# QCE20 Workshop on Quantum Computing Opportunities in Renewable Energy

Organizers: Zach Eldredge (DOE), Annarita Giani (GE Research)

## Times are given in Mountain Time (MT, UTC-6)

### Session 1

**10:45-10:50 Welcome** Zach Eldredge (DOE), Annarita Giani (GE Research)

**10:50-11:20** Invited Talk

***Potential Quantum Computing needs across the Renewable Energy Sector***

Danielle Merfeld, Ph.D., VP and CTO GE Renewable

**Bio:** Dr Merfeld is the Chief Technology Officer of GE Renewable Energy. She leads technical efforts to develop differentiated products and services across the broadest renewable energy portfolio in the industry, which combines onshore and offshore wind, blades, hydro, storage, utility-scale solar, and grid solutions as well as hybrid renewables and digital services offerings. Danielle is the co-leader of the GE Women's Network.

Prior to her role at GE Renewable Energy, Danielle was the Vice President & General Manager at GE Global Research where she advanced disruptive technology platforms across the industrial sector. As a thought leader in the industry, Danielle has delivered remarks and participated on panels at conferences and symposiums on topics like digital platforms, advanced controls, the energy transformation, the future of renewable energy, grid challenges and solutions, and microsystems.

Danielle received her B.S. degree in Electrical Engineering from the University of Notre Dame, and Ph.D. in Electrical Engineering from Northwestern University. She has authored or co-authored over 70 papers in refereed technical journals and has given presentations at conferences and symposiums around the world. Danielle is a member of several technical associations and on the Board of Trustees at the University of Notre Dame. She also is on the board of Advanced Energy Economy, an organization of businesses working to make energy secure, clean, and affordable.

**11:20-11:50** Invited Talk

***Computing Advancements for Renewable Energy Integration – will there be a quantum leap?***

Zhenyu (Henry) Huang, Ph.D., P.E., F. IEEE Laboratory Fellow, PNNL; Research Professor, Washington State University

**Bio:** Dr. Zhenyu (Henry) Huang is Laboratory Fellow at Pacific Northwest National Laboratory (PNNL), Richland, WA, USA, and Research Professor at Washington State University, Pullman, WA, USA. He just completed an assignment as Technical Advisor at the US DOE EERE Solar Energy Technologies Office (SETO). His research focuses on developing and adapting latest math, computing, and data analytical techniques to understand and manage the emerging complexity in the power grid and other associated infrastructures.

Dr. Huang has over 190 peer-reviewed publications in the areas of high performance computing, power system modeling and simulation, and optimization and control for power and energy systems. He is a Fellow of IEEE and is active in several IEEE Power and Energy Society (PES) technical committees, including officer roles at committee, subcommittee, and working group levels. He is recipient of the 2008 PNNL Ronald L. Brodzinski's Award for Early Career Exceptional Achievement and the 2009 IEEE Power and Energy Society Outstanding Young Engineer Award. Dr. Huang is a registered Professional Engineer in Washington State. Dr. Huang received his B. Eng. from Huazhong University of Science and Technology, Wuhan, China, and Ph.D. degree from Tsinghua University, Beijing, China.

**11:50-12:15 Quantum Computing Opportunities for Renewable Energy**, Zach Eldredge (DOE), Annarita Giani (GE Research)

**12:15-13:00 Break**

## Session 2

**13:00-13:15** ***Quantum Computing of Aluminium Fumarate as a Model for CO2 Capture by Metal Organic Frameworks***, Gabriel Greene-Diniz, David Zsolt Manrique, David Muñoz Ramo, Cambridge Quantum Computing, Elvira Shishenina, Philip Llewellyn, Total SA

