Quantum technologies for climate change: Preliminary assessment

Potential high-impact use-cases of quantum technologies for climate change with a focus on four main areas: **simulating physical systems, combinatorial optimization, sensing, and energy efficiency**.[1]

Studying the quantum scale with classical computers faces major obstacles, as the time and memory required for exact simulation increases exponentially with the size of the system. For instance, in order to perform an exact simulation of N quantum particles with d states each, one generally needs to store and do linear-algebra operations on at least a dN-dimensional space. For a relatively small problem of 100 quantum particles, this would require a memory size of at least 2^100 ≈ 10^30, a quantity equivalent to > 10^89 terabytes that one could never hope to even store in a classical computer.

Though there are currently many useful materials and chemical simulations performed on traditional computers, their imprecise results can often be used only for qualitative conclusions or for eliminating poor candidates. Following are ways in which a quantum computer could become a useful tool to help alleviate the climate crisis if a viable machine is built in the next 10-20 years.

The approaches used for finding the ground state of an atomic nucleus are different from those for studying dynamics in a solvated chemical process .One could have linked quantum algorithms to application, chemical or material type to application, or a more general "simulation goal" to application (both target material and desired property), which is presented in the following table,

	Solar energy [11]	Wind energy [12, 13]	Batteries [14]	Industrial processes [15]	Materials for the grid [16]	Synthetic fuels (incl. electrolysis) [17]	CO_2 capture [18, 19]	Atmospheric science [20]	Nuclear power [21]	Structural materials [4]	Biological enzymes [22]	Plastics & circular economy	Agriculture
Gas-phase electronic structure [23]	-	-	-	●	-	●	●	●	-	-	-	•	●
Molecular dynamics [24]	-	-	•	●	-	●	●	●	-	-	●	•	•
Solution chemistry [25]	-	-	●	-	-	●	●	●	-	-	●	●	●
Transition metal elements [26]	●	●	●	●	●	●	-	-	•	•	●	●	-
Lanthanides & actinides [27]	●	●	•	•	•	•	-	-	●	•	-	-	-
Electronic band structure [28]	●	-	●	-	-	●	-	-	-	-	-	-	-
Electron/hole diffusion constants [28]	●	-	●	-	-	●	-	-	-	-	-	-	-
Vibrational and vibronic structure [29, 30]	•	-	•	•	-	•	•	●	-	-	●	-	●
Magnetism [31]	•	●	-	•	●	-	-	-	•	-	-	-	-
Nuclear structure and reactions [32]	-	-	-	-	-	-	-	-	●	-	-	-	-
Excited states of a Hamiltonian [33–36]	●	-	-	•	-	•	-	●	•	-	•	•	•

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It would be useful to determine in detai lwhich climate science applications will be the first to benefit from quantum dimulation. There are approaches based on the phase-esimation algorithm, which are too costly to be implemented on early generations of quantum hardware. An alternative to this approach is the variational quantum eigensolver (VQE), which is a hybrid type of computing.

Two important factors when designing quantum algorithms - circuit depth and system complexity.

At this early stage it remains unclear, however, to what degree quantum computers can provide advantages in optimization over classical algorithms in impactful applications of interest, and at what timeframe we can expect to realize such advantages in terms of both hardware and algorithm development. For example, a recent paper [47] considers quantum approaches to problems related to smart-charging of electric vehicles, and observes performance competitive with classical methods.

Two particular challenges are the capability limitations of existing or near-term hardware, and the fact that in many cases we already have very good polynomial time exact or approximate classical algorithms. On the other hand, as these quantum algorithms are believed to not be efficiently classically simulatable in general, the potential for quantum computational advantage remains tantalizing and further research is required to identify the most promising applications. The first commercial quantum devices, quantum annealers, were deployed to solve certain classes of hard opti mization problems. These devices are severely restricted in the class of algorithms they offer. Despite a decade of experimentation, the scaling advantages offered by such hardware and its future incarnations remains unclear.

