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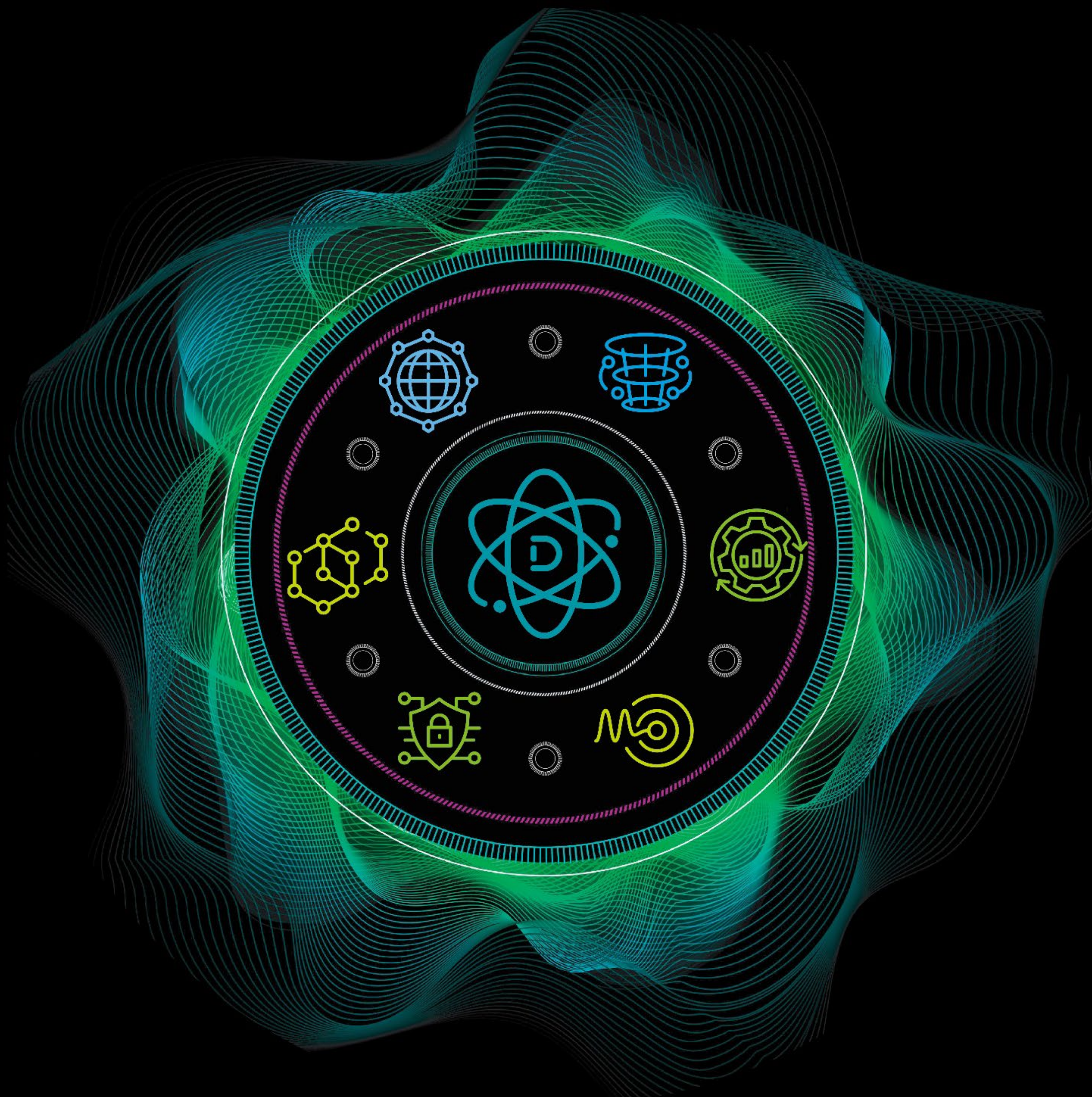

Quantum Computing for Climate Action

September 2023

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Quantum Computing for Climate Action

Quantum computing will likely transform the fight against climate change. By accelerating the development of innovative solutions to address technical challenges, quantum and digital solutions promise the acceleration of solutions to drive progress towards sustainable solutions and informed decision-making.