**Abstract:** At present noisy Intermediate-Scale Quantum (NISQ) technology is limited to relatively small numbers of qubits, low circuit depths and noisy measurement results. For realistic applications, quantum simulations may require several orders of magnitude more qubits and larger circuit depths to provide useful predictions. This reflects the scaling problem of simulations on quantum computers. On the other hand, quantum computation possesses the ability to capture complex chemical properties, possibly to unprecedented accuracies. Hence if the scaling problem can be overcome, there is the potential for large impact in the area of renewable energy. Due to their hydrothermal stability and comparatively easy synthesis, Aluminium based Metal–organic frameworks (Al-MOFs) have received considerable attention as candidates for CO2 capture by adsorption. Accurate characterisation of the electronic and geometric characteristics of adsorption reactions, in particular the local metal-cluster chemistry on the Al-MOF surface, is crucial for further development of this technology. To this end, we implement density matrix embedding theory (DMET) to perform fragmented quantum computations of the Al fumarate molecule. Our calculations, which utilise UCCSD and hardware efficient ansätze, show that energies of carbon-based fragments are calculated to high accuracy relative to FCI-based DMET calculations. Given the significant reduction in the number of qubits and circuit depth of the DMET fragments relative to calculations involving the entire molecule, this work demonstrates an integrated framework of classical and NISQ computer simulations of molecules relevant to applications such as CO2 capture by MOFs.

**Keywords:** CO2 capture, MOF, DMET, VQE, UCCSD, hardware efficient ansatz

**13:15-13:30** ***Quantum Machine Learning for Predictive Analytics*** Himanshu Thapliyal, **Univ. Kentucky**

**Abstract:** Data from smart home can be used with analytic applications for visualizing and predicting energy usage, benchmarking buildings, validating energy savings and supporting green building certifications, etc. Further, in case of emergency they can be used to send alerts and communicate with smart equipment including thermostats, water heaters and the power grid. Data analytics of smart homes can help in managing electricity demand by: (i) effective integration of new energy sources onto the grid. and (ii) enabling homeowners to keep a track of their energy usage. In this talk, we will discuss possible application of quantum machine learning for predictive analytics of energy usage from smart home. Quantum Machine Learning (QML) is an emerging field of research that uses quantum computers for implementing machine learning algorithms. QML uses both classical and quantum processing to increase speed and performance.

**Keywords:** Quantum Machine Learning, Predictive Analytics, Energy Usage

**13:30-13:45** ***Simulating organic semiconductors on a noisy quantum computer: What model Hamiltonians can do for you***, Eric Jones, **NREL**

**Abstract:** Quantum simulation of quantum mechanical systems is thought to be one of the most important applications of eventual fully error-corrected quantum computers. Meanwhile, understanding the detailed dynamics of highly entangled triplet pair states in organic semiconductors could lead to the design of materials important for both solar energy harvesting beyond the Shockley-Queisser limit and high-temperature quantum information processing. Due to the small numbers of qubits and large error rates that characterize noisy intermediate-scale quantum (NISQ) computers, direct simulation of ab initio theories such as electronic structure remains largely out of reach for systems of interest. Instead, phenomenological model Hamiltonians provide for a hybrid computational framework wherein model parameters are calculated via classical computational methods (e.g. density functional theory) or experiment while model degrees of freedom are simulated on a NISQ processor. We propose an experiment that leverages this idea to determine the fate of chromophore triplet pairs in organic semiconductors, which display singlet fission. Frontier orbital spin degrees of freedom are mapped to qubit states and are unitarily evolved under a model Hamiltonian with exchange and zero-field splitting interactions. Such a model is scalable to larger numbers of chromophores and can incorporate additional physics such as dimerization and spin-orbit coupling. The fate of the triplet pair can be elucidated either by Trotterized time evolution or variational state preparation. We discuss how quantum simulation of this model might reveal design principles for either maximizing photo-dissociation or alternatively, stabilization of the quintet states thought to be useful for quantum information processing applications.

**Keywords:** Quantum simulation, Model Hamiltonian, Triplet Evolution, Organic Semiconductor

**13:45-14:00** ***Scalable demand response scheduling for renewable energy integration through Quantum Computing***, Javad Mohammadi, **CMU** and Mohsen Rahmani, **D-Wave System**

