

QuEnergy

Exploring the role of quantum computing for the electric grid



Link to full report including supplemental information: https://quantumconsortium.org/QuEnergy22

Copyright $\ensuremath{\textcircled{O}}$ 2022 SRI International and Accenture. All rights reserved.

Executive Summary

The electric sector is undergoing rapid change. New business models are emerging as larger portions of the economy, such as transportation, are electrified and intermittent resources and new energy storage solutions are developed and incorporated into the electric grid. Quantum computing can play a part in addressing the increasing complexity as the grid evolves to meet changing requirements and goals of the electric sector.

Applications of quantum computing for the electric sector reported here are informed by analysis of perspectives from the quantum computing industry and electric sector. Applications of quantum computing to optimization, machine learning, and simulation may impact all segments of the electric sector. The most prevalent idea is the application of quantum simulation techniques to aid development of battery technologies. Energy Market Optimization is ranked to have the greatest feasibility and the highest impact over the other ideas.

Expert concepts for the application of quantum computing to the electric sector include application to materials discovery, load modeling and management, and the detection and analysis of faults or outages.

From this analysis, the following observations and conclusions emerged:

- 1 In some cases, the quantum industry and electric sector ascribe differing value to applications of quantum computing. This may represent an opportunity to help quantum companies refine their value propositions and focus on challenges industry finds important. For example, we found that energy experts see more value in being able to predict rare events and rolling blackouts than quantum experts.
- 2 Similarly, our data suggest that the electric sector rates the application of quantum

computing as more feasible than the quantum industry finds the same concepts. This may point to a gap in knowledge in quantum computing (by the electricity industry) and expectations by the quantum industry, which has a more conservative outlook. The energy sector may need to temper its expectations regarding quantum solutions disrupting business in the near term.

We identify and assess four key use cases for quantum computing in the electric sector:

- 1 Fault prediction Using quantum annealing, quantum neural networks, and quantum generative adversarial networks to predict when failures could occur in the energy grid and fix them prior to incident.
- 2 Energy market optimization Determining when power generators are switched on vs left idle (unit commitment) is a combinatorial optimization problem that quantum computers are capable of solving. The output helps to minimize costs while still meeting demand and is an important calculation for grid operators, energy traders, and consumers.
- 3 Integrated planning and optimization for reliable and resilient grid – Using continuous variable optimization on quantum computers to balance distributed generation, future energy sources, and placement of equipment to increase grid resilience.
- 4 Quantum chemistry simulation for new materials – Quantum simulation of materials show promise for new battery technologies and increase solar cell efficiency.

This report shares ideas and concepts applicable to the power industry as starting point for further exploration of the application of quantum computing in the electric sector.



Introduction

The electric sector is undergoing rapid change with new business models emerging as larger portions of the economy, such as transportation, are electrified and intermittent resources and new energy storage solutions are developed and incorporated into the electric grid. Quantum computing can play a part in addressing the increasing complexity as the grid evolves to meet changing requirements and goals in the electric sector. New approaches based on quantum computing can offer a stronger, more resilient, and reliable North American energy system while maintaining energy independence.

Quantum computing may impact all segments of the electric sector because it offers broad applicability for optimization, machine learning, and simulation use cases. Grid segments including generation, transmission, distribution, customer load, asset owners, system aggregators, and service providers, each require these types of solutions.

Optimization approaches include both quantum approximate optimization algorithms that run on gate model quantum computers and adiabatic quantum processes that run on quantum annealers. These methods can solve combinatorial optimization problems, which can be intractable on classical computers. Many problems based on optimizing energy grids include discrete variables, making them prime candidates for quantum optimization algorithms. Quantum machine learning has shown promise through proven algorithmic speedup, synthetic data generation for model training and a potential ability to increase the scale and/or performance of certain machine learning algorithms through hybridizing them to include quantum layers. For example, weather prediction models that use synthetic data generated by a quantum computer met classical benchmarks, and even exceeded them when a quantum layer was added into the model.¹

Lastly, using quantum computers to simulate naturally occurring processes and systems, such as atoms and molecules, has the potential to increase our understanding and allow us to create better, more efficient products. For example, researching next-generation batteries through simulations of candidate materials, such as lithium sulfur, on quantum computers may be a necessary step to finding better storage options for renewable energy and electric vehicles.²

There are many examples of energy use cases that could benefit from quantum computers and quantum algorithms. These examples can run on various quantum computer architectures including both gate-based universal quantum computers and analog quantum computers, such as quantum annealers. Learning about the board applicability of quantum to the electric sector can push the boundaries of quantum technology as it stands today, create new collaborations between the electric sector and quantum communities, as well as offer new innovation for a more efficient grid.



Key quantum computing use cases in the electric sector

	Use Case	Problem Type	Quantu	m Hardware	Options
			Gate	Annealing	Inspired
1	Real-Time Situational Awareness	Machine learning			X.
2	Energy Market Optimization	Optimization			X .
3	Distribution System Operation after Derecho Storm	Optimization, machine learning		1	×
4	Load Modeling for Efficient and Effective Storage	Optimization, simulation, machine learning			
5	Discrete Choices with Nonlinear AC Physics	Optimization			
6	Prediction, Consistency with Observations	Machine learning			×
7	Demand Modeling (and Prediction)	Simulation			
8	Extreme Event Preparation	Optimization			×
9	Energy Demand Forecasting	Machine learning			
10	Rolling Blackout/Rare Event Prediction	Machine learning			×
11	Quantum Simulation of New Materials	Simulation, optimization			
12	Optimization of Grid Resilience	Optimization			×
13	Day-ahead Market	Optimization			X X
14	Coordinating Weather Events and Network Use Patterns	Optimization, machine learning			
15	Integrated Planning and Optimization	Simulation, optimization			×
16	Integration Operations and Control	Simulation, optimization			×
17	From Materials to Plant and Design	Simulation			

Quantum Use Cases



Points of View 1: Overall Impact/Feasibility

A group of electric and quantum experts were convened to identify the top high-level areas where the electric sector could benefit from current and future quantum computers. These were the resulting top 17 use cases. All 221 use cases are listed in the appendix.

