Quantum FOR CLIMATE & SUSTAINABILITY

# FINAL REPORT

October 4 - 5, 2023


Annarita Giani (GE Vernova Advanced Research),
Karl Thibault (Université de Sherbrooke and Q4Climate)



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GE Vernova Advanced Research

Niskayuna, NY


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Annarita Giani (GE Vernova Advanced Research) and Karl Thibault (Université de Sherbrooke and Q4Climate)



The solution to climate change lies at the intersection of multiple disciplines. Here, the potential contribution of quantum computing is identified, and an outline delineating the essential steps required to bridge the gap between quantum computing and climate change mitigation is presented.

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## PARTICIPANTS AND CONTRIBUTORS

**Iftikhar Ahmed**
GTM & Invent Lead | Quantum Lab
Capgemini

**Reed Anderson**
Manager
Scientific Computing Support
& Technology, Naval Nuclear
Laboratory

**Ali Arabnya**
Director of Infrastructure Finance &
Climate Risk
Quanta Technology

**Mostafa Ardakani**
Professor
Department of Electrical and
Computer Engineering,
University of Utah

**Richard Arthur**
Senior Principal Engineer
Computational Methods Research
GE Aerospace Research

**Anjuli Bamzai**
Senior Science Advisor
Global Climate Change
National Science Foundation

**Sumit Bose**
Technology Manager
Power Systems-Electric Machines
GE Vernova Research

**Marie-Eve Boulanger**
Program Manager
Pinq2

**Aggie Branczyk**
Senior Research Scientist
IBM Quantum

**Fangyu Cao**
Assistant Director of Research
Operations
Quantum Science and Engineering
Center, George Mason University

**Aranya Chakrabortty**
Professor
Department of Electrical and
Computer Engineering,
North Caroline State University

**Yousu Chen**
Chief Electrical Engineer
Pacific Northwest National Laboratory

**Alexandre Choquette**
Quantum Partnerships Canada
IBM Quantum

**Carleton Coffrin**
Scientist
Los Alamos National Laboratory

**Paul Dabbar**
Chief Executive Officer
Bohr Quantum
Former Under Secretary for Science
United States Department of Energy

**Reuben Demirdjian**
Meteorologist
Marine Meteorology Division
Naval Research Laboratory

**Anil Duggal**
Chief Scientist
GE Vernova Advanced Research

**Nick Farina**
Co-Founder and Chief Executive Officer
EeroQ Quantum Hardware

**Arash Fereidouni**
Application Scientist
Quantum Technologies
Zurich Instruments

**Alberto Figueroa**
Sourcing Manager
On Shore Wind
GE Vernova Advanced Research

**Tracey Forrest**
Program Director
Transformative Quantum Technologies
University of Waterloo

**Yiwei Fu**
Scientist
AI and Machine Learning
GE Vernova Advanced Research

**Dimitrios Giannakis**
Professor
Department of Mathematics
Dartmouth College

**Pierre Gentine**
Maurice Ewing And J. Lamar Worzel
Professor of Geophysics
Department Of Earth And
Environmental Engineering
Professor Of Earth And Environmental
Sciences, Columbia University

**Ali Ghassemian**
Program Manager
Office of Electricity
Department of Energy

**Vlad Gheorghiu**
Co-Founder, President and
Chief Executive Officer
SoftwareQ Inc.

**Justin Ging**
Chief Product Officer
Atom Computing

**Judy Guzzo**
Senior Manager
External Partnership
GE Vernova advanced Research

**Timothy Hansen**
Harold C. Hohbach Endowed Associate
Professor
Electrical Engineering and Computer
Science, South Dakota State University

**Michael Hayduk**
Deputy Director
Air Force Research Lab Information
Directorate

**Reza Hedayati**
Founder and Chief Executive Officer
NubisAI, Inc

**Balaji Jayaraman**
Scientist
Aerodynamics
GE Vernova Advanced Research

**Sonika Johri**
Founder
Coherent Computing Inc

**Christophe Jurczak**
Founder and Partner
Quantonation

**Marna Kagele**
Technical Fellow
Quantum Computing, Strategic
Foresight, Innovation
The Boeing Company

**Janis Klamt**
Climate Models
German Aerospace Center (DLR)

**Peter Koudal**
Scientist
Enterprise Optimization
GE Aerospace Research

**Aditya Kumar**
Senior Principal Engineer
Estimation & Modeling
GE Vernova Research

**Arnoldas Kurbanovas**
Analyst
Atmospheric Sciences Research Center (ASRC), State University of New York (SUNY) at Albany

**Michelle Lampa**
Senior Manager of Strategic Partnerships
North America

**James LeBlanc**
Executive Director
Electrification
GE Vernova Advanced Research

**Robert Ledoux**
Program Director
Advanced Research Projects Agency Energy, (ARPA-E)
United States Department of Energy

**Yan Li**
Charles H. Fetter Endowed Fellow
Assistant Professor
Penn State University

**Frank Liddy**
Executive In Residence
Terranet Ventures Inc.

**Binquan Luan**
Research Staff Member
IBM Watson Research Center

**Michael Marthaler**
Co-Founder and Chief Executive Officer
HQS Quantum Simulations GmbH

**Christian Metzl**
Client Partner | Automotive & Mobility
Client Partner | Quantum Lab
Capgemini

**Shree Mishra**
Acting Deputy Division Director
Atmospheric Scientist
National Science Foundation

**Samuel Mugel**
Chief Technology Officer
Multiverse Computing

**Kouhei Nakaji**
Researcher
University of Toronto

**Souransu Nandi**
Scientist
Model Based Controls
GE Vernova Advanced Research

**Sanjeev Nayak**
Quantum Technology Innovator and Accelerator
University of Connecticut

**Ibrahima Ndiaye**
Scientist
Power Systems
GE Vernova Advanced Research

**Per Nyberg**
Chief Commercial Officer
ORCA Computing Ltd.

**Soronzonbold Otgonbaatar**
Doctoral Candidate
German Aerospace Center (DLR)
LMU Munchen

**Rima Kasia Oueid**
Senior Commercialization Executive
Office of Technology Transitions
U.S. Department of Energy

**Jonathan Owens**
Scientist
Material Chemistry and Physics
GE Vernova Advanced Research

**Paul Parazzoli**
Quantum Engagement Lead
IBM Quantum

**Hari P. Paudel**
Senior Technical Staff
Leidos Inc.
DOE, National Energy Technology Laboratory

**Pierre Louis-Peguy**
Solutions Lead
D-Wave

**Christophe Pere**
Lead Scientist
PINQ2

**Michel Pioro-Ladriere**
Director of Partnerships and Strategy
Nord Quantique

**Daniel Pompa**
Manager
Quantinuum

**Radislav Potyrailo**
Principal Scientist
Microsystems
GE Global Research

**Rakesh Radhakrishnan**
Energy Transition Expert, Investor, Business Leader
Advanced Research Projects Agency Energy, (ARPA-E)
United States Department of Energy

**Shreyas Ramesh**
Global Lead
Quantum Systems Integration
Accenture

**Saikat Ray Majumder**
Senior Data Scientist
Statistical Signal Processing
GE Aerospace Research

**Sanjubala Sahoo**
Professor
Department Of Materials Science And Engineering, University of Connecticut

**Austars Schnore**
Chief Architect IoT/Smart Products
Cognizant

**Travis Scholten**
Technical Lead
IBM Quantum

**Vishal Shrotriya**
Strategy and Business Development
PsiQuantum

**Joanna Slawinska**
Professor
Department of Mathematics
Dartmouth College

**Marlou Slot**
Scientist
NIST and CU Boulder

**Aneesh Subramanian**
Professor
Atmospheric and Oceanic Sciences
University of Colorado at Boulder

**Kara Sulia**
Associate Director
Atmospheric Sciences Research Center
Director xCITE Lab
Research Faculty
Atmospheric Sciences Research Center
University at Albany, SUNY

**Jiacheng Tang**
Scientist
Model Based Controls
GE Vernova Research

**Himanshu Thapliyal**
Professor
Department of Electrical Engineering and Computer Science, University of Tennessee at Knoxville

**Lars Tray**
Manager
D-Wave

**Dimitar Trenev**
Program Lead

ExxonMobil

**Julian Van Velzen**
Head of Quantum Lab
Capgemini

**Blaise Vignon**
Chief Product Officer
Alice&Bob

**Yinan Wang**
Professor
Department of Industrial and Systems Engineering, Rensselaer Polytechnic Institute

**Zongjie Wang**
Professor
Department of Electrical & Computer Engineering, University of Connecticut

**Jan Woodcock**
Director of Operations
Center of Excellence Weather & Climate Analytics
Atmospheric Sciences Research Center
University at Albany, SUNY

**Benjamin Wunsch**
IBM Research

**Masako Yamada**
Director of Applications
IonQ

**Guohui Yuan**
Program Manager
Solar Integration
Solar Energy Technologies Office
U.S. Department of Energy

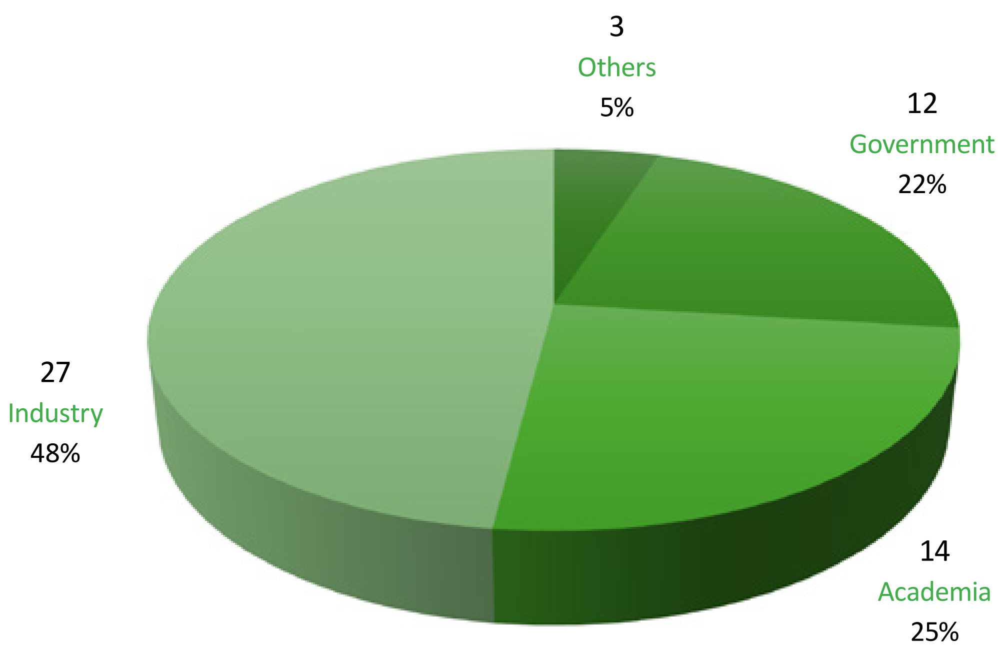
**May Yuan**
National Science Foundation (NSF)

**Peng Zhang**
Professor
Department of Electrical and Computer Engineering,
SUNY Empire Innovation
Stony Brook University

**Yifan Zhou**
Assistant Professor
Department of Electrical and Computer Engineering
Stony Brook University

## 95 Participants from 56 Organizations

The percentage of the different categories of participants is shown in the following table.



# EXECUTIVE SUMMARY

Urgent action is needed to address climate change, driven by significant post-industrial emissions causing severe consequences. Recent extreme weather events underscore the economic and human toll, prompting a focus on immediate measures to reduce greenhouse gas (GHG) emissions in energy and transportation. Current earth system models face constraints on classical computers. Classical computing limitations lead to an experimental search for solutions, while quantum computing (QC) emerges as a potential accelerator.

Addressing climate complexity and scaling quantum tools necessitate interdisciplinary collaboration. This workshop prioritized impactful applications by fostering collaboration among diverse experts from various fields for the benefit of people's lives and the planet's health. Participants shared ideas, explored climate change challenges and quantum technology opportunities, and identify initiatives for convergent acceleration. The aim is to develop prototypes within 3-4 years.

The workshop emphasizes funding programs at the intersection of quantum and sustainability and climate proposing recommendations targeting the Noisy Intermediate-Scale Quantum (NISQ) regime. Workshop discussions expanded to quantum sensing, communication, and networking, considering their collective impact on climate change mitigation. Ensuring equitable solutions across social and economic contexts is crucial, with outlined steps to promote fairness and incl

## Summary of Recommendations

- Craft calls for proposals focusing on quantum problem formulation to drive promising proofs of concept and prototype development.
- Establish interdisciplinary "Centers of Excellence" concentrating on specific problem domains or challenges, utilizing a fail-fast approach due to the inherent research risk.
- Create quantum algorithm libraries tailored to the needs of problem-domain experts.
- Ensure adequate access to quantum computing hardware and software capabilities.
- Provide training for problem domain experts in quantum science and technologies.
- Define application-specific benchmarks to evaluate quantum technologies and algorithms.
- Identify key grand challenges within each problem domain.
- Create a quantum sandbox which connects quantum technologies with energy infrastructure.
- Design innovative and utility-scale algorithms for both immediate and future achievements.
- Expand the workforce and explore international collaboration opportunities.
- Emphasize co-design to optimize both quantum algorithms/software and hardware.
- Clearly describe quantum hardware resource estimates in a consistent and appropriate manner Showcase accelerated performance in proofs of concept in the field of optimization, chemistry and forecasting.
- Recognize the importance of hybrid approaches to formulate use-case-specific strategies and benchmarks.