**Abstract:** It is expected that the electric grid of the future would differ from the current system by the increased integration of distributed generation, distributed storage, demand response and communications and sensing technologies. The consequence of this transition from the operational perspective is that overall, the flexibility in the grid increases; but this also means that more control decisions need to be made. This flexibility is vital not just for balancing the increased variability but also to be able to handle the uncertainty inherent to the non-dispatchable renewable generation resources. A key question that needs to be answered is how flexible resources (such as thermostatic loads) can be efficiently managed and scheduled to ensure a reliable operation of the electric power grid despite the increased challenges imposed on the supply side. The number and heterogeneity of these small-scale flexible resources results in a computationally complex scheduling problem. Quantum computing lend itself very well to address these complexities. Quantum computing's strength in handling binary variables offers a great tool to derive optimal on and off decisions to manage schedulable loads (e.g., electric water heaters, refrigeration system, air conditioning units) for balancing intermittency of renewable resources. In this talk we will present a class of load scheduling problems that can be casted in a form that fully leverages quantum computing's strength. We will also discuss how quantum computing can be integrated with widely used decomposition methods to address a variety of power system problems with binary and continuous variables.

**Keywords:** future electric grid, renewable integration, load scheduling, distributed energy resources

**14:00-14:15** ***Practical implementation of quantum optimization algorithms for wind farms design***, Marouane Salhi, **Qubits Engineering**

**Abstract:** Qubit Engineering is a quantum computing startup with a mission to optimize wind farm energy production by improving the turbine layout in a pre-construction phase and also by optimizing the dynamic control of the fleet of turbines during operations. While the Qubit Engineering team has a genuine interest in promoting renewable energy technology for a better future, the team is also a big advocate of the role quantum computing can play in solving important and practical problems within the industry. The choice of the wind farm design as a first application was the result of an investigation of the type of challenges that are faced by the industry which may benefit from today's quantum computing technology. This was the first step in the progress towards a practical implementation of quantum computing. The second step is to have a deep understanding of the specific problem chosen and plan for a mapping strategy of the problem into the quantum machine. The CEO and co-founder of Qubit Engineering will be joining the IEEE Quantum Week to share more about the two-year long journey in developing practical quantum optimization algorithms for the design of wind farms.

**Keywords:** renewable energy, wind farm layout optimization

**14:15-14:30** ***Designing Energy-Efficient Quantum Computers Through Prediction and Reduction of Cooling Requirements for Cryogenic Electronics***, Michael Martin, Caroline Hughes, Gilberto Moreno, Eric Jones, David Sickinger, Sreekant Narumanchi and Ray Grout, **NREL**

**Abstract**: Data center energy usage is a major contributor to global energy use, leading operators to put effort into both reducing data center energy consumption and using energy from renewable sources. Continuing these efforts in the quantum computing era will be complicated both by the changing technology, and the uncertainty in how widely quantum computers will be adopted. Modeling energy use in quantum computing is key to predicting and reducing energy use. Unlike their classical counterparts, quantum computers need to be maintained at temperatures near absolute zero, requiring energy-intensive cryogenic cooling. Therefore, as quantum computers scale up from existing 50 qubit systems to the 10,000 to 100,000 qubit systems required to solve complex problems, the energy consumption of both the electronics and cooling systems will also increase. To predict this scaling, this work analyzes the energy requirements for both computation and cooling of quantum hardware. We show that the energy requirements for cooling of quantum computers is determined by several computing system parameters, including the number and type of physical qubits, the operating temperature, the packaging efficiency of the system, and the split between circuits operating at cryogenic temperatures and those operating at room temperature. The energy requirements are found based on thermal system parameters such as cooling efficiency and cryostat heat transfer. Analysis of these parameters shows that the energy required for cooling is significantly larger than that required for computation, a reversal from conventional computing. The results and discussions provide a roadmap for creating energy efficient quantum data centers.

**Keywords:** energy efficiency, computer architecture, cryogenics

**14:30-15:15 Break**

## Session 3

**15:15-15:30** ***Quantum Computing for Mixed-Integer Linear Programming,*** Chin-Yao Chang, **NREL**

**Abstract**: Quantum computing (QC) emerges as a new computing resource that can be superior to conventional computing for certain class of optimization problems. However, QC can only solve unconstrained binary programming problem in principle, while in practical power system applications, mixed-integer linear programming (MILP) is of most interest. For example, planning of electric power infrastructures, control of on-load tap changer (OLTC) and static VAr compensator for voltage regulation with presence of renewable generation. We attempt to bridge the gap between capability of QC and the need for power systems by developing a new approach for MILP. The idea is decomposing the MILP into binary programming and linear programming problems, which are respectively solved by QC and conventional computing. We formalize the decomposition approach which ensures that with sufficient number of back-and-forth iterations, the algorithm can reach the optimal solution of the original MILP problem. The new algorithm is an attempt to take the best of the two worlds (QC and conventional computing) and we believe that it has great potential for various applications. The algorithm is tested on Amazon Web Services (AWS) and has shown effective for small-scaled examples. The algorithm still has many limitations and we will also cover those in the presentation.