The workshop goals and methodology as well as all 221 use cases are provided in the supplemental information following this report.

Experts in the quantum computing industry and energy sector assessed each use case in terms of relative feasibility and impact. Energy Market Optimization was ranked to have the greatest feasibility and the highest impact over versus the other ideas. Optimization of Grid Resilience and Quantum Simulation of new Materials were also in the upper right quadrant as show in the figure below.

All Participants



Use Case

- A: Real-time Situational Awareness
- B: Energy Market Optimization
- C: Distribution System Operation After Derecho Storm
- **D**: Load Modeling for Efficient and Effective Storage
- E: Discrete Choices with nonlinear AC physics
- F: Prediction, consistency with observations
- G: Demand Modeling
- H: Extreme event preparation
- I: Energy Demand Forecasting
- J: Rolling Blackout / Rare Event Prediction
- K: Quantum Simulation of new Materials
- L: Optimization of Grid Resilience
- M: Day-ahead Market
- N: Coordinating weather events and network use patterns
- O: Integrated Planning and Optimzation
- P: Integration Operations and Corol
- O: From Materials to Plant and design

Source: QED-C

Points of View 2: All Participants vs Thought Leaders

By looking at the Feasibility vs. Impact matrix (three views below) for different populations of participants, patterns start to emerge. For example, when the scores from workshop observers are removed, 10 ranks higher compared to other concepts. This means that workshop participants who were invited to participate because of their expertise in the energy industry or quantum technology saw more value in being able to predict rare events and rolling blackouts.

All Participants vs. Named Experts





Use Case*

- L: Optimization of Grid Resilience
- E: Discrete Choices with nonlinear AC physics
- I: Energy Demand Forecasting
- M: Day-ahead Market
- G: Demand Modeling
- F: Prediction, consistency with observations
- A: Real-time Situational Awareness
- D: Load Modeling for Efficient and Effective Storage
- H: Extreme event preparation
- N: Coordinating weather events and network use patterns
- P: Integration Operations and Corol
- K: Quantum Simulation of new Materials
- Q: From Materials to Plant and design
- B: Energy Market Optimization
- **O:** Integrated Planning and Optimzation
- J: Rolling Blackout / Rare Event Prediction
- C: Distribution System Operation After Derecho Storm

* Use cases are ordered from least to most disparity between compared groups

Source: QED-C



Points of View 3: Public Sector vs Private Sector

Breaking down the scores further to explore differences between energy public sector participants and quantum industry experts in the private sector reveals more insights. For example, a cluster of ideas was identified as high impact by energy experts, but not quantum industry attendees. These could be use cases that quantum experts are not thinking about because they do not realize how much value they provide.

Public Sector vs. Private Sector

- Energy Attendees (DOE + Labs + Utilities)
 Quantum Industry Attendees
- Quantum Industry Attendees (Quantum companies)



Source: QED-C

Use Case*

- K: Ouantum Simulation of new Materials
- H: Extreme event preparation
- D: Load Modeling for Efficient and Effective Storage
- **O:** Integrated Planning and Optimzation
- J: Rolling Blackout / Rare Event Prediction
- L: Optimization of Grid Resilience
- M: Day-ahead Market
- P: Integration Operations and Corol
- Q: From Materials to Plant and design
- **F:** Prediction, consistency with observations
- I: Energy Demand Forecasting
- N: Coordinating weather events and network use patterns
- A: Real-time Situational Awareness
- E: Discrete Choices with nonlinear AC physics
- B: Energy Market Optimization
- C: Distribution System Operation After Derecho Storm
- G: Demand Modeling

* Use cases are ordered from least to most disparity between compared groups

Points of View 4: Quantum Knowledgeable vs Energy Knowledgeable

Finally, comparing the scores of the quantum experts to those of the energy experts shows that energy experts think many concepts are more feasible than the quantum experts do. This could be due to a gap in knowledge between quantum experts and energy experts on the current state of quantum technology, with the quantum experts opting to be more conservative in their outlook of the feasibility of quantum applications.

Quantum Knowledgeable vs. Energy Knowlegde

- Quantum Attendees (Labs + Companies)
- Energy Attendees (DOE + Labs + Utilities)



Source: QED-C

Use Case*

- K: Ouantum Simulation of new Materials
- B: Energy Market Optimization
- H: Extreme event preparation
- E: Discrete Choices with nonlinear AC physics
- C: Distribution System Operation After Derecho Storm
- P: Integration Operations and Corol
- J: Rolling Blackout / Rare Event Prediction
- N: Coordinating weather events and network use patterns
- Q: From Materials to Plant and design
- **O:** Integrated Planning and Optimzation
- G: Demand Modeling
- I: Energy Demand Forecasting
- F: Prediction, consistency with observations
- D: Load Modeling for Efficient and Effective Storage
- A: Real-time Situational Awareness
- L: Optimization of Grid Resilience
- M: Day-ahead Market

* Use cases are ordered from least to most disparity between compared groups





Top Applications of QC in the Power Industry

Four concepts were prioritized as highest impact among the 221 ideas (see supplemental information) based on input from experts in the quantum industry and electric sector. The types of quantum computers which could be available at the scale required to solve the problem and the availability of people with the skills required to make meaningful progress on creating the solution were considered.

Fault Prediction (Prediction, Consistency with Observations)

This use case focused on developing a fault prediction solution. Today's fault detection systems catch, classify and locate faults for remediation. They do this by recognizing anomalies in data streams picked up by sensors, phasor measurement units (PMUs) and Digital Fault recorders (DFRs). An anomaly will signal the presence of a fault, and the characteristics of the anomaly can be used to deduce the fault's type and location so the appropriate crews can be dispatched.³ However, these methods depend on high grid observability, and the lack thereof is a leading cause of underperforming fault detection systems.³ For example, predicting sag in transmission lines require data from thermal sensors, active/reactive power sensors, voltage sensors, among others.