We separate, roughly, these algorithms into two classes: 1) near-term quantum al gorithms, and 2) fault-tolerant algorithms. Similar to the situation with quantum annealing, near-term algorithms (such as, for example, QAOA [50, 51], or related variational approaches) enable mapping optimization problems to near-term quantum hardware. Despite much recent interest the power, potential advantage, and applicability of these algorithms similarly remains unclear, especially in the context of small noisy real-world devices of the foreseeable future. **Hence, we are unable to make concrete claims as to the potential advantages and impact towards climate offered in the near-term by either quantum annealers or gate-model quantum computers.**

Better hardware will allow larger problems to be tackled and larger quantum circuits to be reliably deployed (for example, QAOA on n qubits (variables) with number of layers growing as logn or poly(n)). The case for quantum advantage is theoretically stronger if we consider algorithms allowed to run for longer than polynomial time in the input size.

As these algorithms have stringent quantum hardware requirements (i.e., sufficiently low error rates and long coherence times), they are much less promising to provide a computational advantage in application to climate change within the near term, though remain an important future research direction.

Target for research: problems and application areas that ideally meet two conditions: i) impactful for helping with climate change, and ii) a good fit for quantum resources and potential quantum advantage.

Example applications related to optimization and climate:
• Power and energy: real-time allocation and routing with immediate potential power and energy savings, e.g., static or dynamic grid optimization problems (including load balancing or unit commitment), batteries, renewable energy, and real-time wireless network.
• System layout: design of facilities, manufacturing plants, and supply chains, e.g., wind turbine placement, hybrid energy system design, and in automotive industry applications.
• Transportation networks: improvements offer direct carbon reductions, e.g., traffic flow and navigation.
• Distribution networks: optimized scheduling and allocation of goods and resources, e.g., potential improved efficiencies in shipping, water distribution], buildings and cities
• Climate mitigation and adaptation: climate and weather.

Current state-of-the art sensing technologies are already used to monitor several climate related properties, such as atmospheric levels of select greenhouse gas emissions and optical properties of aerosol particles. Applied to climate change, they are anticipated to have transformative impacts across a variety of domains, from electricity to environmental monitoring.

Through quantum sensors, orders of magnitude improvements in sensitivity, selectivity or resource efficiency can potentially be achieved; the power of quantum effectively translates into a dramatic step-function transformation. For example, quantum sensors allow for the measurement of electric and magnetic fields very accurately across many frequencies; drift-free operation, obviating the need for calibration; the ability to sense changes in gravity to reveal potential climate change indicators; non-line-of-sight imaging; and navigation in GPS denied environments.

As for opportunities for quantum sensing, there are very good classical sensors today. Thus, quantum sensors will be driven by applications where they are found to uniquely meet a need. The opportunity calls for greater precision, selectivity or efficiency. However, quantum technology is often more complex and costly than classical. Demand-side pull provides a focus for technology development, and supports technology validation and commercialization.

Climate change solution domains offer a way of categorizing quantum sensing applications. Five domains have been identified for this purpose as follows:

i) electricity systems,

Quantum sensors offer a pathway to higher efficiency solar cells and higher solar fuel conversion efficiency through improved materials characterization and quantum coherent approaches, enhanced remote-sensing for the identification of promising geothermal sources [76] or other renewable energy resources [77], and more effective monitoring of nuclear plants [78, 79]. Furthermore, while society transitions away from fossil fuels, quantum sensing may help reduce current-system impacts by improving fossil fuel infrastructure maintenance and leak detection.

ii) transportation,

For example, current state-of-the-art procedures to assess Solid Electrolyte Interphase- a key parameter in battery performance- do not provide an adequate understanding due to measurement difficulties [81]. Quantum sensors may help to alleviate these challenges by improving our understanding of battery degradation mechanisms [82]. It's worth noting that neutron interferometry is already applied to battery diagnostics today.

iii) industry,

. Some promising applications include precision agriculture [90] and cattle management [91]. For example, measuring biomarkers of methane emissions in cattle may enable the selection of cattle for breeding which emit less methane and ultimately may lower agricultural greenhouse gas emissions [92]. Quantum sensors can be used to image magnetic fields with unprecedented performance, which may in turn lead to an acceleration in the development of smart materials for a variety of applications highly relevant to climate change.