**Keywords:** Mixed-integer programming, Benders decomposition

**15:30-15:45** ***The Quantum Approximation Optimization Algorithm Applied to the Unit Commitment Problem,*** Samantha Koretsky, Pranav Gokhale, Jonathan Baker, Madeline DeVoe, Fred Chong, **Univ. Chicago**, Olivia Del Guercio, Honghao Zheng, Niroj Gurung, **Commonwealth Edison**, Amin Khodaei, **Univ. Denver**

**Abstract**: The unit commitment (UC) problem is a vital optimization problem in the electrical power industry. It aims to minimize operational cost while meeting a given power load using a number of power-generating units that are subject to constraints. In the problem, the cost of each power unit is given by a quadratic polynomial dependent on the power it generates. However, individual units may be turned on or off, adding another layer of complexity. Classical optimizers, while frequently used to solve quadratic optimization problems, are not well equipped to solve the more complex UC problem.

Quantum machines provide novel approaches to this problem. In particular, the Quantum Approximation Optimization Algorithm (QAOA) was designed to approximate solutions to similar problems and can easily be adapted to the UC problem. We aim to solve the UC problem more efficiently than previous methods, and we develop a hybrid architecture that combines QAOA with classical methods to this end. Our technique uses QAOA to handle the discrete variables of the problem—the status of a unit being on or off—while using a classical optimizer to handle the continuous variables. The combination of classical and quantum algorithms both limits the number of gates used in the quantum computation, which limits noise and error in the quantum machine, and allows for a quantum advantage that classical computing alone cannot achieve. We expect our approach to be more efficient than classical methods in the 10-50 qubit range.

**Keywords:** quantum computing, quantum approximation optimization algorithm, smart grid optimization, unit commitment, hybrid architecture

**15:45-16:00** ***A Quantum Chance Constrained Binary Optimization (QCCBO) Algorithm***, Peter Graf and Eric Jones, **NREL**

**Abstract**: Many problems in renewable energy systems design and control involve stochastic optimization. Because the squared amplitudes of a quantum superposition state represent probabilities, classical probability distributions can be embedded as superpositions in a quantum computer. Here we present a quantum algorithm for solving so-called "chance constrained" binary optimization problems. Such problems have the form

min_x f(x)

s.t. P_xi[g(x,xi) == 0] < eps.

That is, we seek to minimize f(x) over binary strings x subject to a constraint g==0 that we allow to be violated, but only with small probability (i.e. small "chance" of violation). The random variable xi represents an exogenous input that we have to "plan for" in our choice of x. Our quantum algorithm consists of three parts. First, we "prepare the state" representing the probability distribution of xi. Next, we describe a quantum circuit that implements g(x,xi) (e.g., for g composed of CNOT gates) and how, when given x and the superposition xi as input, its output can be used to estimate P_xi[g(x,xi) == 0]. Finally, we discuss first steps of embedding this process into a QAOA-like optimization scheme. The intuition behind the potential benefit is that a probability over 2^n possible states is evaluated using unitary operators on only n qubits. This work represents a step toward solving on a quantum computer a class of stochastic optimization problems encountered frequently in energy systems design and control.

**Keywords:** quantum chance-constrained optimization, quantum binary optimization, quantum stochastic optimization

**16:00-16:40 Panel Discussion**

- Ceren Susut-Bennet, DOE
- Laurent White, ExxonMobil (Dual Energy Challenge)
- Witold Kowalczyk, Zapata Computing (Sustainability)
- Karl Thibault, Q4Climate Initiative

Presentations - 20 mins
Discussion - 10 mins
Questions from audience - 10 mins

**16:40-16:45** ***Final remarks, next steps***, Zach Eldredge (DOE), Annarita Giani (GE Research)