Even when fault detection systems are working properly, they are inherently a reactive system; the fault has already occurred; the only action that can be taken is to minimize the impact.

Predicting faults before they occur would be much more valuable than learning about them after an outage. If a grid operator could be informed that a fault was likely, the necessary reconfiguration of operations could be executed so that the fault would not affect end users of the grid-or given enough time, a crew could remediate the cause of the impending fault. This kind of prediction would require a machine learning model to be trained to predict anomalies from waveform data supplied by the sensors and PMUs. Quantum machine learning methods have the potential to decrease the training time and increase the prediction power of these types of models. Annealing methods, guantum neural networks and quantum generative adversarial networks (to reduce the problem space) are suggested as a starting place for further analysis.

Quantum machine learning methods have been tested for fault detection and diagnosis of industrial process systems. For example, there exists a

generative quantum algorithm that leverages guantum sampling and annealing to generate fault indications based on data from reactors used in chemical and industrial engineering.⁴ When classical classifiers used these guantum-generated indicators, they outperformed traditional fault detection techniques for most types of faults.⁴ Furthermore, the researchers demonstrated that the guantum techniques scale more efficiently than classical ones, enabling more data to be processed in less time.⁴

Applying this work to energy grid faults could enable faults to be predicted before they happen. The success of this use case could be measured by the reduction in outages. Noted that a potential barrier to success is the need for more sensors. phasor measurement units (PMUs), and digital fault recorders (DFRs) to ensure sufficient quality and granularity of the data. However, guantum optimization methods have been suggested as a possible solution to optimize the positioning of existing sensors and PMUs. It is also suggested that the implementation of quantum machine learning methods would be best within an existing classical pipeline where the results can be easily compared to the existing solution as a benchmark.



Energy Market Optimization

This use case is based on the "popular unit commitment problem" where a set of energy generators are coordinated to meet energy demand while minimizing costs or maximizing revenue. Several inputs are used for the optimization problem, starting with the bids provided by the various energy sources (generators). Next, load demands are modeled, considering current weather forecasts. Finally, the network operator runs the optimization and selects the generation resources that minimize the total energy cost.

Currently, a typical solution for this type of unit commitment problem would be based solely on customer demand and generation costs. However, as grids evolve, innovations like bi-directional energy flow and combined cycle units mean that finding the absolutely optimal solution will require incorporating other stages of the energy value chain into the model, such as distribution or even consumer generation.

For example, in 2021, California created the Emergency Load Reduction Program (ELRP), the first energy demand response program to allow behind-the-meter batteries and electric vehicles send power back to the grid.⁵ In order to take full advantage of programs such as ELRP, intermittent renewable energy sources and alternative storage technologies should also be incorporated into upstream planning systems. However, certain classical solutions scale exponentially with the size of combinatorial problems such as this one and can guickly meet their limits as more variables and constraints are added. The scalability that gubits afford may mean that guantum computers can find better and/or faster solutions.

The next steps in this area could be explored in two phases: first, a proof of principle of the core algorithmic solution to the unit commitment problem, followed by a longer implementation phase during which necessary features to take the solution to

Energy Market Optimization

To advance this concept beyond the idea a sample set of skills and rough timeline are shown here.

This multiphase effort could be categorized as "Research then Development".

Phase 1 - Proof of Principle (core algorithmic solution to unit commitment problem of linear DC approximation with discrete variables)







production are developed, such as time-expanded models, data ingestion, post processing, and possibly quantum-enhanced machine learning methods for forecasting. The proof of principle phase focuses initially on a linear DC approximation model with discrete variables but may be expanded to other versions of the unit commitment problem, such as AC equations, depending on the discovered value.

This use case impacts several personas across the energy supply chain, including energy traders, grid

operators and consumers. The success of this use case can be measured by runtime improvements or solution quality improvements. The authors of this concept noted that even an improvement on the order of just 1 percent could save hundreds of millions of dollars annually.

Additional quantum relevant concepts within Energy Market Optimization include distributed AC/DC power flow optimization, stochastic power grid analytics, and decentralized marketing clearing.



Integrated Planning and Optimization for Reliable and Resilient Grid

This use case is about integrating the many optimization calculations that happen up, down and across the power supply chain. From generation to consumption, the use of all types of resources must be optimized to minimize costs and maximize profits while providing reliable service. Maintenance schedules, load distribution, and storage options are all examples of optimization problems that affect the reliability and resiliency of the grid. Integrating these problems into a holistic planning system would help ensure resource adequacy against stressors and enable grids to evolve to efficiently deliver electricity to future generations. An economic optimization problem that includes production cost is necessary to plan future power grids. These are typically performed by either holding lines or generation sources constant and varying other grid infrastructure. Co-optimization would be more beneficial to yield a more resilient and reliable power grid while saving costs. In the economic optimization problem, constraints at different timescales need to be considered. The timescales may range from sub-microseconds to hours as more power electronics are integrated in the power grid. Optimal placement and options of distributed energy resources (DERs) and switches, network





reconfiguration and switching control, as well as power system restoration optimization can also increase resilience.

As more distributed energy resources are built, and bi-directional power flow increases, holistic transmission-distribution planning will be more important than ever. This concept includes multi-physical scale modeling (in addition to the multiple timescale modeling) to encompass requirements for large transmission networks to plants as well as individual houses.

Integrated optimizations like the one just described have been demonstrated on quantum computers for other industries. For example, the different stages of a manufacturing supply chain—from sourcing to consumer distribution—have been modeled for and run on a quantum computer. Furthermore, the biggest port in the United States, the Port of Los Angeles, deployed, an optimization engine powered by artificial intelligence and quantum technology from D-Wave systems in June 2020. The company reported that the engine "doubled cargo handling equipment productivity and produced more predictable cargo flows."⁶

Energy supply chain enhancements have the potential to drive major cost savings and more efficient integration of renewable energy sources. Integrated planning and optimization could inform the decisions of planners (such as transmission planners and reliability coordinators) and policy makers. The success of this use case can be measured by economic improvements and enhanced reliability and resilience of the grid.