This publication aims to **explore the potential of quantum computing to solve specific climate-relevant issues** and will help those who are interested in the science and engineering behind the solutions. Our goal is to encourage the quantum computing community to focus on climate-related use cases, while inspiring climate practitioners to approach the quantum community with curiosity and enthusiasm. Thus, it is connected to our overall mission to bridge the gap in the under-explored intersection of climate challenges and quantum computing solutions.

Shifting Computational Paradigms – Key to Fighting Climate Change

The promise of quantum computing

Quantum computers are not just faster computers. In contrast to classical computers, they operate on a completely different computational paradigm. Instead of utilizing Boolean logic based on bits, quantum computers leverage the power of quantum-mechanical effects. As a result, the mathematical space in which problems can be solved is fundamentally broader. In today's understanding, this different solution space is where many of the computational advantages of quantum computers originate.

As is the case for many emerging computational paradigms, the technology to build quantum computers, as well as effective quantum algorithms must be developed in conjunction with each other.

The chances to effectively tackle climate-related challenges are in many cases greatly impacted by the capabilities of computational systems. To develop innovative solutions, knowledge and understanding are key as is the ability to **simulate** and **analyze complex systems** crucial to comprehend intricate dependencies. Highly advanced computers are required to **simulate** environmental systems, to **optimize** resource consumption and to accelerate **material development**. However, these advancements will require entirely new computing paradigms as classical computing systems approach their physical and economical limits. A sample of the potential solutions is outlined in the table below:

Simulation	Optimization	Machine Learning
• Catalysts • Batteries • Carbon capture materials	• Electrical grid • Vehicle routing • Transportation space usage	• Earth system modeling • Materials discovery • Policy decision support

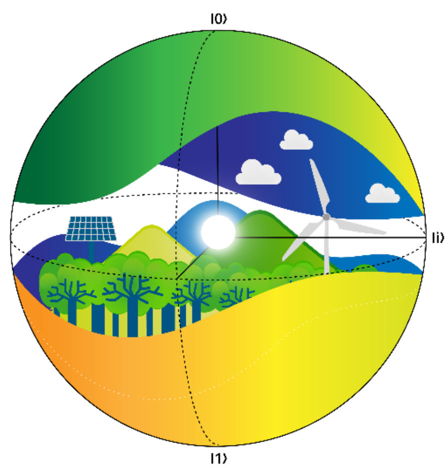
Several new paradigms have emerged over the past decades, promising to provide novel solutions to challenging scientific and technological problems. Among these paradigms are *neuromorphic computing, in-memory computing*, and *quantum computing*. They all have their unique advantages for unique challenges and their parallel existence in the future is to be expected.

Beyond improvements in computational performance, the new supercomputer must also consider the carbon footprint of their operations. Global information and communications infrastructure is expected to consume 21% (8000 TWh) of all global electric energy production in 2031. [1] Finding ways to make computation less energy-intense (Green-IT) is therefore a highly relevant challenge to reduce the overall carbon footprint. Quantum computers show great potential to improve computational performance and at the same time decrease the required energy to solve a given problem. Quantum computers show great potential to improve computational performance while also decreasing the required energy to solve a given problem.

At Deloitte Quantum, our aim is to build an ecosystem that bridges the gap between quantum developers and climate practitioners. With climate change and quantum expertise, Deloitte is a trusted guide and valuable resource for both innovators tackling climate issues and cutting-edge quantum solution designers. Our unique position allows us to be the link between these two communities, providing inspiring insights, practical guidance, and meaningful use cases for successful collaboration.

