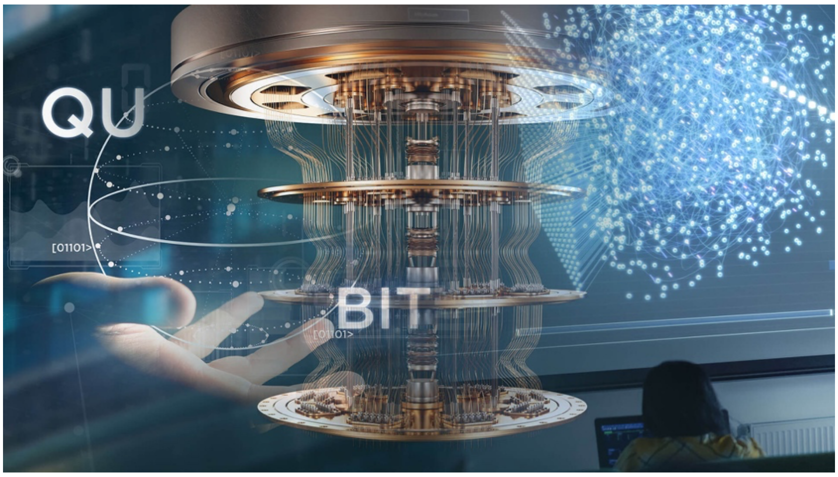

White Paper
on
Quantum Computing and Quantum Machine Learning for Climate Science

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Executive Summary

Climate change stands as one of the most formidable challenges of the 21st century, requiring innovative approaches to address the complexity of modeling the Earth's climate system, predicting future changes, and devising sustainable solutions. As classical computing approaches its limits in handling the intricate dynamics of climate systems, Quantum Computing (QC) and Quantum Machine learning (QML) are emerging as transformative technologies. These technologies offer the potential to revolutionize climate change efforts by introducing unprecedented computational power and advanced algorithms.

This white paper assesses the current state of QC and QML in climate-related research. It explores key applications, technological advancements, challenges, and future directions, with a particular emphasis on critical areas such as climate modeling, climate data forecasting, extreme event prediction, energy systems optimization, materials discovery, and predictive analytics.
Additionally, it explores the current limitations, future directions, and the anticipated impact of quantum technologies in mitigating and adapting to climate change.

Clearly, the aim of this White Paper is not to provide comprehensive overview of quantum computing and quantum machine learning—an unfeasible task given the breadth and complexity of the topics involved. Instead, its purpose is to highlight key aspects of the field and its application to climate change, also offering guidance on scientific journals that can be consulted for further, in-depth exploration of the subject.

The White Paper is divided into three parts: **Part I** and **Part II** focus on the role of **QC** and **QML** respectively in the development of Climate Change applications, while **Part III** presents the challenges of **QC** and **QML** and their possible solutions.

In the first part (**Part I**), after a short introduction (**Sect.1**) on the strategic role that Quantum Computing can play in the development of Climate Change applications, the challenges of climate change models are briefly summarized (**Sect.2**), followed by a short overview of Quantum Computing and its theoretical aspects (**Sect.3**). Finally, **Sections 4.1 to 4.4** describe the role that **QC** can play in various areas of Climate Change, particularly for climate modeling and simulation (**Sect.4.1**), the optimization of energy systems (**Sect.4.2**), environmental monitoring (**Sect.4.3**), and the development of efficient communication technologies due to their impact on climate change (**Sect.4.4**). For each of these sections, recent scientific contributions from literature are also reported and commented upon.

The second part (**Part II**) is dedicated to the strategic role that **QML** can play in Climate Data Forecasting (**Sect.5.1**), along with the prediction of climate hazards (**Sect.5.2**), climate monitoring (**Sect.5.3**), and in accelerating decarbonization (**Sect.5.4**). Recent scientific contributions from literature on the use of QML in the development of climate change applications are reported and commented upon (**Sect.5.5**). Finally, a specific section is dedicated to the description of the currently available QML software and simulation tools (**Sect.5.6**), analyzing the critical factors that need to be considered when choosing a specific tool (**Sect.5.6.1**).

The last part of the White Paper (**Part III**) is dedicated to analyzing the significant challenges that Quantum Computing and Quantum Machine Learning must overcome to fully achieve their potential.

The White Paper also contains 10 important **Appendices** for further details, in particular:

Appendices A to E provide references from scientific literature related to the topics discussed in Parts I and II.
Information on actively available quantum computers and quantum technologies is provided in **Appendices F and G,** respectively.

Appendix H offers an in-depth analysis of the Koopman operator, which can play a significant role in Quantum Computing and Quantum Machine Learning.

Appendix I provides an in-depth look at Variational Quantum Algorithms (VQA), an important and strategic class of quantum algorithms capable of solving complex problems using both classical and quantum computation.

Finally, **Appendix J** includes comments on the frequently mentioned Noisy Intermediate-Scale Quantum (NISQ) era, which refers to the current stage in the development of quantum computing, where quantum devices with around 50 to a few hundred qubits are available.

Given the rapid and continuous evolution of quantum computing and quantum machine learning technologies, this White Paper should be regarded as a living reference rather than a static document. In particular, the scientific literature cited herein reflects the state of research at the time of writing and is expected to evolve significantly. For this reason, the list of publications and technical references should be periodically reviewed and updated to ensure continued alignment with the latest peer-reviewed research and technological developments in the field.

Part I - Quantum Computing for Climate Change

1. Introduction

Climate change is one of the most pressing global challenges, requiring complex simulations and data processing to understand its intricacies and predict future scenarios.
The growing urgency of climate change mitigation requires innovative tools that can enhance predictive models, optimize resources, and generate novel solutions for reducing carbon emissions.
Traditional supercomputers, while powerful, struggle with the immense computational demands of climate modeling, which involves nonlinear dynamics, multiple variables, and chaotic systems. They are not able to efficiently solve the highly complex and multivariate problems that climate change poses, such as simulating the Earth's climate systems, managing energy resources, and analyzing vast datasets from satellites and sensors.
Quantum computing, based on the principles of quantum mechanics, leverages *superposition*, *entanglement*, and *interference* to solve complex problems exponentially faster than classical computers, showing promise in addressing problems that are otherwise intractable for classical supercomputers.

2. Challenges in Climate Models

Climate models are essential for understanding and predicting the behavior of Earth's climate system. These models simulate interactions between the atmosphere, oceans, ice, and land. They are based on solving partial differential equations (PDEs) to forecast how variables like temperature, humidity, and wind will evolve over time.
However, despite their sophistication, they face several challenges, that can be summarized in the following points:

Uncertainty in Climate Sensitivity

- *Definition*: Climate sensitivity refers to how much the Earth's temperature will increase in response to a doubling of carbon dioxide (CO_2) levels.
- *Challenge*: There is still uncertainty in predicting the exact response of the climate system to greenhouse gas emissions. Different models produce varying estimates, leading to a range of possible temperature increases.

Complexity of Earth Systems

- *Atmosphere, Oceans, and Land Interactions*: Climate models must account for complex feedbacks between different components of the Earth's system. Interactions between the atmosphere, oceans, cryosphere (ice sheets and glaciers), and land surface are difficult to represent fully, as they involve many small-scale processes.
- *Biosphere Feedbacks*: Feedback mechanisms such as changes in vegetation, carbon uptake by the oceans and forests, or permafrost thawing add further complexity, which is hard to model accurately.

Resolution Limitations

- *Spatial Resolution*: Models operate on grids that divide the Earth into segments. The size of these grid cells impacts the model's resolution. Current models often have grid sizes on the order of tens or hundreds of kilometers, which can limit the ability to simulate localized phenomena like storms or specific regional climate effects.
- *Temporal Resolution*: Some climate processes operate on very short timescales (e.g., thunderstorms), while others (e.g., ocean circulation) evolve over centuries. Capturing the wide range of timescales accurately is computationally demanding.

Cloud Representation

- *Cloud Formation and Behavior*: Clouds are one of the most challenging elements to model. They influence both warming (by trapping heat) and cooling (by reflecting sunlight), making them a crucial part of the climate system. Small errors in cloud representation can lead to significant differences in climate projections.
- *Sub-grid Scale Phenomena*: Cloud dynamics often happen at smaller scales than most climate model grid cells can capture, requiring approximations that introduce uncertainties.

Aerosols and Other Short-lived Forcings

- *Aerosol Impacts*: Aerosols, like soot or sulfate particles, affect the climate by reflecting or absorbing sunlight and influencing cloud formation. Their distribution is highly variable, and they have a much shorter atmospheric lifetime than greenhouse gases, making their effects more challenging to model.
- *Natural Variability*: Events like volcanic eruptions or wildfires release large quantities of aerosols and other particulates, which can temporarily cool the planet or disrupt weather patterns.

Non-linear Feedback and Tipping Points

- *Positive Feedback*: Certain processes, such as ice-albedo feedback, where melting ice reduces reflectivity and accelerates further warming, are difficult to predict in terms of when they will occur or how strong they will be.
- *Tipping Points*: Abrupt changes in the climate, such as the collapse of ice sheets or shifts in ocean circulation, are inherently difficult to model. These events may trigger significant, rapid changes, but their likelihood and timing are uncertain.

Data Availability and Quality

- *Historical Data Gaps*: Climate models rely on historical data to validate their predictions, but in many parts of the world, particularly in the oceans and the polar regions, long-term high-quality data is sparse or nonexistent.
- *Future Emissions Scenarios*: Predictions depend on assumptions about future human activity, such as fossil fuel use, technological advancements, and policy decisions. These are inherently uncertain, and models must use different scenarios to capture a range of possibilities.

Regional and Localized Predictions

- *Downscaling*: Global climate models often struggle to make accurate predictions at regional or local scales due to their coarse resolution. To address this, "downscaling" techniques are used, but these introduce their own uncertainties.
- *Extreme Events*: Predicting the frequency, intensity, and location of extreme events such as hurricanes, floods, or heatwaves remains a major challenge, as they are influenced by small-scale atmospheric and oceanic processes.

Computational Constraints

- *Processing Power*: Climate models require massive computational resources, especially high-resolution models or those running long-term projections. This limits how many simulations can be run and restricts sensitivity testing or scenario analysis.
- *Long-term Projections*: Simulating climate over centuries or millennia to understand the full impacts of greenhouse gases is computationally intense, leading to challenges in generating long-term projections.

Parameterization

- *Simplifying Complex Processes*: Many small-scale processes (e.g., turbulence, convection) cannot be directly simulated at the scale of global climate models and are instead approximated or "parameterized." These approximations introduce uncertainties and can differ across models.
- *Tuning*: Some models are "tuned" to match observed climate variables, which can lead to uncertainties when trying to predict future conditions under novel circumstances.

Model Uncertainty and Bias

- *Inter-model Differences*: Different models may produce different outcomes for the same scenario due to variations in the way they simulate processes. This creates a range of outcomes that increases uncertainty.
- *Model Biases*: Systematic errors in the models, such as overestimating or underestimating certain variables (e.g., precipitation or temperature), lead to biases that can propagate through projections.

Despite these challenges, climate models remain vital tools for understanding climate change, guiding policy, and planning adaptation strategies.
As climate models grow more detailed, the need for enhanced computational power becomes paramount. Anyway, advances in computing power, data collection, and scientific understanding continue to improve model accuracy over time.

Quantum Computing offers a new paradigm where large-scale simulations can be executed more efficiently. Indeed, as quantum computing emerges with its unique computational capabilities, researchers are increasingly investigating how quantum computing, in contrast to classical computing, could address pressing these challenges for generating accurate climate projections and informing effective policymaking to address climate change.

3. Overview of Quantum Computing and its Theoretical Background

Quantum computing is a rapidly developing field that leverages the principles of quantum mechanics to process information in ways fundamentally different from classical computing. At its core, quantum computing harnesses the phenomena of *superposition*, *entanglement*, and *quantum interference* making them theoretically capable of solving problems exponentially faster than classical computers.
Several quantum algorithms, such as Shor's algorithm for factoring and Grover's algorithm for search optimization, have demonstrated the potential of quantum speedup. While quantum computing is still in the experimental phase with noisy intermediate-scale quantum (**NISQ**) devices (see **Appendix J** for info on **NISC**), the technology is progressing rapidly.

- **Classical vs. Quantum Computing**
  - *Classical Computing*: Traditional computers use bits as the fundamental unit of information, which can be either 0 or 1. Operations on bits follow deterministic logic (AND, OR, NOT gates) to perform computations.
  - *Quantum Computing*: Quantum computers use *quantum bits* or *qubits*, which, unlike classical bits, can exist in a superposition of both 0 and 1 simultaneously due to the principles of quantum mechanics. This allows quantum computers to process a massive amount of information in parallel.

  In the following a short summary of quantum principles is reported.

- **Quantum Mechanical Principles**: The power of quantum computing arises from the following key principles of quantum mechanics:
  - *Quantum states*: Unlike classical bits, which are binary (0 or 1), qubits exist in a two-dimensional linear vector (Hilbert) space, allowing them to represent states of both $|0\rangle$ and $|1\rangle$ simultaneously. ($'|\quad\rangle'$ is the Dirac notation used to represent states in quantum mechanics). The two computational basis states of a qubit are expressed as:

    $$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}, |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$$

    So, the state of a qubit is a vector in a two-dimensional complex vector space. The special states $|0\rangle$ and $|1\rangle$ are known as computational basis states and form an orthonormal basis for this vector space.
  - *Superposition* and *entanglement*: Quantum computing operates on two fundamental principles of quantum mechanics: *Superposition* and *Entanglement.*
    - *Superposition*: Superposition extends the classical idea of a bit to its quantum counterpart, the qubit. While a traditional bit exists in only one of two possible states, a qubit can exist in both states at once due to superposition. When multiple qubits are combined, they form quantum registers. This ability to exist in multiple states simultaneously is the foundation of quantum computing’s remarkable power, allowing quantum computers to operate in many states at the same time rather than just one. A microscopic object can exist in a "hazy" state, occupying more than one position at once. Instead of being in a single location, the object is said to be in a "superposition," meaning it is, in some sense, in multiple places simultaneously. This "haziness" applies not only to spatial position but also to other physical properties such as energy, momentum, and unique quantum characteristics like "spin." When a superposition of states is measured, to which specific state it will collapse is unpredictable. In contrast to other branches of physics where the laws are deterministic—yielding a unique outcome for every experiment—the laws of quantum mechanics only provide the probability of each possible outcome. For

instance, a photon does not exist in a single, fixed position but rather in a superposition of many positions. This idea might seem counterintuitive, as our everyday experience suggests that objects are always in one place or another, never in multiple places at once. The reason we observe particles in a specific position is because measurement collapses the quantum superposition into a single classical state. The concept of superposition is what gives quantum computing its extraordinary potential. Classical computers operate in one state at any given moment. Now, imagine a computer existing in many states simultaneously and processing information across all those states at once. This would represent the ultimate form of parallel processing—something achievable only in the quantum realm. Although we do not directly observe superposition, when we measure it, the superposition collapses into a single, well-defined state. However, until that measurement is made, the object exists in many states at the same time.

From a mathematical point of view, a qubit can exist in a linear combination of both the 0 and 1 states, represented as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where α and β are complex numbers often referred as complex probability amplitudes and must satisfy:

$$|\alpha|^2 + |\beta|^2 = 1$$

In this equation, $|\alpha|^2$ represents the probability of the qubit collapsing to the state $|0\rangle$ upon measurement, while $|\beta|^2$ is the probability of collapsing to $|1\rangle$.

When measured, the qubit collapses to either 0 or 1 with probabilities $|\alpha|^2$and $|\beta|^2$, respectively. Superposition allows quantum computers to explore multiple solutions simultaneously.

This principle allows qubits to store and process information exponentially faster than classical bits, potentially leading to significant energy efficiency.

- *Entanglement*: Entanglement also plays a crucial role in quantum computing, as qubits can become entangled, meaning the state of one qubit is directly related to the state of another, regardless of distance. When a system S consists of two subsystems, S1 and S2, their states can become linked or entangled and the state of one subsystem cannot be described independently of the state of the other, as long as their evolution. Measuring one subsystem will instantly affect the state of the other, aligning them in a desired way. This leads to strong correlations that are essential for many quantum algorithms. A measurement performed on one system instantly affects the state of the other, no matter how far apart they are—what Albert Einstein famously called "spooky action at a distance". Entangled qubits act as a single system, providing exponential parallelism. Indeed, in quantum computing, entanglement is essential because it allows qubits to share information instantaneously. This interconnectedness enables powerful computational processes that are impossible in classical computers. For instance, when qubits are entangled, a change or measurement in one qubit immediately influences the state of its entangled partner, allowing quantum computers to process and transfer data with remarkable efficiency. In essence, entanglement is a key resource that distinguishes quantum computing from classical computing, enabling phenomena like instantaneous correlations and enhanced processing power.

- *Quantum Interference*: Quantum interference is a fundamental phenomenon in quantum mechanics where the probability amplitudes of different quantum states combine, leading to constructive or destructive interference. This behavior is essential for the operation of quantum computers and quantum phenomena in general. In quantum mechanics, particles such as electrons or photons can exist in a superposition of multiple states at once. Each of these possible states is described by a wave function or probability amplitude - a complex number whose squared magnitude represents the probability of observing the system in that specific state. In classical probability, probabilities are added directly. However, in quantum mechanics, *probability amplitudes* are combined, and when different paths (or quantum states) interfere, their amplitudes can result in two types of interference:
  - *Constructive Interference:* Occurs when amplitudes reinforce one another, increasing the probability of observing the system in a particular state.
  - *Destructive Interference:* Happens when amplitudes cancel each other out, decreasing or eliminating the probability of a specific outcome.

  This is analogous to the interaction of waves, such as water or light waves: when they are in phase, they amplify each other, leading to constructive interference, while out of phase, they cancel each other out, resulting in destructive interference.

  A classic example of quantum interference is the *double-slit experiment*, where particles such as photons or electrons are directed at a barrier with two slits. When both slits are open:
  - If the particles are treated as classical objects, they will pass through either one slit or the other, forming two distinct impact patterns.
  - In quantum mechanics, however, each particle behaves like a wave, passing through both slits simultaneously (a superposition of passing through slit 1 and slit 2). The wave functions for the two paths interfere, resulting in an interference pattern of alternating bright and dark regions, indicating where particles are more or less likely to be detected. This interference pattern is a direct consequence of the superposition of quantum states corresponding to each possible path the particle could take.