# BACKGROUND

There is an urgent need to mitigate the root causes of climate change. Post-industrial human activities are releasing enormous amount of carbon dioxide, methane, and other GHG emissions to the atmosphere *(EPA, 2022).* The energy and transportation sectors are the main sources of GHG emissions. Consequences include droughts, water scarcity, fires, rising sea levels, falling lake levels, flooding, melting polar ice caps, storms with catastrophic effect on biodiversity, people's health, ability to grow food, housing, and safety. The total cost of extreme weather events in the United States, for the last five years ($742.1 billion) is more than one-third of the disaster cost total of the prior 42 years ($2.155 trillion). This reflects a five-year cost average of nearly $148.4 billion per year. In 2020 these events resulted in the deaths of 262 people *(NOAA, 2022).*

These deleterious effects will continue unless we take measures to reduce emissions and consider carbon capture technologies *(Policymakers, 2018).* There is an immediate need to quickly reduce these sectors' GHG footprint by accelerating research into energy systems (e.g., renewable electricity, smart grid deployment, industrial processes, carbon capture and sequestration, etc.) and in transportation systems (e.g., improved battery performance *(Garcia, 2020)* and lower carbon production footprint, energy reduction from scheduling efficiency, etc.). Presently many developments in GHG reduction are inhibited by the limitations of classical computing making the search for solutions "Edisonian", not systematic but based on experiments and trial and error approach *(Hotz, 2022).* Quantum computing QC could significantly hasten the development of technologies to reduce and capture GHG emission *(O'Brien, 2019).*

Global earth system models have been developed to determine the climate effects of GHG including the prediction of high-impact events such as hurricanes, tornadoes, and heatwaves *(Ornes, 2018)*. These models require vast amounts of data such as air temperature, pressure, and density. Classical computers, even high-performance computers, cannot perform high fidelity climate predictions in a reasonable time or at a granular enough spatial scale. This is a fundamental limitation of classical computers given the high dimensionality of these models *(Hotz, 2022)*.

Developing technologies for sustainability *(Foster, 2021)* and reducing GHG emissions to mitigate climate change would greatly benefit from high-fidelity simulations of complex chemical processes and optimization of the design and control of large-scale energy and transportation systems. Quantum computers and associated algorithms may provide a means of accelerating the development of these technologies in regimes where such calculations are unachievable with classical computing.

Much research is still needed to develop applicable quantum algorithms and realize scalable quantum computers. It is important to keep in mind the potential of QC for sustainability and climate (S&C) related problems, as that will inform the development of new algorithms and hardware. Specific funding at the interface between QC and S&C would be useful incentive for researchers to step outside their current boundaries. In order to devise such funding programs, we organized a workshop that helped identify a vision and roadmap for an NSF program funded by the Convergence Accelerator program. The workshop provided insight to other government agencies for parallel or joint programs. The proposed program would focus on improving algorithms that can achieve computational advantage in the near-term Noisy Intermediate-Scale Quantum (NISQ) regime *(Preskill, 2018)*. Engaged disciplines include QC algorithm and hardware development and their counterparts in classical computing as well as quantum sens*ing (Crawford, et al., 2021) (Degen, Reinhard, & Cappelaro, 2017) and networking (Wilkinson, Pope, & Pirandola, 2020) (Cacciapuoti, et al., 2020)*. Assessments of the most important problems to tackle was guided by experts in energy, transportation, and climate simulation. We explored the opportunities of this new computational paradigm based on QC and its potential to solve problems related to renewable energy transition that are computationally infeasible classically.

While the focus of the workshop was QC, there were discussions related to other quantum technologies like quantum sensing, quantum communication and quantum networking and how these impact our ability to tackle climate change.

Another important aspect to consider is that advancements related to the application of quantum technologies for addressing climate change should be equally distributed and should not be impacted by different social and economic environments. The workshop included a discussion in this regard and outlined steps to ensure that this approach will help to fight global climate and weather challenges.

We believe in the value of each person's unique identity, background, and experiences and affiliation. The workshop was created with an inclusive culture in mind, so we hope we succeeded in creating a space where everyone felt empowered to participate and get involved because they felt accepted, respected, and that they belonged.

## MOTIVATION

The development of quantum technologies is rapidly reaching the point of usefulness *(Kim, et al., 2023)*. They promise applications in a wide range of domains such as finance, logistics, pharmaceuticals, mining, defense, etc. However, we believe their most useful application for humanity lies in addressing issues related to climate and sustainability. In order to allow this to happen, the quantum community must reach out to S&C related communities and discuss possible applications of quantum technologies on their specific problems.

Quantum computing technologies are quickly becoming useful computational tools, and our climate is deteriorating at an even more rapid pace. This workshop aimed to understand the computational challenges related to the fight against climate change, the benefits that QC bring to the field *(Berger, et al., 2021) (Oddersede, 2021)*, to find the most promising applications in the next three to five years, and to propose formulate focused funding programs to accelerate their deployment.

More specifically, workshop goals included establishing the state-of-the-art in quantum computation (hardware and software), identifying the most important computational challenges related to understanding and mitigating climate change, quantifying the benefits that QC could bring to these challenges, and making recommendations on the best strategy to fund the research and to implement these new tools.

Government and private funds have enabled exciting advances in QC hardware *(Kjaergaard, et al., 2020)* and QC software and applications *(Bova, Goldfarb, & Melko, 2021)* in the last decade *(Zhang & Ni, 2020).* A relatively small fraction of these funds has been allocated to specific applications in the climate and energy fields. We believe the reason is that it was only until recently that quantum computers could be put to work for tasks which are beyond what classical computers can do and consequently there is a lack of connection between the quantum and climate communities. There are thus "application gaps" not addressed by existing government basic science research investments or industry R&D which views such research as too risky to pursue on its own. This current funding gap for QC applications in the climate and energy space will cause an unacceptable delay in applying this potentially disruptive technology for climate change solutions. Such a delay is unacceptable given the promise of near term advantages and, even more so, the urgent and critical need to mitigate climate change. Existing quantum computer hardware and software can be used now to develop QC applications for high impact solutions that will yield near-term advantages that can also be scaled up in far-future quantum computers leading to "quantum advantage".

### Convergence Aspect

Given the complexity climate change, the difficulty of scaling quantum tools and the wide array of S&C challenges these new tools might help solve, this research requires interdisciplinarity and the integration of different knowledge and solutions from natural sciences (physics, chemistry, biology, earth science, etc.), as well as social, health, and engineering sciences, behavioral science, economics, and policy making. The need for cooperation for fighting climate change has been demonstrated *(Rudall, 2021)* and will always be crucial. This workshop brought together experts from these diverse scientific disciplines that are not used to interact with each other. Typical scientific conferences usually bring together experts from academia, industry and government in a single discipline or even in a specific narrow domain within a discipline. Here, brainstorming sessions among participants from multiple scientific domains and prioritizing a maximum positive impact in people's lives and/or health of the planet helped identify specific applications that are the 'low-hanging fruit' for quantum accelerations.

### Acceleration Aspect

The participants were encouraged to share ideas, establish a broad understanding of the climate change challenges and quantum technology opportunities, identify initiatives that are ready for convergent acceleration that will provide prototypes in 3-4 years and will be ready to be scaled up to achieve full quantum advantage when fully functional quantum computers become available.

## CLIMATE CHANGE PRIORITIES

The United Nations has outlined several sustainable development goals, including targets related to Energy, Climate Action, and Sustainable Cities and Communities *(Sustainable Develpment Goals, n.d.)*.

In April 2023, leaders of the Major Economies Forum on Energy and Climate (MEF) convened at the White House to deliberate on the necessary actions to address the climate crisis. The focus of the meeting was on achieving the ambitious goal of limiting global warming to 1.5°C, with a commitment to reducing emissions by 50-52 percent by 2030 *(The White House, n.d.)*.

The Nature Conservancy stated six climate goals for 2030 1) reduce emission or store 3 billion metric tons of carbon dioxide yearly 2) protecting and restoring the health of natural habitats that help protect communities from storm surge, extreme rainfall, severe wildfires and sea level rise 3) conserve 4 billion hectares (9.9 billion acres) of ocean through new and better-managed protected areas, global-scale sustainable fishing, innovative financing, and positive policy changes 4) conserve 650 million hectares (about 1.6 billion acres) of land 5) conserve 1 million kilometers (621,000 miles) of river systems and 30 million hectares (74 million acres) of lakes and wetlands 6) support 45 million people whose well-being and livelihoods depend on healthy oceans, freshwater, and lands. *(Conservancy, n.d.).*

The Intergovernmental panel on climate change (IPCC) 2023 Climate Change 2023 Synthesis Report *(IPCC, 2023)* states that "Human activities, principally through emissions of greenhouse gases, have unequivocally caused global warming [...]." and that "Widespread and rapid changes in the atmosphere, ocean, cryosphere and biosphere have occurred. Human-caused climate change is already affecting many weather and climate extremes in every region across the globe." Adaptation to and mitigation of the effects of climate change can both benefit from new technological advancements, which can in turn benefit from well thought-out policy instruments (such as R&D funding programs) : "From 2010 to 2019 there have been sustained decreases in the unit costs of solar energy (85%), wind energy (55%), and lithium-ion batteries (85%), and large increases in their deployment, e.g., >10× for solar and >100× for electric vehicles (EVs), varying widely across regions. The mix of policy instruments that reduced costs and stimulated adoption includes public R&D, funding for demonstration and pilot projects, and demand-pull instruments such as deployment subsidies to attain scale." Despite these new developments, it is crucial to do further research aiming at reducing our GHG emissions as "All global modelled pathways that limit warming to 1.5°C (>50%) with no or limited overshoot, and those that limit warming to 2°C (>67%), involve rapid and deep and, in most cases, immediate greenhouse gas emissions reductions in all sectors this decade.", as shown on Figure 1.

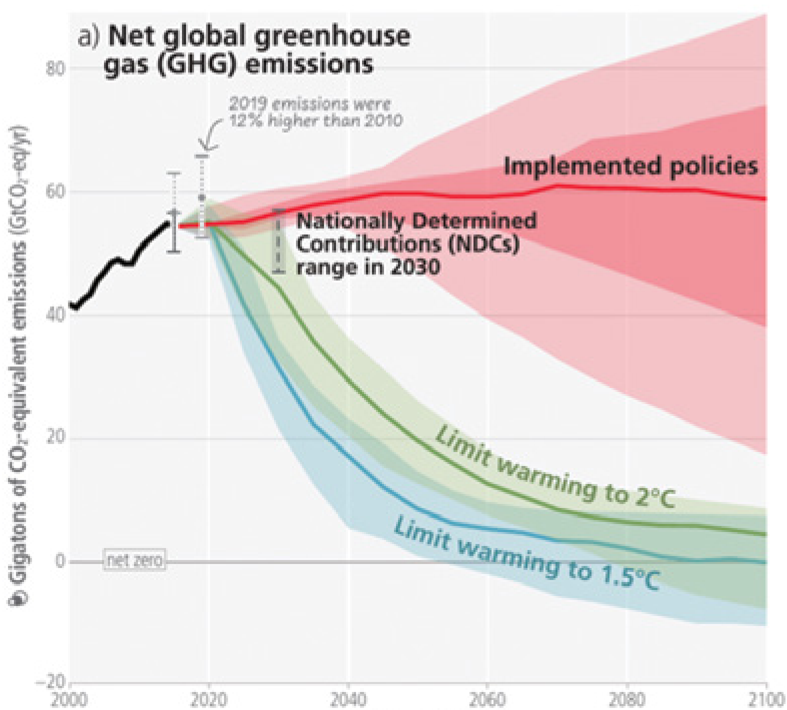



FIGURE 1. (IPCC)

# BACKGROUND ON QUANTUM COMPUTING

Much like classical computing, the field of quantum computing is distinctly divided in two core domains: the physical hardware and the software stack. This duality is crucial for comprehending the multifaceted nature of quantum computing advancements.

### HARDWARE

The advent of quantum computers as accessible tools for both public and private use started around 2015 with a limited number of available qubits. Since then, quantum computing has witnessed an extraordinary surge in computational power, soaring from fewer than 10 qubits to the order of 1000 qubits in contemporary state-of-the-art gate-based quantum computers.

Nevertheless, these devices currently reside within the domain known as the near-future quantum computers era. In this phase, the inherent noise and susceptibility to errors in their qubits impose constraints on the complexity and duration of algorithms that can be effectively implemented. Noise accumulates as the circuit depth increases, and this brings constraints on the number of operations that can be performed reliably. There is the need of developing new techniques for managing the impact of noise, whether it be through error mitigation or novel error correction schemes. Consequently, today's quantum computers cannot be used yet for tackling at scale large real-world problem instances. In contrast, future quantum computers will offer qubits of higher quality using methods to minimize errors, offering a promising solution to overcome current limitations and tackle concrete large-scale problems.

### SOFTWARE

Within the scope of this workshop, our primary focus revolved around the algorithmic layer of the software stack. Quantum algorithms research stands out as a dynamic field dedicated to addressing diverse problem types through the utilization of quantum hardware and quantum programming languages. The act in concert to accelerate certain basic calculations, such as optimization, sampling, matrix inversion, and list searching. Although these results are still theoretical, it is generally accepted that quantum computing will become industrially relevant around the hundred logical qubit mark.

The applications of quantum computing extend across diverse domains, encompassing areas such as combinatorial optimization, chemistry simulations, condensed matter physics, forecasting, and finance. Survey papers *(Dalzell, 2023)* show the current state of the art in quantum algorithms.

Quantum machine learning is an active area of research and development *(Wallner & Clements, 2023)*. The field aims to leverage the unique properties of quantum systems to improve the efficiency of solving certain computational tasks involved in machine learning. Some potential advantages include the ability to handle large datasets more efficiently, solve complex optimization problems faster, and provide novel algorithms for specific machine learning tasks.

## WORKSHOP VISION AND DIFFERENTIATION FROM RELATED ACTIVITIES

Over the past few years, numerous events focusing on the intersection of quantum computing and climate change have been organized. These gatherings have assumed diverse formats, incorporating a range of technical presentations on specific applications of quantum computing relevant to climate-related challenges. Simultaneously, some events have featured high-level discussions. In this context, we highlight three such events below:

### IEEE Quantum and Climate Summit *(Summit, n.d.)* (March 2022)

A single-day event, the summit comprised keynote presentations and technical talks that at the intersection of quantum computing and climate-related challenges. It included a roundtable discussion on the role of quantum technologies in addressing climate issues.

### Q4Climate *(Q4Climate, n.d.)* Workshop *(Berger, et al., 2021) (Feb 2022)*

This workshop spanned two afternoons. The workshop was separated into four sessions covering four domain areas closely linked to climate change: energy, environmental monitoring, transportation, and information and communication technologies. Each of these sessions was respectively paired with a topic where quantum technologies might provide solutions: simulation, sensing, optimization and energy efficiency. Each day started with a keynote presentation followed by breakout sessions, facilitating interactive discussions among small groups of 5-6 participants interested in each topic. The event followed the publication of a report *(Berger, et al., 2021)* by the same organization that identified potential high-impact use cases of quantum technologies in addressing climate change.