Deloitte's annual **Quantum Climate Challenge** is open to participants around the globe. In the first installment of the challenge in 2022, concepts for flight route optimization were developed with a focus on reducing the negative impact of air travel on the environment. In 2023, participants leveraged quantum computing for materials research, investigating binding characteristics and selectivity of metal organic frameworks that are used to filter carbon dioxide out of the atmosphere.

To further raise awareness of high-impact use cases, we intend to highlight **promising industry applications**, showcasing not only aspirational ideas but already ongoing explorations in this emerging field. These use cases serve as valuable sources of inspiration, providing meaningful starting points for deeper investigations into the potential of quantum computing. They specifically highlight areas that pose significant challenges for traditional algorithms and where quantum computing holds tremendous promise in surpassing current computational limitations. Find out more here.



High Impact Climate-Related Use Cases

Quantum computers are generally thought to have the greatest potential in the area of *simulation (of physical systems), optimization,* and *machine learning*. For each of these areas, the following sections describe the key limitations of classical computing, how quantum computing may solve these issues, and provides real-world examples of use cases for quantum computing in the context of climate and sustainability.

Simulation of Physical Systems

Many solutions to climate change require technical advancement in areas such as renewable energy systems (solar, wind, and waterpower), carbon capture, and energy storage. While the development of these solutions eventually requires building prototypes and synthesizing materials in the real world, the simulation of physical systems and chemical materials can significantly accelerate technological advancements. Simulations provide a platform to design and optimize new technologies, allowing for much faster development cycles than a trial-and-error based approach in the lab, resulting in cost savings.

The simulation of quantum mechanical systems, such as molecules and materials, requires the use of approximations on classical computers. The fact that all nuclei and electrons in a molecule influence all other nuclei and electrons within that molecule is one of the critical aspects in computational chemistry.

To solve or approximate the *Schrödinger equation*, which governs material properties, specialized methods are required on classical computers. Without approximation, the computational complexity can increase exponentially with the system size. It is therefore virtually impossible to calculate the properties of large molecules or molecular assemblies with great accuracy. Over the last few decades, a plethora of methods have emerged in computational chemistry – historically summarized under the term *quantum chemistry*. These methods utilize approximations and specialized knowledge about the system's chemistry to reduce computational complexity – often at the cost of accuracy of the solution.

Systems that are particularly difficult to simulate using classical quantum chemistry are highly correlated electron systems and systems where the so called Born-Oppenheimer approximation.

With quantum computing, classical approximations would not be necessary, enabling more precise calculations of molecules and materials' properties. Ultimately, this will accelerate the material discovery cycle, which today still heavily relies on lab testing.

Furthermore, quantum computers may **enable the precise calculation of systems** where approximations of well-established computational chemistry methods lead to a significant error in the result. Systems that are particularly difficult to simulate using classical quantum chemistry are highly correlated electron systems where the so called *Born-Oppenheimer approximation* (which assumes nuclei as fixed, independent of where electrons are) is not valid. This is particularly interesting for the development of climate-friendly technologies since highly correlated electron systems show promising applications, such as in electrode materials in batteries or as catalysts. The Born-Oppenheimer approximation was found to be invalid, e.g., in some biological systems that use photosynthesis. Getting rid of the necessity of this approximation could therefore lead to a better understanding of natural photosynthesis.