    Quantum interference is crucial to the operation of quantum computers and their ability to achieve speedups over classical systems. Here's why it's important:

- *Superposition of States:* As already said, in quantum computing, qubits can exist in a superposition of $|0\rangle$ and $|1\rangle$ states, allowing a quantum computer to process many inputs simultaneously by evolving multiple quantum states at once.

- *Quantum Algorithms:* Algorithms like Grover's and Shor's rely on quantum interference. For instance, in Grover's algorithm, destructive interference reduces the amplitude of incorrect answers, while constructive interference amplifies the correct one, increasing its probability during measurement.

- *Quantum Gate Operations:* Quantum gates (such as the *Hadamard* and *controlled-NOT* gates) modify qubit amplitudes to manipulate quantum states. These gates harness interference to favor certain computation paths, leading to the desired outcomes.

- *Speedup Mechanism:* Quantum interference allows quantum algorithms to explore multiple computational paths at once, eliminating incorrect solutions through destructive interference and amplifying correct ones via constructive interference. This mechanism contributes to the significant speedup seen in specific quantum problems.

In Grover's search algorithm (see below), quantum interference is utilized to search an unsorted database faster than classical algorithms. The process begins by creating a superposition of all possible solutions. Then, through a series of iterative steps:

- *Oracle calls* flip the sign of the amplitude associated with the correct solution, effectively marking the correct answer.
- The *Grover diffusion operator* (which performs an inversion about the mean) applies constructive interference, increasing the amplitude of the correct answer.
- Simultaneously, *destructive interference* reduces the amplitudes of incorrect solutions.

After enough iterations, the amplitude of the correct solution becomes large enough to be measured with high probability.

The *Quantum Fourier Transform (QFT*) (see below) relies on quantum interference as well. It maps quantum states to their frequency components through a sequence of Hadamard and controlled phase gates. These operations manipulate the amplitudes of qubits, causing interference between different computational paths. This interference is key to extracting periodicity in algorithms such as Shor's algorithm.

Although quantum interference has similarities to classical wave interference (like light and sound waves), in quantum mechanics, interference involves probability amplitudes rather than physical waves.

This distinction gives rise to non-intuitive phenomena such as superposition and wave function collapse upon measurement.

In conclusion, Quantum interference is a fundamental phenomenon that enables quantum systems to behave in ways classical systems cannot. By harnessing interference, quantum computers can enhance the probabilities of correct outcomes and suppress incorrect ones. This allows for efficient solutions to complex problems, such as factoring large numbers or searching unsorted databases. Without interference, quantum algorithms like Grover's search or Shor's factorization wouldn't outperform their classical counterparts.

- *Measurement*: Quantum measurement is a fundamental process in quantum mechanics that refers to the act of observing or measuring a quantum system, which affects the system in a unique way. Unlike classical systems, where measurement simply reveals an already well-defined property of the system, in quantum mechanics, measurement plays an active role in determining the state of the system.
  In quantum mechanics, measurable quantities (such as position, momentum, or the spin of a particle) are represented by mathematical operators called *observables*. Each observable has a set of *eigenstates*, which are the possible states the system can collapse into when that observable is measured. For example, the observable corresponding to measuring the state of a qubit has two eigenstates: $|0\rangle$ and $|1\rangle$. When a measurement is performed, the system collapses into one of these eigenstates. The *Born rule* is a principle in quantum mechanics that provides the probabilities of different measurement outcomes. It states that the probability of obtaining a specific measurement result is the square of the absolute value of the probability amplitude for that result.
  As already said, in quantum mechanics, particles like electrons, photons, or qubits (in quantum computing) can exist in a superposition of multiple states simultaneously. A qubit can be in a superposition of the basis states $|0\rangle$ and $|1\rangle$, represented as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

  where α and β are complex numbers often referred as complex probability amplitudes.
  When a measurement is performed on a quantum system, the system's *wave function* collapses to one of the possible *eigenstates* of the observable being measured. For example, if the state of a qubit is measured, it will collapse into either $|0\rangle$ or $|1\rangle$, and following *Born rule,* the probabilities are determined by the squared magnitudes of the corresponding amplitudes:

$$P(|0\rangle) = |\alpha|^2 \text{ , } P(|1\rangle) = |\beta|^2$$

  Then for a quantum state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, the probability of measuring $|0\rangle$ is $|\alpha|^2$ and the probability of measuring $|1\rangle$ is $|\beta|^2$.
  The measurement outcome is probabilistic, and the wave function no longer remains in a superposition after the measurement-it collapses to a definite state corresponding to the measurement result.

A crucial aspect of quantum measurement is that it *disturbs* the system. Before the measurement, the system exists in a superposition of states, but once measured, it collapses into a definite state. After this collapse, the system no longer retains information about the original superposition. This disturbance is a consequence of the *Heisenberg uncertainty principle*, which states that certain pairs of properties (like position and momentum) cannot both be measured precisely at the same time.
In conclusion, quantum measurement is a unique and non-classical process where the act of observing a system plays a central role in determining its outcome. Measurement causes the collapse of a quantum system's superposition into one of its possible states, and the probabilities of the outcomes are governed by the quantum state's probability amplitudes. Quantum measurement is not only key to understanding fundamental physics but also crucial for practical applications, such as quantum computing and quantum communication.

- **Quantum Gates and Circuits:** Similar to classical logic gates, quantum computers use *quantum gates* to manipulate *qubits*. However, these gates are *unitary operators* that preserve the probability amplitudes.

    - *Common Quantum Gates*

        - *Hadamard Gate (H)*: Creates a superposition state by applying equal probabilities to both 0 and 1.

        - *Pauli-X, Y, Z Gates*: Analogous to classical NOT gates, these gates apply specific transformations to qubit states.

        - *Controlled-Not Gate (CNOT)*: Entangles two qubits by flipping the second qubit (target) if the first qubit (control) is 1.

        - *Phase Gates*: Shift the phase of a qubit's state.

    - *Quantum Circuits*: Quantum algorithms are implemented through circuits made up of a series of quantum gates. Quantum circuits evolve qubit states over time, eventually producing an output through measurement.

- **Quantum Algorithms:** Several algorithms have been developed that take advantage of quantum mechanical principles to outperform their classical counterparts in specific tasks.

    - *Grover's Algorithm*: is one of the first quantum algorithms, designed to solve unstructured search problems faster than any known classical algorithm. It is particularly useful for searching through an unsorted database or finding solutions to certain types of computational problems where brute-force searching is needed. Discovered by Lov Grover in 1996 it represents one of the most important algorithms in quantum computing due to its quadratic speedup over classical algorithms. Suppose we have an unsorted list of *n* elements, and we are trying to find a particular element in the list. A classical algorithm would check the first entry, then the second, and would continue until the object is found or all *n* elements are checked. In the worst-case scenario, the algorithm examines all *n* entries. This gives a time complexity of O(n). Now, imagine a quantum computer using superposition. Instead of looking at one entry after another, it can search all entries simultaneously, leading to a significant speedup. Such a quantum computer could find the object in *n* queries. Grover's algorithm can solve this search problem in $O(\sqrt{n}$ time, compared to $O(n)$ classically, providing a quadratic speedup compared to classical algorithms.

- *Shor's Algorithm*: Shor's algorithm is one of the most famous and impactful quantum algorithms, discovered by Peter Shor in 1994. It solves the problem of integer factorization exponentially faster than the best-known classical algorithms. This breakthrough has significant implications for cryptography, especially for public-key encryption systems like RSA, which rely on the difficulty of factorizing large integers. Given a large composite integer *N*, the goal is to find its prime factors. For instance, if *N=15* the factors are 3 and 5. While factoring small integers is trivial, factoring very large numbers (with hundreds or thousands of digits) is computationally hard using classical algorithms. This difficulty underpins the security of widely used encryption schemes. The best-known classical algorithm for factorizing large numbers is the *General Number Field Sieve (GNFS)*, which runs in sub-exponential time

$$O\left(e^{(c(logN)^{\frac{1}{3}}(loglogN)^{\frac{2}{3}}}\right)$$

where *N* is the number to be factored. While this is better than brute force (which runs in exponential time for an *n-bit* number), it is still infeasible for very large numbers, like those used in RSA encryption.

Shor's algorithm factors an *n-bit* integer *N* in polynomial time $O(n^3)$, which is exponentially faster than any known classical algorithm. Specifically, it uses *quantum phase estimation* and the *Quantum Fourier Transform (QFT)* to find the period of a function related to the factors of *N*, from which the factors can be derived. Shor's algorithm builds on earlier quantum algorithms, such as Deutsch, Deutsch-Jozsa, and Simon's periodicity algorithm. While these early algorithms solve more abstract problems, they offer valuable insights into the principles of quantum software design. This algorithm can efficiently factor large integers into primes, providing an exponential speedup over classical factoring algorithms.

- *Quantum Fourier Transform (QFT)*: QFT provides an efficient way to compute the discrete Fourier transform, crucial for solving problems like period finding. QFT is the quantum analogue of the classical Discrete Fourier Transform (DFT). It's a fundamental algorithm in quantum computing and plays a crucial role in many quantum algorithms. The QFT transforms a quantum state into a superposition of its frequency components, which is analogous to how the classical Fourier transform decomposes a signal into its constituent frequencies.

From a mathematical point of view, given a quantum state $|x\rangle$, where x is an *n-bit* integer (i.e., $x \in \{0,1, \dots 2^{n-1}\}$), the Quantum Fourier Transform is defined as:

$$QFT(|x\rangle) = \frac{1}{\sqrt{N}} \sum_{y=0}^{N-1} e^{2\pi i \frac{x \cdot y}{N}} \; |y\rangle$$

where:

$N = 2^n$ is the total number of possible states (the size of the computational basis.

$e^{2\pi i \frac{xy}{N}}$ is the complex phase factor associated with the transformation, representing a rotation in the complex plane.

In essence, the QFT transforms the computational basis state $|x\rangle$ into a superposition of all possible basis states $|y\rangle$, weighted by complex phase factors determined by $x \cdot y$.

It should be noted that, given a vector of size *N*, a *Classical Discrete Fourier Transform (DFT)* computes the frequency representation of that vector. The *classical DFT* requires $O(N)$ time using the standard algorithm, or $O(NlogN)$ using the *Fast Fourier Transform (FFT)*. The *Quantum Fourier Transform (QFT)*, on the other hand, acts on quantum states and requires only $O(n^2)$quantum gates (where n is the number of qubits, and $N = 2^n$). This is exponentially faster compared to the classical FFT for large *N*.

- *Variational Quantum Algorithms (VQE, QAOA)*: These algorithms are designed to run on noisy intermediate-scale quantum (NISQ) devices, combining quantum circuits with classical optimization techniques to solve practical problems such as optimization, chemistry, and machine learning tasks. More info on *Variational Quantum Algorithms* is reported in ***Appendix I***.

- **Quantum Computing Models:** Several theoretical models define how quantum computation can be structured:

  - *Gate-Based Quantum Computing*: The most widely studied model, where quantum algorithms are represented by circuits composed of quantum gates.

  - *Adiabatic Quantum Computing (AQC)*: A different model where computation is performed by slowly evolving a quantum system from an initial ground state to a final ground state that encodes the solution. AQC is theoretically equivalent to the gate model but operates on different principles.

  - *Quantum Annealing*: A special case of AQC, used to solve optimization problems by finding the global minimum of a function.

- **Quantum Error Correction:** One of the significant challenges in quantum computing is *quantum decoherence* and *noise*, which arise due to the fragile nature of qubit states. Quantum error correction codes (such as the *Shor Code*, *Steane Code*, and *Surface Codes*) have been developed to protect quantum information from errors.

  - *Fault-Tolerant Quantum Computing*: A critical goal for the field is to develop quantum computers that can perform large-scale computations reliably by implementing error-correcting codes that mitigate noise.

- **Quantum Computing Platforms:** Various physical systems are being explored as potential platforms for building quantum computers, including:

  - *Superconducting Qubits*: These qubits are based on superconducting circuits that exhibit quantum properties at very low temperatures.

  - *Trapped Ions*: Trapped ion quantum computers use ions trapped in electromagnetic fields and manipulated with lasers. They have high-fidelity gate operations and long coherence times.

- *Photonic Quantum Computers*: These use photons to encode qubits and can leverage the speed of light for fast information transfer.

- *Topological Quantum Computing*: A more theoretical approach, which aims to encode *qubits* in *anyons*, particles that exhibit topological properties, providing inherent error resistance.

More information on Available Quantum Computers and related Quantum Technologies can be found in **Appendices F and G**.

Furthermore, for a deeper understanding of the principles of quantum computing, it is recommended to consult the following books and their related bibliographic:

Title: *Quantum Computing for Computer Scientists*
Authors: Noson S. Yanofsky, Mirco A. Mannucci
Publisher: Cambridge University Press
Publication Year: 2008
ISBN: 978-0521879965

Title: *Quantum Computation and Quantum Information*
Authors: Michael A. Nielsen & Isaac L. Chuang
Publisher: Cambridge University Press
Publication Year: 2010
ISBN: 978-1-107-00217-3

These books provide a broad perspective on the basic principles of quantum computing and an entryway for further investigation of the latest research literature.

- **Current Challenges and Future Outlook**

  - *Noisy Intermediate-Scale Quantum (NISQ) Era*: The current generation of quantum devices is noisy and error-prone, limiting the types of algorithms that can be run efficiently. The focus is on developing practical algorithms that can be implemented on these imperfect machines. More information on NISQ can be found in **Appendix J**.

  - *Quantum Supremacy*: Achieved in 2019 by Google, this milestone demonstrated that quantum computers could solve certain problems faster than classical supercomputers. However, the task solved (random circuit sampling) was not practically useful, and much work remains to achieve practical quantum advantage.

  - *Scalability*: Building a large-scale, fault-tolerant quantum computer is the ultimate goal, requiring breakthroughs in qubit coherence, error correction, and qubit interconnects.

In conclusion, Quantum Computing represents a paradigm shift in computation, with the potential to revolutionize fields such as cryptography, materials science, machine learning, and more. While there are significant challenges to overcome, the theoretical foundations of quantum mechanics provide a solid basis for future advancements in this exciting and rapidly growing field.

4. Quantum Computing for Climate Change

Quantum computing (QC) has recently garnered substantial attention in data science and computational problem-solving, with promising applications in addressing climate change.

Key areas where QC could play a transformative role include:

- **Climate Modeling and Simulation**: climate models are complex systems that simulate interactions between the atmosphere, oceans, and land. These models rely on solving non-linear partial differential equations (PDEs) across massive datasets, a computationally expensive process. QC offers the potential to significantly reduce the time required for climate simulations, by solving complex equations more efficiently, so allowing for more accurate models of Earth's systems.
  Moreover, Quantum Computers (using quantum algorithms, such as quantum Monte Carlo), can tackle problems involving high-dimensional spaces (like weather patterns and ocean currents), chaotic behaviors and probabilistic phenomena that are currently intractable for classical systems.

- **Optimization of Energy Systems:** Quantum Computing's ability to solve optimization problems at scale has implications for managing energy systems, which is crucial for climate mitigation. Renewable energy sources like solar and wind are intermittent, creating challenges for grid optimization and energy storage. Quantum optimization algorithms can help balance energy supply and demand in real-time, optimizing power grids and energy storage solutions to maximize the use of renewable energy. Additionally, Quantum Computers can optimize the design and operation of carbon capture systems, reducing the carbon footprint of industrial processes and energy generation. QC can optimize complex energy systems such as electricity grids, renewable energy resources, and storage systems. Using quantum annealing and variational quantum algorithms, it is possible to solve complex optimization problems like reducing carbon emissions or optimizing renewable energy supply networks. Additionally, QC's optimization algorithms present solutions for reducing energy consumption and emissions in transportation and contribute to advancements in lightweight material development and battery design. Finally, QC's combinatorial optimization abilities also enable better resource allocation for renewable energy networks and carbon capture infrastructures.

- **Material Science for Sustainable Technologies:** developing new materials for clean energy technologies— such as more efficient solar cells, batteries, and catalysts for hydrogen production —can be accelerated using QC. Simulating molecular interactions and designing materials at the quantum level holds great promise for breakthroughs in energy efficiency and storage. Quantum simulations allow for accurate predictions of molecular properties and behaviors, making QC ideal for discovering new materials for renewable energy technologies that could revolutionize clean energy production and storage. Moreover, in the field of materials science, QC aids in designing eco-friendly construction materials, while also contributing to the reduction of carbon emissions from cement production.

- **Quantum Sensing:** quantum sensing refers to the use of quantum phenomena, such as *superposition* and *entanglement*, to measure physical quantities with unprecedented precision. In the context of climate change, quantum sensing offers significant advantages for environmental monitoring and the measurement of climate variables. QC's enhanced data processing capabilities can be utilized for real-time global carbon monitoring, by processing vast quantities of satellite and sensor data. This can improve decision-making for emission reduction strategies by governments and industries worldwide.

- **Quantum Communication technologies:** Quantum communication, particularly through quantum key distribution (QKD), offers a way to ensure secure transmission of climate-related data. Given the growing reliance on digital infrastructure for climate monitoring, resource management, and environmental governance, ensuring data security is critical.

The following sections delve into the specific roles of QC in these major application areas.

4.1 Quantum Computing for Climate Modeling and Simulation

Quantum Computing holds tremendous potential for enhancing climate modeling and simulation, offering the capability to process vast amounts of data and simulate highly complex systems more efficiently than classical computers. Climate models require the analysis of a wide array of interdependent processes that occur in the atmosphere, oceans, cryosphere, and biosphere, and quantum computing could provide breakthroughs in this field.

- **QC for Simulating Complex Climate Systems**
  Climate models are inherently complex because they involve multiple interacting systems operating on different spatial and temporal scales. Accurately simulating the Earth's climate requires massive computational power to model these intricate interactions, including:

  - *Atmospheric dynamics*: Modeling the movement of air masses, temperature changes, and energy exchanges.

  - *Ocean currents*: Understanding how ocean circulation patterns distribute heat and impact global weather.

  - *Cloud formation and behavior*: Clouds have a significant but difficult-to-predict impact on climate due to their role in both cooling (by reflecting sunlight) and warming (by trapping heat).