### Workshop on Quantum Computing and Renewable Energy at the IEEE Quantum Week (Sept 2020, 2021, 2022, 2023)

This is a one-day workshop, that include keynote presentations, followed by distinct sections featuring technical talks centered around quantum computing applications for energy transition and climate change. The workshop finished with a panel discussion. The summary of the first two editions of the workshop was documented in both a comprehensive report *(Giani, 2021)* and a detailed assessment *(Giani & Eldredge, 2021).* This annual workshop has been organized for the past four years.

### Uniqueness of this workshop

This workshop's objective was to foster a collaborative exchange between climate scientists, varied problem-domain experts and quantum researchers, with a specific focus on the tangible identification of climate and energy applications that have the potential to benefit from the acceleration provided by quantum computing and broader quantum technologies. Emphasizing short and medium-term objectives, the primary aim was to establish a roadmap that dynamically integrates anticipated advancements in quantum hardware.

In delineating the workshop's scope, efforts were directed towards pinpointing existing gaps in quantum computing research relevant to climate and energy applications. The collective vision formulated during the workshop aimed at outlining concrete deliverables achievable within the next 3-4 years. The interactive sessions facilitated both directional discussions, exploring approaches, and in-depth exploration of selected technical topics through breakout rooms.

Prior to the workshop, a strategic pre-outreach initiative was undertaken, involving an initial broad selection of the most relevant areas. This selection process was refined to align with the constraints of a two-day workshop format, ensuring a focused and impactful engagement.

## THE RIGHT TIME

As mentioned before, in 2021, an initial evaluation of potential domains linked to climate and sustainability that could be influenced by quantum technologies was conducted *(Berger et al., 2021)*. Over the subsequent years, there has been a growing consensus that chemistry and energy simulations are poised to experience the earliest and most pronounced impact *(Montgomery, et al., 2023), (Kim, et al., 2021), (Zhao, et al., 2023), (Kuhn, Zanker, Deglmann, Marthaler, & Weiss, 2018), (Gujarati, et al.), (Di Paola, et al., 2023), (Kanno, et al., 2023), (Stober, et al., 2020), (Bassman, Metcalf, Carter, Kemper, & de Jong, 2021), (Kerzer, et al., 2023), (Chen, Stein, Li, & Huang, 2023).* Additionally, optimization *(Amaro, Rosenkranz, Fitzpatrick, Hirano, & Fiorentini, 2022), (Fuller, et al., 2021), (Bentley, Marsh, Carvalho, Philip, & Biercuk, 2022), (Chai, et al., 2023) (Guijo, et al., 2024), (Malcolm, et al., 2022)* along with modeling, simulation and forecasting *(Frolov, 2017), (Zubov, Volponi, & Khosravy, 2015), (Palmer & Tennie, 2023),* stand out as two other domains with significant potential for transformative influence by quantum computational tools.

The current state of quantum technology development calls for discussions on strategically prioritizing problem domains, ensuring that quantum can harness its potential in the most impactful manner. Interdisciplinary dialogues, like the one facilitated by this workshop, are imperative to lay the groundwork for research projects at the intersection of QC and S&C. Some early efforts in this area have already resulted in published works, underscoring the momentum in this critical intersection of quantum technology and environmental challenges *(Singh, Dhara, Kumar, Singh Gill, & Uhlig, 2021) (Babin, 2023)*.

Acknowledging the early stage of quantum technologies, we recognize that the realization of real-world applications for solving climate and sustainability challenges at scale in the next 3-5 years may be unlikely. Nevertheless, we contend that the present moment is opportune for investing in research at the intersection of quantum computing and these critical issues. By focusing on specific problems with the highest potential in terms of feasibility, impact, and efficiency, we can lay the foundations for future solutions. The field is evolving rapidly, and some result of utility scale experiments have already been conducted *(Yu, Zhao, & Wei, 2023), (Shtanko, Wang, Zhang, Harke, & Seif, 2023), (Chen, et al., 2023), (Farrell, Illa, Ciavarella, & Savage, 2023), (Baumer, et al., 2023).* Even if a full quantum solution at scale is not achievable, the effort enables us to explore problem formulation for quantum hardware and create prototypes, thereby advancing our understanding and paving the way for future breakthroughs. Given that private companies are actively investing in becoming quantum-ready, it is fitting and timely for the government to do the same.

## HIGH LEVEL WORKSHOP OUTCOMES

This workshop selected the climate and energy applications for which quantum technologies provide a fundamentally new, productive and potentially disruptive tool in the fight against climate change. Applications and specific use cases that have potential for short term (3-4 years) testing and prototyping were investigated, with a roadmap for scale applications to follow the future advancements in quantum computer capabilities. The following is a list of workshop outcomes:

- Quantum can become a **strong enabler** for fighting climate change.
- Highlighted the importance of **immediately** developing quantum applications to accelerate solutions for the urgent global societal damage caused by climate change.
- Identified **use case applications** with associated near term algorithms that will provide significant impact in a three-year program that can be further refined with advances in quantum infrastructure.
- Discussed the **benefits** and the **impact** to society at scale of quantum solutions. This involves considering various factors and collaboration between researchers, industries, and policymakers will play a crucial role.
- Demonstrated that in a short term applied **research** program, a **multidisciplinary team** can advance the fight to address the root causes of climate change with the use of quantum computing.
- Created a **community** of people interested in climate change and the opportunity quantum technologies bring, as well as facilitated a connection between these two large scientific domains and developed strategies to bridge them.
- Initiated plans for a pipeline of HR and **work force training.** This involves an initial reflection on a strategic and comprehensive approach that includes define training objectives, provide access to quantum technology resources, establish certification programs, and implement strategies to attract individuals from diverse backgrounds to the field.
- Identified **gaps** in government fund that can be filled by new funding programs.

Potential deliverables for new research programs included near term QC algorithms in quantum chemistry and optimization with benchmarks against associated classical computing algorithms. Fundamental research in QC algorithms in these areas has been already performed so it is likely that focused work on applying and extending them will produce impactful results within three years. An example of a successful deliverable in chemistry was the predictions of a chemical process that significantly reduces the GHG emissions from a globally important process such as Haber-Bosch. Other deliverables were related to new materials for energy storage and solar panels. Examples of deliverables in the optimization space were resource allocation, logistics and high-fidelity simulations of a smart grid design that has significant advantages for performance and resiliency, and real-time dispatch algorithms that dramatically reduce intermodal freight GHG footprint. Given the broad impact that QC could have in the energy and transportation sector (see introductory paragraph), many important deliverables were presented. In simulation and forecasting to assess short-term and long-term projection of weather or climate prediction. Hybrid approaches of classical and quantum computation were considered.

# VALUE OF THE WORKSHOP TO NSF AND OTHER AGENCIES

## Intellectual Merit

Quantum technologies have the potential to accelerate the development of solutions to climate change. The workshop objective was to develop a deep understanding of the government funding, commercial investments and applications that would benefit from quantum computing acceleration in a short term (3-4 years). Understanding the gaps within the funding landscape would give recommendation to NSF and other government agencies for future impactful and timely programs.

In the following paragraphs, we highlight specific areas of the intersection of quantum technologies and climate change mitigation technologies which were the focus of the workshop.

### Chemistry

An early motivation for the development of quantum computing was to simulate quantum systems. The intrinsic features of a quantum computer could in principle lead to the full-time evolution of quantum systems without approximations. In quantum chemistry *(Yudong Cao, 2019)* the underlying physics is understood; the Schrodinger Equation (SE) is the quantum characterization of physical systems. The limitation in obtaining non-approximate solutions to the SE lies in the exponentially increasing number of basis states as a function of the number of interacting electrons and nuclei. This requires a prohibitively high classical computer computational resource (memory and computation time), which is a significant burden for other than the smallest molecular structures or those with particularly simple electron configurations. Density Functional Theory (DFT) is the dominant approximate (although in principle exact) quantum chemistry model run on classical computers. It has had success in understanding and developing new materials and pharmaceuticals. However, it has not been as successful in accurately predicting the properties of strongly interacting molecular systems or multistep chemical processes. Many catalytic processes, high temperature superconductors, some semi-conductors, etc. often fall into these categories. Developing QC algorithms that can overcome some of DFT's shortcomings through leveraging current or near-term quantum hardware could have a profound impact on accelerating developments in these areas important to climate and energy issues.

The workshop had a breakout room focused on identifying specific chemical processes that are crucial to climate change mitigation. These processes would benefit from the application of quantum chemistry on quantum computers in the near term era and beyond.

### Optimization

Optimization is central to solving problems related to global logistics, supply and demand, resource allocations, multibody simulation, renewable resource integration *(Ajagekar & You, 2019).* Given the high dimensionality of the problems, approximate models are used. In the near term, quantum computing and hybrid approaches may enable us to improve upon state-of-the-solvers, and potentially yield a problem-specific benefit *(Abbas, et al., 2023).* During the workshop, breakout room discussions on the most urgent and promising applications resulted in recommendation for future programs.

### Forecasting

Quantum computing will accelerate weather forecasting at both local and global scale *(Frolov, 2017) (Rigetti, 2021) (Graham R. Enos, 2021)*. Accurate climate simulations and forecasting will produce precise warning of extreme weather events and give projection for decision making potentially saving thousands of lives and millions of dollars. But weather forecasting requires a large amount of data with many dynamic parameters that constantly change and interact. This results in limitation in classical computation. Even high-performance computers have reached their limit in this regard. Quantum computers can work with a large amount of data, offering promising solutions to accelerate and improve forecasting. The workshop included a breakout room focused on simulation, modeling and forecasting.

Machine learning is an example of another technology that could be improved with the use of quantum computers with impact in forecasting, optimization, and chemistry.

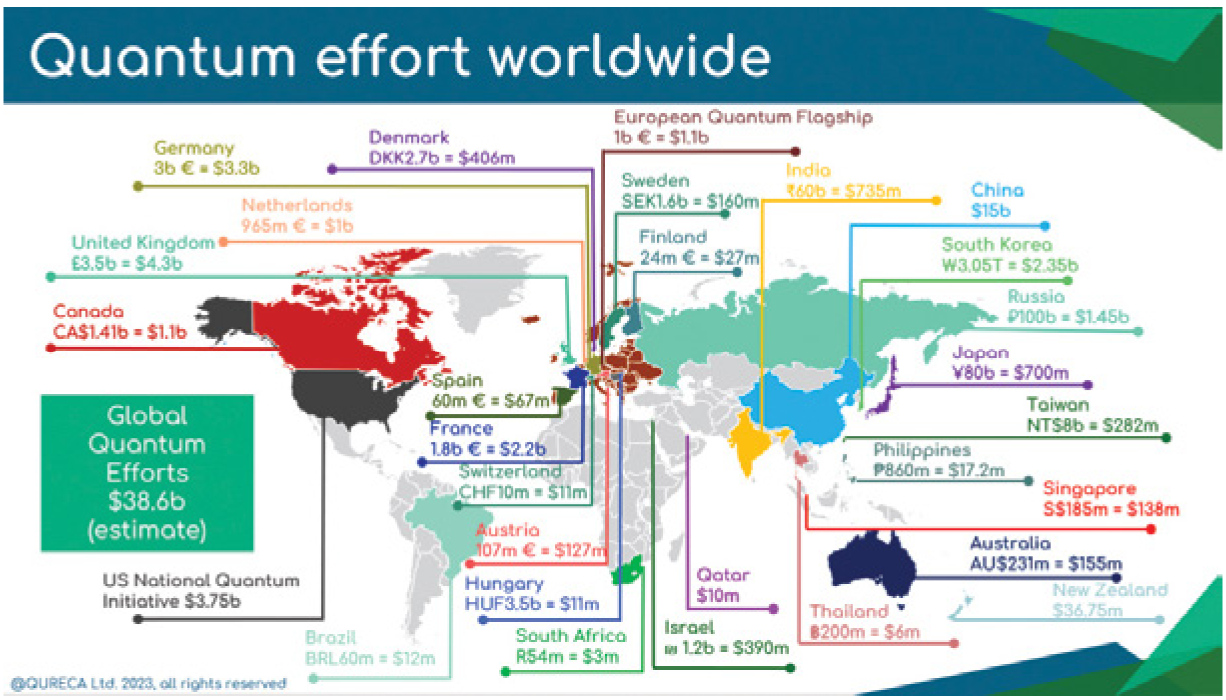
## Broader Impacts

The intent is to develop strategies to bridge these two fields (climate change and quantum computing) that are on opposite sides of the spectrum in terms of timeline of impact and technology. Problems related to climate change stem from industrial human activity, while quantum computing represents cutting-edge technology currently under development. Researchers in these two worlds often speak different languages. For a successful outcome it was required that scientists from the climate change domain quantify and prioritize the problems, while understanding the opportunities quantum computing brings. On the other hand, scientists in quantum computing needed to understand the challenges faced by climate scientists and to explain their new tools in an easily understandable manner. A continuous dialogue between these two communities is needed. This workshop provided an opportunity to promote collaborations that result in accelerated translations of efforts on short time scales. This report is intended to convey recommendations to shape future programs for the NSF Convergence Accelerator and other government agencies from key actors in both quantum and S&C ecosystems.

The broader impact of this work in the area of chemistry – beyond climate change - is certain to be demonstrated in all areas where quantum chemistry is foundational. This includes new pharmaceutical development, more efficient industrial processes, new material development. Advances in the area of optimization will impact domains like energy *(Paudel, et al., 2022) (Giani & Eldredge, 2021)*, transportations, finance, aerospace, manufacturing. New developments in simulation and forecasting will bring benefits in climate modeling, finance, and manufacturing, among other domains.

# OTHER EFFORTS, RELATED WORK, RELATED FUNDED PROJECTS

The global momentum behind the quantum effort, fueling research and innovation in quantum science and technology, is experiencing a continuous upsurge. Presently, global investments in this field have exceeded an impressive $38.6 billion. This substantial financial commitment is indicative of the growing significance and potential of quantum technologies. Projections suggest that the overall global quantum technology market is anticipated to reach a substantial value of $106 billion by the year 2040 [1]. This trajectory underscores the increasing recognition and strategic importance of quantum advancements on a global scale. Studies conducted by different agencies show the investments in the various countries *(Qureca), (IBM & SandboxAQ, 2024)*. The figure below outlines the primary programs and initiatives taking place worldwide *(Qureca).*




The figure comes from here: https://qureca.com/overview-of-quantum-initiatives-worldwide-2023/

The majority of investments in the quantum realm are predominantly directed towards the creation of a quantum computer, rather than being allocated to substantive research projects aimed at addressing crucial societal issues. Achieving this objective is precisely the purpose of our role.