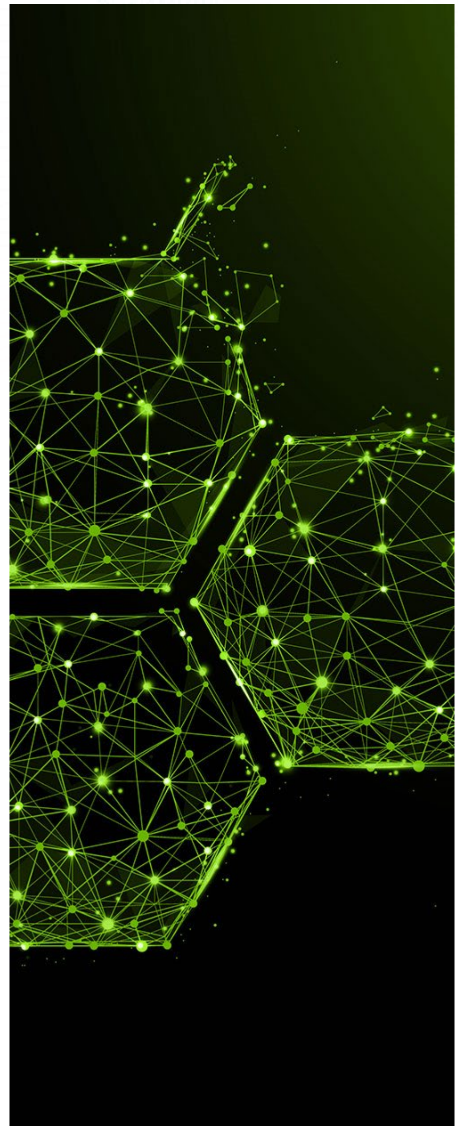
In the context of fighting climate change, some high-impact use cases for chemical simulations on quantum computers are:

- **Catalysts.** Catalysts are materials that increase the rate of a chemical reaction without being consumed in the reaction itself. By developing advanced catalysts, chemical reactions can be optimized to require less energy and fewer resources. This in turn leads to a significant reduction in global energy consumption and in the emission of greenhouse gases. Enzymes are biocatalysts. Advances in their development show great potential to improve bioprocesses that turn biological waste into basic chemicals. This could accelerate the process of liberating the chemical industry from its dependence on petro-chemistry, thereby enabling it to transition towards more sustainable, eco- and climate-friendly alternative base-chemicals. [2]

- **(Bio-)photoelectrochemistry.** Natural photosynthesis can be understood as a solar-to-chemical conversion, where chemical compounds are transformed to fuels with the help of sunlight. Artificial photosynthesis is a process that converts solar energy directly into fuels, instead of turning sunlight to electrical energy (via solar cells) and then storing that electrical energy in chemical bonds. Since current classical algorithms cannot accurately describe the light-harvesting process, quantum computing may significantly accelerate the development of artificial photosynthesis. This is especially true for biophotoelectrochemical (BPEC) systems, where light harvesters and biocatalysts are combined to yield solar-driven biochemical reactors. Examples for the use of BPEC systems include H2 production, CO2 reduction, synthesis of value-added chemicals, and pollution control. [3] [4] [5] [6] [7]

- **Batteries.** To further improve energy density and life cycle of batteries, novel electrode materials as well as a better understanding of the electrode-electrolyte interface are needed. Some of the most promising candidates for electrodes, such as transition metal oxides, can exhibit highly correlated electron systems. For these materials, their properties are strongly influenced by the interactions between electrons, giving rise to a variety of interesting physical phenomena. The presence of correlated electron systems makes materials particularly difficult to simulate using classical methods. Further, the solid electrolyte interphase forming at the electrode-electrolyte interface is crucial for the long-term performance of many types of batteries. The understanding of both electrode and interface is bound by the limitations of existing modeling techniques. Quantum computing may offer a way to overcome these challenges and gain unique insights into the properties relevant to battery performance, paving the way to more efficient batteries with extended lifespans. More efficient batteries, could in turn, enable the increased use of renewable energy sources. [8] [9]

- **Metal organic frameworks as carbon capture materials.** In order to capture and remove CO2 from the atmosphere, nano porous adsorbent materials can be deployed. Metal organic frameworks (MOFs) are promising candidates for such sorbents due to their low energy requirements and their unique tunability. To accelerate material development, electronic and structural information obtained via computational chemistry are crucial. It is computationally demanding to identify specific CO2 sorption mechanisms in such systems. Today, classical quantum chemical computations often yield imprecise solutions for the CO2 binding capacity of MOFs. Precise, quantum-enabled simulations may significantly speed up material development and the large-scale, economic deployment of carbon capture facilities. [10] [11]