Quantum computers, with their ability to process exponentially large datasets and perform complex simulations in parallel, could dramatically improve the accuracy of these models. They excel at solving the types of differential equations that describe fluid dynamics, heat transfer, and the chemical processes involved in climate systems, providing more detailed and accurate projections.

- **QC for Improving Resolution and Detail**
  Classical climate models often suffer from limited resolution due to the constraints of current computational power. This means that small-scale processes, such as cloud microphysics or localized weather phenomena, are often approximated, leading to uncertainties in predictions. QC can simulate these small-scale processes at higher resolutions, potentially capturing more detailed dynamics, leading to:

  - More accurate predictions of extreme weather events (e.g., hurricanes, heatwaves, and floods).

  - Better understanding of regional climate effects, which is crucial for localized climate adaptation strategies.

- Enhanced ability to simulate feedback loops and tipping points, such as ice-albedo feedback or the collapse of ocean currents.

These improvements in model resolution could provide critical insights for policymakers and businesses to develop more effective climate mitigation and adaptation plans.

- **QC for Faster Processing of Climate Data**
  One of the significant bottlenecks in climate modeling is the sheer amount of data required to simulate future climate scenarios. Data from satellites, ground-based sensors, and historical climate records must be processed to initialize models and validate their predictions. Quantum computers can process these massive datasets faster than classical computers, speeding up the time it takes to run climate simulations. This allows scientists to:

  - Run more frequent simulations, exploring a wider range of possible future scenarios.
  - Test a larger number of variables to assess uncertainties in model predictions.
  - Improve the accuracy of near-term climate forecasts, which are important for guiding short-term policy decisions.

By reducing the computational time needed to simulate climate processes, QC could significantly accelerate climate research and lead to more timely insights.

- **QC for Modeling Nonlinear Climate Feedback and Tipping Points**
  Climate systems are characterized by numerous nonlinear feedback mechanisms, which can amplify or dampen the effects of climate change. This feedback are difficult to model due to their complexity and potential to cause abrupt changes in the system.
  Examples include:

  - *Ice-albedo feedback*: As ice melts, the Earth's surface absorbs more sunlight, leading to further warming and more ice melt.
  - *Permafrost thawing*: The thawing of permafrost releases methane, a potent greenhouse gas, which accelerates warming.
  - *Ocean circulation* shifts: Changes in ocean circulation, such as the weakening of the Atlantic Meridional Overturning Circulation (AMOC), could drastically alter global weather patterns.

  The capability of Quantum Computers to handle complex, multi-variable systems allows them to simulate this nonlinear feedback more accurately. By doing so, they can help scientists better predict potential "tipping points" where the climate system could shift rapidly into a new state. This is critical for understanding the risks of sudden and irreversible changes in the climate.

Conclusion
Climate modeling involves predicting Earth's climate through grid cells with varying spatial and temporal resolutions. Although finer resolutions yield better results, they come with higher computational costs. Quantum algorithms, such as **Variational Quantum Algorithms** (**VQAs**) for

solving partial differential equations (PDEs), demonstrate superior expressive power compared to classical methods in solving climate PDEs. Despite the challenges posed by the **NISQ** (Noisy Intermediate-Scale Quantum) era, quantum computers may complement classical resources by handling specific NWP or climate model tasks that require higher resolution.
Then, quantum computing has the potential to revolutionize climate modeling and simulation by improving the accuracy, resolution, and speed of climate predictions. With its ability to handle complex, multi-variable systems and simulate nonlinear feedback, quantum computing could offer deeper insights into the Earth's climate system, enhance predictions of extreme weather events, and provide more reliable long-term forecasts. These advances could play a vital role in shaping global climate policy and guiding efforts to mitigate and adapt to climate change.

*Additional details on Variational Quantum Algorithms (**VQAs**), along with relevant scientific references, can be found in **Appendix I**.*

*Additional details on the **NISQ** era can be found in **Appendix J**.*

4.1.1 Recent scientific contributions on QC for Climate Modeling and Simulation

Numerous contributions on the application of quantum computing to climate modeling and simulation have appeared in scientific journals in recent years. In particular:

In **[Schwabe, M.; Pastori, L.; de Vega, I.; Gentine, P. et al, (2025)]**, building on the work of hybrid (physics + AI) ESMs, the additional potential of further improving and accelerating climate models with quantum computing and obstacles facing current quantum computing paradigms are discussed. It is also shown how a strong interdisciplinary collaboration between climate scientists and quantum computing experts is needed to overcome these hurdles and harness the potential of quantum computing.

In **[Liu, Y. Y.; Chen, Z.** et al., **(2024)]**, a numerical method based on the variational quantum algorithm to solve potential and Stokes flow problems is presented. This work brings quantum computing to the field of computational fluid dynamics, showing how, by virtue of quantum advantage over classical methods, promising advances in solving large-scale fluid mechanics problems of engineering interest may be prompted.

In **[Syed Masiur Rahman et al., (2024)]**, the potential role of QC in advancing climate change-related research, focusing on areas where quantum supremacy is expected to have the most impact is critically examined.

In **[Soronzonbold Otgonbaatar, Olli Nurmi, Mikael Johansson, et al., (2023)]**, a survey on existing literature that applies quantum computing to solve climate change and sustainability-related problems is given.

In **[Díez-Valle et al., (2023)]**, it is shown that quantum optimization could enhance weather and climate models by improving parameter tuning and uncertainty quantification processes. It is shown that techniques, such as the *Quantum Approximate Optimization Algorithm (QAOA)*, could optimize parameters in models like the Weather Research and Forecasting (WRF) model, leading to better regional simulations and improved model performance across various climatic regimes and spatial scales.

In **[Tennie and Palmer (2023)]**, a quantum algorithm for solving non-linear differential equations in numerical weather prediction models is proposed. The authors suggest that integrating stochastic differential equations with quantum solvers the efficiency and accuracy of weather modeling could be enhanced.

In **[Giani and Goff-Eldredge, (2022)]**, it is shown that quantum computers could run global climate simulations faster and with higher precision, enabling more accurate predictions of climate change impacts, offering deeper insights into complex climate systems, such as atmospheric circulation patterns and ocean dynamics, which are critical for climate research.

In **[Frolov (2017]**, the constraints that limit the performance of silicon transistor-based supercomputers and hinder the development of numerical weather and climate prediction models are explored. This research highlights the shift from fundamental science to technical solutions, with the computing industry aiming to develop a general-purpose quantum computer in the near future. The study suggests that the effectiveness of quantum computations and quantum computers for addressing numerical weather and climate prediction problems needs careful evaluation.

More references on the use of Quantum Computing for Climate Change Modeling and Simulation can be found ***in Appendix A****.*

4.2 Quantum Computing for the Optimization of Energy Systems

Quantum Computing has the potential to revolutionize the optimization of energy systems by leveraging its ability to process large amounts of data and solve complex optimization problems more efficiently than classical computers.
Moreover, Quantum Computing offers immense potential for advancing material science, especially in the development of sustainable technologies. Its ability to model and simulate complex quantum systems—such as atomic and molecular interactions—makes it ideal for studying new materials that are difficult to investigate using classical computing. These materials could enable breakthroughs in renewable energy, energy storage, carbon capture, and efficient catalysis, all of which are critical for sustainability.

In the following the areas in which Quantum Computing can be applied in **energy system optimization** and **sustainable technologies** are reported.

- **Energy system optimization and management**

  Quantum computing can optimize the operation and management of electrical grids, particularly in scenarios involving:

  - *Power Flow Optimization*
    Managing the distribution of electricity across a grid to minimize losses and improve efficiency. Classical methods use complex algorithms like linear programming or heuristic approaches, but quantum computing can handle the nonlinearities and combinatorial complexities more effectively.

  - *Load Balancing and Demand Forecasting*
    Quantum algorithms can enhance demand prediction accuracy and optimize load balancing in real-time, reducing energy waste and improving reliability.

        - For example, *Quantum annealing* algorithms for *Optimal Power Flow* (*OPF*) can minimize power losses, reduce grid congestion, and ensure voltage stability across different time horizons, crucial for modern grids integrating renewable sources like wind and solar.

- *Renewable Energy Integration*
  As the share of renewable energy sources (like solar and wind) in grids increases, so does the complexity of managing intermittent generation and ensuring reliable supply.

  Quantum computing can help with:

    - *Unit Commitment Problem (UCP)*: this involves determining the most cost-effective combination of power generation units that should be active at any time while adhering to demand and operational constraints. Quantum computers could solve this problem more efficiently by searching through vast solution spaces faster than classical approaches.

    - *Energy Storage Optimization*: efficiently managing energy storage systems, such as batteries, is crucial to balance renewable energy supply with fluctuating demand. Quantum algorithms can help determine optimal charge/discharge cycles to maximize the use of renewable energy.
        - For example, by solving optimization problems with complex constraints, quantum-enabled Battery Optimizations could enhance energy storage systems, making them more cost-efficient and improving the overall grid's reliability in managing renewable energy.

- *Energy Market Optimization*
  In deregulated energy markets, optimizing the trading of energy in real-time markets, day-ahead markets, and futures markets is computationally intense.

  Quantum computing can aid in:

    - *Optimal Bidding Strategies*: Quantum computers can optimize bidding strategies for energy producers and consumers in competitive markets, considering real-time price changes, supply-demand balance, and environmental constraints.

    - *Risk Analysis and Portfolio Optimization*: Energy companies can use quantum computers to optimize energy portfolios, considering the risks of fluctuating prices and changes in demand.
        - For example, Quantum-assisted Trading Algorithms can improve decision-making processes in energy trading by finding optimal strategies in less time compared to classical models, leading to better prices and improved profits.

- *Optimization of Supply Chains and Energy Infrastructure*
  The logistics of energy supply chains, including fuel transportation, refinery operations, and delivery of power, involve multiple stages and actors.

  Quantum computing can:

- *Optimize Supply Chain Operations*: Quantum algorithms can streamline fuel supply chains, optimizing routing, storage, and transport to minimize costs and carbon emissions.

- *Infrastructure Planning*: Quantum computers can optimize the location and scale of new energy infrastructure, such as renewable power plants, based on factors like geography, weather patterns, and grid connectivity.

- *Climate and Energy System Modeling*
  Energy system models that consider climate variables can become highly complex, requiring significant computational resources.
  Quantum computing can enable better modeling and simulation of:

  - *Climate-Energy Interaction*: Quantum algorithms can handle the massive datasets required for climate forecasting and predict how climate change impacts energy systems, allowing for more proactive strategies in renewable energy adoption and grid management.
    - For example, Quantum-enhanced Climate Models would allow scientists to simulate energy systems under different climate scenarios with higher accuracy, improving policy and investment decisions regarding energy infrastructure.

- *Efficient Optimization Algorithms*
  The two main quantum algorithms applicable to energy system optimization include:

  - *Quantum Annealing*: Well-suited for solving combinatorial optimization problems, such as scheduling, grid management, or logistics in energy systems. Quantum annealers from companies like D-Wave are already being explored for these purposes.

  - *Quantum Approximate Optimization Algorithm (QAOA)*: This algorithm can solve constrained optimization problems, such as minimizing the cost of energy while ensuring supply reliability. It's particularly useful for high-dimensional problems where classical algorithms struggle.

- *Quantum Hardware Limitations*
  Current quantum computers are still in the "noisy intermediate-scale quantum" (NISQ) era (*see Appendix J for more detail on NISC*), meaning they are susceptible to errors and have limited qubit counts. However, as the technology matures, these limitations will gradually reduce, enabling more complex and practical applications.

- *Algorithm Development*
  Specialized quantum algorithms for energy optimization are still being developed. Significant progress is required before quantum computing becomes a mainstream tool in the energy sector.

- *Integration with Classical Systems*

Hybrid systems that combine quantum and classical computing are likely to emerge in the near term, using quantum computing to accelerate specific sub-tasks while classical computers handle the rest of the process.

- **Sustainable technologies**
    - *Design of New Materials for Energy Storage*
        - *Batteries and Supercapacitors*: Quantum computing can help simulate and discover new materials for high-efficiency batteries, such as solid-state electrolytes, advanced lithium-ion batteries, or alternative battery chemistries like sodium-ion and aluminum-ion batteries. This could lead to safer, longer-lasting energy storage solutions for renewable energy grids and electric vehicles.
        - *Material Discovery*: Quantum computers can simulate quantum behaviors in materials, such as the electron dynamics in battery electrodes, leading to the discovery of new materials with superior energy density, fast-charging capabilities, and longer lifespans.
            - For example: using Quantum Simulations of Battery Materials, Quantum computers could model the behavior of lithium ions in battery materials more accurately, leading to the discovery of better-performing and more sustainable materials for future batteries.
    - *Efficient Catalysis for Green Chemistry*
        - *Catalyst Discovery*: catalysts are critical for chemical reactions in industries such as manufacturing, energy, and transportation. Quantum computers can simulate catalytic processes at the atomic level, enabling the discovery of new, highly efficient catalysts that can reduce energy consumption and minimize the need for harmful chemicals in processes like hydrogen production, fuel synthesis, and carbon capture.
        - *Ammonia Production (Haber-Bosch Process)*: Quantum computing could lead to new catalysts for more energy-efficient production of ammonia, an essential component for fertilizers, which currently consumes significant amounts of energy globally.
            - For example: using Quantum Simulations for Hydrogen Production, Quantum computers can help design catalysts that improve the efficiency of water-splitting reactions for hydrogen production, reducing the need for rare or expensive materials like platinum.
    - *Photovoltaic Materials for Solar Energy*
        - *Optimizing Solar Cells*: Quantum computing can simulate the electronic properties of photovoltaic materials, helping to discover more efficient materials for solar cells. This includes investigating materials like perovskites, which have shown

great potential for high-efficiency, low-cost solar energy conversion but still face stability and scalability challenges.

- *Next-Generation Solar Materials*: by leveraging quantum mechanics simulations, researchers can better understand exciton dynamics and electron-hole interactions in novel materials, pushing the limits of solar energy efficiency beyond what classical computers can achieve.
  - For example, in the production of Perovskite Solar Cells, Quantum computers could model complex phenomena such as defect states and stability mechanisms in perovskite solar cells, leading to materials with higher efficiencies and longer lifetimes.

- *Materials for Carbon Capture and Storage (CCS)*

  - *Carbon Adsorption Materials*: Quantum computing can be used to design new materials for carbon capture, including metal-organic frameworks (MOFs) and zeolites. These materials need to be highly selective and efficient in adsorbing CO_2 from the atmosphere or industrial emissions.

  - *Simulating Adsorption Properties*: Quantum computers can simulate how different molecular structures interact with CO_2 at the atomic level, enabling the design of materials that are optimized for carbon capture and more cost-effective than current technologies.
    - For example, Quantum computers can help discover or improve MOFs that selectively bind CO_2 molecules, facilitating carbon sequestration and removal technologies.

- *Superconductors for Energy Efficiency*

  - *High-Temperature Superconductors*: Superconductors offer the potential to transmit electricity without loss, which could drastically improve the efficiency of power grids. Quantum computers are well-suited to simulate the electron pairing mechanisms that lead to superconductivity, especially in high-temperature superconductors, which are still not fully understood.

  - *Quantum Simulations for Power Grids*: Finding materials that exhibit superconductivity at room temperature would revolutionize energy transmission and storage, significantly reducing energy loss and improving the efficiency of energy distribution systems.
    - For example: Quantum computing can be used to produce efficient Room-Temperature Superconductors, by understanding the quantum mechanics behind electron pairing in superconducting materials, allowing to accelerate the discovery of materials that conduct electricity without resistance at higher temperatures.

- *Sustainable Polymers and Plastics*

  - *Biodegradable and Recyclable Materials*: Quantum computing can assist in the design of new polymers that are more easily recyclable or biodegradable, helping to reduce the environmental impact of plastics. Simulating the polymerization processes at the quantum level can provide insights into how to control material properties like strength, flexibility, and degradation.

- *Green Chemistry for Plastics*: Quantum simulations could guide the development of new polymerization catalysts that enable more sustainable production of plastics from renewable resources, like biomass, instead of petroleum.
  - For example, Quantum computing cab be used to produce Biodegradable Plastics, by simulating the interaction of biodegradable materials with different environments, helping to design polymers that degrade faster in natural settings, thereby reducing plastic pollution.

- *Fuel Cells and Hydrogen Economy*

  - *Fuel Cell Materials*: Quantum computing could help develop more efficient proton exchange membranes (PEMs) or new catalysts for fuel cells, which are crucial for generating clean energy through hydrogen. Better fuel cell materials could lead to more efficient hydrogen production, storage, and utilization.

  - *Hydrogen Storage Materials*: Quantum computers can aid in finding lightweight, high-density materials for hydrogen storage, a major challenge for the widespread adoption of hydrogen fuel.
    - For example: quantum computing can be used to produce Hydrogen Storage Materials, by identifying new materials that enable safer and more efficient hydrogen storage, a critical need for the hydrogen economy to become viable.

- *Sustainable Mining and Resource Extraction*

  - *Quantum Chemistry for Efficient Mining*: Quantum simulations can help optimize chemical processes in mining, leading to more efficient and environmentally friendly extraction of metals and minerals used in technologies like batteries, solar panels, and wind turbines.

  - *Reduced Environmental Impact*: by identifying alternative extraction processes, quantum computing can help reduce the environmental footprint of mining, minimizing energy consumption, water usage, and waste generation.
    - For example: quantum computing can be used for efficient Metal Extraction Processes, by improving the design of solvents or other agents that efficiently extract rare earth metals from ores, reducing the environmental impact of mining operations.

Conclusion

Quantum Computing offers transformative potential for optimizing energy systems, from grid management to renewable integration and market trading. Although still in its early stages, Quantum Computing could lead to more efficient, resilient, and sustainable energy infrastructures in the coming decades as the technology matures and quantum algorithms become more specialized.

Moreover, Quantum Computing has the potential to transform material science in the context of sustainable technologies by enabling faster, more accurate simulations of atomic and molecular processes. This could lead to significant breakthroughs in developing energy-efficient materials, improving renewable energy technologies, and reducing the environmental impact of industries through more efficient chemical processes.

As quantum hardware and algorithms continue to improve, Quantum Computing's role in the design and discovery of sustainable materials will likely expand, making it a key tool in the global transition to a more sustainable energy system.