Quantum Chemistry Simulation for New Materials

A wildly anticipated use case across all the experts was using quantum simulation methods to explore new materials. It was discussed in all but one group and was the subject of two concept cards. At the root of this idea is the fact that materials science depends on our understanding of the fundamental building blocks of the natural world, like atoms and molecules. The behaviors of these particles follow the laws of quantum mechanics, making quantum computers an ideal medium to analyze them.

This concept is material to the evolution of the electric grid. For example, as electric vehicles

become more popular, larger and more efficient batteries will be necessary. For example, the lithium-ion batteries in current electric vehicles do not have enough capacity to enable the same range as traditional combustion engines, thus limiting the use of electric vehicles.⁷

Quantum computing has the potential to accelerate research into alternatives to the lithium-ion battery. Specifically, quantum computers have been used to simulate the four molecules that are relevant to lithium sulfur, a top contender for next-generation battery technology.²





Increasing pressure to ease reliance on fossil fuels in favor of renewable energy necessitates other types of new materials as well. Despite the promise of photovoltaics for the conversion of sunlight into electricity with up to 86 percent efficiency, modern solar cells typically achieve around 20 percent efficiency.^{8,9} Quantum computing may be used to analyze the crystalline structures that underlie photovoltaics to "computationally explore the landscape of useful chemistries."¹⁰ Perovskite photovoltaics, multi-junction cells, hot-carrier solar cells, intermediate band solar cells and multiple exciton generation are also potential areas of research with quantum considerations.¹⁰

Using quantum chemistry for the simulation of new materials could impact several stages of the energy value chain, from generation to consumer, and on both large and small scales. It could lead to not only cost savings through increased efficiency, but also accelerate the transition to clean energy and diminish the impacts of climate change.



Examples of Applicability for the Top Concepts Across the United States



1	Washington relies primarily on hydro electric power and in times of drought can leverage energy market optimization	5	After the 2021 Freeze-Out Texas are increasing residential solar installations meaning integrated planning optimization will be needed
2	California passed a plan to pay consumers to discharge their EVs back to the grid, further increasing the complexity of unit commitment optimizations ²	6	Crucial for a resilient grid, Illinois plays a key roll in the energy supply chain as a key hub (road, rail, waterways) for moving crude oil and natural gas, producing feedstock for ethanol and biodiesel, and has chemical facilities for uranium conversions
3	Wyoming produces 13 more times energy than it consumes and exports raw materials for generation (coal, natural gas, uranium), both factors play into national resilience	7	Control room of PJM, where a change in the optimization method used to allocate generation units to energy demand led to 10 s of millions of dollars in savings annually for the 65M customers in the mid-Atlantic region ¹

8

Quantum computers can simulate molecules for exploration of new solar cell technology - for every 1% increase in efficiency at the Agua Caliente Solar Project in Nevada, 1000 more average homes can be powered³

4

Data collected from sensors and PMUs, like the large cluster in New England, may be able to be used to predict faults before they happen



Conclusion

The data shows that there are opportunities to improve the quantum industry's understanding of the impact it could have on the electric sector. Additionally, there are opportunities to increase awareness within the electric sector on the feasibility of quantum systems in the short and long term. Further engagement between the quantum and energy communities, including through consortia like QED-C, could provide useful cross pollination.

Four key use cases could be used as starting points for further research to apply quantum computing and analytics, inform algorithm development and applications of quantum algorithms and/or quantum computers. These top use cases were distributed across quantum optimization, machine learning, and simulation which shows utility and versatility of quantum computers in the electric sector. While timelines for studying the top four use cases have been created, there is opportunity to explore additional ideas and create projections for when quantum computing would be practical for those topics as well. There is a bright future for quantum and energy.

Together, this cross-industry collaboration can continue working toward a stronger, more resilient, and reliable North American energy system while maintaining energy independence.



Works Cited

1 Rigetti enhances predictive weather modeling with quantum machine learning. (2021, December 1). HPC Wire. https://www.hpcwire.com/off-the-wire/ rigetti-enhances-predictive-weather-modeling-withquantum-machine-learning/

2 Rice, J., Gujarati, T., Motta, M., Takeshita, T., Lee, E., Latone, J., & Garcia, J. (2021, April 7). Quantum computation of dominant products in lithium–sulfur batteries. The Journal of Chemical Physics, 154, 134115. https://aip.scitation.org/ doi/10.1063/5.0044068

3 Taft, J. (2017, September). Fault intelligence: distribution grid fault detection and classification. U.S. Department of Energy: https://gridarchitecture. pnnl.gov/media/white-papers/FaultIntelligence_ PNNL.pdf

4 Ajagekar, A., and You, F. (n.d.). Quantum computing assisted deep learning for fault detection and diagnosis in industrial process systems. https://arxiv. org/pdf/2003.00264.pdf

5 St. John, J. (2021, March 10). California's latest demand-side emergency plan draws criticism from providers. Green Tech Media: https://www. greentechmedia.com/articles/read/californiaslatest-demand-side-emergency-plan-takes-heatfrom-providers 6 Quantum computing application sees real world success at pier 300 at The Port of Los Angeles. (2022, January 5). PR Newswire: https://www.prnewswire. com/news-releases/quantum-computingapplication-sees-real-world-success-at-pier-300-atthe-port-of-los-angeles-301455106.html

7 Benveniste, G., Rallo, H., Canals Casals, L., Merino, A., and Amante, B. (n.d.). Comparison of the state of lithium-sulphur and lithium-ion batteries applied to electromobility. ScienceDirect: https:// www.sciencedirect.com/science/article/pii/ S0301479718308776#

8 Svarc, Jason. (2022, March 22). Most efficient solar panels 2022. Clean Energy Reviews: https://www. cleanenergyreviews.info/blog/most-efficient-solarpanels

g Photovoltaic research. (n.d.). Imperial College London: https://www.imperial.ac.uk/quantumphotovoltaics/research/

10 Giani, A. (2021). Quantum computing opportunities in renewable energy. Nature Computational Science: 1, 90–91. https://www.nature.com/articles/s43588-021-00032-z



Acknowledgments

The following individuals are acknowledged for their generous contributions to this report and their participation in the workshop that informed it. We greatly appreciate their time and critical thinking. Please note that the contents of this report do not necessarily reflect the views of specific institutions. Additionally, the views of participating federal officials do not necessarily reflect positions or policies of the federal government or its agencies.