Many efforts have emerged in the last few years at the burgeoning interface between quantum and climate. We state many of them, as well as their main goals, so that interested readers can contact them, and to point out that there are still not enough dedicated organized efforts in this field.

The first mover in this space was Q4Climate, a collaborator for this workshop, which aims to gather a community of experts to identify the most promising use cases for quantum technologies targeting the mitigation, adaptation and prediction of climate change, in order for research projects to emerge to solve those issues.

Qlimate is an initiative led by PsiQuantum, with Quantum Delta from the Netherlands as partners. They are mostly interested in applications of fault-tolerant quantum computing to drive large-scale decarbonization.

QC4EO, *(Agency, n.d.)* led by the European Space Agency (ESA) in collaboration with CERN, and QA4EO, ((DE), n.d.) led by the German Aerospace Center and funded by the ESA, are two research projects from Europe which aim to identify earth observation practical use-cases that can be solved using quantum computing.

In Denmark, a project focused on quantum computing for modelling climate *(SDU, n.d.)* is led by the Danis Meteorological Institute and the SDU climate cluster.

A total of 13 Spanish entities, including companies such as Repsol, BBVA, and Multiverse Computing, are collaborating to develop quantum solutions to fight climate change and enable the environmental transition, one of the strategic lines of research of the CUCO project. *(News, n.d.)*

The Blaise Pascal [re]Generative Quantum Challenge, *(Challenge T. B., n.d.)* hosted by PASQAL in 2023, was a Hackathon pushing participants to prove that quantum solutions can provide large-scale energy solutions today.

For the past 2 years, Deloitte has hosted its Quantum Climate Challenge, *(Challenge D. Q., n.d.)* where participants were asking to explore how quantum computing can impact a specific climate change related issue, namely the optimization of flight paths and carbon capture using metal organic frameworks.

The IBM Working Group on Sustainability using quantum computing is a brand-new initiative which will kick-off in April 2024. Its goal is to assemble teams of researchers working on concrete research projects solving issues related to sustainability and climate change with quantum computing.

The Government of Canada released in 2022 a call for projects called Quantum computing for climate, *(climate, n.d.)* which asked SMEs and startups to demonstrate a potential application of their technology to climate change by reducing emissions.

# WORKSHOP ORGANIZATION AND FORMAT

## Pre-Workshop Activities

We promoted the workshop through our personal networks within the scientific community, utilizing the workshop's webpage for dissemination *(GE, n .d.)*, and through GE website and social media (e.g., Twitter, LinkedIn, Facebook). The website created before the workshop will be maintained and will be used as a repository of information related to climate change and quantum computing. It will contain the final report that will be also shared with NSF.

To better identify how to maximize the outcomes, meetings with individual participants were organized before the workshop. The goal was to strategize on how to best achieve the desired outcome and to meet each other before the event.

## The Workshop Agenda

The workshop took place October 4th and 5th 2023 with the following agenda. Please note that the agenda underwent last-minute adjustments. On the second day, Misty Wahl delivered the keynote presentation at 8:10, discussing "Democratizing Quantum Computing," stepping in for Catherine Lefebvre. Rima Oueid participated in the panel discussion at 8:30 am on “The Economy, Equity, and Democracy of quantum Solutions”. Sayon Chanda was absent from the “Chemistry and Energy Application” panel at 10am. Yousu Chen and Travis Scholten participated in the panel 10:30am on Optimization Application. Amin Khodaei, Rozhin Eskandarpour and Davide Venturelli did not join the panel discussion.

Quantum FOR CLIMATE & SUSTAINABILITY

# AGENDA - DAY 1

Wednesday, October 4th

2023 NSF Sponsored Climate, Sustainability & Quantum Computing Workshop

7:00 – 8:00 am Breakfast in the Gallery

## SESSION 1: CHALLENGES - STEINMETZ AUDITORIUM

7:50 – 8:00 a.m. Welcome - Annarita Giani - GE Research

8:00 – 8:05 a.m. Q4Climate - Karl Thibault - Université de Sherbrooke,

8:05 – 8:10 a.m. Decarbonization Effort at GE Research - Anil Duggal, GE Research

8:10 – 8:30 a.m. Keynote: Challenges in Sustainability and Climate Change - Pierre Gentine - Columbia University

## PANEL DISCUSSIONS

8:30 – 9:00 a.m. Challenges in Chemistry & Energy

- Bob Ledoux, ARPA-E (Lead)
- Dimitar Trenev, ExxonMobil
- Julian Van Velzen, Capgemini
- Jon Owens, GE Research
- Yifan Zhou, Stony Brook University

9:00 – 9:30a.m. Challenges in Optimization & Energy

- Aussie Schnore, Cognizant (Lead)
- Guohui Yuan, SETO, DOE
- Yan Li, Penn State University
- Ibrahima Ndiaye, GE Research

9:30 – 10:00 a.m. Challenges in Simulation/Modeling & Forecasting

- Per Nyberg, Orca Computing (Lead)
- Aneesh Subramanian, University of Colorado Boulder
- Jerrold Cline, GE Research
- Reed Anderson, Naval Nuclear Laboratory
- Balaji Jayaraman, GE Research

10:00 – 10:05 a.m. Reminder of objectives and execution of breakouts

10:05 – 10:20 a.m. Break

10:20 – 11:45 a.m. Parallel breakout rooms: Challenge identification

| CHEMISTRY & ENERGY (CR 9) | OPTIMIZATION (CR 4) | MODELING & FORECASTING (CR 5) |
| --- | --- | --- |
| Moderator: Bob Ledoux (ARPA-E)<br>Facilitator: Marlou Slot (Nist, Womanium ) | Moderator: Aggie Branczyk (IBM)<br>Facilitator: **Carleton Coffrin** (LANL) | Moderator: **Per Nyberg** (ORCA Comp)<br>Facilitator: Baiaji Jayaraman (GE Research) |

NSF GE



continued

# AGENDA - DAY 1

Quantum FOR CLIMATE & SUSTAINABILITY

Wednesday, October 4th

2023 NSF Sponsored Climate, Sustainability & Quantum Computing Workshop

11:45 a.m. – 12:15 p.m. Report out and summary of the discussions (10 min each breakout room)

12:15 – 1:20 p.m. Group photo and Lunch in the Gallery

## SESSION 2: POTENTIAL OF QUANTUM, 3-5 YEAR HORIZON - STEINMETZ AUDITORIUM

1:20 p.m. Welcome - Annarita Giani, GE Research

1:20 – 1:40 p.m. Talk: Quantum Materials - Marlou Slot, NIST and Womanium

## PANEL DISCUSSIONS

1:40 – 2:10 p.m. Quantum Hardware
- Travis Scholten, IBM (Lead)
- Masako Yamada, IonQ
- Pierre-Louis Peguy, D-Wave
- Blaise Vignon, Alice&Bob
- Michel Pioro-Ladrière, Nord Quantique

2:10 – 2:40p.m. Quantum Algorithms & Software (NISQ/Fundamental/Hybrid)
- Sam Mugel, Multiverse (Lead)
- Jhonathan Romero Fontalvo, Zapata
- Sonika Johri, Coherent Computing Inc
- Vlad Gheorghiu, SoftwareQ
- Dominic Marchand, 1Qbit

2:40 – 3:10p.m. Quantum Sensing & Networking
- Tracey Forrest, University of Waterloo (Lead)
- Paul Dabbar, Bohr Quantum Technology
- Marlou Slot, NIST and Womanium
- Hari Paudel, National Energy Technology Laboratory (NETL)

3:10 – 3:30 p.m. Break

3:30 – 5:00 p.m. Parallel breakout rooms: Quantum Approach Discussion

| CHEMISTRY & ENERGY (CR 9) | OPTIMIZATION (CR 4) | MODELING & FORECASTING (CR 5) |
|---|---|---|
| Moderator: Bob Ledoux (ARPA-E)<br>Facilitator: **Marlou Slot** (Nist, Womanium) | Moderator: **Aggie Branczyk** (IBM)<br>Facilitator: **Carleton Coffrin** (LANL) | Moderator: **Per Nyberg** (ORCA Comp)<br>Facilitator: **Hari Paudel** (NETL) |

5:00 – 5:30 p.m. Report out and summary of the discussions

6:00 – 8:00 p.m. Dinner in the Gallery

ORGANIZERS: ANNARITA GIANI (GE RESEARCH), KARL THIBAULT (UNIV. SHERBROOKE)

# AGENDA - DAY 2

Quantum FOR CLIMATE & SUSTAINABILITY

Thursday, October 5th

2023 NSF Sponsored Climate, Sustainability & Quantum Computing Workshop

7:00 – 8:00 am Breakfast in the Gallery

## SESSION 3: PROMISING APPLICATIONS - STEINMETZ AUDITORIUM

8:00 – 8:10 a.m. Welcome - Annarita Giani, GE Research

8:10 – 8:30 a.m. Keynote: Democratize Quantum Computing for the Sustainable Development Goals (SDGs)
Catherine Lefebvre, Geneva Science and Diplomacy Anticipator GESDA

8:30 – 9:15 a.m. The Economy, Equity, and Democracy of Quantum Solutions
Ali Arabnya, Quanta Technology (Lead)
Nick Farina, EeroQ
Will Farina, EeroQ
Misty Wahl, Unitary Fund

9:15 – 9:35 a.m. Talk: How to Invest in Quantum Technologies - Christophe Jurczak, Quantonation

9:35 – 10:00 a.m. Break

## PANEL DISCUSSIONS

10:00 – 10:30 a.m. Chemistry & Energy Applications
Justin Ging, Atom Computing (Lead)
Christian Metzl, Capgemini
Sayon Chanda, NREL
Michael Marthaler, HQS Quantum Simulation

10:30 – 11:00 a.m. Optimization Applications
Amin Khodaei, University of Denver (Lead)
Rozhin Eskandarpour, Resilient Entaglement
Davide Venturelli, NASA (tentative)
Carleton Coffrin, Los Alamos National Laboratory
Mike Hayduk, Air Force Research Laboratory

11:00 – 11:30 a.m. Modeling/Simulation & Forecasting Applications
Shreyas Ramesh, Accenture (Lead)
Soronzonbold Otgonbaatar, QC4EO Europe
Kara Sulia, Univ. Albany
Reuben Demirdjian, U.S. Naval Research. Laboratory

11:30 – 12:15 p.m. Organizational meeting on report writing and roles.

12:15 – 1:15 p.m. Lunch in the Gallery

ORGANIZERS: ANNARITA GIANI (GE RESEARCH), KARL THIBAULT (UNIV. SHERBROOKE)

continued

## SESSION 4: IDENTIFICATION OF A PROGRAM TO DELIVER SUCCESSFUL PROTOTYPES IN 3-5 YEARS - STEINMETZ AUDITORIUM

1:15 – 2:45 p.m. Parallel breakout rooms. Formulate priority and a program.

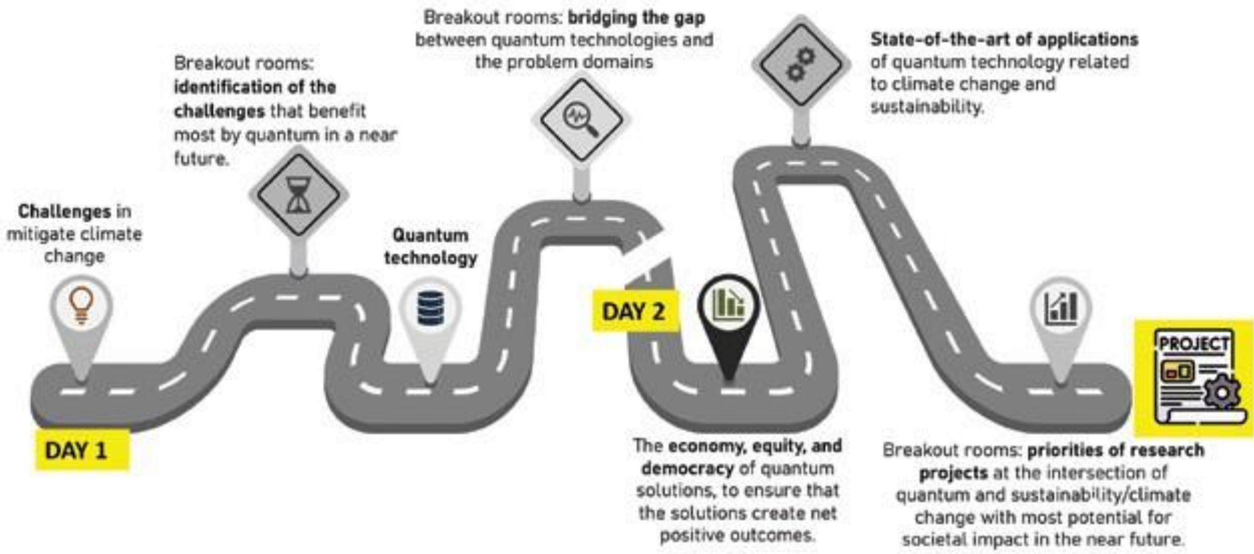
| CHEMISTRY & ENERGY (CR 9) | OPTIMIZATION (CR 4) | MODELING & FORECASTING (CR 5) |
|---|---|---|
| Moderator: **Bob Ledoux** (ARPA-E)<br>Facilitator: **Marlou Slot** (Nist, Woma-nium) | Moderator: **Aggie Branczyk** (IBM)<br>Facilitator: **Carleton Coffrin** (LANL) | Moderator: **Per Nyberg** (ORCA Comp)<br>Facilitator: **TBD** |

2:45 – 3:15 p.m. Report out of the three working groups

Recommendation for a program in climate change and quantum computing

3:15 – 3:20 p.m. Adjourn

The workshop was distributed over two days. The overall flow of the event is shown in the following figure.




The workshop started by addressing real challenges that stakeholders face in dealing with climate change. We identified energy, chemistry, and optimization as key areas were advanced technologies, like quantum computing, could be beneficial. Prof. Pierre Gentine, a professor in the department of Earth and Environmental Engineering and in the department of Earth and Environmental Sciences from Columbia University, who gave a keynote talk on challenges in sustainability and climate change. Climate models are characterized by uncertainty, and their current runtime is extensive. Introducing higher resolution for improved modeling will further prolong the duration of simulations. Another factor to contemplate is the examination of extremes. Presently, it remains uncertain whether these extremes are attributable to climate change or inadequate modeling. So, it is timely to investigate if quantum computing has the potential to bring advantages.