4.2.1 Recent scientific contributions on QC for the Optimization of Energy Systems

Numerous contributions on the application of quantum computing for Sustainable Technologies and Optimization of Energy Systems have appeared in scientific journals in recent years. In particular:

In **[Liu, M.; Liao, M.; Zhang, R.; Yuan, X.; Zhu, Z.; Wu, Z., (2025)],** a groundbreaking framework for optimizing microgrid operations using the Quantum Approximate Optimization Algorithm (QAOA) is presented. The increasing integration of decentralized energy systems, characterized by their reliance on renewable energy sources, presents unique challenges, including the stochastic nature of energy supply-and-demand management. The study leverages quantum computing to enhance the operational efficiency and resilience of microgrids, transcending the limitations of traditional computational methods. The proposed QAOA-based model formulates the microgrid scheduling problem as a Quadratic Unconstrained Binary Optimization (QUBO) problem, suitable for quantum computation. This approach not only accommodates complex operational constraints—such as energy conservation, peak load management, and cost efficiency—but also dynamically adapts to the variability inherent in renewable energy sources. By encoding these constraints into a quantum-friendly Hamiltonian, QAOA facilitates a parallel exploration of multiple potential solutions, enhancing the probability of reaching an optimal solution within a feasible time frame. The proposed model is validated through a comprehensive simulation using real-world data from a microgrid equipped with photovoltaic systems, wind turbines, and energy storage units. The results demonstrate that QAOA outperforms conventional optimization techniques in terms of cost reduction, energy efficiency, and system reliability. Furthermore, the study explores the scalability of quantum algorithms in energy systems, providing insights into their potential to handle larger, more complex grid architectures as quantum technology advances. This research not only underscores the viability of quantum algorithms in real-world applications but also sets a precedent for future studies on the integration of quantum computing into energy management systems, paving the way for more sustainable, efficient, and resilient energy infrastructures.

In **[Blenninger, J.; Bucher, D.; Cortiana, G.; Ghosh, K.; Mohseni, N.; Nüßlein, J.; O'Meara, C.; Porawski, D.; Wimmer, B. (2024)]**, the key results and use-cases explored in the German Federal Ministry of Education and Research (BMBF) funded project "Q-GRID" (which aims to assess potential quantum utility optimization applications in the electrical grid) are summarized. The project focuses on two layers of optimization problems relevant to decentralized energy generation and transmission as well as novel energy transportation/exchange methods such as Peer-2-Peer energy trading and microgrid formation. For select energy grid optimization problems, it is demonstrated that exponential classical optimizer runtime scales even for small problem instances. It is also shown that variational quantum algorithms such as QAOA and hybrid quantum annealing solvers may provide more favourable runtime scaling to obtain similar solution quality. These initial results suggest that quantum computing may be a key enabling technology in the future energy transition insofar that they may be able to solve business problems which are already challenging at small problem instance sizes.

In **[Śmierzchalski, T., Mzaouali, Z., Deffner, S. et al, (2024)]**, strategies and reproducible results for optimizing the performance and energy consumption of quantum annealing systems (employing reverse-annealing protocols) are presented.

In **[V. Malathy, Vivek Veeraiah, T. Jayapratha, Rakesh Chandrashekar, S. Aswini, (2023)]**, the potential of quantum computing to address the complex optimization challenges in energy systems is investigated-.

In **[the book, Advances in Smart Energy Systems, Biplab Das et al., (2023)]**, smart computing techniques which offer an effective solution for investigating and modeling the stochastic behavior of renewable energy generation, operation of grid-connected renewable energy systems, and smart decision-making among alternatives are presented.

In **[Ajagekar A, You F, (2022)]**, the prospects of Quantum Computing for various areas of applications in energy sustainability to help address climate change are discussed. Furthermore, sustainable energy applications that may draw advantages from QC-based strategies are identified while simultaneously setting realistic expectations over the potential improvements offered over classical techniques.

In **[Sherbert, K., Jayaraj, A. & Buongiorno Nardelli, M., (2022)]**, a novel approach to electronic band structure calculations in a quantum computer by adopting a basis of local atomic orbitals is presented.

In [**Bauer, B., Bravyi, S., Motta, M. & Kin-Lic Chan, G, [2020]**, the central problems in chemistry and materials science, in areas of electronic structure, quantum statistical mechanics, and quantum dynamics that are of potential interest for solution on a quantum computer are reviewed. A detailed snapshot of current progress in quantum algorithms for ground-state, dynamics, and thermal-state simulation is also presented, analyzing their strengths and weaknesses for future developments.

In **[Akshay Ajagekar, Fengqi You, (2019]**, the applications of quantum computing to energy systems optimization problems are explored, discussing some of the challenges faced by quantum computers and techniques to overcome them.

More references on the use of Quantum Computing for Sustainable Technologies and Optimization of Energy Systems can be found in ***Appendix B.***

4.3 Quantum Sensing for Climate Change

Quantum Sensing is an emerging technology with the potential to significantly impact climate change research and environmental monitoring. By leveraging the principles of quantum mechanics, quantum sensors can achieve ultra-precise measurements that surpass the capabilities of classical sensors.

Quantum Sensing could be applied to address the following climate change applications:

- *High-Precision Environmental Monitoring*
  Quantum sensors can detect minute changes in environmental variables such as temperature, humidity, and atmospheric composition. This allows for:
  - *Better Greenhouse Gas Monitoring*: Quantum-based gas sensors can detect extremely low concentrations of gases like carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) in the atmosphere. These sensors could be used in satellite or drone-based platforms

to provide more accurate and real-time data on greenhouse gas emissions, improving climate models.

- *Accurate Ocean and Atmospheric Measurements*: Quantum sensors can measure changes in temperature, pressure, and chemical composition in oceans and the atmosphere. This could help scientists track global warming patterns and the dynamics of ocean currents, which play a significant role in regulating Earth's climate.

- *Quantum Gravimetry for Ice and Sea-Level Monitoring*
  Quantum gravimeters measure minute changes in the Earth's gravitational field. These measurements can help in:

  - *Glacier and Ice Sheet Monitoring*: As glaciers and ice sheets melt due to rising temperatures, the distribution of mass on Earth changes. Quantum gravimeters can detect these changes with high precision, providing data to track the rate of ice melt and predict its impact on sea levels.

  - *Sea-Level Rise Tracking*: Subtle shifts in the Earth's mass distribution, caused by ice melt and water movement, can be measured using quantum gravimetry. This can give scientists better predictions about rising sea levels and their effects on coastal communities.

- *Magnetometry for Geophysical Surveys*
  Quantum magnetometers, which measure the Earth's magnetic field with high precision, can be used to:

  - *Monitor Underground Water Resources*: Changes in underground water resources, such as aquifers, can be monitored by detecting subtle magnetic field variations. This can help in understanding how climate change impacts water availability in drought-prone regions.

  - *Detect Seismic Activity and Volcanic Eruptions*: by sensing minute magnetic field variations, quantum sensors can provide early warnings of seismic activities and volcanic eruptions, helping vulnerable populations prepare for natural disasters that could be exacerbated by climate change.

- *Quantum LIDAR for Deforestation and Carbon Sequestration*
  LIDAR (Light Detection and Ranging) systems based on quantum technologies can provide highly accurate 3D mapping of forests and other carbon sinks.
  This has several applications for climate change:

  - *Mapping Forest Degradation and Deforestation*: Accurate, high-resolution data from quantum LIDAR systems can help track deforestation rates and the health of forests, which are critical in carbon sequestration and biodiversity preservation.

  - *Monitoring Carbon Storage*: Forests and soils store large amounts of carbon. Quantum LIDAR can assess how much carbon is sequestered and help in developing strategies for carbon offset programs.

- *Quantum Clocks for Precise Timekeeping in Climate Studies*

Quantum clocks, which are among the most accurate timekeeping devices, could improve global positioning systems (GPS) and enhance the precision of environmental data collection. They could assist in:

  - *Improved Climate Modeling*: Accurate timing data is crucial in climate simulations and models. Quantum clocks could synchronize sensors globally, enabling more precise data collection and improving predictions of future climate scenarios.

  - *Satellite-Based Climate Observation*: Many climate monitoring satellites rely on precise timing to gather data about Earth's systems. Quantum clocks could improve the synchronization of these satellite networks, leading to better coordination and more accurate climate data.

- *Quantum Imaging for Remote Sensing*
  Quantum-enhanced imaging techniques, such as quantum radar or quantum-enhanced cameras, can increase the resolution and sensitivity of remote sensing systems, enabling:

  - *Enhanced Atmospheric Observation*: These imaging systems could detect subtle changes in cloud formation, particulate matter, or aerosols in the atmosphere, all of which are important in understanding climate change dynamics.

  - *Improved Agricultural Monitoring*: Quantum imaging can help monitor soil moisture, crop health, and other agricultural parameters with high accuracy, providing critical data for sustainable land management in a changing climate.

Potential Benefits:

- *Increased Sensitivity and Accuracy*: Quantum sensors provide unprecedented precision, allowing for the detection of tiny changes that classical sensors may miss. This can lead to better tracking of climate-related variables.

- *Real-Time Data Collection*: Many quantum sensors are capable of real-time measurements, providing instantaneous insights that can help inform climate action decisions.

- *More Robust Climate Models*: Improved data from quantum sensors will enhance the accuracy of climate models, leading to better predictions and more effective mitigation strategies.

Challenges:

- *Scaling and Deployment*: Quantum sensing technologies are still largely in the research phase, and their widespread deployment may take time. Scaling these systems to the levels needed for global climate monitoring presents technical and logistical challenges.

- *Cost*: The development and implementation of quantum sensors may be expensive, although costs are expected to decrease as the technology matures.

Conclusion

Quantum Sensing has the potential to transform how we monitor and understand climate change by providing more accurate, sensitive, and real-time data on various environmental variables. Its role in improving climate models, tracking carbon sinks, and detecting subtle environmental changes makes it a promising tool for addressing global climate challenges.

4.3.1 Recent scientific contributions on Quantum Sensing for Climate Change

Numerous contributions on the application of Quantum Sensing to the climate change have appeared in scientific journals in recent years. In particular:

In **[Luiz Davidovich, (2024)]**, Quantum sensors allowing the estimation of parameters with precision higher than that obtained with classical strategies are reviewed, emphasizing recent results regarding noisy systems.

In **[Kantsepolsky, B. and Aviv, I, (2024)]**, the potential applications of quantum sensing in four critical urban infrastructure domains: water, energy, transport, and construction are presented.

In **[Martina, Gschwendtner., Yannick, Bormuth., Henning, Soller., Amanda, Stein., Ronald, L., Walsworth, (2024)]**, it is shown that quantum sensing technologies can enhance climate research and renewable energy by accurately measuring environmental parameters like temperature, pressure, and magnetic fields, leading to improved data collection and analysis.

In **[Xiang, Li., (2023)]**, it is shown that quantum sensing can enhance climate research and renewable energy by enabling highly sensitive measurements of environmental parameters, improving data accuracy for modeling and optimizing energy systems.

In **[Kantsepolsky, I. Aviv, R. Weitzfeld and E. Bordo, (2023]**, a comprehensive review of quantum sensing state-of-practice is presented with a detailed analysis of how quantum sensing overcomes the existing limitations of sensor-driven systems' precision and performance.

In **[Marián, Mešter, (2023]**, a technological summary of research needs and activities to support the operation and management of energy systems until 2050, and the latest findings from the world of quantum technologies

More references on the use of Quantum Sensing for Climate Change can be found in ***Appendix C****.*

4.4 Quantum Communication Technologies for Climate Change

Quantum communication technologies have direct and indirect benefits for climate change mitigation efforts.

In particular, they will allow:

- *Secure Transmission of Environmental Data*
  Monitoring and modeling climate change requires the collection of vast amounts of sensitive data from satellites, ocean buoys, and ground-based sensors. Using quantum communication to secure this data ensures that it can be transmitted without the risk of interference or manipulation. This is crucial for international collaborations where data accuracy and integrity are paramount.

- *Facilitating International Climate Agreements*
  Secure communication is vital for international climate negotiations, where data about emissions, environmental impact, and mitigation efforts are shared between nations. Quantum communication can ensure that sensitive data exchanged during climate talks is protected from cyberattacks or leaks, enabling more trustworthy collaboration between nations.

- *Optimizing Resource Management and Energy Grids*
  Quantum communication could enable distributed quantum computing to help optimize energy systems, improve renewable energy integration, and enhance resource management strategies. Secure data transfer between different parts of the world ensures that climate efforts, such as emissions monitoring or carbon trading, are more efficient and less vulnerable to tampering.

Challenges and Future Outlook

Despite its promise, quantum communication faces several challenges:

- *Technological Maturity*: Quantum communication technologies are still in the research and development phase. Scaling them for widespread use, especially over long distances, requires further breakthroughs in quantum repeaters and error correction.

- *Infrastructure Development*: Deploying quantum networks on a global scale requires significant infrastructure investment, including building quantum repeaters, satellites, and fiber-optic quantum channels.

- *Cost*: The cost of developing quantum communication systems is currently high, although prices are expected to drop as the technology matures.

Conclusion
Quantum communication represents the future of secure data transmission and has wide-ranging applications, from unbreakable encryption to climate change monitoring. By providing highly secure communication channels and enabling new forms of quantum networks, quantum communication can help address some of the most pressing challenges of the digital age, including cyber-security and climate change.

4.4.1 Recent scientific contributions on Quantum Communication Technologies for Climate Change

Numerous contributions on the application of quantum communication technologies to the climate change have appeared in scientific journals in recent years. In particular:

In **[Hafiz, M.W., Hwang, S.O (2023)]**, an arbitrary quantum signature scheme that does not require the establishment of entangled states to authenticate users to transmit and receive arbitrated states to retrieve classical data is presented. The consequences of the probabilistic model indicate that the quantum-assisted classical framework substantially enhances the performance and security of digital data and paves the way toward real-world applications.

In **[Paudel, H.P., Crawford, S.E., Duan, Y., et al. (2023)]**, the current status of quantum communications and networking and their applications in the energy sector are discussed. Moreover the emerging op opportunities for innovation to ensure clean, secure, and reliable energy production, transportation, and consumption are presented.

In **[Brijwani, G.N., Ajmire, P.E., Thawani, P.V, (2023)]**, quantum computing in the context of cybersecurity is explored, showing how modern cryptographic schemes can be significantly improved with quantum computers.

In **[Khan, S., Jain, C., Rathi, S., Maravi, P.K., Jhapate, A., Joshi, D., (2023]**, the vulnerability of Public Key Infrastructure (PKI) and its key exchange mechanisms to quantum computing attacks is demonstrated, along with a proposed solution to secure key exchange protocols. The solution involves the use of Quantum Key Distribution (QKD), which ensures a secure exchange of keys between the sender and the intended recipient.

In **[Chen, Y.A., Zhang, Q., Chen, T.Y., et al., (2021]**, the development of a quantum communication network using satellites is presented. Such networks can securely transmit environmental and climate-related data across the globe, offering secure communication solutions for global climate monitoring and international climate agreements.

In **[Pirandola, S., et al. (2020)]**, recent advances in quantum cryptography, including quantum key distribution (QKD), are presented. The secure transmission of sensitive climate data is crucial in international collaborations on climate monitoring, and QKD can offer unhackable channels for such exchanges.

More references on Quantum communication technologies for climate change *can be found in* ***Appendix D****.*

Part II - Quantum Machine Learning for Climate Change

5. The role of Quantum Machine Learning in Climate Science

Quantum Machine Learning (QML) is an emerging field that combines the principles of Quantum computing(QC) and Machine Learning (ML) to solve complex problems. When applied to climate change, QML offers unique advantages to gain deeper insights into the complexities of climate dynamics. Its ability to process and analyze vast, intricate datasets at unprecedented speeds could significantly enhance the accuracy of climate models, providing better predictive insights. QML approaches offer the potential for significant advances in predictive modeling and optimization, both of which are critical for climate science, and more informed decision-making support.

QML presents a promising alternative by utilizing the power of quantum computing to overcome the limitations of traditional ML methods in climate change research.
Two primary challenges limit the performance of classical ML algorithms in climate science: (i) the availability of high-quality training data and (ii) the computational resources required to process the vast amounts of data generated by planetary-scale climate models.

QML leverages the unique properties of quantum computing to tackle these complex problems more efficiently than classical computers. In climate science, QML can significantly enhance our understanding of climate patterns, improve the accuracy of climate models, and optimize strategies for mitigating the impacts of climate change. By utilizing quantum algorithms and quantum annealers, QML can process enormous datasets, simulate highly complex climate systems, and optimize resource allocation for sustainable energy production.
These capabilities open new pathways for more effective climate action, enabling faster and more precise modeling, better resource management, and more informed policy decisions to address the global climate crisis.

Key areas where QML could play a transformative role include:

- *Climate data forecasting*: covering areas like *weather prediction*, *energy load forecasting*, *renewable energy forecasting*, and *carbon price forecasting*. These focus on improving the accuracy of predictive models through QML.

- *Climate hazard prediction*: aimed at improving the ability to predict climate-related hazards such as hurricanes, floods, and other extreme weather events.

- *Climate monitoring*: which involve *earth observation*, *satellite imagery analysis*, and *real-time environmental monitoring* to track climate changes.

- *Mitigation applications for decarbonization acceleration*: which include sectors such as *energy systems*, *transportation*, and *agriculture*. These applications focus on reducing carbon emissions and transitioning toward sustainable systems.

The following sections delve into the specific roles of QC in these major application areas.

5.1. QML for Climate Data Forecasting

Quantum Machine Learning algorithms allow to improve the accuracy of predictive models in *weather prediction, renewable energy forecasting,* and *carbon price forecasting*.