Of course, significantly improved materials and chemistry simulations have a plethora of use cases as materials science drives technological advancement in multiple areas. For instance, improved understanding of magnetism could result in more efficient wind turbines and improved power transformers. A better understanding of transition metal elements could lead to advances in solar cells, batteries, or the generation of synthetic fuels via electrolysis.

Beyond the issues related to calculating properties of single molecules, computational chemistry faces great challenges with scaling. As the complexity of the calculations of material properties increase with the number of electrons and nuclei involved, problems are typically simulated using an increasing amount of approximation at increasing problem scale.

Approaches to handle the computational complexity to make calculations on classical computers tangible have been developed for each of these scales. However, for many problems in the field of materials science, the necessary approximations in smaller scale calculations carry over to the macroscopic scale. Quantum computers potentially collapse this 'simulation hierarchy,' getting rid of approximation-induced errors. When macroscopic properties can be calculated directly from atomistic information, more accurate simulations of technologically relevant systems become possible, while reducing the number of lab feedback cycles.

Physical simulations beyond chemistry

Even beyond chemical simulation, quantum computing may have a significant impact on the simulation of other physical systems. This is mainly since differential equations are ubiquitous in mathematical descriptions of physical systems which quantum computers are particularly suited to solve. Differential equations have, for instance, been solved in order to optimize wind turbines, energy systems, and battery charging.

To solve differential equations, most classical algorithms rely on sequential integration of time steps. The high degree of interdependence of the equations significantly hinders the acceleration of differential equation solvers using highly parallel computing architectures.

Further, for large, complex systems, a large system of these equations must be solved computationally, which becomes exponentially difficult. First promising results of quantum algorithms solving prototypical (partial) differential equations for some use cases are already available. [12] [13] [14] [15]

- **Thermal management.** Heat conduction, the transfer of thermal energy through physical interconnections, significantly affects the efficiency and lifespan of various technological systems. Batteries for instance are characterized by heat-dependent efficiency and degradation. By optimizing heat flow in systems of multiple batteries, battery temperature can be controlled, minimizing the negative effects of high temperatures across battery cells. The mathematical description of heat conduction is a challenging differential equation that is traditionally difficult to solve, but quantum algorithms have shown promising speed-ups. These enhanced calculations have the potential to improve battery efficiency, extend their lifespan, and promote more efficient resource utilization. [16] [17]

- **Weather forecasting.** Accurate weather forecasting is essential in combating climate change. It enables the assessment of how climate change impacts the frequency, intensity, and duration of weather events. This understanding is crucial for gauging the effects on human societies. Improved weather forecasting also aids in designing and evaluating adaptation strategies, such as addressing the increased occurrence of heatwaves. Weather-forecasting models heavily rely on complex fluid dynamics. These dynamics are by a set of differential equations, known as the Navier-Stokes equations. Recent advancements in quantum algorithm development point towards significant speed-up using quantum algorithms solving these equations which may greatly enhance weather-forecasting models. [18] [19]

Optimization

To effectively mitigate climate change, it is crucial to optimize processes and systems in a way that minimizes their environmental and climatic impact while optimizing the consumption of available resources.

Many optimization problems can be formulated in a way that allows them to be efficiently solved on a quantum computer, resulting in reduced overhead compared to classical solutions.