Pierre Gentine

After the key note speech panels discussions on chemistry and optimization for energy and simulation and modeling presented challenges in these fields.

Breakout sessions were dedicated to pinpointing which of the previously mentioned challenges (as well as others that emerged during these discussions) were most likely or held the greatest potential to be solved by quantum computing in the near future.

In the afternoon, the spotlight shifted to panels featuring diverse quantum stakeholders showcasing their technology and its current or imminent capabilities. This emphasis proved crucial, particularly for participants with limited quantum knowledge, as it provided a clear understanding of the present state of quantum technology. Marlou Slot, a Quantum Materials Physicist at the National Institute of Standards and technology (NIST), started the session with a keynote talk on quantum materials and quantum sensing. Classical physics, rooted in principles that govern macroscopic objects, proves inadequate when attempting to approximate the intricate behavior of quantum materials. The unique and non-intuitive characteristics inherent in quantum systems, such as superposition and entanglement, elude the grasp of classical theories. Consequently, a more sophisticated and quantum-mechanical framework is essential to accurately describe the properties and phenomena exhibited by these materials at the quantum level. Also, further research is needed to extend the exploration of applications for quantum sensing. Following the keynote address, panels delved into quantum hardware, software, and algorithms, showing roadmaps and cutting-edge software advancements.

Subsequent breakout sessions were centered on bridging the gap between the discussed quantum technologies and the problem domains highlighted earlier in the day. A dinner on-site provided an additional opportunity for participants to engage in further interactions.

The second day started with a keynote talk by Misty Wahl from Unitary Fund, a non-profit organization dedicated to cultivating a quantum technology ecosystem designed to benefit a broad spectrum of individuals. The focus of the session revolved around the economic, equitable, ethical, and democratic aspects of quantum solutions.

Travis Scholten, Blaise Vignon, Pierre-Louis Peguy, Masako Yamada, Michel Pioro-Ladrière

Sam Mugel, Vlad Gheorghiu, Dominic Marchand, Jhonathan Romero Fontalvo, Sonika Johri

Misty Wahl

A panel discussion revolved around strategies to ensure that the solutions we pursue result in net positive outcomes. This panel was succeeded by a keynote delivered by Christophe Jurczak from Quantonation, the premier early-stage VC fund exclusively committed to deep physics and quantum technologies. Jurczak's talks explained the fund's pivotal role in fostering innovation at the intersection of deep physics and quantum advancements, emphasizing its commitment to shaping the future landscape of these cutting-edge fields through strategic investments and support for groundbreaking projects.

The following session's main goal was to identify research projects with great potential in the near future. Presentations focused on real-world uses of quantum technology for climate change, providing a clear view of what can be achieved with the latest quantum advancements. Breakout sessions were devoted to shaping and defining research projects at the intersection of quantum technology and sustainability or climate change, with a focus on those likely to make significant contributions soon.

The day concluded with a comprehensive recap of each topic and an overview of the research projects that each topic suggests can be realistically accomplished in the near term.


Christophe Jurczak


Shreyas Ramesh, Kara Sulia,
Soronzonbold Otgonbaatar, Reuben Demirdjian

# QUESTIONS IN CLIMATE AND SUSTAINABILITY

Climate and sustainability science and technology involve answering to a wide range of questions across various disciplines. Some of the main computational challenges in climate and sustainability are found in the following areas. Although discussions during this workshop addressed many of these questions, our focus was not to dive deeply into any of them.

## Climate Science

How are global temperature patterns changing over time, and what are the primary drivers of these changes?

What are the regional impacts of climate change, including shifts in precipitation patterns, sea level rise, and extreme weather events?

How do natural climate variations, such as natural climate patterns like El Niño and La Niña, interact with human-induced climate change?

## Oceanography and Climate

What role do oceans play in regulating the Earth's climate, and how are ocean currents and temperatures changing?

How is ocean acidification affecting marine ecosystems, and what are the consequences for biodiversity?

## Carbon Cycle and Greenhouse Gases

What are the sources and sinks of greenhouse gases, including carbon dioxide and methane, and how do they contribute to climate change?

How effective are natural and human-made processes in sequestering carbon, and how can these processes be enhanced for climate mitigation?

## Renewable Energy

What are the most efficient and sustainable technologies for harnessing renewable energy sources such as solar, wind, and tidal power?

How can energy storage technologies be improved to address the intermittency of renewable energy sources?

How can we make better forecasting models for solar and wind energy generation

## Biodiversity and Conservation

How is climate change impacting biodiversity, and what are the key vulnerabilities of different species and ecosystems?

What conservation strategies are most effective in preserving biodiversity and promoting ecosystem resilience in the face of climate change?

## Sustainable Agriculture

How can agricultural practices be optimized to enhance food security while minimizing environmental impacts such as deforestation, water use, and greenhouse gas emissions?

What role do soil health and carbon sequestration play in sustainable agriculture and climate mitigation?

## Urban Sustainability

How can urban planning and design be adapted to mitigate the urban heat island effect and enhance resilience to extreme weather events?

What are the most effective strategies for sustainable urban transportation and waste management?

## Climate Policy and Economics

What policy measures and economic incentives are most effective in reducing carbon emissions and promoting sustainable practices?

How do climate policies impact different socio-economic groups, and what are the equity considerations in climate action?

## Human Behavior and Climate Change

What psychological and social factors influence individual and collective behavior related to climate change, and how can this knowledge inform effective climate communication and education?

How can behavioral economics be leveraged to encourage sustainable choices and lifestyles?

## Technological Innovations

What emerging technologies hold promise for addressing climate and sustainability challenges, such as carbon capture and utilization, advanced recycling methods, and sustainable materials development?

These questions represent a snapshot of the diverse and interdisciplinary nature of research in climate and sustainability science. Ongoing scientific investigations aim to deepen our understanding of these issues and inform evidence-based solutions for a more sustainable future.

# BREAKOUT ROOM DISCUSSIONS & RECOMMENDATIONS

Each of the three main workshop parts began with expert panels discussing the topic at hand. This was then followed by smaller group discussions in separate breakout rooms, categorized by the specific problem domains. Most recommendations crossed multiple domains. The organizers provided guidelines to the breakout group session moderators but left it to them and the participants to determine the most suitable course of action. This approach aimed to foster a collaborative and dynamic environment where diverse perspectives could be considered. Consequently, the recommendations are summarized in a distinct manner mirroring the structure of each breakout session.

## CHEMISTRY AND MATERIALS

Moderators: Robert Ledoux, ARPA-E and Marlou Slot, NIST

### INTRO

Robert Ledoux, Marlou Slot

At the core of our modern society lies chemicals and materials pivotal to creating the solutions to our energy needs. As we work towards a clean energy transition, the requirement to rapidly innovate in this space is critical. This ranges from clean energy generation and energy storage to the optimization of industrial processes. For example, solar cells accounted for three-quarters of renewable capacity additions worldwide in 2023 [IEA, 2024], and novel materials promise to further increase the efficiency. Similarly, the development of nuclear fusion relies on new materials and solving engineering challenges and would change the paradigm of energy generation. Batteries will play a vital role in achieving renewable energy goals, with new battery storage solutions that are more energy dense, safe and less resource intensive being crucial for the success of the clean energy transition. As another example, global energy consumption is heavily influenced by industrial processes, with the concrete industry alone utilizing approximately 7% of worldwide energy *(Uratani, 2023)*, and the fertilizer industry contributing around 2% *(Rosa, 2023).* These sectors employ intricate and energy-intensive chemical processes, and an enhanced comprehension of these processes has the potential to drive reductions in energy costs for these industries.

## QUANTUM CHEMISTRY AND ITS LIMITATIONS

Computational quantum chemistry involves the application of computational techniques to understand and predict chemical phenomena and electronic structures, which underpin the key areas for the clean energy transition. Various challenges arise in this field, spanning from the complexity of quantum mechanical calculations to the simulation of large molecular systems. The boundaries of what is computationally feasible in understanding molecular and material structures and interactions are continuously pushed. However, the exponential nature of many-body quantum systems places severe and fundamental limitations on truly ab initio calculations on a classical computer.

## QUANTUM COMPUTING AS A FUTURE SOLUTION

Quantum computing holds significant promise for addressing these issues, leveraging the principles of quantum mechanics that govern the behavior of molecules, their interactions, and properties. One of the foundational motivations of quantum computing is to simulate quantum systems on quantum computers where the "curse of dimensionality" is mitigated by the intrinsic quantum correlations inherent in quantum computers. Therefore, it is expected that fault-tolerant quantum computing will be uniquely suited to transform the power of quantum chemistry simulations.

Gate-based and analog quantum computers as well as quantum annealers are poised to play a key role in modeling and emulating interactions within quantum systems. Within a hybrid approach, classical computers and quantum computers will work towards their respective strengths throughout the computational process. The prospect of having fault-tolerant computers with sufficient qubits within the next five years is unlikely but not impossible. However, demonstrating proof-of-concepts and their speed-up and scalability on the currently available quantum hardware will be a crucial step toward realizing the potential of quantum computation for molecule and material simulations. It is also imperative that teams bridge the full quantum computational stack from chemical/materials applications through algorithmic and compiler levels to direct optimization with quantum hardware.



BACK TO TOC

## EXAMPLES OF APPLICATIONS/IMPACT

Major computational challenges could be overcome by quantum computing, paving the way to impact major sectors. A few examples are presented in the table below.

| Computational Challenge | Description | Example Applications |
|---|---|---|
| Quantum Mechanical Calculations | Performing accurate quantum mechanical calculations, especially for large molecular systems, is computationally intensive and exponential in the number of degrees of freedom. The trade-off between accuracy and computational cost poses a significant challenge, and approximations are often necessary. | **Battery design:** simulating electromechanical reactions in electrolytes using more accurate methods than the Born-Oppenheimer approximation typically used in state-of-the-art classical methods (such as density functional theory)<br>**Solar cell design:** simulating novel materi-als such as organic semiconductors or by understanding novel mechanisms such as singlet fission |
| Electronic Correlations | Accurately capturing electronic correlation effects, such as electron-electron interactions, is crucial for describing atomic and molecular properties. However, these correlations are challenging to model, particularly for strongly correlated systems. | **High-temperature superconductor research:** solving the Fermi-Hubbard model or simulating complex electronic correlations (e.g. spin-orbit)<br>Transition metal chemistry for a wide variety of energy materials. |
| Reaction Pathways | Studying chemical reactions and determining reaction pathways involves exploring potential energy surfaces. Locating transition states and characterizing reaction intermediates computationally can be challenging, especially for complex reactions. | **Catalytic system simulations:** Accurately determining reaction pathways in catalytic processes is crucial in determining reaction rates. One example is replacing the Haber-Bosch process with a more energy-efficient alternative found through new algorithms simulating nitrogen fixation.<br>Understanding interface dynamics such as the boundaries to electrolytes and cathode/anodes for better performance |
| Large Molecular Systems | Simulating large molecular systems, such as proteins or polymers, poses computational challenges due to the vast number of atoms involved. Developing efficient algorithms and parallel computing techniques is essential for handling large-scale simulations. | Rapidly searching for and determining properties of multi-scale large molecular configurations such as high-entropy alloys<br>Understanding and utilizing optical molecular excitation states important to optical excitations in photonic devices. |
| Dynamics & Time Scales | Simulating molecular dynamics over atomic time scales is computationally demanding. Bridging the gap between the time scales of molecular processes and the computational time required to simulate them is a challenge. | Understanding and exploiting energy transfer in photo-initiated reactions such as photosynthesis.<br>Optimizing pathways in molecular synthesis for better materials production at lower energy usage and better performance. |

## SUMMARY/RECOMMENDATIONS

To summarize, quantum computing's main application lies in tackling high-dimensional computational challenges and intricate electronic configurations that classical computers struggle to address. In the next 3-5 years, quantum hardware will steadily gain the capability to simulate increasingly intricate processes. Within this timeframe, we recommend:

- Enhancing or creating scalable algorithms within the NISQ (Noisy Intermediate-Scale Quantum) and early fault-tolerant era will be a crucial focus.
- Co-design is imperative, necessitating the optimization of both quantum algorithms and quantum hardware. Teams should include experts on applications, algorithms and hardware.
- Proofs of concept and demonstration of their speed-up and scalability for chemistry and materials use cases will pave the way for a future quantum advantage in these domains.
- Comparison with existing state-of-the-art quantum chemistry calculations on classical computers is essential to determine where quantum computers have the greatest advantage.
- In the foreseeable future, hybrid computing, combining classical and quantum paradigms, will prevail.

# OPTIMIZATION

Moderators: Aggie Branczyk, IBM and Carleton Coffrin, LANL

Optimization involves finding the best solution to a problem among a set of possible solutions. The following is a list of examples of climate and sustainability problems, which if solved can lead to significant societal benefits by promoting sustainability, resilience to climate change, and responsible resource management.

| Climate and Sustainability Challenges in Optimization | Example |
|---|---|
| Renewable Energy Resource Allocation | Optimization of the placement and distribution of renewable energy sources, such as wind turbines and solar panels, to maximize energy output while considering environmental impact and land use efficiency. |
| Carbon Capture & Storage (CCS) | Optimization of the deployment of carbon capture and storage technologies to identify optimal locations for capturing and storing carbon dioxide emissions, minimizing costs, and maximizing effectiveness in mitigating climate change. |
| Supply Chain Sustainability | Optimization of supply chain networks for sustainable practices, considering factors like transportation routes, manufacturing processes, and resource utilization to minimize carbon footprint and environmental impact. |
| Urban Planning for Climate Resilience | Optimization of urban development and planning to enhance climate resilience, including optimizing infrastructure design, green spaces, and disaster response strategies to minimize the impact of extreme weather events. |
| Water Resource Management | Optimization of water resource allocation and management to address challenges such as droughts and water scarcity, considering factors like agricultural needs, population growth, and ecosystem preservation. |
| Biodiversity Conservation Planning | Optimization of conservation strategies to protect biodiversity, involving the identification of optimal areas for reserves, wildlife corridors, and habitat restoration to maintain ecosystem health and balance. |
| Circular Economy Implementation | Optimization of circular economy practices to minimize waste and promote recycling and reuse, considering factors such as material flows, product life cycles, and sustainable consumption patterns. |
| Climate-Resilient Agriculture | Optimization of agricultural practices to enhance resilience to climate change, including crop selection, irrigation strategies, and pest management to ensure food security in the face of changing climate conditions. |
| Smart Grid Optimization | Optimization of energy distribution networks (smart grids) to improve efficiency, reduce energy losses, and integrate renewable energy sources effectively, contributing to a more sustainable and resilient energy infrastructure. |
| Natural Disaster Response Planning | Optimization of emergency response plans for natural disasters, such as hurricanes, floods, and wildfires, to minimize the impact on communities and enhance preparedness and recovery efforts. |

Solving these optimization problems can lead to significant societal benefits by promoting sustainability, resilience to climate change, and responsible resource management. Computational challenges in optimization can arise from various factors, and here are some key considerations:

Carleton Coffrin, Aggie Branczyk

**Dimensionality:** As the number of decision variables in an optimization problem increases, the solution space becomes larger and more complex. Searching through high-dimensional spaces poses computational challenges, requiring efficient algorithms to explore and find optimal solutions.