- *Weather prediction*: accurate weather forecasting is crucial for a range of applications, from daily weather predictions to long-term climate modeling. Traditional supercomputers, based on silicon transistors, face fundamental limitations that impede performance improvements, impacting the accuracy and resolution of numerical weather and climate prediction models. As global meteorological centers strive to enhance forecast accuracy and model resolution, they often encounter significant challenges due to the excessive computing power required. Recent advancements in Quantum Machine Learning offer promising alternatives to traditional approaches. In particular, Quantum Support Vector Machine (QSVM) algorithms have been recently developed to enhance the efficiency and accuracy of support vector machines (SVMs) in processing complex data sets. QSVM algorithms are used for forecasting solar irradiation and have the potential for improving predictions related to weather forecasting. Moreover, exploiting quantum phenomena, particularly *superposition* and *entanglement*, models based on *Variational Quantum Circuits (VQCs*) have been developed for efficient weather forecasting. Specifically, in these models, an *entanglement* layer between the variational layers is added to significantly improve circuit performance. Additionally, a superposition layer before the data encoding layer is used to reduce the number of required variational layers, allowing to enhance the overall performance of the model. Finally, QML algorithms like quantum neural networks (QNNs) have been also developed to improve the predictive capabilities of machine learning models. They can more effectively capture the nonlinear relationships in climate data, potentially reducing the uncertainty in climate predictions. Quantum Neural Networks (QNN), combined with other techniques, have been investigated to achieve highly accurate and rapid weather forecasts. In particular, Quantum Physics-Informed Neural Networks (QPINNs) have emerged as a promising approach to solving complex quantum systems by integrating the principles of quantum mechanics into machine learning models. QPINNs for small datasets, and quantum machine learning (QML) models for interpolation tasks, offer potential solutions and can improve generalization where classical deep learning models struggle due to limited datasets. Attention-Enhanced Quantum Physics-Informed Neural Networks (AQ-PINNs) models have been designed to improve the computational efficiency of climate models, specifically targeting fluid dynamics governed by the Navier-Stokes equations, which are essential in climate modeling. The key innovation is the integration of quantum computing techniques with attention mechanisms to reduce the computational burden while maintaining high predictive accuracy. AQ-PINNs, in particular, were found to reduce model parameters by over 50% compared to classical approaches, without sacrificing convergence or accuracy. By reducing resource consumption and enhancing efficiency, these models address concerns about the environmental impact of AI in climate research, making it a potential tool for more sustainable climate modeling.

- *Renewable energy forecasting*: accurate forecasting of renewable energy sources, such as wind and solar power, is essential for optimizing grid stability and energy management. Recent advancements in quantum machine learning (QML) are making significant strides in this area. In particular for:

    - *Wind speed forecasting*: hybrid models that integrate quantum processes with residual Long Short-Term Memory (LSTM) networks have been introduced. These models exploit Particle Swarm Optimization (PSO) approaches for one-day-ahead spatiotemporal wind speed forecasting. These hybrid approaches demonstrate superior performance compared to traditional methods like GRU, KELM, CNN, BLSTM, SVRM, and ANN, in terms of accuracy. However, these models suffer of the extended training duration, due to the quantum embedding layer and the exclusive use of a quantum simulator. Despite these models are efficient enough for 24-hour wind power and speed forecasting.

    - *Solar Irradiance Forecasting*: high-precision hybrid prediction models combining a Variational Quantum Circuit (VQC) and a Long Short-Term Memory (LSTM) network for one-hour-ahead solar irradiance forecasting have been developed. The innovative Quantum LSTM (QLSTM) model architecture incorporates the VQC into the LSTM framework. Compared with traditional models such as SARIMA, CNN, RNN, GRU, and LSTM, the QLSTM models demonstrated superior performance in terms of annual average mean absolute error and other metrics. These models address the challenge of fluctuating solar energy output due to varying weather conditions, thus improving forecast accuracy and grid stability.

- *Carbon price forecasting*: Carbon pricing is a mechanism that assigns a monetary value to carbon emissions, encouraging reductions in carbon footprints. Pioneering attempts are reported in the scientific literature aimed at applying hybrid quantum methods to carbon price forecasting. They allow to provide businesses and policymakers with better tools for making informed decisions about investments in cleaner technologies and practices. In particular, hybrid quantum computing models, like L-QLSTM, have been designed for predicting carbon prices. These models build upon the QLSTM framework by incorporating linear layers to improve the quantum model's learning capability. L-QLSTM models offer accuracy comparable to classical LSTM models for carbon price predictions. The integration of linear embedding layers and an optimized variational quantum circuit contributes to its enhanced performance.

5.2. QML for Climate Hazards Predictions

Predicting climate-related hazards such as earthquakes and asteroid impacts is crucial for disaster preparedness and risk mitigation. QML offers innovative approaches to enhance prediction accuracy for these natural hazards.

- *Earthquake Prediction:* models based on Quantum Support Vector Machines (QSVM) for earthquake prediction have been developed. These models seek to advance predictive tools for natural disaster mitigation, emphasizing the need for efficient and accurate forecasting methods.

- *Asteroid Hazard Prediction*: QML-based models for predicting asteroid hazards using Variational Quantum Circuits (VQC) and Quantum Support Vector Classifiers (QSVCs) algorithms have been developed. In some of these models, an impressive accuracy of 98.11% and an average F1-score of 92.69% is reached, demonstrating the potential of QML in enhancing real-time risk detection and mitigation for asteroid impacts.

These advancements highlight the growing impact of QML on climate monitoring and hazard prediction, offering new tools and techniques for improving our understanding and response to climate-related challenges.

5.3. QML for Climate Monitoring

Climate monitoring relies on satellite image classification to track environmental changes, validate scientific models, and guide climate-related policies. The need for efficient processing of vast amounts of high-resolution data is critical in this field. Quantum Machine Learning (QML) has shown promising potential in enhancing climate monitoring applications, as demonstrated by recent research for satellite image classification:

- *Satellite Image Classification*: QML models have been developed for classifying satellite-observed hyperspectral images. These models focus on distinguishing vegetation from other land types, which is crucial for understanding land use changes and monitoring ecosystems. In particular, hybrid quantum-classical models have been proposed to improve traditional image classification approaches. These models include a neural network with parallel quantum layers and a neural network with a quanvolutional layer, which leverage quantum effects to enhance classification accuracy. Hybrid Quantum Convolutional Neural Networks (QCNNs) models for remote sensing applications have been also developed, highlighting the superior performance of QCNNs over classical methods in Earth Observation tasks. In some studies, it is shown that quantum circuits utilizing quantum entanglement achieved the highest classification scores. Furthermore, in a recent work, the integration of Projected Quantum Kernels (PQK) in classical machine learning algorithms has been evaluated on the Copernicus Sentinel-2 dataset. The achieved results indicate that PQK features significantly improved the classification accuracy. Finally, quantum circuit-based neural network classifiers for multi-spectral data classification investigated. Although their results showed promise, the overall classification performance was less competitive compared to state-of-the-art classical systems.

5.4. QML for Decarbonization Acceleration

Decarbonization acceleration focuses on rapidly reducing carbon emissions and transitioning to a low-carbon or carbon-neutral economy. It is a critical strategy for mitigating the impacts of global warming. Key sectors driving this transition include *energy systems*, *transportation*, and *agriculture*, which collectively account for a significant portion of global emissions. Quantum Machine Learning (QML) can significantly contribute to the acceleration of decarbonization efforts by optimizing key systems and processes in these high-emission sectors.

- *Energy Systems*: efficient energy production, distribution, and consumption are essential to reducing carbon emissions. Transitioning from fossil fuels to renewable energy-based systems and establishing optimized, sustainable management systems are essential steps toward achieving climate neutrality. Quantum Machine Learning offers promising solutions for optimizing energy systems in ways that classical algorithms may struggle to achieve. QML has been applied to optimize grid management, enhance the efficiency of renewable energy integration, and develop quantum-based algorithms for energy resource allocation. Several contributions on QML for energy systems can be found in the scientific literature. In particular:

    - *Data-driven approaches* combining multi-agent quantum deep reinforcement learning have been proposed for distributed frequency control in islanded microgrids. These hybrid models merge traditional deep reinforcement learning (DRL) with QML to determine the optimal cooperative control strategy. The results achieved by these models show reduced parameter requirements and improved training efficiency, ultimately enhancing the sustainability and performance of microgrids by offering eco-friendly services to residents.

    - *Quantum Reinforcement Learning (QRL)* models have been proposed for energy-efficient control in domains such as HVAC systems, electric vehicle energy management, and profit optimization for charging stations. The results scieved by these models demonstrated that quantum neural networks outperform classical models in terms of accuracy and rewards, despite a slower learning process. QRL models required fewer parameters, showing potential for enhancing energy efficiency across various sectors.

    - *Quantum Neural Networks (QNNs)* have been designed as controllers for photovoltaic solar systems, aiming to track the maximum power point and minimize energy losses. Quantum-driven controllers rapidly adapted to changing environmental conditions, surpassing classical methods and achieving greater efficiency in optimizing solar energy.

    - *Distributed Area Autonomy Load Frequency Control (DAA-LFC)* techniques have been proposed. These techniques use quantum-based algorithms (DQMA-DMDPG) for balancing interests among grid operators while restoring frequency across multi-area microgrids. These models integrated meta-learning and large-scale learning, showing empirical success in minimizing frequency deviations, reducing power generation costs, and aligning operator interests effectively.

- *Lightweight robust quantum Q-learning (LRQQL)* methods have been proposed to address challenges in smart generation control (SGC) for zero-carbon power systems. The LRQQL algorithm outperform classical methods such as SARSA and Q-learning in reducing control error, frequency error, and convergence time, showing promise for improving energy management in zero-carbon power grids.

In conclusion, QML has proved in enhancing energy system management and optimization, from microgrids to renewable energy generation and smart control systems. While some quantum models may experience slower learning processes compared to classical counterparts, the overall efficiency gains in accuracy, adaptability, and computational resource optimization offer a compelling case for the integration of QML in the energy sector. As renewable energy systems continue to scale, QML will likely play a pivotal role in achieving global decarbonization goals.

- *Transportation*: the transportation sector is another major contributo*r* to carbon emissions. The transportation sector, particularly vehicle electrification, has been significantly impacted by economic and environmental concerns related to the continued use of fossil fuels. As nations worldwide aim to reduce carbon emissions, the transition to electric vehicles (EVs) and the optimization of supporting infrastructure have become critical areas of research. Recent advancements in Quantum Machine Learning (QML) are beginning to shape new approaches to solving these challenges. QML has been explored for optimizing route planning, improving electric vehicle battery performance, and enhancing traffic management systems to reduce fuel consumption and emissions. Several contributions on QML for the transportation sector can be found in the scientific literature. In particular for:

  - *Optimizing Electric Vehicle Charging Station Placement*: hybrid approaches that combines the Eurasian Oystercatcher Optimizer (EOO) with Quantum Neural Networks (QNN) have been proposed. These models aim at optimizing the placement of electric vehicle charging stations (EVCS) and capacitors within distribution systems (DS). EOO-QNN models regulate capacitor placement to maintain voltage profiles, increase net energy gain, and reduce active power loss. It has been demonstrated that EOO-QNN models offer better voltage stability compared to traditional optimization techniques, such as the Salp Swarm Algorithm (SSA) and Particle Swarm Optimization (PSO).

  - *Energy Trading*: Blockchain and Quantum Reinforcement Learning (QRL) models for Energy Trading have been proposed to optimize energy trading in the context of e-mobility and microgrids (MGs). These models address the challenge of determining optimal electricity pricing for electric vehicles (EVs) charging through a double-auction mechanism, which sets market-trading prices for electricity generated by MGs. Smart contracts are used on a consortium blockchain to transform the problem into a Markov Decision Process (MDP) and employs QRL for policy optimization. The achieved results show that these models converge more quickly, maximizes utility for both MG operators and EV users, and reduces transaction confirmation times while optimizing market prices. These improvements help ensure the efficient and sustainable charging of EVs, promoting the wider adoption of electric mobility.

In conclusion, the application of QML in the transportation sector, particularly for vehicle electrification and EV infrastructure, holds great promise for improving energy efficiency and optimizing critical systems. By integrating quantum-based approaches, such as QNN and QRL, with classical optimization and blockchain technologies, QML can enhance EV charging infrastructure and energy trading mechanisms, pushing forward the electrification of transportation in an environmentally sustainable way.

- *Agriculture*: sustainable agriculture practices are essential for decarbonization, and QML techniques have been used to optimize crop management, reduce the carbon footprint of agricultural operations, and improve precision farming methods by analyzing large datasets for resource efficiency. Recent advancements in deep learning, both classical and quantum, have shown substantial promise in enhancing agricultural practices. These methods are increasingly being explored to improve predictions and decision-making in agriculture, particularly concerning crop health and disease management. Several contributions on QML for can be found in the scientific literature. In particular:

    - Various neural network models for predicting wheat plant diseases have been compared. The models evaluated include Convolutional Neural Networks (CNNs), traditional Neural Networks (NNs), Quantum Neural Networks (QNNs), and Quantum Convolutional Neural Networks (QCNNs). The study found that the classical CNN model achieved an accuracy of 91.32%, surpassing the quantum models.

In conclusion, this result challenges the assumption that quantum-based approaches are inherently superior for machine learning tasks. Anyway, the findings suggest that, without the infrastructure of a true quantum computing platform, the benefits of QNNs may not be fully realized on conventional hardware. This underscores a critical observation: while quantum methods are promising, their advantages are not always evident when implemented or simulated on classical systems, which may not fully harness the unique properties of quantum mechanics, such as *superposition* and *entanglement*.

5.5 Recent scientific contributions on QML for Climate Change

Numerous contributions on the application of Quantum Machine Learning to the climate change have appeared in scientific journals in recent years. In particular:

In **[Kin Tung Michael Ho, Kuan-Cheng Chen, Lily Lee, Felix Burt, Shang Yu, Po-Heng (Henry)Lee, (2025)]**, the application of quantum machine learning and optimization techniques for climate change prediction and enhancing sustainable development are presented in this review. The paper highlights how QC and quantum machine learning can optimize multi-infrastructure systems towards climate neutrality, evaluating the performance of current quantum algorithms and hardware in practical applications and presents realistic cases, i.e., waste-to-energy in anaerobic digestion, disaster prevention in flooding prediction, and new material development for carbon capture.

In [da Silva, M. H. F.; de Jesus, G. F.; Nascimento, C. M. S.; da Silva, V. L.; Cruz, C, (2025)], the emerging intersection between quantum machine learning (QML) and climate forecasting is explored, presenting the implementation of a Quantum Neural Network (QNN) trained on real meteorological data from NASA's Prediction of Worldwide Energy Resources (POWER) database. It is shown that QNN has the potential to outperform a classical Recurrent Neural Network (RNN) in terms of accuracy and adaptability to abrupt data shifts, particularly in wind speed prediction. Despite observed nonlinearities and architectural sensitivities, the QNN demonstrated robustness in handling temporal variability and faster convergence in temperature prediction. These findings highlight the potential of quantum models in short- and medium-term climate prediction, while also revealing key challenges and future directions for optimization and broader applicability.

In [Pandey, T. N.; Ravalekar, V.; Nair, S. D.; Pradhan, S. K., [2025)], a comprehensive study on the use of quantum machine learning (QML) on time-series data is presented. The primary objective is to compare the results and time complexity of classical machine learning algorithms on traditional hardware to their quantum counterparts on quantum computers. As the amount and complexity of time-series data in numerous fields continues to expand, the investigation of advanced computational models becomes critical for efficient analysis and prediction. A time-series dataset that include temperature records from different nations throughout the world spanning the previous half of the century is used. The study compares the performance of classical machine learning algorithms to quantum algorithms, which use the concepts of superposition and entanglement to handle subtle temporal patterns in time-series data. This study attempts to reveal the different benefits and drawbacks of quantum machine learning in the time-series domain through rigorous empirical analysis. The findings of this study not only help to comprehend the applicability of quantum algorithms in real-world contexts, but they also open the way for future advances in utilizing quantum computing for increased time-series analysis and prediction.

In **[Amal Nammouchi et al., 2023]**, an extensive review on the use of QML for climate change is reported.

In **[Siddhant Dutta et al. (2024)]**, the use of Quantum Physics-Informed Neural Networks (QPINNs) for climate change is explored.

In **[Besir Ogur (2023)]**, the impact of quantum phenomena, particularly superposition and entanglement, on weather forecasting using a Variational Quantum Circuit model is presented.
*(Additional details on Quantum Algorithms (VQAs), along with relevant scientific references, can be found in **Appendix I**).*

In **[Hong and Santos (2023)]**, a novel hybrid model that integrates quantum processes with residual Long Short-Term Memory (LSTM) networks is presented. This model demonstrates superior performance compared to traditional methods in terms of accuracy for speed forecasting.

In **[Yu et al. (2023)]**, A high-precision hybrid prediction model combining a Variational Quantum Circuit (VQC) and a Long Short-Term Memory (LSTM) network for one-hour-ahead solar irradiance forecasting is presented.

In **[Cao et al. (2023)]**, a hybrid quantum computing framework for predicting carbon prices is designed.

In **[Bhavsar et al. (2023)]**, a QML-based approach for predicting asteroid hazards using Variational Quantum Circuits (VQC) and the Quantum Support Vector Classifier algorithm (Pegasos QSVC) is presented.

In **[Dhotre et al. (2022)]**, the use of Quantum Support Vector Machines (QSVM) for earthquake prediction is presented.

More references on Quantum Machine Learning for Climate Change *can be found in **Appendix E**.*

5.6 QML Software tools

Several companies, research institutions, and governments are developing quantum computers, using various technologies, each with unique capabilities. In ***Appendix F*** an overview of the most notable quantum computers currently available, categorized by their underlying technology, access methods, and key providers is reported.
Anyway, number of software tools and simulators have been developed specifically for quantum machine learning or can be adapted for this purpose.
Quantum computing simulators can be used to emulate the behavior of quantum computers on classical systems. They allow researchers, developers, and students to experiment with quantum algorithms, test theories, and develop quantum software without requiring access to an actual quantum computer. These simulators are crucial for exploring quantum algorithms and advancing quantum research since real quantum hardware is still in its early stages and can be expensive or difficult to access.

In the following are reported some of the leading frameworks and libraries.

1. PennyLane

- *Description*: PennyLane is a quantum computing library that focuses on quantum machine learning and quantum neural networks. It allows users to implement hybrid quantum-classical models by integrating with both quantum computing hardware and machine learning libraries such as TensorFlow and PyTorch.

- *Features*:
    - Support for multiple quantum hardware platforms (IBM Q, Rigetti, Xanadu, etc.)
    - Integration with classical ML libraries (TensorFlow, PyTorch, JAX)
    - Automatic differentiation of quantum circuits

- *Best For*: Researchers looking to work with hybrid quantum-classical algorithms in machine learning, variational quantum algorithms (VQAs), and quantum neural networks.