Utility / Energy

Bonneville Power Administration (BPA)

Cindy Polsky ComEd, Honghao Zheng EPB Jim Glass Exelon Chris Moyer GE Annarita Giani GreenMountain Power Stephanie Ross Tennessee Valley Authority (TVA) Tom Butler

National Laboratories

Argonne National Laboratory (ANL) Kumarsinh Jhala Alinson Xavier Brookhaven National Laboratory (BNL) Meng Yue Peng Zhang Fermilab (FNAL) Adam Lyon Los Alamos National Lab (LANL) Carleton Coffrin Lawrence Berkeley National Laboratory (LBNL) Bert de Jong Lawrence Livermore National Laboratory (LLNL) Ignacio Aravena Jean-Paul Watson National Renewable Energy Laboratory (NREL) Peter Graf Eric Jones Oak Ridge National Laboratory (ORNL) Suman Debnath Pacific Northwest National Laboratory (PNNL) Yousu Chen Henry Huang Kevin Schneider Sandia National Laboratories (SNL) Ojas Parekh

Quantum

AccentureCarl Dukatz
Rajiv MistryAWSSebastian HassingerD-WavePeguy Pierre-LouisIBMJoe Broz and Nicolas Robles

IonQSonika JohriMicrosoftAlex BocharovNVIDIAJin-Sung KimQuantumTom LubinskiCircuitsMichal Stechly

Additionally, the event was open to a broader set of 'observers' including QED-C Members and government agencies. Observers had the opportunity to participate in limited activities after idea generation was complete.

Planning and Facilitation

The following individuals were invaluable in organizing the workshop and preparing this report.

QED-C - Quantum Computing

QED-C

Celia Merzbacher Jonathan Felbinger Krystal Bouverot Mary Scott Barbara Heydorn

Department of Energy

Rima Oueid Alireza Ghassemian **Use Case TAC Members** Mark Danchak, Aspirant Ventures (Use Cases Chair) Carl Dukatz, Accenture (Use Cases Compute Chair) Santanu Basu, Corning Terry Cronin, Toshiba Jon Felbinger, SRI Jim Gable, Anametric Paul Gleichauf, ARM Kevin Glynn, Northwestern Suresh Nair, Ina Solutions Rima Oueid, DOE Joanna Peters, StratConGlobal Keeper Sharkey, Odestar Damian Watkins, Aperio Global Ellen Winsor, EMW Consulting

Accenture | Accenture Federal Services

> Carl Dukatz Nathan Shetterley Julianna Harwood Kung-Chuan Hsu Anita Puri Mimi Whitehouse Nicole Varela Sarah Krisher Sarah Hewson Kathryn Wayman











Supplementary Information: Workshop Goals and Methodology

Workshop Goals

- Identify ways quantum computing and analytics can help address the electric sector's most pressing problems today and into the future, including currently intractable problems that classical computing has not been able to address effectively
- Help inform quantum algorithm development by gaining insights from energy applied mathematics and optimization experts (e.g., combinatorial optimization to serve as a bridge to quantum algorithms)
- Inform development or application of quantum algorithms and/or quantum computers (including near term quantum computers such as quantum gate model and annealers)

Collaboration and Workshop Structure

The workshop was designed to create the maximum number of collaboration opportunities between attendees with knowledge of the electric sector and attendees familiar with quantum technologies. With up to five slots available for each brainstorming group, the workshop encouraged interaction between participants with energy expertise and participants with quantum expertise. Facilitators and attendees from the quantum sector were briefed on the workshop several days before the event took place to ensure smooth operations. Participants from the electric sector did not receive a detailed briefing to encourage fresh thinking and new ideas.

As shown in the illustration below, each group included a facilitator, who acted as a note taker and timekeeper, along with participants representing different sectors. Each group was configured to include members that could answer questions pertaining to quantum and energy. It was important that the groups be self sufficient finding answers quickly to their own questions so that they could complete all of the exercises.



Value Chain Matrix

The primary tool to guide conversations during the ideation session was the Electricity Industry Value Chain – Matrix:

Categories of Quantum Approaches	A. Customer Load/Energy Asset Owner • Identification and prioritization of primary bidirectional assets (bidirectional EVs, storage, PV, microgrid) • Dc power transformed to AC power via invertors • Efficiency factor assessment and improvement	B. Aggregator/Service Provider • Connect generation plant to power grid • Rely on transformers • Increase voltage to transmission network levels • Monitor flow of electricity, monitor reactive power flow, reactive power compensation, improve power factors	 C. Distribution Realtime voltage and frequency control across home, buildings, and energy resources Radial Distribution Networks Distributed control Dynamics and stability Large scale coordination Events and outages 	 D. Transmission Occur over one of four power grids (interconnections) that make up North America's power system Supply at average current of 60 Hertz Generation facilities dictate power dispatched to grid based on demand predictions Use Base-Loading and Peaking power plants to manage demand 	 E. Generation Identification of primary fuel and supply chain of resource as a result of two-way flow network (coal, gas, nuclear, hydro, wind) Mechanical power transformed to electrical power through generator Efficiency factor (usually thermal but can be other) assessment and improvement
Optimization					
Machine Learning					
Simulation					
Operatio	ns and Markets: Other acti	vities which enable the val	ue chain to run efficiently		

The columns at the top of the matrix describe stages of the electricity supply chain: customer load/ energy asset owner, aggregator/service provider, distribution, transmission and generation. This organizational structure provided participants with starting points to think of specific use cases that could benefit from quantum computing. The pieces of the value chain were not meant to be thought of as independent of each other. Attendees were also encouraged to think about how the five categories interact and which processes and operations touch multiple parts of the value chain.