**Search Space Complexity:** The structure of the optimization search space can vary, and some problems exhibit rugged landscapes with numerous local optima. Navigating such complex spaces demands robust algorithms capable of avoiding getting stuck in suboptimal solutions.

**Nonlinearity:** Many real-world optimization problems involve nonlinear objective functions or constraints. Nonlinearity adds complexity, making it challenging to develop algorithms that efficiently converge to the global optimum.

**Discrete Variables:** Problems with discrete decision variables introduce combinatorial complexity. Finding the best combination among discrete options can be computationally demanding, and specialized algorithms like genetic algorithms or simulated annealing are often employed.

**Constraint Handling:** Optimization problems often include constraints that the solution must satisfy. Dealing with equality and inequality constraints efficiently requires specialized algorithms, such as penalty methods or constraint-handling techniques.

**Stochasticity:** Optimization problems in uncertain or dynamic environments may have stochastic components. Stochastic optimization algorithms must be employed to handle randomness and variability in objective functions or constraints.

**Scalability:** The ability of an optimization algorithm to handle larger problem sizes is crucial. Scalability issues arise when the computational resources required grow significantly with the size of the problem.

**Multi-Objective Optimization:** When dealing with conflicting objectives, multi-objective optimization seeks to find a set of solutions representing a trade-off. It introduces the challenge of defining and navigating the Pareto front efficiently.

**Global vs. Local Optimization:** Distinguishing between global and local optima is a common challenge. Many algorithms might converge to a local optimum, and ensuring global convergence is a non-trivial task.

**Dynamic Optimization:** Problems that change over time introduce the challenge of dynamic optimization. Adapting optimization strategies in real-time to changing conditions requires sophisticated algorithms.

Addressing these computational challenges is crucial for effectively solving a wide range of optimization problems across diverse fields, including engineering, finance, logistics, and machine learning. Researchers continuously work on developing algorithms and techniques to overcome these challenges and improve optimization efficiency.

Numerous industries face complex optimization challenges related to their energy consumption, spanning domains like airport traffic, transport logistics, and manufacturing chains. Conventional optimization algorithms are frequently employed to minimize variables such as cost and energy usage in these diverse scenarios. Quantum computers, and the use of novel algorithms, present a cutting-edge tool capable of enhancing the optimization of problem types traditionally deemed challenging for classical solutions. Unlike classical computers, which struggle to solve certain problems within constrained time frames, quantum computers have the potential to transcend these limitations. A recent survey compared quantum solutions against state-of-the-art classical methods and complexity-theoretic limitations to evaluate possible quantum speed ups *(Dalzell, 2023).* A comprehensive catalog of quantum algorithm is the quantum zoo (https://quantumalgorithmzoo.org/).

It is important to keep in mind that optimizing processes typically leads to an increase in their use, counteracting the foreseen decrease in energy use.

## RECOMMENDATIONS

- Need to identify class of problems in relation to the desired speed-up (e.g., quadratic vs exponential).
- There's a demand for research and design in algorithm development.
- Overcoming the barrier of limited access to quantum processing unit (QPU) time requires institutional solutions rather than a case-by-case or project-by-project approach.
- Establishing bridging events is crucial to facilitate the connection between experts in quantum technology and specialists in various applications. This approach serves as a pivotal means to foster collaboration, knowledge exchange, and synergies between the quantum technology community and professionals in diverse fields of application.
- Establish effective coordination between basic research offices and applied research offices at the governmental level, such as SC, OE, and ARPA-E. This collaboration is crucial for optimizing the synergy between fundamental research and practical applications, ensuring a more streamlined and impactful research and development ecosystem.
- Address the existing shortfall in workforce capacity, specifically in the ability to foresee and respond to short-term advancements. Implementing measures to enhance workforce skills, training programs, and strategic recruitment efforts should be prioritized.
- Plan a follow-up workshop with a narrower focus, such as quantum optimization or quantum simulation, tailored to specific domains like energy systems or chemistry.
- Develop a research topic aligned with the expertise of existing climate scientists or ongoing energy projects. This targeted approach ensures that the research agenda is closely tied to the knowledge and capabilities of current experts, maximizing the potential for meaningful contributions and advancements in the respective fields.
- Adopt a targeted strategy similar to the one already employed by certain DOE programs, which involves allocating "seed money" for initiatives. This approach can effectively catalyze and support the initial stages of projects, fostering innovation and providing a solid foundation for further development and success. This investment aims to ensure a workforce ready to apply quantum computing approaches to solutions within 2-5 years.

# MODELING AND FORECASTING

Moderator: Per Nyberg, OrcaComputing

Per Nyberg guided the breakout session on forecasting and modeling, centering the discussions around a series of questions posed to the participants. The initial panel discussion specifically addressed the identification of challenges through a series of questions.

## Challenge Identification

**Which climate/sustainability challenges do you believe are the most likely to be unsolvable by classical means?**

Computational challenges in climate and sustainability forecasting and modeling arise from the complexity of the Earth system, the vast amount of data involved, and the need for high-resolution simulations. Some key computational challenges are included in the following table:

| Climate and Sustainability Challenges in Modeling and Forecasting | Example |
|---|---|
| High-Resolution Models | Achieving high spatial and temporal resolution in climate models is computationally demanding. The Earth's climate system operates at various scales, and capturing fine-scale details, such as local weather patterns, alongside large-scale global phenomena, requires simulations with high resolution, leading to increased computational demands. A big challenge is high resolution regional predictions. |
| Ensemble Simulations | To account for uncertainties and variability, climate models often employ ensemble simulations. Running multiple simulations with different initial conditions and model parameters significantly increases computational requirements. |
| Coupled Earth System Models | Climate models must simulate interactions between the atmosphere, oceans, land surface, and ice. Coordinating these components and ensuring accurate data exchange between them requires complex and computationally intensive models. |
| Data Integration | Incorporating observational data into models for improved accuracy involves complex data assimilation techniques. Efficiently assimilating diverse data sources while maintaining model stability is a computational challenge. |
| Long-Term Simulations | Simulating climate over extended time periods, such as centuries, demands stable and efficient algorithms. Managing computational resources over extended runs is crucial for long-term climate modeling. |
| Extreme Events Modeling | Modeling extreme weather events, such as hurricanes, floods, and heatwaves, requires high-resolution simulations and specialized algorithms to capture the intricate dynamics involved. |

| Climate and Sustainability Challenges in Modeling and Forecasting | Example |
|---|---|
| Biogeochemical Cycling | Incorporating biogeochemical processes, such as carbon and nutrient cycling, into climate models adds complexity. Modeling the interactions between physical and biological components demands advanced computational approaches. |
| Dynamic Earth System Models | Earth system models that include interactions between the atmosphere, oceans, land surface, and living organisms require advanced computational frameworks to handle the diverse processes involved. |
| Modeling multi-scale physics | The study of physical phenomena that occur at multiple spatial and temporal scales is computationally challenging. For example, modeling convection is a process of heat transfer that occurs in fluids (liquids or gases) when there is a temperature difference within the fluid. This process involves the movement of the fluid itself, leading to the transfer of heat from hotter regions to cooler ones. |
| Dynamic Nature of Earth's Systems | Earth's systems are dynamic and constantly changing. Modeling dynamic processes such as atmospheric circulation, ocean currents, and ice melting involves solving complex equations that demand substantial computational power. Regional models require more detailed data and can strain computational resources. |
| Modeling stochastic and uncertain scenarios | Assessing and quantifying uncertainties in climate models involves running ensembles of simulations with varied initial conditions and model parameters. This introduces additional computational demands to explore the range of possible outcomes. |
| Machine Learning Model Training | Incorporating machine learning techniques for data analysis and model optimization adds complexity. Training and implementing machine learning models to improve climate simulations require significant computational resources. |
| Digital Twin Creation | Creating digital twins at a resolution that can be used to model different climate change scenarios, exploring the potential impacts of temperature changes, sea level rise, and altered precipitation patterns under various emissions scenarios requires very high computational resources. Digital Twins are important for condition monitoring in fact they facilitate continuous monitoring of the condition and performance of physical entities and anomalies or deviations from normal behavior can be identified, enabling predictive maintenance strategies and real time policy monitoring and enforcement. |

Addressing these computational challenges is essential for advancing climate and sustainability modeling, enabling scientists to better understand Earth's complex systems and make more accurate predictions for future climate scenarios. Ongoing research focuses on developing innovative algorithms and leveraging high-performance computing to overcome these challenges.

### Which challenges do you believe have the greatest impact on society from a sustainability/ climate change standpoint?

Several challenges related to sustainability and climate change have significant impacts on society. Identifying the most impactful challenges can be subjective and context-dependent, but some widely recognized issues include the following.

| Challenges Related to Sustainability and Climate Change with Significant Impacts on Society | Example |
|---|---|
| Greenhouse Gas Emissions | High levels of greenhouse gas emissions, primarily carbon dioxide from burning fossil fuels, contribute to global warming. Reducing emissions is crucial for mitigating climate change. |
| Loss of Biodiversity | Habitat destruction, pollution, and climate change contribute to the loss of biodiversity. This has profound implications for ecosystems, food security, and the overall health of the planet |
| Deforestation | Deforestation, driven by agriculture, logging, and urbanization, results in the loss of crucial carbon sinks and biodiversity. It also contributes to climate change and disrupts ecosystems. |
| Water Scarcity | Increasing demands for water, coupled with the impacts of climate change, lead to water scarcity in many regions. This affects agriculture, industry, and human populations. |
| Rising Sea Levels | The melting of polar ice caps and glaciers contributes to rising sea levels, posing threats to coastal communities, ecosystems, and infrastructure. |
| Extreme Weather Events | More frequent and intense extreme weather events, such as hurricanes, droughts, and heatwaves, are linked to climate change. These events have immediate and long-term impacts on communities and economies. |
| Social Inequities and Vulnerability | Vulnerable populations, often with fewer resources, are disproportionately affected by the impacts of climate change. Addressing social inequities is crucial for building resilience and ensuring a just transition to a sustainable future. |
| Food Insecurity | Changes in temperature and precipitation patterns, along with extreme weather events, affect agricultural productivity, leading to food insecurity. This is a pressing issue with global implications. |
| Ocean Acidification | Increased carbon dioxide levels not only contribute to global warming but also lead to ocean acidification, harming marine life and ecosystems, especially coral reefs. |
| Waste Management | Improper waste disposal and excessive consumption contribute to pollution and environmental degradation. Developing sustainable waste management practices is essential for a circular economy. |

| Challenges Related to Sustainability and Climate Change with Significant Impacts on Society | Example |
|---|---|
| Energy Transition | Transitioning from fossil fuels to renewable energy sources is critical for reducing greenhouse gas emissions and ensuring a sustainable and resilient energy future. |
| Lack of Climate Action | Global efforts to address climate change often face political, economic, and social challenges. A lack of comprehensive and timely climate action poses a significant risk to the planet's future.<br>Addressing these challenges requires concerted efforts at local, national, and international levels. Collaboration between governments, businesses, communities, and individuals is essential for achieving sustainable and climate-resilient societies. |

Among the scientific and technical challenges that could bring benefit to the problems and have potential to be bring benefit to the society are multi-scale physics, non-linear optimization.

**Multiscale physics** refers to the study of physical processes that occur at various spatial and temporal scales. For example, global ocean circulation models that simulate large-scale ocean circulation patterns, like the Atlantic Meridional Overturning Circulation (AMOC). These models struggle to represent and include smaller-scale processes, such as coastal upwelling, eddies and the interactions between ocean and land crucial for the marine ecosystem. Another example is the inclusion of extreme events, these models usually lack the resolution to accurately simulate the intensity and local impacts of specific events like hurricanes or tornadoes. Understanding multiscale physics is essential for developing more accurate and comprehensive models, improving predictions, and informing sustainable practices in climate science and environmental management. An example is stochastic energy modeling considering different scenarios for the future deployment of renewable energy source considering variability in solar and wind energy generation, informing energy system planning and grid integration.

**Non-linear optimization problems** are characterized by complex, non-linear relationships between variables and objectives. For example, optimizing the configuration of an energy system, considering renewable energy sources, storage technologies, and demand-side management, involves non-linearities due to the intermittent nature of renewables, energy storage constraints, and dynamic energy demand patterns. Another example is developing integrated climate-economic models to inform policy decisions involves non-linear optimization. The interactions between economic variables, carbon pricing mechanisms, and climate feedback can exhibit non-linearities that impact the optimal pathways for achieving climate and economic goals.

### Can you estimate the resources (money, manpower, computation, time) needed to areas achieve a reasonable solution to these challenges?

Estimating the resources required to address climate and sustainability challenges is a complex task and depends on various factors, including the specific goals, the scale of interventions, technological advancements, and the global and local contexts. The following needs were discussed.