- Website: [PennyLane]

2. TensorFlow Quantum (TFQ)

- *Description*: TensorFlow Quantum is a library that integrates quantum computing with Google's TensorFlow machine learning framework. It enables the construction of quantum models for machine learning tasks and provides the tools for quantum data processing.

- *Features*:
    - Integration with TensorFlow for hybrid quantum-classical models
    - Support for parameterized quantum circuits
    - Quantum data preprocessing

- *Best For*: Deep learning practitioners who are already familiar with TensorFlow and want to extend their models to quantum computing.

- *Website*: [TensorFlow Quantum]

3. Qiskit Machine Learning

- *Description*: Qiskit is an open-source quantum computing framework by IBM, and it includes a machine learning module for building quantum machine learning algorithms. It allows integration with quantum computers available via the IBM Quantum Experience platform.

- *Features*:
    - Pre-built quantum machine learning algorithms like quantum support vector machines (QSVMs) and quantum neural networks (QNNs)
    - Integration with classical ML models in Scikit-learn
    - Support for running on IBM's quantum hardware
- *Best For*: Users looking to leverage IBM's quantum computing hardware with machine learning algorithms.

- *Website*: [Qiskit Machine Learning]

4. Cirq + TensorFlow Quantum

- Description: Cirq is a Python framework for building and simulating quantum circuits, developed by Google. When used with TensorFlow Quantum, it enables creating quantum machine learning applications that can be run on quantum hardware or simulators.

- *Features*:
    - Ideal for simulating near-term quantum algorithms (NISQ devices)
    - Tight integration with TensorFlow Quantum

- *Best For*: Google Quantum AI researchers and developers working on quantum ML experiments and simulations.

- *Website*: [Cirq]

5. PyQuil + Rigetti Forest

- *Description*: PyQuil is a Python library that helps in writing and running quantum programs using Quil, a quantum instruction language. With PyQuil, users can also simulate quantum algorithms, including those related to machine learning, and run them on Rigetti's quantum processors via the Forest platform.

- *Features*:
    - Hybrid quantum-classical integration for machine learning algorithms
    - Quantum machine learning library with pre-built algorithms (like VQE, QAOA)
    - Access to Rigetti's quantum processors through the Forest API

- Best For: Developers interested in working with Rigetti's cloud quantum infrastructure.

- *Website*: [PyQuil]

6. D-Wave Ocean SDK

- *Description*: The D-Wave Ocean SDK is a software development kit that allows users to develop quantum algorithms for D-Wave's quantum annealing hardware. It includes modules for creating machine learning models optimized for quantum annealing, such as quantum Boltzmann machines and variational algorithms.

- *Features*:
    - Specializes in quantum annealing, suitable for optimization tasks
    - Ready-made tools for quantum machine learning (e.g., Boltzmann Machines)
- *Best For*: Users interested in quantum annealing-based machine learning applications, especially in optimization-heavy domains like combinatorial optimization.

- *Website*: [D-Wave Ocean SDK]

7. Strawberry Fields

- *Description*: Strawberry Fields is a quantum software platform focused on photonic quantum computing, developed by Xanadu. It is designed for building quantum algorithms, including those for quantum machine learning, based on continuous-variable (CV) quantum systems.

- *Features*:
    - Ideal for researchers working on continuous-variable quantum systems
    - Integration with PennyLane for quantum ML tasks

- *Best For*: Photonic quantum computing and quantum machine learning in continuous-variable systems.

- *Website*: [Strawberry Fields]

8. Quantum Development Kit (QDK)

- *Description*: Microsoft's Quantum Development Kit includes Q#, a quantum programming language, and libraries that support quantum machine learning. It integrates with machine learning frameworks like PyTorch and is designed to work with both simulators and quantum hardware.

- *Features*:
    - Integration with machine learning frameworks and cloud services
    - Includes libraries for hybrid quantum-classical models

- *Best For*: Developers familiar with Microsoft's ecosystem, interested in building QML models with Q#.

- *Website*: [Microsoft Quantum Development Kit]

9. QuTip (Quantum Toolbox in Python

- *Description:* QuTip is an open-source software framework designed to simulate the dynamics of quantum systems. It is highly flexible and focuses on solving problems related to quantum mechanics, quantum optics, and open quantum systems. Developed primarily for research and education, QuTiP provides an extensive set of tools to model and analyze quantum systems in various contexts.

- *Features*:
    - Simulations of the time evolution of both closed and open quantum systems
    - Allows users to design and optimize control pulses for quantum systems
    - Can create custom Hamiltonians and wavefunctions, defining the system's quantum state and its evolution over time
    - Offers advanced solvers for both time-dependent and time-independent quantum systems
    - Seamless integration with other scientific computing libraries like NumPy, SciPy, and Matplotlib
    - Provides specialized modules for quantum optics simulations
    - Supported by an active community of quantum researchers and contributors

- *Best For*: research and education communities

- *Website*: [QuTip]

These tools vary in complexity and focus on different quantum paradigms, such as gate-based, annealing, or photonic quantum computing. Depending on your interest and the hardware you aim to use, you can choose the most suitable framework for your quantum machine learning experiments.

5.6.1 Critical factors to consider when evaluating a framework for Quantum Machine Learning

These factors help assess the suitability of the framework for different use cases, such as scalability, hardware compatibility, ease of use, and integration with classical machine learning tools. In the following is a breakdown of the most important criteria:

1. Quantum Hardware Compatibility

- *Key Question*: Does the framework support the quantum hardware you plan to use (gate-based, annealing, photonic, etc.)?

- *Why It Matters*: Different frameworks are designed to work with specific quantum hardware platforms (e.g., IBM, Google, Rigetti, D-Wave). Ensure the framework supports the hardware or simulators relevant to your research or application.

- *Evaluation*:
    - *Examples*:
        - PennyLane: Supports multiple platforms (IBM Q, Rigetti, Xanadu).
        - Qiskit: Primarily designed for IBM Quantum devices.

  - D-Wave Ocean SDK: Specializes in D-Wave quantum annealing hardware.

- *Recommendation*: Choose a framework that aligns with the quantum hardware or simulator you intend to use.

2. Integration with Classical Machine Learning Tools

- *Key Question*: How well does the framework integrate with classical ML libraries like TensorFlow, PyTorch, or Scikit-learn?

- *Why It Matters*: QML often involves hybrid quantum-classical models where classical computing handles part of the computation. Seamless integration with classical ML libraries simplifies workflows, allowing for easier model development and optimization.

- *Evaluation*:
  - *Examples*:
    - TensorFlow Quantum: Built to integrate directly with TensorFlow.
    - PennyLane: Supports PyTorch, TensorFlow, and JAX.
    - Qiskit: Includes modules that interface with Scikit-learn.

- *Recommendation*: Select frameworks that integrate with the ML tools you're already familiar with or planning to use.

3. Type of Quantum Computing Paradigm

- *Key Question*: Is the framework focused on a particular quantum paradigm (e.g., gate-based, quantum annealing, continuous-variable)?

- *Why It Matters*: Different quantum paradigms are suited to different types of problems. For example, quantum annealing is typically better for optimization problems, while gate-based quantum computing is more flexible for general-purpose algorithms.

- *Evaluation*:
  - *Examples*:
    - D-Wave Ocean SDK: Specializes in quantum annealing.
    - Cirq and Qiskit: Focus on gate-based quantum computing.
    - Strawberry Fields: Tailored for photonic quantum computing (continuous-variable).

- *Recommendation*: Choose a framework that supports the quantum computing paradigm relevant to your problem domain.

4. Usability and Developer Ecosystem

- *Key Question*: How easy is the framework to use for quantum and machine learning researchers? Is there strong community support and good documentation?

- *Why It Matters*: Usability can significantly impact the learning curve and productivity. If a framework has a strong developer community and comprehensive tutorials, you'll be able to get up to speed more quickly and troubleshoot issues more effectively.

- *Evaluation*:
  - *Examples*:
    - Qiskit: Extensive community, tutorials, and learning resources.
    - PennyLane: Good documentation, strong focus on ease of use, and community support.
    - TensorFlow Quantum: Benefits from the large TensorFlow ecosystem.

- *Recommendation*: Prioritize frameworks with active community support, detailed documentation, and a rich set of tutorials and code examples.

5. Support for Hybrid Quantum-Classical Algorithms

- *Key Question*: Does the framework support variational quantum algorithms (VQAs), quantum neural networks (QNNs), or other hybrid quantum-classical approaches?

- *Why It Matters*: Many current quantum algorithms rely on a hybrid approach to optimize classical and quantum components together, especially in the noisy intermediate-scale quantum (NISQ) era.

- *Evaluation*:
  - *Examples:*
    - PennyLane: Designed for hybrid quantum-classical computations, especially variational quantum algorithms.
    - TensorFlow Quantum: Focused on quantum-classical hybrid models.
    - Qiskit: Supports variational algorithms like VQE and QAOA.

- *Recommendation*: If your goal is to develop and optimize hybrid models, ensure the framework offers tools and libraries to facilitate this.

6. Performance and Scalability

- *Key Question*: How well does the framework scale with problem size and complexity? What is the performance like when using quantum simulators vs. real hardware?

- *Why It Matters*: QML frameworks often rely on simulators for testing since quantum hardware is still limited. Performance on these simulators and the scalability of the quantum circuits are critical factors, especially as you handle larger data sets or more complex models.

- *Evaluation*:
  - *Examples:*
    - Cirq and Qiskit: Well-optimized simulators for gate-based algorithms.

    - PennyLane: Good support for both simulators and hardware, with efficient backpropagation methods for hybrid models.
    - D-Wave Ocean: Focused on scaling up optimization problems for annealing.

- *Recommendation*: Evaluate the framework's performance on both simulators and hardware for your specific use case.

7. Quantum Data Handling and Preprocessing

- *Key Question*: Does the framework provide tools for handling quantum data (e.g., encoding classical data into quantum states)?

- *Why It Matters*: Quantum machine learning often requires encoding classical data into quantum states, and different frameworks may offer various strategies for this. Some also provide tools for managing quantum data and handling measurement outputs efficiently.

- *Evaluation*:
  - *Examples*:
    - TensorFlow Quantum: Specialized in quantum data handling and preprocessing.
    - Qiskit: Provides tools for quantum feature maps and data encoding.
    - PennyLane: Supports a variety of data encoding methods for quantum circuits.

- *Recommendation*: If your focus is on encoding and processing large amounts of classical data into quantum states, choose a framework with built-in tools for efficient data handling.

8. Flexibility and Customization

- *Key Question*: How customizable is the framework for developing new quantum algorithms or modifying existing ones?

- *Why It Matters*: As the field of QML is still evolving, researchers may need to customize or experiment with novel algorithms. A flexible framework allows you to modify quantum circuits, change optimization strategies, or design new quantum gates.

- *Evaluation*:
  - *Examples*:
    - Cirq: Provides low-level access to quantum circuits and gate-level operations.
    - Qiskit: Offers both high-level tools and low-level customization for quantum algorithms.
    - PennyLane: Offers flexibility in creating custom quantum nodes and hybrid models.

- *Recommendation*: If you need a high level of control over quantum circuit design and the flexibility to implement custom algorithms, ensure the framework supports this.

9. Simulation Capabilities

- *Key Question*: How robust are the quantum simulation tools provided by the framework? Does it support noise models or near-term quantum device characteristics?

- *Why It Matters*: Quantum simulators are essential for developing and testing algorithms before deploying them on actual quantum hardware. Simulating noise and other device-specific limitations is crucial when working in the NISQ era.

- *Evaluation*:
    - *Examples*:
        - Cirq: Strong simulation capabilities with noise models and fidelity measures.
        - Qiskit: Supports noise models and backend simulators to mimic real devices.
        - PennyLane: Can simulate both ideal and noisy quantum circuits.

- *Recommendation*: Ensure the framework's simulation environment aligns with the type of quantum systems you're working with, particularly if you're targeting NISQ devices.

10. Cost and Licensing

- *Key Question*: What are the licensing requirements and costs associated with using the framework? Are there any restrictions for academic or commercial use?

- *Why It Matters*: While most QML frameworks are open-source, access to hardware or cloud-based simulators may come with costs. It's essential to understand the pricing models and any restrictions.

- *Evaluation*:
    - Examples:
        - IBM Quantum and Qiskit: Free for limited access to hardware, but higher usage incurs costs.
        - D-Wave: Requires payment for accessing larger quantum annealers.

- *Recommendation*: Assess whether the licensing terms and costs align with your usage requirements, especially if you're planning for commercial applications.

By carefully considering these factors, the best framework that aligns with the specific quantum machine learning goals, hardware preferences, and technical capabilities can be selected.

Part III - Quantum Computing and Quantum Machine Learning Challenges

Quantum Computing (QC) represents a revolutionary shift in the way we process information, leveraging the principles of quantum mechanics to solve problems that are currently infeasible for classical computers.

Quantum Machine Learning (QML) holds great promise for enhancing the capabilities of classical machine learning by leveraging quantum computing's unique properties. However, there are significant challenges that need to be addressed for QC and QML to reach their full potential. In the following some of these challenges are reported.

1. Linear-Non Linear Compatibility

- *Problem*: Neural networks rely on non-linear activation functions to introduce complexity and enable learning. In contrast, quantum systems inherently operate linearly due to the nature of quantum mechanics. This mismatch creates challenges in integrating non-linear neural network functions with linear quantum operations.

- *Impact*: The lack of direct compatibility can limit the effectiveness of Quantum Neural Networks (QNNs) and may require innovative approaches to bridge this gap.

- *Possible Solution*: Various solutions have been identified to address the challenges associated with applying Quantum Computing and Quantum Machine Learning to non-linear systems. In particular, the **Koopman Operator**, used to analyze nonlinear dynamical systems by representing them in terms of a linear operator in an infinite-dimensional space, plays a key role. Its relevance to Quantum Computing, along with further scientific references, is discussed in ***Appendix H***.

2. Noisy Quantum Hardware (NISQ era)

- *Problem*: Current quantum computers are in the Noisy Intermediate-Scale Quantum (NISQ) era, meaning they have a limited number of qubits, are prone to noise, and often suffer from errors in quantum gates and measurements.

- *Impact*: These noise levels affect the reliability and scalability of QML algorithms, limiting the size and complexity of the machine learning models that can be run on real quantum hardware.

- *Possible Solution*: Error correction techniques and noise mitigation strategies are being developed, but they are computationally expensive and not yet fully practical for large-scale QML tasks.

3. Limited Qubit Count and Connectivity

- *Problem*: Current quantum hardware has a limited number of qubits (tens to hundreds), and not all qubits are fully connected (i.e., able to directly interact with one another).

- *Impact*: Many QML algorithms require large numbers of qubits and strong connectivity between them, especially for complex datasets or deep learning models. This limits the scalability of QML models.

- *Possible Solution*: Advances in quantum hardware (more qubits, better connectivity) and hybrid quantum-classical algorithms are being explored to overcome this challenge.

4. Lack of Efficient Quantum Data Input (Quantum Data Encoding)

- *Problem*: Encoding classical data into quantum states (quantum feature mapping) is often inefficient and resource-intensive, especially for high-dimensional datasets.

- *Impact*: The bottleneck of loading data into a quantum computer, known as the "data input problem," reduces the potential speedup of quantum algorithms and poses challenges in handling large datasets.

- *Possible Solution*: Research is focusing on developing more efficient quantum encoding schemes and finding quantum-native data (such as data from quantum chemistry or physics) to directly work with.

5. Training and Optimization Challenges

- *Problem*: Training quantum models often involves optimization processes that are inherently difficult. Many QML models use variational quantum circuits, which require optimizing parameters in high-dimensional, non-convex landscapes that can suffer from issues like barren plateaus (regions where the gradient is almost zero).

- *Impact*: This makes it hard for QML models to converge to good solutions, leading to inefficient training and poor model performance.

- *Possible Solution*: Improved optimization techniques, such as quantum-aware optimizers, hybrid classical-quantum approaches, and strategies to mitigate barren plateaus, are being developed to enhance the training process.

6. Quantum Algorithm Development and Interpretability

- *Problem*: Many quantum algorithms are still in the early stages of development, and it is not always clear how and when they will outperform classical machine learning algorithms. Additionally, QML models can be hard to interpret, and the theoretical understanding of their advantages is still evolving.

- *Impact*: This leads to uncertainty about when QML will provide practical advantages over classical approaches, especially in real-world applications. Interpretability, which is key for many industries (e.g., healthcare, finance), is also a challenge since quantum states are not easily interpretable.

- Possible Solution: Ongoing research is needed to develop more robust quantum algorithms and methods to interpret quantum models, as well as benchmarking quantum and classical performance.

7. Hybrid Quantum-Classical Integration

- *Problem*: Many current QML approaches use hybrid quantum-classical models where part of the computation is done on quantum hardware and part on classical systems. Integrating these systems seamlessly is a major challenge due to the different architectures, communication overhead, and data transfer bottlenecks.

- *Impact*: This integration challenge limits the efficiency and scalability of hybrid models, which are seen as the most promising route in the NISQ era.

- *Possible Solution*: Optimizing the quantum-classical interface, minimizing communication overhead, and using efficient partitioning of tasks between quantum and classical components can help mitigate these issues.

8. Algorithmic Scalability and Quantum Advantage

- *Problem*: While some quantum algorithms theoretically offer exponential speedups over classical ones (like Grover's and Shor's algorithms), it's still unclear how and when QML algorithms will demonstrate clear quantum advantage (i.e., solving problems faster than classical methods).

- *Impact*: The lack of a demonstrable, practical quantum advantage limits the current enthusiasm and investment in QML, particularly in industries where near-term benefits are crucial.

- *Possible Solution*: Focusing on quantum-inspired algorithms or developing quantum algorithms for problems where classical methods struggle, such as optimization, might help showcase early examples of quantum advantage.

9. Quantum Computing Software Ecosystem

- *Problem*: The software ecosystem for quantum computing, including development tools, libraries, and frameworks, is still in its infancy. Many quantum programming languages (e.g., Qiskit, Cirq, PennyLane) are evolving rapidly, but there is no clear standard yet.

- *Impact*: This fragmentation makes it harder for developers and researchers to choose the right tools for their projects, leading to issues with interoperability and steep learning curves.

- *Possible Solution*: A more mature, standardized software ecosystem, along with better documentation and education resources, will help bridge this gap and make QML development more accessible.