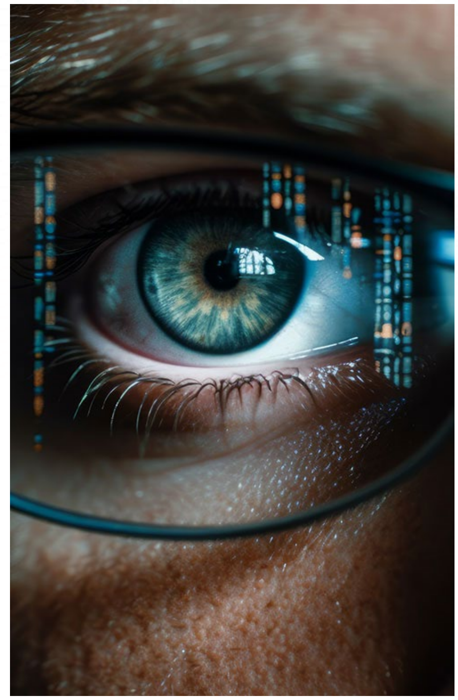
Classical optimization algorithms have become increasingly sophisticated, but still struggle to efficiently solve certain types of problems, particularly those that involve a large number of variables or constraints. Specifically, an increase in the number of parameters increases the complexity of calculating the objective function – the error in each iteration. This can potentially result in the algorithm taking longer to converge to an optimal solution or, in some cases, not reaching it within a reasonable time. Additionally, optimization problems with many parameters often have intricate solution spaces with many local minima. This is often dealt with by dividing the solution space into different sub-spaces, running optimization algorithms on all of them, and then picking the overall best solution from all optimizations. Still, this is computationally expensive and finding the global optimum is not guaranteed.

The limitations of classical algorithms have motivated the search for new optimization methods and quantum computing has emerged as a promising candidate. Conceptually, quantum computers are thought to be advantageous for solving optimization problems with many parameters because of their unique ability to explore a large solution space efficiently as well as escaping local minima. Many optimization problems can be formulated in a way that allows them to be efficiently solved on a quantum computer, resulting in reduced overhead compared to classical solutions. In essence, this implies that quantum computers possess a remarkable ability to tackle specific optimization problems that would otherwise be intractable on classical computers.

To tackle climate change problems, there are several optimization use cases where quantum computers can play an important role:

- **Electrical grid optimization.** In electrical grids, supply and demand have to be carefully managed to match at all times. This is especially difficult in situations where demand fluctuates rapidly. Load balancing and the unit commitment problem are two demanding problems in this area. Load balancing refers to matching supply with demand in real-time, while the unit commitment problem refers to the process of determining which generators to use when to meet the expected demand. Classical algorithms can struggle to solve these problems due to the large number of variables and constraints involved. Quantum optimization algorithms offer the potential to solve these problems more efficiently and more accurately while exploring a larger solution space. This could reduce the need for backup power sources as well as support the utilization of decentralized, renewable energy sources, which can be demanding to integrate into traditional grids. [20] [21]

- **Vehicle routing optimization.** Transportation is closely associated with greenhouse gas emissions. When vehicles are stuck in traffic or driving inefficient routes, they consume more energy – often in the form of fossil fuels - and emit more pollutants into the atmosphere than necessary. Optimizing traffic flow and considering energy consumption in routing can lead to a reduction in harmful emissions and fuel consumption, resulting in a more sustainable transportation system. As a side-effect, this may also improve air quality, which in turn can help protect ecosystems



and promote human health, both of which are important to mitigate the effects of climate change. Similar to ground-based transportation, the optimization of flight trajectories can significantly decrease climate effects from air travel by considering fuel burn, geographical location, altitude, weather conditions and timing. [22] [23] [24] [25]

- **Efficient use of transportation space.** The carbon footprint associated with transporting an individual good is closely tied to two factors: the capacity of the vehicle, e.g., boat, aircraft, or truck, to carry goods and the route taken by the vehicle. When it comes to transporting goods within a single container, there is a wide range of shapes and sizes to consider. Consequently, efficiently packing multiple goods into multiple containers while also accounting for the distribution plan becomes an intricate and highly challenging combinatorial optimization problem. Quantum computers display promising potential in discovering improved packing solutions for these scenarios. [26]

Machine Learning

Machine learning has emerged as a formidable tool for addressing specific problems, leveraging algorithms trained on preexisting data to make predictions or classify new inputs within the same category. Today, supervised learning, which entails training from pre-labeled data, has achieved remarkable progress. It has shown exceptional proficiency in image classification applications, from detecting objects in photographs to medical imaging and autonomous vehicles.