- Need for interdisciplinary teams. Collaborate with experts in quantum computing, as well as specialists in climate science and sustainability. Interdisciplinary collaboration can lead to innovative solutions and insights. Allocating human resources to advance technologies in renewable energy, carbon capture, sustainable agriculture, and ecosystem restoration requires collaboration between governments, industries, and academia covering different scientific domains. It is important to include skilled personnel to design, implement, and monitor regulations and policy. This includes professionals in environmental science, law, economics, and public policy. Also involving communities and fostering behavioral change requires a significant investment in outreach programs, education, and community development. This involves a diverse workforce, including educators, community organizers, and communication specialists.
- Quantum approaches to accelerating classical implementations and quantum native implementations. Quantum computing can be applied to accelerate parts of existing classical algorithms. These could be the early wins with quantum. Full realization of quantum will require development of quantum native algorithms which are designed from the start to leverage the unique characteristics and capabilities of quantum computers. Identify the quantum analog of the classical problem you are trying to solve. This involves mapping your problem to a quantum representation. Hybrids approaches leverage the strengths of both classical and quantum computation, with some parts of the algorithm executed on a quantum computer (if available) and others on classical hardware.
- Develop clear understanding of where new technology should be applied. Need to understand the promising use cases, understand bottlenecks, costs and appropriate benchmarks, tools and data sets.
- Enable a broader/broadest section of the climate science community. In order to empower a broader section of the climate science community, the integration of quantum technologies plays a pivotal role. Various initiatives can be undertaken to leverage quantum algorithms, libraries, and hardware for advancing climate research. Here are key strategies to enable the climate science community through quantum technologies.
  - Cultivate collaboration by creating open-source quantum algorithms and libraries tailored for climate science applications. This initiative promotes the sharing of resources and expertise, contributing to a collaborative environment for advancing quantum solutions in the realm of climate science.
  - Formulate backend algorithms that are optimized for quantum hardware to augment computational efficiency. This strategy aims to harness the capabilities of quantum systems effectively, contributing to improved performance in computational tasks.

- Establish standards for quantum information storage, particularly for new quantum sensor data in climate science. Establish repositories that adhere to specified standards, facilitating the efficient sharing and access of quantum-generated climate data among researchers. This approach enhances collaboration and accessibility, fostering a more streamlined and effective exchange of valuable information.
- Promote the cultivation of an “Open-Source Quantum” ethos within the climate science community, encouraging collaborative efforts in developing quantum tools, algorithms, and software. Emphasize accessibility and transparency in quantum computing resources to enhance the collective progress and understanding in the field.
- Invest in quantum skills development programs tailored for climate scientists. Offer training and resources to empower researchers with the knowledge and skills to comprehend, implement, and effectively leverage quantum algorithms. This initiative aims to promote the broader adoption of quantum technologies within the realm of climate science.

### Which challenges do you believe are the most likely to be solvable by quantum technologies before they are solved by classical methods?

It is crucial to allocate resources and investments to research programs dedicated to identifying and uncovering potential breakthroughs in the application of quantum technologies. A sustained commitment to scientific exploration and innovation is essential to fully grasp and harness the transformative capabilities of quantum advancements.

### Are there urgent challenges we should prioritize in the coming 5 years? Focus on areas with the greatest ROI to science community:

The participant felt that the applications that mostly benefit from quantum acceleration in the next 3-5 years are those that need multiscale physics (e.g.: convection), non-linear optimization and the modeling of ensembles/stochastic scenarios.

## Quantum Solution

The second breakout room focused on identifying the quantum approach to accelerate specific problems.

### What is the likelihood that this morning’s challenges will see quantum advantage before fault-tolerant error correction?

The likelihood of climate challenges experiencing quantum advantage before the implementation of fault-tolerant error correction is uncertain and depends on the progress of quantum technologies and research in addressing specific climate-related problems. It’s an area that requires ongoing exploration and development to better understand the potential timelines and advancements in both quantum computing and error correction methodologies.

### How likely will we achieve quantum advantage with near term vs future quantum computers on each challenge?

Currently, hybrid models show the most significant potential. This is particularly evident in addressing sub grid scale processes and leveraging Quantum Machine Learning, where parts of the training occur on a quantum machine and inference is executed on a classical computer.

### What is the best balance of hybrid classical and QC for achieving quantum advantage?

Determining the optimal balance between hybrid classical and quantum computing to achieve quantum advantage is still in its early stages. To establish this balance, it is essential to develop use-case-dependent strategies and benchmarks.

### Where are near term approximate algorithms likely to provide advantage?

- Quantum machine learning for image processing.
- Applications where data is naturally represented in a quantum way in a way that the structure can be preserved. Identifying these domains is still an open question.
- Greenhouse chemistry / reaction chemistry

### How can we apply quantum computing to the challenges presented this morning? What theoretical/algorithmic techniques should theorists be focusing on?

As mentioned before, multiscale physics (e.g.: convection), Optimization problems (non-linear), Ensembles/ stochastic scenarios incl. model initialization, Uncertainty quantification
Then in a more general discussion quantum sensors as source of data and process that naturally fit quantum computation was identified. In particular greenhouse gas detection and lower level methane detection Also, higher level abstraction layers that capture the essence of the problems are promising. Together with transport equations for power distribution (operators and distributors) and interactions of radiation with clouds

### Which hardware design choices will be most important, depending on (a) the challenge and (b) whether NISQ or FTQC is required?

It is too early to access the choice of hardware. Benchmarking projects are necessary to arrive to an answer.

### Given a and b above, what would be the hardware requirements of a given quantum computer?

- Deployment of quantum sensing/networking devices
- Hybrid integrated with HPC.
- Need complex systems analysis of the applications and workloads to understand.

### What are useful metrics to benchmark algorithmic and hardware developments to measure progress?

Meaningful metrics for gauging progress in algorithmic and hardware advancements include fidelity, the resilience of algorithms to noise and accuracy, and benchmarks tailored to specific applications.

## Priorities for a Program

During the third breakout room it was discussed what the priorities for a program are.

### If you were to build a 2-to-5-year research project on one topic, which topic would you choose and why?

**Research Project Title:** Probabilistic forecasts that are beyond the reach of classical

- 5-10 year funding timeframe

**Requisites:**

- Ensure that improved high fidelity data is available to support those capabilities when quantum model is ready
- Quantum computer hardware access

**Objectives:**

- Build foundational elements:
  - Libraries, abstraction layers, benchmarks providing greatest ROI and economies of scale
- Build science exploration models.
  - quantum “shallow water model”
  - Physics informed AI model
  - Low TRL to begin with and then transition into production
- Workflow characterization

All objectives requires interdisciplinary teams with complementary skills

### Who are the relevant research groups and/or organizations to your selected project?

Approaches to solve climate applications with quantum require a multi-disciplinary team encompassing expertise in mathematics, applied mathematics, computer science, quantum information science, engineering, physics, and domain sciences, with a focus on incorporating use-case, end-user, and stakeholder perspectives, along with trainers and workforce developers; ensure representation from multiple institutions, including government agencies (NOAA, NASA, DOE, DOD), private/public foundations, and quantum hardware/software companies; and leverage international collaborations, such as with DLR, to maximize impact.

**What do you see as the major challenges/risks towards advancing your selected research project (technical, financial, other)?**

Potential challenges and risks include issues related to organizational structure, size, and focus; the identification of quantum-native thinkers; the adoption of open source and vendor-agnostic approaches; addressing gaps in the software stack; uncertainties in the clarity of quantum science; and technical concerns regarding hardware maturity and performance.

**How should the government structure their funding programs? In other words, how do you foresee projects such as those discussed before to be funded?**

A government-funded project should maintain a structured organizational framework that ensures rigorous development and advancement, fosters agility, and encourages high-risk approaches, drawing inspiration from initiatives like the Small Business Innovation Research (SBIR) program at NSF; the project should actively involve large companies with only one of few lead institutes.

**What are the next steps to refine this program?**

To strategize for a successful program, it is essential to identify key science questions, assess the current state of the art, formulate a comprehensive position paper and plan for future events that bring together climate, sustainability, and quantum communities.

Notion of Quantum Institute for Climate. Establish a quantum institute dedicated to addressing climate and sustainability challenges. Secure a total funding of $20 million over the course of five years, with an openness to private investments. The institute's primary focus will be on building a national testbed for quantum applications aimed at contributing innovative solutions to environmental issues.

## QUANTUM SENSING

Opportunities to apply quantum sensors to climate and sustainability were discussed as part of the Chemistry and Energy break-out room. Applications of quantum sensors extend across terrestrial, marine and air environments. Already there are examples of quantum sensors being applied to measure geophysical targets (such as gravitational changes through atomic gravimeters) and greenhouse gases (such as methane through optical methods). Participants noted the potential of quantum sensors to elucidate material properties of interest to climate and sustainability, improve critical mineral detection, monitor underground geothermal resources and $CO_2$ storage, and support secure smart grids and mobility. Quantum sensors could also be used for improving synchronization of DER assets to better optimize the energy grid.

Tracey Forrest, Paul Dabbar, Marlou Slot, Hari Paudel

### Suggestion To Advance The Field

Quantum sensors have existed on the market for over a decade, and quantum advantage in sensing can be realized today. The key is in finding new use cases that could benefit from even slight improvements in the size, weight, power, and cost (SWAP-C). This technology offers unprecedented sensitivity and resolution, promising to revolutionize fields like earth and emissions monitoring. Improvements in position, navigation, and timing are also critical to synchronizing distributed renewable energy resources. Transitioning from the lab to scalable deployment requires overcoming hurdles in achieving target sensitivities, miniaturizing devices for field deployment, and reductions in cost and power. Sensitivities refers to required sensitivity/ resolution/selectivity. Improving SWAP-C could lead to economies of scale and wider adoption. Given the potential for dual-use, responsible development of quantum sensors needs to consider ethical implications, governance, and potential misuse. Multidisciplinary and international collaboration is key to development. Realizing quantum sensor's potential requires early adopters, use cases that are scalable and deliver business value and increased public literacy in quantum impact.

## THE ECONOMY, DEMOCRACY AND EQUITY OF QUANTUM SOLUTIONS

Ali Arabnya, Rima Kasia Oueid, Misty Wahl, Nick Farina

The broader impact of quantum technologies extends beyond technological advancements and encompasses the critical domains of diversity, equity, and inclusion. As we explore the potential of quantum technologies, it becomes imperative to ensure that the benefits and opportunities they bring are accessible to diverse communities. Embracing diversity in the development, deployment, and utilization of quantum technologies not only promotes social equity but also enhances innovation by incorporating a wide range of perspectives and experiences.

Fostering an inclusive environment within the quantum technology ecosystem is essential for addressing systemic disparities. This involves not only addressing representation gaps within the workforce but also considering the broader societal implications of quantum advancements. Proactive measures in education, outreach, and community engagement can contribute to creating an inclusive landscape where the benefits of quantum technologies are shared equitably, ensuring that no community is left behind in the transformative journey ushered in by these advancements. In essence, the broader impact on diversity, equity, and inclusion is a pivotal aspect that should be conscientiously integrated into the development and application of quantum technologies.

Ensuring equitable access to quantum resources and knowledge is crucial. There is a risk that quantum computing technologies may not be equally accessible globally, creating global disparity and leading to a potential technology divide between developed and developing nations. Certain under-represented groups or regions may face disparities in education and training opportunities, leading to an uneven distribution of quantum expertise. There is a need for inclusion and inclusive policymaking that accounts for a variety of techno-socio-economic concerns and that considers the perspectives and needs of different stakeholders. During this session we also discussed the need to reaffirm our principles and values to ensure we are sharing knowledge with parties that uphold and demonstrate a profound respect for human rights and democracy.

Quantum technologies, with their unprecedented capabilities, hold the potential to shape a resilient and advanced future. However, it is crucial to recognize that this tremendous potential also carries the inherent risk of misuse. The very same advancements that promise groundbreaking solutions may, if mishandled, pose significant ethical challenges. Thus, while navigating the frontier of quantum technologies, it is imperative to adopt responsible practices and ethical frameworks to ensure their positive contributions while safeguarding against unintended negative consequences. A balanced approach that fosters innovation alongside ethical considerations will be instrumental in maximizing the benefits of quantum technologies while minimizing potential risks.

As broader impact, stakeholders can contribute to reducing the equity gap in quantum computing and ensure that the benefits of quantum technologies are accessible to researchers and professionals in developing regions and countries by implementing a set of policies and strategies. Collaboration, education, and resource-sharing are essential components of promoting equity in this rapidly advancing field. Open-source initiatives and collaborative research provide access to quantum computers, software, and resources through collaborations, partnerships, or shared initiatives. Open-Source Software promotes collaboration and allows researchers in developing countries to access and contribute to quantum computing projects. There is the need for promotion of initiatives to support underrepresented groups in STEM fields (such as women and historically underrepresented minorities), in pursuing education and careers in quantum computing. From an economic perspective, we should take into account the impacts of quantum solutions on the economy, and the role of the economy in developing quantum technologies. Areas of consideration include but are not limited to economic growth at local, national, and global scale using economic metrics such as GDP, employment, and productivity. Policymakers should also consider what sectors of the economy are impacted the most by quantum technologies, and who are the winners and the losers of this emerging technology. Finally, understanding that how the quality of democracies can shape the future of quantum technologies and how this emerging technology can advance (or harm) democracies in general, are important dimension of a sustainable quantum solution development.

The following three examples are designed with the intention of making quantum concepts more accessible to the community, enhancing inclusivity, and mitigating obstacles that may hinder entry into the realm of quantum technologies. These initiatives aim to close gaps in both comprehension and involvement, ensuring that the advantages and opportunities arising from quantum advancements are distributed equitably and made accessible to a broad audience.

The Open Quantum Institute (www.oqi.gesda.global), an international multistakeholder initiative hosted at CERN, born at the Geneva Science and Diplomacy Anticipator, ambitions to respond to the above-described challenges. Its core activities consist in developing applications of quantum computing serving the UN Sustainable Development Goals, whilst fostering inclusivity in the development of the technology by leveraging diplomacy. The Geneva Science and Diplomacy Anticipator (GESDA) Foundation was created in 2019 in Geneva to fully leveraging the potential of new science and technology advances to improve well-being and promote inclusive development. One of the driving inquiries guiding the efforts revolves around discovering methods to safeguard the welfare of humanity and promote the sustainable future of our planet. Exploring strategies to provide the global population with essential food and energy, all the while rejuvenating our planet, is a key focus. The guiding vision is to “Harness the future to construct the present” by uniting diverse communities to collaboratively foresee scientific and technological progress. Building upon these advancements, the aim is to formulate inclusive and global solutions for a sustainable future.

Unitary fund is a non-profit organization dedicated to fostering the development of a quantum technology ecosystem that serves the broader population. An avenue involves the provision of micrograants, which support researchers globally in their efforts to advance quantum technologies.

Conducting in-house research on an open-source compiler for error-mitigated quantum programming, along with establishing an open community platform for sharing benchmarks in quantum technology, contributes to the enhancement of the overall ecosystems.

Additionally, they manage an open-source quantum technology community that organizes hackathons and events through Discord.

