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RESEARCH PAPER

# *Application Overview of Quantum Computing for Gas Turbine Design and Optimization*

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## *Abstract*

Conceptual designs require optimization methods to identify the best fit in the system. The article investigates the application of quantum computation in gas turbine design and simulation problems with current technologies, approaches and potential capabilities. Quantum optimization algorithms and quantum annealers help in predicting overall efficiency and optimizing various operating parameters of the gas turbine. A comparison of both classical and quantum computers has been discussed briefly. The classical model challenges are mitigated with the use of quantum computation. A novel hybrid model for simulating gas turbines has been proposed, which consists of a combination of both physics and machine learning to eliminate few of the critical problems faced. This review elaborates application of quantum computing based machine learning for design and optimization of a gas turbine. The overall states of the gas paths of gas turbines could be analyzed using the quantum computing model in the future.

*Keywords:* machine learning, quantum computing, optimization, thermodynamic analysis

*Citation*
Aurthur Vimalachandran Thomas Jayachandran (2022), Application Overview of Quantum Computing for Gas Turbine Design and Optimization. *AI, Computer Science and Robotics Technology* 2022(0), 1–12.

*DOI*
https://doi.org/10.5772/acrt.10



*Published*
2 August 2022

## *1. Introduction*

According to a Bloomberg study, investments in alternative energy will reach 10 trillion dollars by 2050 and the world's energy consumption would grow at 2.3% [1]. To address problems facing climate change investments would focus on environmentally friendly sources for producing power as published in energy transition investment of 2021 [2]. The demand for conceptual designs in power plants to reduce pollution has led to creation of new energy simulation and energy system optimization models. A novel conceptual gas turbine requires systems that could predict and simulate the system under various operating conditions. To simulate a gas turbine operating at various altitudes, there are numerous factors to consider such as wind speed, air temperature, humidity etc. To improve the efficiency, gas turbines utilize various combinations of heat exchangers, intercoolers and solar heaters. Conceptual designs require optimization methods to identify the best fit in the system.

Gas turbine models and simulators help in the trade-off between efficiency and cost to design a gas turbine. Numerous researchers have studied gas turbine problems which include conventional multivariate interpolation, steepest ascent method and other nature-inspired gradient-free methods algorithm based on Bee colony, Cuckoo search, Genetic, grasshopper, and Covariance matrix details of these algorithms are available here [3–10]. In the energy sector, quantum based optimization has been done to predict the placement of oil well reservoirs using Quantum particle swarm optimization and was found to perform better than the other optimization methods [11]. Quantum particle swarm optimization (QPSO), widely used to solve multi variables optimization problems in estimating Q factor in circuits has been explored [12] for performance control of gas turbines and to predict gas turbine controls without the required rotor speed conversion [13]. Gas turbine simulations are required to create operating curve at steady state conditions [14], to study designs with intercoolers and recuperators [15, 16], to increase efficiency [17], to investigate off-design performance, transient states and analyze Gas Turbine Gas Path Fault Diagnosis [18–20].

## 2. *Application of quantum computing in aerospace*

Quantum computing is rapidly changing various research studies in superconductivity, laser communication, encryption, imaging and many more. It provides insight for non-chemical approaches in the field of energy generation and storage. Aerospace applications in obtaining knowledge of transition between boundary and initial conditions even for minute changes and requires precision knowledge for induced disturbances [21].

The ability to use fuzzy logic in quantum computing for solving vector/scalar helps in reducing the multi-year calculation problems to a fraction of a minute through higher order magnitude calculations. The advantage of quantum entanglement finds various applications in quantum computing, quantum cryptography, quantum teleportation, and quantum sensors. The reversible gates when reversible allow quantum gain [22].