iv) environmental monitoring

The monitoring of greenhouse gases is critical to assess the state of climate change [83–85]. Satellites are used in a variety of settings to monitor methane, carbon dioxide and other gases. Accurate readings of methane, in particular, are difficult to obtain because of spectral interference from other gases in spectroscopy, a challenge quantum sensors may overcome. Quantum sensors may also be used to identify and monitor greenhouse gas emissions via satellite over large areas such as peatlands [86]. Moreover, aerosols, which play an important role in climate change, also currently suffer from sensing limitations that may be addressed through quantum technologies [87]. Ice sheet melting dynamics and sea-level rise are crucial parts of climate change models. Their monitoring, through optical properties suitable for quantum sensing, would provide important data to climate modelers [88]. In addition, quantum gravimeters deployed via satellite may lead to a better understanding of a broader set of indicators and mechanisms of the global climate system including global mass variations, earth's response to natural and human induced forces and monitoring of polar regions for example [89].

v) society.

Quantum gravimeters are already being studied for use in volcano hazard assessments and mitigation plans [94].

One of the factors which make quantum computers a potentially ecological choice is its energy efficiency. D-Wave device and a supercomputer differ significantly in the type of problems they can solve. We classify quantum computing devices in three categories: single-purpose devices, Noisy Intermediate-Scale Quantum (NISQ) devices [1] and fault-tolerant devices. Single-purpose devices, such as the D Wave 2000Q, are designed to implement a specific algorithm, in this case quantum annealing. NISQ devices are made up of, as their name implies, a limited amount of imperfect qubits over which we exercise imperfect control. Finally, a fault-tolerant quantum computer's qubits are protected from errors using quantum error correction and an appropriate hardware design. Fault-tolerant devices are the most directly comparable to today's supercomputers, but unfortunately remain far from attainable in the near term.

In the study, where Google claimed that their quantum computer provided a speedup over Summit HPC, comparing the efficiency of two different devices is a complex task. To simplify it, the lifetime of a specific device can be split into three parts: production, operation and end-of-life. Operating costs can be separated into four categories: electricity, facilities, personnel and hardware/software. chip with some thousands of qubits can still fit in a dilution fridge. One specific area which might be worth studying in more details, because of its environmental impact, is the difference in water consumption for cooling and other purposes such as fabrication. This is however out of the scope of this report. Summit for example is composed of 27648 GPUs and 9216 CPUs, for which the total cost amounts to ~ 325 M$ [96]. Quantum computers, on the other hand, cannot yet simply be bought. One can estimate the costs of all the cooling (~ 1 M$) and electronics to operate them (10-20 M$), but the cost of the actual chip is yet undetermined.

This assessment covers only a small portion of the footprint of quantum computers. In particular, it highlights the reduction in electricity consumption that could be achieved from operating quantum computers versus classical supercomputers. Even if chips themselves need approximately the same amount of heavy or non-renewable materials to create, quantum computers of today have only one chip compared to the tens of thousands of chips in supercomputers. This could be a huge reduction in the use of those materials but, in the long-term, quantum error correction schemes might need a very large number of classical and/or quantum chips to operate, counterbalancing this reduction.

the advent of largeand accurate quantum computers could provide efficient methods to simulate a host of challenging physical systems that are crucial to tackle climate-change related problems in energy, industrial processes, atmospheric science, and other sectors. Renewable energy, systems layout, transportation, distribution, and direct climate modeling and mitigation, though their precise advantages over classical computers requires further investigation. Quantum sensors could be relevant for climate mitigation, as they can provide improved sensitivity, selectivity and efficiency gains across a wide variety of application domains. **Promising areas not discussed in this preliminary assessment include quantum machine learning and quantum approaches for solving differential equations, among others.**

Variational Quantum Solutions to the Advection - Diffusion Equation for Applications in Fluid Dynamics

Reliable solutions of the equation can be obtained on even the noisy quantum computers available today. This and other methods that exploit quantum computers could replace some of our traditional methods in numerical weather prediction as quantum hardware continues to improve.

From Richardson's proposal (6 hours ahead prediction, done in 6 weeks), to Robinson's vision for NWP

Numerical Weather Prediction (NWP) is a subset of the broader field of fluid dynamics that seeks to provide solutions to systems of partial differential equations (PDEs), namely the Navier-Stokes equations, ultimately amounting to solving an initial value problem.