Quantum computing as an accelerator for classical machine learning may put problems that are just beyond the capabilities of today's systems into reach.

Some high-impact climate use cases that fall in this category are:

- **Earth system modeling.** Earth system modeling is the process of using computer models to simulate intricate interactions between various components of our planet, including the atmosphere, oceans, land surface, and ice sheets. Historically, earth system modeling has pushed the limits of computing power, relying on the most advanced supercomputers. In recent years, the amount of high-quality Earth system data generated has far surpassed our capacity to process and comprehend it through traditional means. This is where machine learning models have emerged as promising tools.

  A key application of these models is improving the predictability of weather and climate. Machine learning models are applied to large volumes of historical data to identify relationships that are indicative of weather or climate conditions. Additionally, AI-based Earth system modeling addresses the challenge of uncertainty quantification. Earth system models are inherently complex and involve a large number of parameters fraught with uncertainties that carry through into the predictions of the model. Machine learning algorithms offer the potential to identify the sources of these uncertainties, leading to improved prediction accuracy and reliability.

- **Training Earth system models is often time-consuming and difficult.** However, the use of machine learning and quantum-accelerated machine learning holds great promise for improving our understanding of the Earth system and our ability to make accurate and reliable predictions regarding weather and climate dynamics. By leveraging these cutting-edge technologies, we can unlock new insights and empower humanity to navigate the complexities of our dynamic planet more effectively. [27] [28] [29] [30] [31]

- **Development of novel materials.** Classical machine learning models have shown their capacity to learn from precisely calculated properties of molecules, greatly advancing the field of chemical space exploration. Chemical space exploration is the process of systematically exploring the space of possible chemical compounds that exhibit desired properties. Machine learning algorithms can be used to predict the properties of new molecules based on their structural features. [32] [33] With the development of quantum machine learning, it is expected that we will be able to explore a much larger space of materials and accelerate the discovery of new compounds with desirable properties, leading to the development of sustainable and more efficient technologies.

- **Decision support for biodiversity protection policies.** Biodiversity decline and climate change are a mutually-reinforcing phenomena – climate change contributes to a decline in biodiversity and unhealthy ecosystems accelerate climate change. With the urgent need for conservation policies that maximize the protection of biodiversity, there has been increasing interest in using machine learning to address this issue. [34] As recently demonstrated, reinforcement learning may, for instance, help to optimize spatial conservation prioritization policies. [35] Quantum-enhanced approaches have the capacity to augment the performance of classical machine learning models, enabling them to capture and analyze intricate interconnections and dependencies in the realm of biodiversity and ecosystems. By leveraging these advanced techniques, we can unlock new insights and develop more effective strategies for conservation, leading to improved preservation of biodiversity and a more sustainable approach to mitigating the impacts of climate change.

Harnessing the potential of quantum-accelerated machine learning offers immense potential in advancing our comprehension and capacity to deliver more precise forecasts.

The reason to expect that these use cases are possible is the field of **quantum machine learning**. Quantum machine learning ranges from enhancing classical machine learning algorithms via running computationally costly subroutines on quantum computers to the translation of stochastic learning methods into the language of quantum computers.