Aerospace industry faces optimization problems as a major concern especially for parameters related to design or control. Quantum computing provides optimization solutions from numerous sensors that may aid in propulsion control, navigation control, trajectory and attitude control. It also helps in solving non-linear problems in aerodynamics, airflow and thermodynamics cycle calculations [23]. Properties of quantum computing aid in stochastic processes and for calculating molecular energy states for chemical reactions. One such application was to estimate the potential energy of dimethyl ether (DME) reacting with oxygen resulting in the combustion temperature range of 800–1350 K at the total pressure exhibited on a combustion chamber similar to that of high altitude flight. Using quantum optimization the energy value obtained at operating pressure was used to study the thermodynamic cycle of a 6 kW micro gas turbine power plant for high altitude flight systems which aids in fuel geometry optimization value process [24].

## 3. Quantum computing

Gas Turbine operations create terabytes of data that were difficult to collect and sort data, however, with the help of machine learning (ML) and artificial intelligence (AI), analyzing and managing such data has become easier [25]. For solving complex parametric optimization problems quantum computing provides new insights as it processes the information unlike classical binary computing methods. Quantum computing uses physics, data and coding to perform calculation simultaneously rather than the classical iterative method to solve a problem. The minimum information required for processing is known as qubits [26, 27].

The figure 1 represents the conceptual illustration of the classical method bits and quantum computational method qubit. Bits have two states 1 and 0 while the qubits have superimposition states where it can be both 1 and zero at the same time thus allowing simultaneously to explore various different solutions and converging to one optimum solution [28]. Quantum computing performs faster due to quantum entanglement where one qubit can understand the data of a distant qubit without sending any signals. The illustration also states the point representation of a point in a unit sphere using North and South poles [29]. Bloch Sphere representation of a qubit's state space by interpreting $\theta$ and $\phi$ as polar coordinates.

## 4. Key highlights of quantum computing

Quantum Computing (QC) is the field of research that studies the algorithms and systems that apply quantum phenomena to the solution of complex mathematical problems. The minimum quantity of processable information is known as qubit which is 2-D mechanical system that encodes $|0\rangle$ and $|1\rangle$. The key concepts of quantum computing are superposition state, entanglement, interference, measurement and no duplicates (not possible to clone). The quantum state of a quantum bit (qubit) is represented by $|\psi\rangle$ and they could have simultaneously be represented as $|0\rangle$ and $|1\rangle$ known as super position [30, 31]. The equation (1) shows the mathematical representation of it.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{1}$$

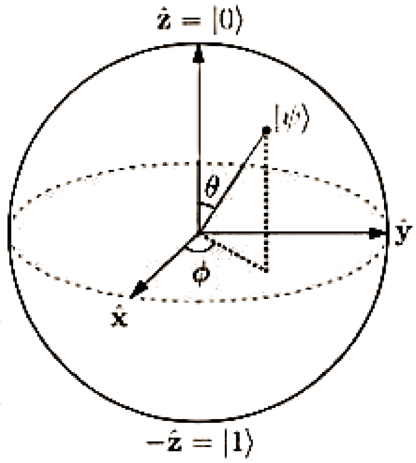


*Figure 1.* Conceptual illustration of bit vs. qubit is represented. The qubit states can be represented by a point on the unit sphere with the North and South poles corresponding to the states classical bit 0&1. Bloch sphere representation of a qubit's state space [25].

where, α and β are two coefficients from equation (1) to represent $|\psi\rangle$ that helps in parallel computing.

In a physical model, the particles interact with each other and could be represented in a quantum state on their dependence known as quantum entanglement. α and β which are complex probability amplitudes are constrained by the equation (2).

$$|\alpha|^2 + |\beta|^2 = 1 \tag{2}$$

The quantum state for two qubits is given by $|\psi\rangle_{12}$ and is represented in four ways

(1) $|0\rangle_1 \ \ |0\rangle_2$,
(2) $|0\rangle_1 \ \ |1\rangle_2$,
(3) $|1\rangle_1 \ \ |0\rangle_2$,
(4) $|1\rangle_1 \ \ |1\rangle_2$,

where, the subscript '*i*, denotes the *i*th quantum bit in this case '*i*' = 1 & 2. Using equation (1) results in

$$|\psi\rangle_{12} = 2^{-1/2}(|0\rangle_1|0\rangle_2 + |1\rangle_1|1\rangle_2) \tag{3}$$