The value chain was intended to be thought of as bi-directional, rather than a one-way flow from generation to end customer. As Rima Oueid, Commercialization Executive with the U.S Department of Energy's Office of Technology Transitions, stated in her opening remarks, "The grid is becoming a two-way flow electric and data network." This bi-directional flow is realized through the evolution of smart grids, which are electricity networks enabled with sensors and digital communication technologies that allow grid operators to monitor usage and network health while ensuring the grid's stable operation. This increasingly complex grid system has ushered in a need for more advanced technologies, such as quantum and edge computing. Participants were prompted to think of the emerging Internet of Things (IoT) and requirements for the future grid, and not just solve for pain points in today's electric grid.

The left side of the matrix shows categories of quantum approaches, including optimization, machine learning and simulation.



Workshop Process

The workshop was designed to create as many ideas as possible up front, methodically select ideas that the participants thought would be the most important, and then develop the remaining ideas into meaningful and actionable concepts. This process yielded three content pieces: Ideas, Concept Cards based on the ideas, and Concept Posters built from the concept cards.

Idea Generation and Analysis

Workshop participants were placed into groups to complete a 45-minute ideation session. For the first step, each participant generated ideas in a 15-minute individual brainstorm and placed their ideas onto the Value Chain – Matrix. The groups then took 25 minutes to discuss their ideas, and finally five minutes to vote for the ideas they thought had the most potential.

The workshop groups came up with a total of 258 ideas. Of these, several were duplicates, resulting in 221 unique ideas (see supplemental information). As depicted in Chart 1, optimization was the most popular problem type, accounting for 42% of ideas, followed by machine learning (29%) and simulation (28%). As can be seen in Chart 2, transmission was the most popular part of the energy value chain, accounting for 28% of ideas, followed by distribution (24%), generation (19%), aggregator (11%) and customer (13%).

The most common idea was using quantum simulation techniques to discover new battery technologies. The biggest clusters of ideas included materials discovery, load modeling and management and fault/outage detection and analysis.



Chart 1: Ideas by Problem Type

Chart 2: Ideas by Position in the Value Chain



Concept Cards

Each group selected the ideas that had the most votes and created a "Concept Card" for each idea. As depicted in the figure below, these Concept Cards included the name of the concept, the type of idea (optimization, simulation, or machine learning), the quantum technology best suited to execute the idea (gate, annealing, quantum inspired or other), a description of the concept and the pain points for the concept addressed. The groups had 15 minutes to fill out the Concept Cards. Most groups ended up with between one and three cards that they then presented to the whole workshop audience.

As shown in Table 1, 18 ideas were selected to be expanded into concept cards (between one and three for each group). Optimization was again the most popular problem domain, followed by machine learning and simulation. The top idea clusters (new materials discovery, load modeling and management and fault/outage detection and analysis) were all represented in one or more Concept Cards.

Some idea clusters did not become Concept Cards. For example, several ideation groups explored how quantum computing could be used to enable electric vehicles (EV) to interact with the grid. Specific ideas included optimizing where EV charging stations are located and installing bi-directional chargers so car batteries could increase grid resiliency. However, none of these ideas were chosen to be expanded into a Concept Card. Similarly, several groups explored optimizing the placement of resources, such as phasor measurement units and other sensors, and analyzing and predicting cascading failures through machine learning and simulation; however, no Concept Cards were created around these ideas either.

Voting

Seventeen of the Concept Cards were rated based on impact and feasibility. One Concept Card, Distributed, Decentralized and Emergent Computing, was



mislabeled during the workshop and inadvertently excluded from the rating process.

It is important to note that although all attendees voted on a scale of 1 to 10, the levels of each dimension were not universally defined, and each attendee used their own relative scale. For example, some attendees reported that they scored feasibility by how quickly quantum hardware would reach the level of maturity needed to run the use case, while others thought of feasibility in terms of which use cases are best to research and test on today's devices.

This empowered the attendees with new flexibility to expand or limit the scope of the original concept based on what they thought was possible to accomplish given a scope and timeframe they set based on the required fields in the Concept Poster.



This resulted in changes to the concepts names and attributes in several ways. The details of the Concept Posters in this report were further expanded after performing a series of post-workshop interviews with attendees. In addition, after the workshop, a fourth use case was developed on Quantum Chemistry Simulation for New Materials. This topic played a critical role in conversation throughout the event and in post-workshop interviews.

Concept Poster

After further discussing the feasibility and impact of the Concept Cards, the workshop attendees agreed to focus on three top concepts to develop into "Concept Posters." Attendees were instructed to use the original Concept Card as a basis for the Concept Poster. As shown in the following chart, the Concept Posters included a description of the concept, how it works, the problem space it occupies, key features, types of personas the concept will affect (consumers, grid operators, policy makers, etc.), and key metrics and outcomes to measure success. The Concept Posters also included a Collaboration Plan, which identified potential team members and suggested a timeline to complete the project.

Conclusion

The workshop enabled experts in energy and quantum computing to share perspectives, generate ideas and explore use cases that could benefit from near-term quantum computers and quantum algorithms. Attendees also investigated applications that could demonstrate the efficacy of near-term quantum technologies, as well as ways to accelerate answers to intractable problems and help optimize the evolving energy grid. The 221 unique ideas (see supplemental information) generated show the potential for a vast number for industry and government projects and collaborations.