Today, there are three areas where quantum computing is anticipated to greatly improve machine learning:

- **Quantum-based optimizers.** To learn the weights of deep neural networks they have to be optimized with respect to the objective. Each epoch the weights are updated and a new error with respect to the objective is calculated. The update of the weights from epoch to epoch is handled by an optimizer. The choice of optimizer therefore greatly impacts how many epochs are required to reach convergence, i.e., the training time is directly connected to the choice of optimizer. As outlined above, quantum computers are particularly good at optimization tasks and could hence lend themselves to optimize neural networks. In fact, the first investigations have shown that quantum-based optimizers can outperform classical ones by hundreds of required epochs. Thus, training of neural networks might be sped up significantly. [36] [37]

- **Hyperparameter tuning**. Neural networks are characterized by multiple so-called hyperparameters. Hyperparameters are set before training and describe the behavior of the network during training and significantly impact the network's performance. Some examples of hyperparameters in neural networks include learning rate, number of hidden layers, number of neurons in each layer as well as type of activation functions. Tuning those parameters to build a neural network that performs well is a daunting task, since any given hyperparameter combination must be evaluated by optimizing the resulting network. Quantum computing is thought to be particularly good at this, due to its proposed ability to efficiently explore the hyperparameter space. [38] [39]

- **Quantum-enhanced feature space**. In certain neural network topologies, a specialized layer is incorporated to extract specific features, such as in the case of convolutional neural networks (CNNs). CNNs typically begin with multiple convolutional layers that serve as self-learning filters, acquiring capabilities such as edge detection and orientation detection. The idea of introducing a quantum layer follows a similar approach, where a layer of quantum gates is inserted into the neural network architecture to enhance its learning capabilities. The quantum layer can act as a sort of quantum feature extractor, allowing the neural network to learn more intricate and nuanced features from the input data. This can potentially improve the accuracy and efficiency of the neural network on specific tasks. [40] [41] [42]

By capitalizing on these state-of-the-art technologies, we unveil fresh perspectives and equip humanity with greater proficiency in maneuvering through the intricacies of our ever-changing planet.

Conclusion

Quantum computing holds immense potential to address sustainability and environmental challenges. To harness this potential, interdisciplinary collaborations between experts in the quantum domain and other scientific disciplines is crucial to develop meaningful solutions. By prioritizing climate-relevant problems when developing new quantum algorithms, we can ensure quantum computing will have a positive impact on the environment already at an early stage. With some of the known use cases of quantum computing requiring large-scale fault-tolerant devices, it is important to keep the focus on climate-relevant application in mind, also when developing smaller scale hardware and software co-design solutions for near term implementation.

In this publication, we outlined several effective areas where the intersection of climate change and quantum computing can bring about effective solutions. While the journey to achieve quantum advantage in these areas may be challenging, concerted efforts to focus on climate change solutioning will ultimately lead to significant milestones being achieved along the way. The examples described in this publication are not intended to be exhaustive, and other important sustainability applications will undoubtedly emerge as the technology matures in the near future.

At Deloitte, we are committed to driving innovation in collaboration with a wide range of clients, partners, and other external innovators. If you are excited to be at the forefront of quantum computing for climate actions, we encourage you to reach out and join us in this exciting endeavor! Together, we can harness the power of quantum computing to make substantial contributions towards addressing climate change and creating a more sustainable future.

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Contacts

Scott Buchholz

Managing Director,
Global Quantum Computing Lead

Deloitte Consulting US

Tel. +1 571 814 7110
sbuchholz@deloitte.com

Dr. Barbara Wellmann

Director,
Quantum.Link Lead

Deloitte Consulting Germany

Tel. +49 30 254 682 857
bwellmann@deloitte.de

Dr. Julian M. Dlugosch

Consultant,
Quantum.Link

Deloitte Consulting Germany

Tel. +49 89 290 365 827
jdlugosch@deloitte.de

Lydia Neuhuber

Director,
Sustainability & Climate Lead

Deloitte Consulting Germany

Tel. +49 89 290 367 447
lneuhuber@deloitte.de

Eike Petersen

Senior Consultant,
Technology Strategy & Performance

Deloitte Consulting Canada

Tel. +1 306 343 4455
eikpetersen@deloitte.ca

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