10. Hardware-Specific Limitations

- *Problem*: Different quantum hardware platforms (e.g., superconducting qubits, trapped ions, photonic qubits) have their own unique characteristics and limitations. Certain QML algorithms may perform well on one type of hardware but poorly on another due to differences in gate fidelities, coherence times, and operational speed.

- *Impact*: The variety of hardware architectures adds complexity to the development of portable, hardware-agnostic QML algorithms.
- Possible Solution: Developing more hardware-agnostic quantum algorithms and improving hardware-specific optimization techniques will help mitigate this challenge.

11. Talent Shortage and Educational Barriers

- *Problem*: There is a shortage of professionals skilled in both quantum computing and machine learning. Quantum mechanics is a complex field that requires significant expertise, making it difficult to build cross-disciplinary teams that can work on QML.

- *Impact*: The talent shortage slows the pace of research and development in QML, as companies and academic institutions struggle to find qualified individuals who can work at the intersection of these fields.

- *Possible Solution*: Increasing educational programs, workshops, and collaborations between universities and industry can help develop the next generation of quantum machine learning experts.

In conclusion, Quantum Machine Learning has the potential to revolutionize the field of machine learning by solving problems that are intractable for classical algorithms. However, many challenges—ranging from hardware limitations to algorithmic scalability—need to be overcome before this vision can be fully realized. Continued research, better tools, and improved hardware will be essential to address these hurdles and unlock the true potential of QML.

Appendix A – Scientific references on Quantum Computing for Climate Modeling and Simulation

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These are only some scientific references available in literature. They offer valuable insights for understanding how quantum communication technologies could be applied to climate change research.

Appendix E – Scientific references on Quantum Machine Learning for Climate Change

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These are only some scientific references on Quantum Machine Learning available in literature. They offer valuable insights into the expanding role of quantum machine learning in climate change applications.

Appendix F – Available Quantum Computers (Updated 2024–2026)

This appendix provides an updated overview of major quantum computing platforms available as of 2024–2026, categorized by technology, access model, maturity, and relevance for climate and Earth-system applications.

A. Providers and Platforms

1. IBM Quantum

- *Technology*: Superconducting (gate-based)
- *Hardware*: **Eagle** (127 physical qubits, legacy), **Osprey** (433 physical qubits), **Condor** (1,121 physical qubits, experimental), **Heron** (133 physical qubits)
- *Access*: IBM Quantum Platform; IBM Quantum Network
- *Notes*: Emphasis on error mitigation, modular scaling, and utility-era workloads.

2. Google Quantum AI

- *Technology*: Superconducting (gate-based)
- *Hardware*: **Sycamore** (53 physical qubits)
- *Access*: Primarily internal/collaborative research; Cirq software ecosystem
- *Notes*: Strong focus on fault tolerance and logical-qubit roadmaps rather than broad public access.

3. Rigetti Computing

- *Technology*: Superconducting (gate-based)
- *Hardware*: **Aspen-M** (80 physical qubits), **Ankaa** (84 physical qubits)
- *Access*: Rigetti QCS; Amazon Braket; Microsoft Azure Quantum
- Notes: Focus on improving gate fidelity and hybrid quantum–classical workflows.

4. D-Wave Systems

- *Technology*: Quantum annealing (optimization-focused)
- *Hardware*: **Advantage** (~5,000+ qubits), **Advantage2** (7,000+ qubits)
- *Access*: D-Wave Leap; Amazon Braket; Microsoft Azure Quantum
- *Notes*: Mature hybrid solvers for optimization (scheduling, routing, grid/portfolio problems).

5. Quantinuum

- *Technology*: Trapped-ion (gate-based)
- *Hardware*: **H1 series** (10–20 physical qubits, legacy); **H2 series** (32 physical qubits, fully connected)
- *Access*: Microsoft Azure Quantum; direct enterprise access
- *Notes*: High fidelity and strong error-correction demonstrations; reports progress toward logical qubits.

6. IonQ

- *Technology*: Trapped-ion (gate-based)
- *Hardware*: **Harmony** (11 physical qubits, legacy); **Aria** (25 physical qubits; also marketed as ~20 algorithmic qubits); **Forte** (32 physical qubits)
- *Access*: Amazon Braket; Microsoft Azure Quantum; Google Cloud Marketplace
- *Notes*: IonQ often reports an application-oriented performance metric ("algorithmic qubits") alongside physical qubits.

7. Pasqal

- *Technology*: Neutral atoms (Rydberg arrays; analog / hybrid)
- *Hardware*: 100–200+ atom processors (analog mode)
- *Access*: Microsoft Azure Quantum; direct partnerships
- *Notes*: Particularly relevant for many-body simulation and some optimization-style formulations.

8. Xanadu

- *Technology*: Photonic (continuous-variable)
- *Hardware*: **Borealis** (Gaussian boson sampling); **X-Series** (CV quantum ML systems)
- *Access*: Xanadu Cloud
- *Notes*: Strong in sampling/ML; fault-tolerant photonic roadmaps are longer-term.

9. Amazon Braket

- *Role*: Cloud access and orchestration platform (multi-vendor)
- *Providers commonly available*: IonQ, Rigetti, D-Wave, QuEra (+ simulators)
- *Notes*: Unified access layer rather than a hardware provider.

10. Microsoft Azure Quantum

- *Role*: Cloud access and orchestration platform (multi-vendor)
- *Providers commonly available*: IonQ, Quantinuum, Rigetti, Pasqal, QCI (+ simulators and resource estimation)
- *Notes*: Includes tooling to estimate logical- and physical-qubit resources for fault-tolerant workloads.

11. QuEra

- *Technology*: Neutral atoms (analog / hybrid)
- *Hardware*: **Aquila** (256+ atoms)
- *Access*: Amazon Braket
- *Notes*: Strong for analog simulation and some combinatorial optimization mappings.

B. Comparison Table (Technology × Qubits × Maturity × Climate Relevance)

Provider / Platform	Technology (policy term)	Representative systems / qubits[1]	Maturity	Climate relevance (examples)
IBM Quantum	Gate-based superconducting	Heron (133 physical); Osprey (433 physical); Condor (1,121 physical, experimental)	Commercial cloud access (NISQ → utility)	Medium–High: algorithm prototyping, error mitigation studies, QML baselines
Google Quantum AI	Gate-based superconducting	Sycamore (53 physical)	Research (limited access)	Medium: methods research (QEC, algorithms); less direct for applied workloads
Rigetti	Gate-based superconducting	Ankaa (84 physical); Aspen-M (80 physical)	Commercial cloud access (early)	Medium: hybrid optimization / ML prototypes; benchmarking
D-Wave	Quantum annealing (optimization)	Advantage (~5,000+); Advantage2 (7,000+)	Commercial cloud access (mature)	High for optimization: grid ops, routing, scheduling, portfolio / planning
Quantinuum	Gate-based trapped ions	H2 (32 physical); H1 (10–20 physical, legacy)	Commercial cloud access (high fidelity)	Medium–High: chemistry/optimization pilots; error-correction demonstrations relevant to scale-up
IonQ	Gate-based trapped ions	Aria (25 physical; ~20 AQ); Forte (32 physical); Harmony (11 physical, legacy)	Commercial cloud access (early)	Medium–High: QML pilots; optimization; application-oriented benchmarking
Pasqal	Neutral atoms (analog / hybrid)	100–200+ atoms (analog)	Commercial / research access (growing)	High for simulation-style tasks: many-body models; some optimization mappings
Xanadu	Photonic (continuous-variable)	Borealis (GBS); X-Series (CV platforms)	Commercial / research access (niche)	Medium: sampling/QML research; potential for climate uncertainty quantification
QuEra	Neutral atoms (analog / hybrid)	Aquila (256+ atoms)	Commercial / research access (growing)	High for analog simulation and some optimization; good for exploratory climate-physics surrogates
Amazon Braket	Cloud access platform (multi-vendor)	Access layer to multiple backends (provider-dependent)	Commercial cloud platform	High as an enabler: procurement and experimentation across vendors
Azure Quantum	Cloud access platform (multi-vendor)	Access layer + resource estimation (logical/physical qubits)	Commercial cloud platform	High as an enabler: fault-tolerant resource estimation; multi-vendor access

[1] Footnote (metrics terminology used in EU/US policy reporting):
A "physical qubit" is a single hardware qubit (e.g., a superconducting circuit, trapped ion, or atom). Because physical qubits are noisy, many applications ultimately require "logical qubits" (also called "error-corrected qubits"), which encode one robust qubit across many physical qubits using quantum error correction. Some vendors also publish application-oriented performance metrics (e.g., IonQ's "algorithmic qubits") that summarize how effectively a device can run selected benchmark algorithms; these are not the same as physical or logical qubit counts. In policy-facing documents, prefer reporting: (1) physical qubits, (2) gate/measurement fidelity or error rates where available, (3) any demonstrated logical-qubit capability, and (4) clearly labeled vendor-specific composite metrics.

C. Recommended Reporting Format (EU / US Policy-Aligned)

For policy-facing white papers, roadmaps, and strategy documents, quantum-computing capabilities should be reported using a clear, technology-neutral structure that avoids overreliance on vendor-specific marketing metrics.

Recommended minimum reporting elements:

1. **Technology class** – Specify the hardware paradigm using standard policy terminology (gate-based superconducting, gate-based trapped ions, neutral atoms, photonic, or quantum annealing).

2. **Physical qubit count** – Report the number of physical qubits available on the system as the primary quantitative metric.

3. **Fidelity and error characteristics** – Where available, report representative single- and two-qubit gate fidelities, measurement fidelity, or error rates.

4. **Connectivity and architecture** – Describe qubit connectivity (fully connected, nearest-neighbor, modular, lattice-based), as this strongly affects algorithm mapping and scalability.

5. **Logical or error-corrected qubit capability** – Clearly state whether logical qubits have been demonstrated, how many, and under what conditions. Distinguish demonstrated capability from roadmap targets.

6. **Vendor-specific composite metrics** – If metrics such as "algorithmic qubits" are cited, label them explicitly as vendor-defined indicators and do not equate them with physical or logical qubit counts.

7. **Access model and maturity** – Specify whether access is public cloud, restricted research, or internal-only, and characterize maturity (exploratory research, early commercial access, or production-scale pilot).

8. **Application relevance** – Qualitatively map platforms to application classes (optimization, simulation, quantum machine learning) and to climate-relevant use cases such as energy optimization, digital twins, uncertainty quantification, and surrogate modeling.

This reporting structure is consistent with practices used in **EU programs** (e.g., *Quantum Flagship, Destination Earth*) and **US federal initiatives** (e.g., *DOE, NSF, NIST*), supporting transparent and comparable assessment of quantum technologies.

Appendix G – Quantum Computers Technologies

Quantum computers are built using various technologies that differ in how they represent and manipulate quantum bits (qubits). Each technology has unique characteristics, advantages, and challenges. Below are the most prominent quantum computing technologies:

1. Superconducting Qubits

- *Description*: Superconducting qubits are circuits made from superconducting materials that can conduct electricity without resistance at very low temperatures. They form the basis of gate-based quantum computing, where qubits are manipulated using microwave pulses.

- *Key Companies:*
  - IBM Quantum (e.g., Eagle, Osprey processors)
  - Google Quantum AI (e.g., Sycamore)
  - Rigetti Computing**

- *Advantages:*
  - Mature technology with high scalability potential.
  - Widely used in research and commercial applications.
  - Fast gate operation times (~nanoseconds).

- *Challenges:*
  - High error rates, requiring extensive quantum error correction.
  - Needs extreme cooling (cryogenic temperatures).
  - Limited coherence times (how long a qubit can retain its quantum state).

2. Trapped Ion Qubits

- *Description*: Trapped ion qubits are individual atoms (ions) held in place by electromagnetic fields. Lasers are used to manipulate their energy levels, representing qubit states.

- *Key Companies*:
  - IonQ
  - Honeywell Quantum Solutions (Quantinuum)**

- *Advantages:*
  - Long coherence times (good for maintaining quantum states).
  - High-fidelity gate operations, meaning lower error rates.
  - Fully connected qubits (any qubit can interact with any other qubit directly).

- *Challenges:*
  - Slower gate speeds compared to superconducting qubits.
  - More complex hardware setup.
  - Scalability is still being tested, though improving with modular designs.

3. Quantum Annealing

- *Description*: Quantum annealers solve optimization problems by evolving a system into its lowest energy state. Unlike gate-based systems, quantum annealers are specialized machines for specific tasks like combinatorial optimization.

- *Key Companies:*
  - D-Wave Systems

- *Advantages:*
  - Specialized for solving optimization problems, such as logistics, portfolio optimization, and machine learning.
  - Scalable to thousands of qubits (D-Wave's Advantage system has 5,000+ qubits).

- *Challenges:*
  - Limited to specific types of problems (optimization) and not suitable for general-purpose quantum computing.
  - Qubits in quantum annealers have limited flexibility compared to gate-based systems.

4. Photonic Quantum Computing

- *Description*: Photonic quantum computers use photons (particles of light) as qubits. These qubits are manipulated through interferometers and other optical components like beam splitters, phase shifters, and detectors.

- *Key Companies:*
  - Xanadu

- *Advantages:*
  - Photons travel at the speed of light, enabling fast quantum information transmission.
  - Room-temperature operation (unlike superconducting qubits that require cryogenic temperatures).
  - High potential for integration with existing fiber-optic communications.

- *Challenges:*
  - Creating reliable single-photon sources and detectors is difficult.
  - Photonic gates are probabilistic, meaning success rates of operations are not deterministic without extra work.

5. Neutral Atom Quantum Computing

- *Description*: Neutral atoms, particularly Rydberg atoms (atoms in highly excited states), are trapped and manipulated using laser beams. These qubits are controlled by changing the energy states of the atoms.

- *Key Companies:*
  - Pasqal
  - QuEra

- *Advantages:*
  - Highly scalable due to the ability to manipulate many atoms simultaneously.
  - Can be arranged in arbitrary geometries, offering flexibility in designing qubit connectivity.
  - Potential for very high qubit densities, with hundreds of qubits already demonstrated.

- *Challenges:*
  - Coherence times and error rates still need improvement.
  - Laser control and trapping technology are complex.

6. Topological Qubits

- *Description*: Topological qubits are based on exotic particles called anyons and leverage topological states of matter, which are inherently protected from environmental noise. This is a highly theoretical approach, and no large-scale topological quantum computer exists yet.

- *Key Companies:*
  - (investing heavily in research)

- *Advantages:*
  - Inherent error resistance, potentially reducing the need for quantum error correction.

- *Challenges:*
- This technology is still in the experimental stage, with no successful large-scale demonstrations.
- Extremely complex to implement and requires new materials and physics to be fully understood.

7. Quantum Dots

- *Description*: Quantum dots are semiconductor particles that can confine electrons or holes, allowing for manipulation of their quantum states (spin). Quantum dots can serve as qubits, where the spin of the electron represents the quantum state.

- *Key Companies*:
    - Intel (conducting significant research in this area)

- Advantages:
    - Integrates well with existing semiconductor fabrication technology, promising for large-scale integration.
    - Potential for fast gate operations.

- *Challenges:*
    - Maintaining coherence in quantum dots is challenging due to their sensitivity to the environment.
    - Scalability beyond a few qubits is still under development.

8. Superconducting Flux Qubits

- *Description*: Flux qubits are superconducting loops where the quantum state is represented by the direction of the current flow (clockwise or counterclockwise). This is a type of superconducting qubit, but it operates differently from the transmon qubits used by companies like IBM and Google.

- *Key Companies:*
- Some university and research labs are exploring flux qubits, but they are less common than transmon qubits.

- *Advantages:*
    - Potential for faster operations than some other qubit technologies.
    - Could be more stable than transmon-based qubits under certain conditions.

- *Challenges:*
    - Complexity in fabrication and controlling the quantum state.
    - Less mature than other superconducting qubit designs.

Comparison of Technologies

Technology	Qubit Type	Advantages	Challenges	Companies
Superconducting Qubits	Superconducting circuits	Scalable, fast gates, mature ecosystem	High error rates, cryogenic cooling	IBM, Google, Rigetti
Trapped Ion Qubits	Ions (electrically charged atoms)	High fidelity, long coherence times	Slower gate speeds, complex setup	IonQ, Honeywell (Quantinuum)
Quantum Annealing	Annealing qubits	Scalable, optimized for specific problems	Not general-purpose, limited flexibility	D-Wave Systems
Photonic Qubits	Light (photons)	Room-temperature operation, fast information transmission	Probabilistic operations, complex photon control	Xanadu
Neutral Atom Qubits	Rydberg atoms	Scalable, flexible qubit arrangements	Coherence and error rates need improvement	Pasqal, QuEra
Topological Qubits	Anyons	Inherent error resistance	Experimental, no large-scale demonstrations yet	Microsoft (research stage)
Quantum Dots	Electron spins in semiconductors	Compatible with semiconductor tech, potential for speed	Sensitivity to environment, coherence issues	Intel (research)
Superconducting Flux Qubits	Superconducting loops	Fast operations, potential for stability	Complexity in control, less mature	Research labs, universities

Choosing the Right Technology

- *Superconducting and Trapped Ion Qubits* are the most mature for general-purpose quantum computing, making them ideal for early-stage experimentation and development.

- *Quantum Annealing (D-Wave)* is ideal for solving large-scale optimization problems but not for general algorithms.

- *Photonic and Neutral Atom Qubits* are promising for scalability and speed, though they are still in developmental stages.

- *Topological Qubits* represent a more speculative but potentially revolutionary approach due to their resistance to errors, though practical systems are still in research.

Each quantum computing technology has distinct advantages based on the type of problem you wish to solve and the maturity of the ecosystem surrounding it.

Appendix H – Koopman operator and Quantum Computing

The Koopman operator is a powerful mathematical framework that provides insights into nonlinear dynamical systems by transforming the problem into a linear setting. Indeed, the Koopman operator allows to analyze nonlinear dynamical systems by representing them in terms of a linear operator in an infinite-dimensional space. It essentially transforms a nonlinear system into a linear one in a higher-dimensional space by acting on functions of the system's state, rather than directly on the state itself.

This approach has been widely applied in areas like fluid dynamics, machine learning, and control systems and is increasingly being explored for solving nonlinear equations.