		Cor	ncept	Post	er &	Coll	abo	orati	on	Pla	n	
Concep	ot Name					Descri	ption					
Person	la											
How it	works					Featu	res					
Proble	m Space					Succes	ss metr	rics/outo	omes			
Team M	Mathe-	Physics	Scientific	Modeling	CADD	Comp	Chamis	. Interf	ace	Data	Backend	ML
Project Sponsor	Project Lead	Theorist Business Specialist	Q Algos Designer	& Sim Quantum Developer	IT Architect	Chem	Green	Develo	oper 1	Scientist	Developer	Specialist
Timeline	e:											et al al
Ress	aarch	Start	-	-	-	-		-	-	-	-	Finish
So	lve			-	-	-				+		
Dev	elop											

Supplementary Information: Quantum Computing Use Cases in the Electric Sector

This table list each idea identified as an opportunity space to explore the use of quantum computing in the energy sector.

All Unique Ideas (Total 221):



Accurate weather forecasting for Derecho Storm					•				
Data completion (real-time, static assets)		•			•				
Fault detection			•			•			
Fault identification		•			•				
Wildfire detection using line fault type		•			•	•			
Extreme event preparation	•					•			
Network reconfiguration and switching control	•					•			
Optimization of outage recovery/response to failure	•					•			



Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Vulnerability analysis / characterization of extreme events		•					•					
Quantum approaches for simulating transmission networks (i.e., Quantum walks)			•				•					
Single phase AC power flow			•				•					
Three phase phase AC power flow			•				•					
AC optimal power flow												
Security constrained optimal power flow	•						•					
Quantum state estimation for distribution grids			•		•							
Single phase state estimation	•						•					
State estimation							•					
Materials discovery			•					•				
Simulation of superconducting materials for transmission			•					•				
Chemistry simulation for new materials for PV panels, batteries			•					•				
Battery and load modeling for efficient storage			•			•						
Better materials for energy production (solar panels, alloys for wind, etc.)			•					•				
Battery and storage improvement			•	•								
Better materials for transformers?			•		•							

Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Simulation of novel fuel materials/catalysts			•					•				
Optimization problem to minimize power losses		•				•						
Outage forecasting						•						
Outage prediction			•			•						
Outage prediction AI/ML modeling		•			•							
Outage/failure prediction based off of network/sensor data						•						
Simulation of outages and failure propagation		•				•						
Resource adequacy planning												
Resource availability modeling			•					•				
Anomaly localization		•				•	•					
Quantum methods for anomaly detection		•			•							
Demand forecasting		•					•					
Demand modeling			•									
Learn to predict demand from historical data and current trends	•					•						
Quantum methods for short and long term forecasting of energy demand	•											
Improving machine maintenance and generator resilience via identification of clusters of weak-links	•							•				



Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Maintenance scheduling	•							•				
Predictive analytics on device failure at very granular level to optimize maintenance and replacement			•			•						
Predictive maintenance			•				•					
Power restoration	•						•					
Power system restoration optimization (large scale coordination for events and outages) 1) Patroller dispatch 2) Construction crew dispatch 3) Vehicle routing (EV as well)	•					•						
PMU based data analytics												
Prediction (consistency of predictions with observations)												
Inverter-based resources simulations)			•					•				
Optimal power flow	•						•					
Forecast of consumption patterns integrated with weather forecast		•			•							
Model precision connecting weather forecast with demand and optimizing			•			•						
Customer behavior preferences												
Maximize customer preferences	•											
Cascade failure analysis		•					•					
Cascading failure analysis												

Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Capacity expansion planning	•						•	•				
Capacity planning	•											
Generation expansion planning	•							•				
Contingency ranking and screening	•	•					•					
Corrective action designs for contingencies	•	•					•					
Contingency screening		•				•						
N-2, N-3 contingency analysis							•					
Bi-directional EVs												
Bidirectional power distribution optimization between EVs and charging station and power plant	•			•								
EV or smart device optimization (when, how much battery used) HVAC optimal usage policy control	•			•								
EV stations (optimization)	•				•							
EV: forecast impact by location												
Dynamic simulation and modeling			•	•		•	•	•				
Dynamic simulation and stability analysis			•				•					
Load forecasting & DER					•							
Load modeling		•					•					
Load modeling and aggregate response of populations												



Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Optimization of load distribution	•						•					
Residential load management/control	•			•								
DER placement	•					•						
Observability - (e.g., sensor placement)	•	•			•	•						
Optimal phasor measurement unit placement	•					•						
Optimization of resources and design	•											
Optimize automated recloser placement	•					•						
Optimizing placement of the equipment	•			•								
Sensor placement	•					•	•					
Multi-period unit commitment	•											
Quantum algorithm for unit commitment problem		•				•						
Sub-hourly unit commitment and optimal power flow	•											
Security constrained unit commitment and economic dispatch	•						•					
Unit commitment and economic dispatch	•											
Unit commitment with quadratic cost/objective	•							•				
Unit commitment problems with non-linear cost/objective function								•				
Agent-based computation and coordination												

Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Aggregator participation in electricity markets									•			
Analysis of historical data												
Asset investment	•			•								
Autonomous drone inspections: Al: image processing, sensor fusion	•				•							
Biding	•			•								
Building electricity/HVAC control via quantum binary neural networks												
Business Recommendation Engine		•			•							
Capacity expansion			•		•							
Chaos engineering - removal of components (transformers, grids etc)		•		•								
Co-optimization with other infrastructures	•											
Combined cycle generator modeling	•							•				
Communications and differential privacy			•			•						
Condition assessment		•						•				
Condition assessment (lots of data!)		•					•					
Optimal control of distributed resources												
Control of distributed devices based on local parameters		•		•								



Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Control of distributed devices in a mixed	•			•								
Controls of distributed devices based on system characteristics		•				•						
Coordinated control of millions of devices	•						•					
Coordinated transmission and distribution planning	•					•						
Estimating customer participation in transactive control schemes	•		•									
Correlated forecast updates for renewables		•	•		•	•						
Cross-cut across optimization, machine learning, simulations: operations (stability analysis combined with energy optimization)												
Crosscotting activities - (L/C-D-T-G)									•			
Day-ahead market	•							•				
Decentralized ACOPF	•					•						
Decentralized market clearing optimization									•			
Decentralized optimization and emergent computation							•	•				
Decentralized, scalable, and immediate communication and computation	•					•						
Degradation modeling								•				
Demand management												

Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Determination of ideal conditions for burning fuels			•					•				
Determine optimal distribution efficiency over available lines	•				•							
Discrete choices with nonlinear AC physics	•					•						
Disruption monitoring in electrical grid		•					•					
Distributed intelligence optimized edge control of DERs		•			•							
Distribution optimization in grid energy storage system	•					•						
Distribution system restoration						•						
Dynamic security analysis			•				•					
Efficient coordination of non-power utility energy sources	•			•								
Either totally new equipment or adding new equipment to existing networks	•			•								
Either you need miniaturized QC for edge, or quantum networks to connect QC resources to the edge	•			•								
Energy disaggregation		•			•							
EV as energy storage availability forecasting												
EV usage forecasting		•			•							
Forecasting		•			•							
Frequency/voltage/rotor angle simulation												



Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Generation bidding strategy												
Grover's algo			•				•					
Hamiltonian simulation methods for finding stable energy transmission profiles		•				•						
Having localized quantum computing to minimize scope		•			•							
Heat exchanger network synthesis	•							•				
Hierarchical coordinated control of G-T-D-C									•			
Hydropower plant optimization	•							•				
Identification of better fuels			•					•				
Identify sampling problems, amenable to quantum approaches	•							•				
Impact of peer-to-peer energy trading on distribution network			•		•							
Impact of weather changes on load curves			•	•								
Integrated planning - G-T-D-C									•			
Inter-dependency of various energy -related systems (grid, gas, communications, water, weather,)							•					
Interacting agents coordinating (emergent computation)			•	•								
Interdiction / N-K optimization for risk mitigation	•						•					
Island mode-compatible microgrid topology re-optimization	•											

Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Large-scale dynamics simulations												
Learn from weather and other real-time info to efficiently balance generation of renewable vs fossil	•	•										
Learn optimal producer-> consumer distribution profile by time of day and day of week	•			•								
Load curve analysis over time												
Machine learning methods for selecting parameters of the power grids	•					•						
Machine learning on distributed assets behavior to refine load shaping	•		•									
Market structures and variations in participation	•						•					
Markets *are* optimization	•						•	•				
Minimize carbon footprint								•				
Minimizing tap changes for LTC when performing volt-var optimization	•					•						
Modeling CO ₂ phase adsorption for removing greenhouse gas			•					•				
Modeling superconductors for transmission			•				•					
Multi-phase state estimation	•					•						
Network reconfiguration	•					•						
Networked microgrid coordination	•					•						



Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Not sure how dynamics and stability can be solved by QC		•				•						
Nuclear generation: develop models to reduce risk and better manage cost of construction	•					•						
Optimal dynamic grid configuration preparing for Derecho Storm hit	•					•						
Optimal planning to ensure resource adequacy facing compound stressors (weather, wildfires,)	•							•				
Optimizing power generation from renewables	•							•				
Optimization of design for complex generators (tokamaks, stellarators, wind-powered)	•							•				
Optimization of location and number of conversion and distribution centrals	•				•							
Optimization of the internal workings of a power plant	•							•				
Optimization under uncertainty?	•							•				
Optimization use cases related to the supply chain?	•							•				
Optimization with significant number of contingency scenarios		•					•					
Optimize utilization efficiency based on assessment of factors - how to optimize the effectiveness of load shedding	•			•								
Phase balancing	•					•						
Plant design - process systems engineering	•							•				

Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Power grid optimization to make grids cleaner and more efficient	•											
Power network optimization in terms of reliable power flow and ren energy integration	•						•					
Privacy preserving AI for private usage data or other sensitive data (differential privacy, homomorphic encryption, secure multi-party computation, etc.)									•			•
Prognostics-based O&M	•			•								
Prognostics-based O&M	•							•				
Prosumer (EV, PV owners) behavior modelling for transactive energy market participation	•		•									
PV hosting capacity analysis for planning			•			•						
Quantum distributed control for microgrids/DERs			•	•								
Quantum electromagnetic transients simulation			•			•	•					
Quantum error correction		•	•									
Quantum learning based transient stability assessment and security analysis	•					•						
Quantum probabilistic approaches (Quantum Monte Carlo methods) for transmission planning and operations	•				•							
Quantum reinforcement learning for controls	•						•					



Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Quantum sensing & internet for PMU, etc.									•	•	•	
Quantum-inspired optimization methods applied to optimization problems in distribution	•					•						
Related: represent scenarios as superposition of classical states	•					•						
Remedial action schemes/ wildfire response	•						•					
Renewable energy generation estimation		•										
Resources co-optimization												
Rolling blackout problem - predict with sparse data		•				•						
Scalable dynamics simulation			•									
Security and privacy												
Simulate dynamics of Distribution network to examine stability - if this can be done faster than classically to predict problems sooner	•			•								
Simulate unforeseen scenarios that may affect the grid, in order to explore effective ways to address these quickly	•		•									
Simulating enormous number of active edge devices in distribution		•										
Smart sampling-based machine learning		•						•				
Solar technology												

Idea 🍚	Optimization	Machine learning	Simulation	Customer	Aggregator	Distribution	Transmission	Generation	Other	Sensing	Communications	Security
Solutions of linear and												
non-linear differential equations associated with distribution of energy and voltages dynamics	•					•	•					
Stability assessment							•					
Stochastic energy pricing	•					•	•					
Stochastic optimization for control									•			
Stochastic power flow					•							
Stochastic simulation of stress test scenarios and catastrophic events		•										
Thermal and combustion efficiency modeling			•					•				
Three phase: phase AC optimal power flow						•						
Transmission distribution co-optimization	•					•	•					
Transmission topology optimization							•					
What is the right DER asset to implement at any given time based on demand	•											
System planning and operations	•					•						
Which assets are most reliable, resilient, responsive to demand signals. Which are slow or failing to respond	•			•								

