) a climate state.

10 Combining high-performance computing and quantum computing: HPC+QC

There are presently significant ongoing efforts around the globe to connect HPC infrastructure with quantum computers. This is surprising considering that quantum computers presently cannot solve any practical, real-world modeling problem more efficiently than a single node of a supercomputer. At the same time, it is a testament to the potential and the *belief* in the potential of quantum computing for scientific modeling. In Europe, the plans for making quantum computing relevant for research and development in academia and industry alike have been outlined, with the goal of having a European quantum computing infrastructure exhibiting quantum advantage by 2030. The first quantum simulators are already being integrated with HPC infrastructure in the HPCQS project [https://www.hpcqs.eu/]. In June 2023, the EuroHPC Joint Undertaking signed hosting agreements for six different quantum computers to be placed in HPC centers around Europe, with the plan to make these available to European users in 2024. These first quantum computers are only the beginning; several updates and new procurements are already planned. It is crucial to consider the actual (future) HPC infrastructure and its implementation. Already in the near-term, it is expected that individual supercomputers will be connected to several quantum machines of various types and implementations [94]. The initial setups, with individual QPUs distributed throughout the continent, connected to an HPC system, can be seen as precursors to a future where QPUs will be connected in parallel, either entangled or not. Plans for even tighter, on-chip integration of QPUs with classical processing units already exist and may be the way to reach fault-tolerant quantum computing. With this in mind, more emphasis on developing parallel quantum algorithms, which simultaneously utilize several QPUs in an HPC+nQC manner, would seem appropriate. For time-evolution problems like climate modeling, this can be a necessary development at a relatively early stage to enable the quantum processing part to keep up with the classical computing tasks at each time step. Reassuringly, the importance of investing in software development for hybrid HPC+QC applications has been recognized. These developments complement the efforts for developing purely classical software for exascale supercomputers and beyond, exemplified by the Destination Earth initiative. Here, it is apt to note that there is a need for significant classical software development alongside quantum algorithm research. Presently, pre-and post-processing tasks take up a significant portion of the total wall time of executing a quantum algorithm. As an example, in the recent experiment on spin dynamics using IBM's 127 qubits QPU, the actual time spent on the QPU was 5 minutes, while the wall-time of the experiment was a hundred times longer, over 9 hours [95]. These overheads will decrease in the future, but at the same time, increasing the qubit count will again increase the complexity of pre- and post-processing. Part of this overhead lies within the domain of hardware development, e.g., qubit reset and readout. Much of this is, however, classical computing routines, such as compiling, transpiring, qubit routing optimization, error mitigation, and noise canceling, to name a few. All of these will become computationally more demanding with increasing qubit count and will, therefore, require increasing amounts of classical computing power. Thus, efficiently operating the quantum machines of the future will require an HPC infrastructure and the classical software to run on it. For reaching quantum advantage as soon as possible, both in general and especially within climate modeling, it is important to develop quantum algorithms keeping the immense, existing classical supercomputing power in mind. This means, for example, taking full advantage of the available HPC infrastructure for performing the necessary pre-and post-processing of data to and from the quantum machines. For electronic structure problems, as in the case of modeling atmospheric reactions discussed above, HPC resources are needed for providing an initial guess for the quantum computer; in other words, they provide the best approximation to the true electronic structure that classical methods can provide, and refine it further on the quantum computer. This exemplifies the need for a broad, multidisciplinary approach to quantum advantage. We need to combine expertise in quantum algorithms, classical HPC algorithms, computer science, AI/ML, and specific domain expertise, also from the end-user side.

11 SWOT analysis

11.1 Strengths

- Quantum machines could be applied to generate data samples from classically difficult distributions [96].
- Proved exponential speed-up in at least one scenario [97].
- The climate modeling community deeply understands the problem at hand and the bottlenecks present, both from the efficiency and accuracy points of view.
- A recognized high-priority problem: resources available for finding solutions.

11.2 Weaknesses

- Data loading is a major obstacle for achieving exponential speed-up of some QML algorithms [36].
- Measurement error mitigation is strongly limited by the number of qubits and the circuit depth. [98].
- Quantum machines can be difficult to train due to the error correction scheme [99].
- Understanding of the applicability of quantum computing to climate modeling limited.
- Quantum-acceleration is presently not seen as a viable route due to the "big data" nature of digital twins.

11.3 Opportunities

• Major shift in the quality of quantum computers. NISQ machines may be available with less than 100 high-quality error-prone qubits.

- New applications of classical machine learning for quantum computing: compiling, mapping, control, error correction.
- Potential to utilize hybrid approaches that require a relatively small number of qubits (of the order on 10² logical qubits), thereby increasing feasibility.
- Progress in QC hardware and software capacity can enable more accurate models.
- Global drive for supporting hybrid HPC+QC software development.

11.4 Threats

- Fundamental lack of ability to control, mitigate, and correct sources of noise in the quantum machines.
- Novel classical algorithms inspired by quantum computing may outperform some pure quantum algorithms.
- Development of sufficiently powerful QC hardware/software delayed.
- Lack of long-term funding commitment to development, in case near-term gains do not live up to (inflated) expectations.

12 Conclusion

Quantum machines promise to solve a particular class of challenging computational problems faster and more efficiently than conventional machines. In computational complexity theory, the difficulty of computational problems can be measured. Hence, This study identifies climate-related problems and challenges that are intractable on classical supercomputers. However, quantum machines promise to find solutions faster and more energy efficient than their classical counterparts. We examined and assessed distinct quantum machines, including a quantum annealer, a quantum simulator, and universal quantum computers, for their practicality. Toward practical problems, we proposed climate change detection, climate modeling, and climate digital twin use-case instances. In particular, we analyzed and evaluated the hardness of our practical climate challenges based on the computational complexity theory and the computational time and energy consumption required.

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