Strangeworks focuses on making quantum computing accessible and user-friendly. They offer tools and platforms to facilitate quantum programming and enable individuals, researchers, and businesses to work with quantum computers without requiring an in-depth understanding of quantum mechanics. It is a collaboration platform of hardware, software, education, and service providers. Strangeworks provides a cloud-based environment and tools for quantum programming, aiming to lower the barriers to entry into the field of quantum computing. Users can experiment with quantum algorithms, access quantum hardware, and collaborate within the Strangeworks platform.

Quantum Dialogues is a research project aiming to anticipate the impacts of the integration of future quantum technologies led by the Institut Quantique de l’Université de Sherbrooke - in collaboration with the Sherbrooke Quantum Innovation Zone, companies, and universities in the Canadian quantum ecosystem - and financed by the Fonds de recherche du Québec - Nature et Technologie. Both local and national dialogues will make it possible to anticipate the needs of all concerned sectors, and to develop support tools for businesses, research, governments, and civil society groups to maximize the benefits of these disruptive technologies and minimize their negative effects for society as a whole.

## QUANTUM INSPIRED AS A SHORT TERM APPROACH

A quantum-inspired algorithm is a computational approach that draws inspiration from principles used in quantum computing but is implemented on classical computers. These algorithms leverage certain characteristics and strategies inspired by quantum mechanics to solve specific computational problems more efficiently than classical algorithms alone. While they were originally developed to simulate quantum behavior, they have since found a wealth of applications to industrial systems. This can be understood because simulating the quantum world relies on efficiently doing linear algebra on a massive scale, which is also relevant to many industrial applications.

While it is acknowledged that quantum-inspired algorithms do not serve as a direct substitute for the unparalleled computing capabilities promised by fully realized quantum computers, they do offer a practical and promising approach to addressing specific complex problems using classical hardware. These algorithms, inspired by principles from quantum computing, leverage certain quantum properties to enhance classical computing performance in tackling intricate computational challenges.

This approach represents a valuable bridge between classical and quantum computing realms, allowing researchers and practitioners to harness quantum-inspired techniques to achieve advancements in the short term. By capitalizing on the unique characteristics borrowed from quantum principles, such algorithms contribute to solving complex problems efficiently within the current limitations of classical computing resources.

Therefore, while the full realization of quantum computers remains on the horizon, quantum-inspired algorithms play a pivotal role in advancing computational capabilities and finding solutions to intricate problems across diverse fields in the immediate future. It is however important to remember that the development and use of quantum-inspired techniques does not guarantee the further development or use of pure quantum techniques at a later time.

Tensor networks have for instance been shown to efficiently solve partial differential equations *(Patel, et al., 2022).* This allows quantum-inspired algorithms to price exotic options more efficiently than Monte Carlo, which is the industry standard, or efficiently solve the Hamilton-Jacobi-Bellman equation, which is indispensable for solving stochastic control problems. Tensor networks also offer significant opportunities to solve some major climate challenges (Mugel, 2023).

# KEY RECOMMENDATION TO FUNDERS AND THE ROLE OF THE GOVERNMENT

The community recognizes the importance of addressing applications pertaining to climate change and sustainability and the promise of quantum computing for these domains. It is acknowledged that within the 3–5 year timeframe, quantum computing will not resolve these challenges at their full scale and complexity. This is due to the inherent extraordinary complexity of these problems and the fact that quantum computers have not yet reached full maturity. At this stage, research should prioritize a quantum-native perspective when transitioning from classical methods. Waiting for quantum technology to mature would lead to significant time loss in addressing urgent climate issues. The main recommendations are:

- Craft calls for proposals focusing on quantum problem formulation to drive promising proofs of concept and prototype development.
- Establish interdisciplinary “Centers of Excellence” concentrating on specific problem domains or challenges, utilizing a fail-fast approach due to the inherent research risk.
- Create quantum algorithm libraries tailored to the needs of problem-domain experts.
- Ensure adequate access to quantum computing hardware and software capabilities.
- Provide training for problem domain experts in quantum science and technologies.
- Define application-specific benchmarks to evaluate quantum technologies and algorithms.
- Identify key grand challenges within each problem domain.
- Identify optimization problems with a desired speed-up.
- Create a quantum sandbox which connects quantum technologies with energy infrastructure and systems to evaluate the performance of quantum technologies: to tinker, optimize, and collect empirical evidence.
- Design innovative and utility-scale algorithms for both immediate and future achievements.
- Clearly describe quantum hardware resource estimates in a consistent and appropriate manner to facilitate meaningful insights about system capabilities.
- Expand the workforce and explore international collaboration opportunities.
- Emphasize co-design to optimize both quantum algorithms/software and hardware.
- Showcase accelerated performance in proofs of concept for chemistry, materials, optimization and forecasting.
- Focus on hybrid computing recognizing the importance of classical and quantum approaches to formulate use-case-specific strategies and benchmarks.
- Tackle workforce capacity gaps through improved skills, training, and strategic recruitment efforts.
- Align research topics with ongoing climate science endeavors or energy projects to guarantee valuable contributions.
- Execute a focused strategy, directing “seed money” for efficient project initiation and development.
- Coordinate basic and applied research offices at the governmental level for optimized synergy.
- Establish institutional solutions to overcome restricted access to quantum processing unit (QPU) time.

# CLIMATE, SUSTAINABILITY AND QUANTUM COMMUNITY

The success of the workshop depended on having the right attendees. The organizers identified a diverse group of participants; they were intentional in bringing a combination of expertise in S&C and quantum R&D. The goal was to maintain a manageable size and to facilitate input and collaborative discussion from all the participants. In addition to reaching out to personal contacts, we contacted key leaders in S&C related fields (such as climate modeling and simulation) and sent personalized invitations. We engaged with the invitees to articulate the objectives of the event and gather their insights. Their diverse perspectives, expertise, and suggestions enriched the planning process, ensuring that the event was thoughtfully curated to meet its intended objectives successfully. This collaborative approach, involving the contributions of all stakeholders, contributed significantly to the overall success and effectiveness of the event. Many participants also recommended further invitations to other experts.

| Participants Affiliation | | |
|---|---|---|
| **Industry** | **Academia** | **Government / Others** |
| • Quantum technology<br>• Energy<br>• Aerospace<br>• Cybersecurity<br>• Aeronautics<br>• Artificial Intelligence<br>• Electronics<br>• Aerospace<br>• Consulting | • Quantum Technology<br>• Electrical Engineering<br>• Computer Science<br>• Earth and Environmental Science<br>• Atmospheric Science<br>• Mathematics<br>• Physics<br>• Climate | • United States Government Funding Agencies<br>• Venture Capitalist<br>• No-Profit |

The workshop created a community of people interested in climate change and the opportunity quantum technologies bring. Its objective was to foster a strong connection between these two distinct scientific domains and to craft strategies for bridging the gap between them. It became evident that maintaining this dialogue is crucial. As a result, the organizers have initiated a LinkedIn Group and a Box Folder. Beyond this, there is an ongoing effort to establish a more structured mechanism for sustaining and nurturing this community. This may involve regular annual meetings, working groups, or other discussion platforms to ensure continued collaboration and knowledge sharing. There is a clear willingness to continue the discussion through:

- Regular annual workshops. We are looking for a formal mechanism to support this.
- Longer workshops (three to four days) with more time available for free discussion.
- More technical workshops or summer schools.
- Collaborating with existing grand challenge events.
- Hosting ~monthly talks on a chosen topic.

# PARTICIPANTS LOGOS

NSF
WOMANIUM | QUANTUM
Brookhaven National Laboratory
PINQ²
University of Denver
NC State University
University at Albany, State University of New York
IQC Institute for Quantum Computing
softwareQ
GE Vernova
arpa-e
RE
University of Waterloo
Zapata
Los Alamos National Laboratory
ExxonMobil
NREL Transforming ENERGY
Institut Quantique UdeS
U.S. Department of Energy
Unitary Fund
Quantonation
ORCA Computing
UConn University of Connecticut
Dartmouth
Stony Brook University
IonQ
Quantinuum
GE Aerospace
D-Wave The Quantum Computing Company
atom computing
Columbia University
Pacific Northwest National Laboratory
Université de Sherbrooke
Quanta Technology
IBM Quantum
AFRL
Capgemini
Multiverse
Bohr Quantum
South Dakota State University
LMU
The University of Tennessee Knoxville
DLR
USRA
HQS Quantum Simulations
accenture
National Energy Technology Laboratory
Rensselaer
Nord Quantique
TQT Transformative Quantum Technologies
PennState
NUBIS A.I.
The University of Tennessee Knoxville
Zurich Instruments
Boulder
AstroCeNT
Alice & Bob
the matter lab
PsiQuantum

# POST-WORKSHOP SURVEY AND FEEDBACK

During the last session of the workshop, the participants anonymously replied some questions through their phones. The intention was to gather feedback on the workshop itself and this report, identify useful metrics to measure societal impact of quantum solutions and determine which next steps would be most appreciated by people currently active in this field.

Answers could also be liked by participants, leading to a few answers clearly being more appreciated.

Below is a summary of the main themes that emerged from the survey with supporting quotes. The answers are presented in the order of importance as assessed from participant likes.

### Question #1: What are the metrics to measure the societal impact of quantum solutions?

- Quantum solutions that are more efficient for specific types of calculations vs current classical solutions
- Concrete applications for quantum technologies which requires further collaboration between problem-domain experts and quantum scientists.
- Speed and efficiency for decision making due to quantum computing, including problem formulation, computation, and estimation.
- Industry adoption
- Employment generation
- Market value of companies in quantum technology or their products
- Prediction accuracy of quantum solutions, such as in the case of weather forecasting
- Measurable societal benefits, e.g., climate, ocean temperature, GHG reduction, improved quality of life, adoption in third world countries, reduced wealth gap
- Adoption by developing countries
- Number of people learning quantum
- Quantum investment

### Question #2: Do you have any feedback on the workshop (things that you liked or disliked, and/or things that we missed)?

- Breakout sessions were productive and appreciated
- Clearly stating and pursuing a common goal throughout the workshop was useful
- Great community gathered together! Many interesting people
- Fantastic workshop, very well-organized.
- Great structure with talks/panels/breakouts
- Great group of people
- Should have a hands-on session for running a sample application on a quantum computer
- Suggest adding some background technical talks on quantum
- Include more time for informal discussions, as the schedule was quite packed
- Add more networking time, a social activity and a tour of GE Research
- Expand more on democracy and equity of quantum solutions
- Introductive sessions to quantum technology and hands-on sessions would have been useful
- Potential end-users from various industries, in particular chemistry, were lacking

- Fewer panels, more free discussions
- Too short, suggest 2-3 full days

### Question #3: Do you have any suggestions related to the report?

- Ensure the report's public availability by publishing it as a white paper, for example, through platforms like arXiv
- Allow participant to give feedback and contribute
- Precisely identify the target audience for the report
- Clearly express the main message conveyed in the report
- Outline the next steps with clarity and precision.

### Question #4: How can we keep the momentum of this meeting?

- Create a LinkedIn Group to jointly share news and other events (done, contact us to join)
- Make it a regular annual event
- Plan forthcoming workshops to maintain group connectivity.
- Arrange summer schools and additional technical workshops for knowledge enrichment.
- Establish subgroups centered around shared interests for more focused collaboration.
- Create a joint discussion space (Slack, Discord, etc.)
- Have specific working groups that meet regularly
- Organize Tedx Talks
- Send a newsletter

## NEXT STEPS/FUTURE FOLLOW UP EVENTS

In response to participant suggestions, a closed LinkedIn Group has been established named Climate, Sustainability, and Quantum Advancement (CSQA). Workshop participants are automatically enrolled, and those with an interest in the topic are also welcome to join.

1. The workshop participants have begun collaborating thanks to the networking opportunities provided during the event. Through strategic partnerships in government and industry-funded projects, participants have the chance to drive technological advancement and make significant impacts, both in their own sectors and in the wider realms of science and industry. These successes wouldn't be achievable without these strategic collaborations.

2. A follow-up event sponsored by Quantonation, led by Christophe Jurczak, and iXcampus is currently being organized. The event will take place in Europe, outside Paris in the Fall 2024. The event is named after Nobel laureate Prof. Alain Aspect (2022), known for advocating fundamental science in Quantum Physics. Prof. Aspect also encourages practical applications, urging students to engage in industry and entrepreneurship. The 2024 Alain Aspect Symposium centers on quantum technologies for Sustainability and Climate Change. Themes include new energy materials, optimization for energy networks, environmental monitoring, and energy consumption in classical and quantum processors. The majority of keynote speakers are expected to provide a “non-quantum” perspective, emphasizing challenges to overcome and essential requirements.

3. Michelle Lampa launched and plays a leading role managing an organization that brings together key players in industry, government, and academia. The organization aims to promote and facilitate the adoption of quantum technologies, break entry barriers for talent, and foster connections among individuals and organizations. Through this initiative, Michelle plays a crucial role in paving the way for a broader and more inclusive embrace of quantum solutions across different domains and fostering an environment conducive to the widespread adoption of quantum technologies.

4. Building on the valuable discussions and connections forged during our workshops, ARPA-E (Bob Ledoux) is currently in the planning stages of an upcoming event at the Department of Energy (DOE) on Quantum Computing for Energy Innovations with the purpose of developing an ARPA-E program in quantum computing. The event will take place in late April 2024 in Washington, DC. The target of the program is a comprehensive implementation addressing challenges in the realms of quantum chemistry and materials science, with direct relevance to the ARPA-E mission's objectives. The development and execution of solutions will require utilization of quantum hardware. ARPA-E anticipates that achieving this will necessitate collaborative efforts and collaboration among hardware, software, algorithms, and domain expertise. Attendees will have the chance to explore the forefront of quantum computing, pinpoint crucial technical hurdles, suggest possible remedies, engage with relevant stakeholders, and exchange insights and experiences within the domain. This event will provide a platform for further collaboration and discussions on advancing innovations and computational power in energy. The goal is accelerating the path to more reliable, affordable, and

sustainable energy, while helping power economies and deliver the electricity that is vital to health, safety, security, and improved quality of life.

5. Aneesh Subramanian is currently in the process of drafting a proposal for a workshop in Fall 2024, the focus is on submitting it to the US CLIVAR (Climate Variability and Predictability Program). This proposed workshop serves as a follow-up to a preceding event.
6. The findings and suggestions obtained from this workshop will be showcased at conferences focusing on both quantum and climate topics.

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