Mathematical models based on the same physical principles can be used to generate either short-term weather forecasts or longer-term climate predictions. Manipulating the vast datasets and performing the complex calculations necessary to modern numerical weather prediction requires some of the most powerful supercomputers in the world.

The open question is, however, whether Deep Learning can outperform classical methods. apparently, in November 2023 AI outperforms conventional weather forecasting for the first time.

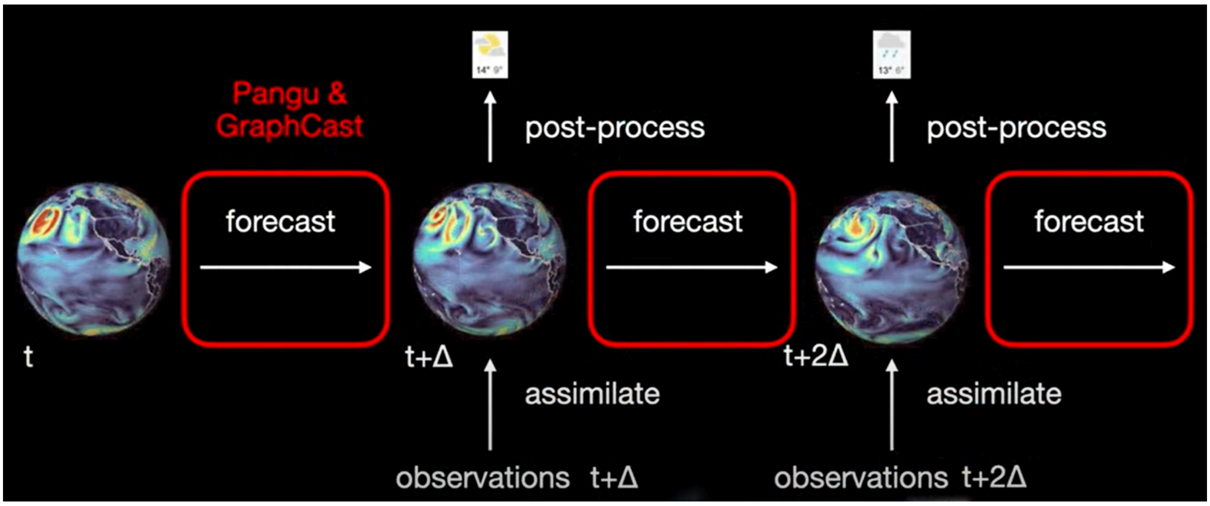
There are different types of forecasting.

- Nowcasting, for example for football game (precipitation, for example_
- Medium-range weather forecasting - days/weeks
  Once a forecast prediction is ready, it is assimilated with observations, and the process keeps in a feedback loop. After each step is a post-processing (like bias correct) - machine learning, small amount of statistics.

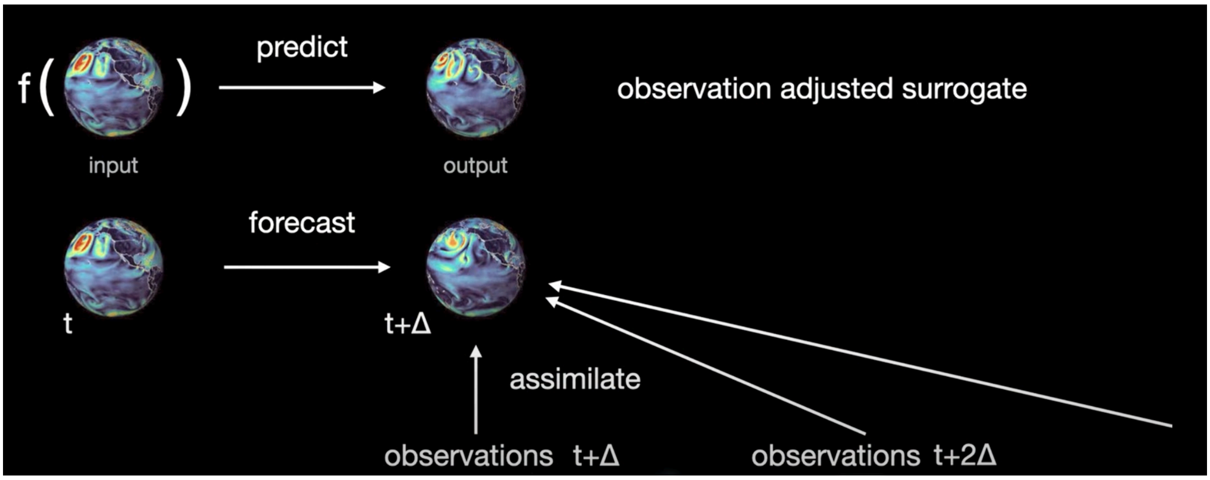
  DeepMind attack forecast step (accelerated by AI). 50% forecast, 50% simulation