In the following a detailed exploration of the Koopman operator, its properties, applications, and relevance in various fields are reported.

1. Mathematical Definition

- ***Nonlinear Dynamical System***: Consider a nonlinear dynamical system described by a state evolution:

$$\boldsymbol{x}(\boldsymbol{t}+\mathbf{1}) = \boldsymbol{f}\big(\boldsymbol{x}(\boldsymbol{t})\big)$$

  where $\boldsymbol{x}(\boldsymbol{t})$ is the state of the system at time $\boldsymbol{t}$ and $\boldsymbol{f}$ is a nonlinear function.

- ***Observables***: An observable is a function $\boldsymbol{g}$ that maps the state space to the real numbers, i.e., $\boldsymbol{g} : \boldsymbol{X} \rightarrow \mathbb{R}$

- ***Koopman Operator***: Given a dynamical system defined by a state $\boldsymbol{x}(\boldsymbol{t})$, the Koopman operator $\boldsymbol{K}$ evolves an observable $\boldsymbol{g}$ as:

$$(\boldsymbol{Kg})(\boldsymbol{x}) = \boldsymbol{g}\,\big(\boldsymbol{f}(\boldsymbol{x})\big)$$

  where $\boldsymbol{f}$ describes the dynamics of the system.

  This means that the operator takes an observable and gives its value at the next time step under the dynamics defined by $\boldsymbol{f}$. Then, the Koopman operator describes how observables evolve over time under the dynamics of the system. It should be noted that the Koopman operator is an infinite-dimension linear operator that acts on observables (functions of the system state) rather than the state itself.

2. Linear Dynamics

- **Infinite-Dimensional Linear Operator**: The Koopman operator is linear, allowing the application of linear analysis techniques. For example, if $\boldsymbol{g_1}$ and $\boldsymbol{g_2}$ are observables, then:

$$\boldsymbol{K}(\boldsymbol{c_1 g_1} + \boldsymbol{c_2 g_2}) = \boldsymbol{c_1 K g_1} + \boldsymbol{c_2 K g_2}$$

  where $\boldsymbol{c_1}$and $\boldsymbol{c_2}$ are constants.

- **Eigenfunctions and Eigenvalues**: An important aspect of the Koopman operator is its eigenfunctions and eigenvalues. If g is an eigenfunction of the Koopman operator with eigenvalue λ:

$$\boldsymbol{Kg = \lambda g}$$

then $\boldsymbol{g}$ evolves in a predictable manner under the dynamics, which helps analyze stability and long-term behavior.

3. Understanding the Equation $\boldsymbol{Kg = \lambda g}$

- **Components of the Equation**

  - $\boldsymbol{K}$: This represents the Koopman operator, which acts on observables (functions of the system state).
  - $\boldsymbol{g}$: This is an observable function (or eigenfunction) that captures some property of the system.
  - $\boldsymbol{\lambda}$: This is the eigenvalue associated with the observable $\boldsymbol{g}$.

- **Interpretation**

  - The equation states that when the Koopman operator $\boldsymbol{K}$ is applied to the observable $\boldsymbol{g}$, the result is simply a scaled version of $\boldsymbol{g}$ itself, scaled by the factor $\boldsymbol{\lambda}$
  - This indicates that $\boldsymbol{g}$ behaves in a predictable manner under the dynamics of the system governed by the Koopman operator.

4. Implications of the Eigenvalue Equation

- **Dynamical Behavior**

  - The eigenvalue $\boldsymbol{\lambda}$ gives insight into how the observable gg evolves over time:
    - **If** $\boldsymbol{|\lambda| < 1}$: The observable $\boldsymbol{g}$ decays over time, indicating stability.
    - **If** $\boldsymbol{|\lambda| = 1}$: The observable remains constant, suggesting a steady state or a periodic behavior.
    - **If** $\boldsymbol{|\lambda| > 1}$: The observable grows over time, indicating instability.

- **Characterization of Dynamics**

  - The eigenfunctions $\boldsymbol{g}$ corresponding to different eigenvalues can characterize various modes of the system's dynamics. These can reveal patterns, such as oscillations or trends, which are essential for understanding complex behaviors.

- **Long-Term Predictions**

  - By identifying the eigenfunctions and their corresponding eigenvalues, one can make long-term predictions about the system's behavior, focusing on specific observables of interest.

5. Properties of the Koopman Operator

- **Linearity**: The operator is linear, allowing the use of tools from linear algebra and functional analysis.

- **Eigenstructure**: It provides a way to analyze the dynamics via its eigenfunctions and eigenvalues, which reveal information about the system's behavior.

- **Invariance**: The Koopman operator can be used to find invariant measures and set structures of the system, which helps in understanding long-term dynamics.

- **Lifted Space**: The state space can be lifted to a higher-dimensional space of observables, allowing for simpler linear analysis.

6. Applications of the Koopman Operator

- **Model Reduction**
  - The Koopman operator allows for the reduction of complex nonlinear systems to a manageable linear form. By focusing on the dominant eigenfunctions, a reduced-order model that captures essential dynamics, while ignoring less significant modes, can be created.

- **Fluid Dynamics**
  - The Koopman operator has found extensive use in fluid dynamics for modeling and controlling complex nonlinear systems, including turbulence. By transforming nonlinear dynamics into a linear framework, the Koopman approach simplifies the analysis of chaotic and intricate fluid flows. This enables deeper insights into underlying dynamics, such as identifying coherent structures and patterns, and understanding turbulence through the evolution of specific observables.

- **Machine Learning and Data Science**
- Recent advancements involve using the Koopman operator in machine learning for system identification and model reduction, enhancing predictive modeling. Data-driven methods can approximate the Koopman operator from empirical data, leading to efficient modeling of dynamical systems.

- **Quantum Mechanics**
  - While the application of the Koopman operator to quantum systems is still an active area of research, it holds potential for understanding the evolution of observables in quantum mechanics, similar to its role in classical systems.

- **Control Systems**
  - In control systems, the Koopman operator is used to design controllers for nonlinear systems by linearizing the system dynamics in a higher-dimensional space, making the system easier to control using standard linear control methods, providing insights into system stability and behavior under feedback

- **Robotics**
  - In robotics, the Koopman operator can aid in trajectory planning and motion control by providing a linear representation of the nonlinear dynamics of robotic systems.

- **Stability and Bifurcation Analysis**
  - *Stability Analysis*: The eigenvalues of the Koopman operator can provide insights into the stability of fixed points in nonlinear systems, where eigenvalues with magnitudes less than one indicate stability.
  - *Bifurcation Analysis*: By studying how the spectrum of the Koopman operator changes with parameters, one can analyze bifurcations and transitions in system behavior.

7. Koopman Operator and Quantum Computing

Quantum computing offers potential advantages for solving problems involving Koopman operators because quantum computers naturally handle high-dimensional linear transformations efficiently. By leveraging quantum algorithms such as quantum phase estimation or quantum matrix inversion, the Koopman operator could be computed and applied to solve nonlinear systems more efficiently than classical methods, especially for large-scale problems.
In the following some key points about how these two fields can be related:

- **State Representation**: Quantum systems are often represented using state vectors in Hilbert space. The Koopman operator can provide insights into the evolution of observables within quantum systems, potentially enabling more efficient simulations.

- **Data-Driven Approaches**: Quantum computing can leverage data-driven methods to approximate the Koopman operator from time series data. This can enhance the ability to model and predict the dynamics of quantum systems.

- **Efficient Algorithms**: Quantum algorithms, such as quantum phase estimation and variational algorithms, could potentially be adapted to compute properties of the Koopman operator or its eigenfunctions, which are crucial for understanding the long-term behavior of dynamical systems.

- **Hybrid Quantum-Classical Approaches**: There is potential for hybrid approaches that combine classical methods for estimating the Koopman operator with quantum algorithms for more efficient computation, particularly in high-dimensional systems.

- **Quantum Control**: The Koopman operator can also play a role in quantum control, where understanding the dynamics of a quantum system is essential for effectively steering its evolution. The operator could help design control strategies that are implemented on quantum hardware.

In conclusion, the connection between the Koopman operator and quantum computing is a promising area of research with the potential to enhance our understanding of complex dynamical systems and improve computational methods in quantum mechanics. As quantum technologies advance, we may see more significant applications of the Koopman operator in quantum computing and related fields.

8. Research Directions and Challenges

- **Data-Driven Techniques**: Developing efficient algorithms for estimating the Koopman operator from data, particularly in high-dimensional systems.

- **Machine Learning Integration**: Integrating Koopman theory with quantum machine learning approaches may allow for more effective data analysis and system identification in quantum contexts.

- **Numerical Methods**: Exploring numerical methods for approximating eigenfunctions and eigenvalues of the Koopman operator. Research is ongoing into using quantum computers to solve eigenvalue problems associated with the Koopman operator, which can provide important insights into the stability and dynamics of non-linear systems

- **Stability Analysis**: Further investigation into how the eigenvalues of the Koopman operator relate to the stability of nonlinear systems.

- **Hybrid Approaches**: Combining classical and quantum computing techniques to leverage the strengths of both paradigms for analyzing complex systems.

- **Applications in Quantum Mechanics**: Applying the Koopman operator framework to quantum mechanics itself can help in understanding complex quantum systems, potentially leading to advancements in quantum simulations and quantum information.

Conclusion

In conclusion, the Koopman operator provides a robust framework for analyzing nonlinear dynamical systems by transforming them into a linear context. Its application spans various fields, including fluid dynamics, control theory, machine learning, and potentially quantum mechanics. As research progresses, the Koopman operator is expected to play an increasingly significant role in understanding and predicting the behavior of complex systems.

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These are only some scientific references on Koopman Operator available in literature. They offer valuable insights into the expanding role of Koopman Operator in climate change applications.

Appendix I - Variational Quantum Algorithms (VQAs)

Variational Quantum Algorithms (VQAs) are a class of quantum algorithms that aim to solve complex problems by using both quantum and classical computation. These algorithms leverage the power of quantum computing for tasks such as optimization, machine learning, and quantum chemistry simulations, while also using classical computers to optimize parameters involved in the quantum computation.

- **Key Concepts in VQAs:**
  - *Parameterized Quantum Circuits (PQCs)*
    - VQAs use parameterized quantum circuits, also known as ansatzes. These circuits have quantum gates whose behavior is controlled by parameters (real numbers), which can be adjusted to minimize a given objective or cost function. The task of a VQA is typically to minimize (or maximize) a cost function, which represents the energy or error of a particular quantum state. The quantum circuit is executed to compute a value that depends on the parameters, and the classical optimizer updates the parameters to minimize this value.
  - *Noisy Intermediate-Scale Quantum (NISQ) devices*
    - VQAs are well-suited for NISQ devices, which are the quantum computers available today. These devices have a limited number of qubits and are prone to errors, but VQAs can tolerate noise better than other quantum algorithms due to their hybrid nature.
  - *Common Types of VQA*
    - *Variational Quantum Eigensolver (VQE)*
      - VQE is used to find the ground state energy of a quantum system, especially in quantum chemistry and materials science. It works by parameterizing a trial quantum state and then minimizing the energy expectation value of this state.
  - *Quantum Approximate Optimization Algorithm (QAOA)*
    - QAOA is designed for solving combinatorial optimization problems, such as Max-Cut or traveling salesman problems. It uses quantum circuits to approximate the optimal solution to these classical problems.
  - *Quantum Neural Networks (QNNs)*
    - QNNs are a form of VQA that applies quantum circuits to perform tasks similar to classical neural networks, like classification and pattern recognition. These are useful in quantum machine learning.
  - *Variational Quantum Linear Solver (VQLS)*
    - VQLS aims to solve linear systems of equations using a variational approach, similar to how classical linear solvers work but taking advantage of quantum computation.

- **Steps in a VQA**
    - *Ansatz Construction*
        - A parameterized quantum circuit (ansatz) is constructed. The choice of ansatz can significantly impact the performance of the algorithm.
    - *Quantum State Preparation and Measurement*
        - The quantum computer prepares the state and measures it based on the current parameters, giving information (like expectation values) that are fed into the cost function.
    - *Classical Optimization*
        - A classical optimizer (e.g., gradient descent, genetic algorithms) adjusts the parameters of the quantum circuit based on the output of the cost function.
    - *Iteration*
        - The process iterates between quantum computations and classical optimizations until the algorithm converges on a solution.
- **Benefits of VQAs**
    - *Noise Tolerance*
        - VQAs are more resilient to noise, as they rely on repeated measurements and classical post-processing, which helps mitigate the errors from noisy quantum devices.
    - *Scalability*
        - They are designed to work with the limited qubits available in NISQ devices, making them practical in the near term.
    - *Flexibility*
        - VQAs can be adapted for various problems, including quantum chemistry, machine learning, and optimization tasks.
- **Challenges**
    - *Optimization Landscape*
        - The cost function may have a complex landscape with local minima, making it hard for classical optimizers to find the global minimum.
    - *Ansatz Design*
        - The choice of ansatz is crucial, but finding an efficient ansatz for a specific problem can be difficult and problem-specific.
    - *Quantum Resources*
        - Despite their efficiency, VQAs still require a significant number of qubits and quantum gate operations, which can be a limitation on current quantum hardware.

In summary, **Variational Quantum Algorithm**s are powerful tools for solving problems by combining quantum computing's ability to manipulate complex states with classical optimization techniques, making them highly valuable for near-term quantum applications.

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These are only some scientific references on Variational Quantum Algorithms available in literature. They offer valuable insights for understanding the role of VQAs for climate modeling and quantum simulations.

Appendix J - The Noisy Intermediate-Scale Quantum (NISQ) Era

The **Noisy Intermediate-Scale Quantum** (**NISQ**) era refers to the current stage in the development of quantum computing, where quantum devices with around 50 to a few hundred qubits are available. These quantum computers are powerful enough to perform computations beyond the reach of classical computers for specific tasks, but they are also limited by several key factors, particularly noise and errors in quantum operations.

The term was coined by physicist John Preskill in 2018 to describe the present state of quantum technology, distinguishing it from the longer-term goal of fault-tolerant quantum computing, which requires much larger, more reliable quantum computers.

- **Key Characteristics of the NISQ Era**

- *Noisy*
  - Current quantum devices are noisy because qubits are prone to errors due to decoherence and gate imperfections. Quantum states are fragile and degrade over time due to environmental interference, making it challenging to maintain accurate quantum information for long computations.

- *Intermediate-Scale*
  - The number of qubits available on current quantum computers typically ranges from 50 to 300 qubits. While this is sufficient for some tasks that classical computers struggle with, it is far from the millions of qubits that are expected to be needed for fully fault-tolerant quantum computing.

- *Non-Error-Corrected*
  - NISQ devices do not yet have error correction that is capable of dealing with the noise effectively for large-scale operations. Although error correction codes exist in theory, they are computationally demanding and require a significant overhead of additional qubits, which NISQ devices lack.

- *Quantum Advantage Demonstrations*
  - NISQ computers are anticipated to show quantum advantage (also called quantum supremacy) for specific problems, meaning they can solve certain tasks faster than classical computers. In 2019, Google's quantum computer, Sycamore, demonstrated quantum supremacy for a specialized problem by performing a task in seconds that would have taken classical supercomputers thousands of years. However, practical and broad quantum advantage for useful problems is still in development.

- **Opportunities in the NISQ Era**

    - *Variational Quantum Algorithms (VQAs)*
        - As discussed in Appendix A, VQAs are well-suited for NISQ devices because they are designed to handle noise by combining quantum circuits with classical optimization techniques. These algorithms have been used for problems in quantum chemistry, optimization, and machine learning.

    - *Quantum Simulations*
        - NISQ devices are promising for simulating quantum systems, such as chemical reactions or materials, that are difficult or impossible for classical computers. Quantum chemistry and condensed matter physics are key areas where quantum simulation is likely to make breakthroughs.

    - *Combinatorial Optimization*
        - Algorithms like the Quantum Approximate Optimization Algorithm (QAOA), which is designed for solving combinatorial optimization problems, are tailored to the capabilities of NISQ devices. These problems are relevant in fields like logistics, finance, and artificial intelligence.

    - Quantum Machine Learning (QML)
        - In quantum machine learning, NISQ devices can be used to accelerate certain types of learning tasks by manipulating data in high-dimensional quantum states. Although still experimental, there is potential for speedups in tasks like pattern recognition, classification, and clustering.

- **Challenges of the NISQ Era:**

- *Noise and Errors*
    - Quantum computations are disrupted by noise, leading to inaccurate results. While quantum error correction is a long-term solution, in the short term, the challenge is to develop quantum algorithms that tolerate noise and exploit the power of quantum systems despite their imperfections.

- *Limited Qubit Count*
    - Although NISQ devices have tens to a few hundred qubits, many practical problems require thousands or millions of qubits for meaningful advantage. The small qubit count restricts the complexity of the problems that NISQ computers can tackle.

- *Algorithm Development*
    - Current quantum algorithms for NISQ devices are not yet mature, and finding the right algorithms to exploit the capabilities of NISQ hardware is an ongoing research challenge. Many of the most famous quantum algorithms, such as Shor's algorithm (for factoring large numbers) and Grover's algorithm (for searching unsorted databases), are not feasible on NISQ devices due to their high resource demands.

- *Scalability*
    - To scale up quantum computers to handle larger, more complex problems, significant advancements are required in qubit quality, quantum error correction, and system integration. Current NISQ devices struggle to scale because each additional qubit introduces more noise and error.

- **Long-Term Outlook Beyond NISQ**

  The NISQ era is seen as a transitional phase in the development of quantum computing. The ultimate goal is to move towards fault-tolerant quantum computing, where qubits can be manipulated with minimal errors over long periods of time. This will require large numbers of qubits with sophisticated quantum error correction to compensate for any noise or faults.

  In the post-NISQ era, we expect quantum computers to achieve universal quantum computing with robust, large-scale systems capable of executing powerful algorithms for cryptography (e.g., Shor's algorithm), complex simulations, and large-scale optimization tasks.

Conclusion

The NISQ era represents an exciting yet challenging time for quantum computing. While quantum computers available today are still small and noisy, they hold the potential to solve certain problems that classical computers cannot. Hybrid algorithms, like VQAs, quantum simulations, and optimization problems are the focus areas for NISQ devices, but achieving practical, widespread quantum advantage will require overcoming significant technical hurdles related to noise, qubit count, and algorithmic development.