- Sub-seasonal forecasting (months)
- Seasonal/Climate (years)

High-Performance Computing scheme for climate change predictions



Rather than focusing on a single area, there is a requirement to join forecasting from different regions. The challenge is that each data point is relatively big, tens of gigabytes, while for example chatgpt was trained on a hige set of small packages.



Machine learning can be applied both for forecast accuracy improvement in near-real time, and for assimilating long-term predictions done in historical data (off-line, smoothed observation adjusted surrogate). They took pictures from around the globe and unwrapped it to form an image of the surface variables and took the pressure levels to the atmosphere and turned it into a cube, and did the same for output side.

The next direction is to use Generative AI / Diffusion models for weather forecasting. As the machine learning diffusion model takes inspiration from physical diffusion, the analogy here may be quite adequate.

Training data is taken from atmosphere observations.
Transforerms, similarly as in ChatGPT, can be used for computer vision, when atmosphere is considered as computer vision problem.

NWP is ready for Deep Learning methods.

Within any modern model is a set of equations, known as the primitive equations, used to predict the future state of the atmosphere. These equations—along with the ideal gas law—are used to evolve the density, pressure, and potential temperature scalar fields and the air velocity (wind) vector field of the atmosphere through time.

Advection-Diffusion Equation

Requires only one boundary condition. Boundry is a physical location where entity exits, when there is flux of quantity. Boundary condition is mathematical condition what is hapeppening at badnary. One boundary condidation per boundry.

In equation - 2 boundary conditions to specify solution.

The Navier-Strokes equations consist of transient, advective, diffusive, and source terms all of which may contain linear and nonlinear terms

The Linear Advection-Diffusion Equation

A linear model equation for the Navier-Stokes is the advection diffusion equation

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \mu\frac{\partial^2 u}{\partial x^2}$$

first derivative - advection, second - diffusion. Advection moves things in space, diffusion spreads things in space. Nonlinear version of this equation, known as the burgers equation, would have a u iver here rather than a constant speed.

$$u(x,0) = A\sin(\omega x)$$

for this initial condition, sin wave to advection and diffusion at the same time, solution - moving wave that is shrinking (X - ct). Exponential decay

$$u(x,t) = A\sin\left[\omega(x-ct)\right]e^{-\mu\omega^2 t}$$

take initial condition and move it in space at the speed C, and scale it with an exponential term: -Miu (diffusion coefficient), omega squared - if I had higher frequency and omega is 100pi, then it will dissipate much faster than in case of 2pi.

$$\left.\frac{\partial u}{\partial t}\right|_i^n = -c\left.\frac{\partial u}{\partial x}\right|_i^n + \mu\left.\frac{\partial^2 u}{\partial x^2}\right|_i^n$$

if we dont have diffusion scheme blow up the solution, solution is unstable. olution is just going to grow in time. Once we add a diffusion term to the governing equation, this term is gonna combat negative diffusion introduced by this.
this combat the instability that came about from the diffusion of using central scheme on the advection term

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} + \mu\frac{u_{i+1}^n - 2u_i^n - u_{i-1}^n}{\Delta x^2}$$

$$\boxed{u_i^{n+1} = u_i^n - c\frac{\Delta t}{2\Delta x}\left(u_{i+1}^n - u_{i-1}^n\right) + \mu\frac{\Delta t}{\Delta x^2}\left(u_{i+1}^n - 2u_i^n - u_{i-1}^n\right)}$$

[saadtony/uCFD: CFD course that I teach in the Chemical Engineering Department at the University of Utah - CHEN6355. (github.com)]

[6. The Advection Diffusion Equation (numerical solution with FDM) (youtube.com)]