The qubits could pass their own trajectory crossing their paths known as interference which helps in speedup via parallel computing. The qubits measurement is very fragile due to superposition, which helps in encryption applications. The state of the qubit cannot be copied or duplicated into another qubit thus preventing data theft [32].

$$\text{Superposition States} \quad \begin{aligned} &\delta|1, 1\rangle \\ &\gamma|0, 1\rangle \\ &\beta|1, 0\rangle \\ &\alpha|0, 0\rangle \end{aligned}$$

The state of a 2-bit digital system is determined by 2 binary digits that is determined using the states of a 2-bit quantum system which is determined by 4 coefficients: $\alpha$, $\beta$, $\gamma$, $\delta$, normalized where the $N$-qubits contain 2 $N$ units of classical information. The qubit simultaneously exhibits in two states $|0\rangle$ and $|1\rangle$ known as superposition that helps in performing parallel computations on a large scale. Factorization of qubit as a product of tensors cannot be done due to this multi-state configuration thus, when the state is true it is then the state is referred to as entangled [33, 34].

## 5. *Quantum programming*

Quantum programming usually concentrates into major categories as Quantum cryptography which deals with distribution of secret keys using quantum entanglement feature. The transfer of data from one quantum system to another quantum over a distance is known as Quantum teleportation which uses symmetry properties of entangled states [35].

To implement numerically, a formula has to be created for computing coherence vectors and correlating matrices [36] following procedures could be performed as shown in figure 2. The measurement must agree with the desired result and quantum algorithms are performed numerous times repeatedly for attaining a higher probability and could be represented as

$$M = (H, O, T, \delta, \beta) \tag{4}$$

where, $H$ is the state space of the quantum system operated on, $O$ a set of (deterministic) unitary transformations, $T$ a set of (probabilistic) measurement commands, $\delta$ is the initialization operator and $\beta$ describes the final measurement [37]. The figure 2 represent the various steps and procedures required for applying a quantum algorithm. The inputs are encoded in the form of state of qubits. Superposition are enabled allowing the qubits to be present in multiple states. Simultaneously the computation algorithm is applied to all the states to obtain true (quantum entanglement). In order to improve the probability of measuring the

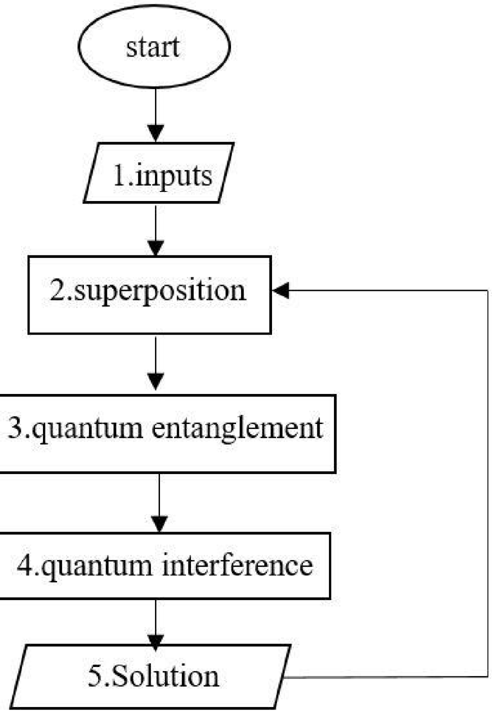


*Figure 2.* Procedures to apply a quantum algorithm.

true/correct state quantum interference is performed. The last step measures and encodes qubits for interpreting the solution.

## 6. *Quantum optimization and machine learning*

The quantum registers hold the input data of all possible configurations and randomize the possible outcome as the likelihood of measuring the desired solution. Aerospace industries require solutions for multi-disciplinary design optimization problems which require numerous target variables. Usually, the best solution would be the triggering of a cost function with minimum computational costs [38]. One common unstructured search optimization method is Grover's algorithm applied to the function $f(x)$ for evaluating the circuit on input $x \in \{0, 1\}n$. The time taken to evaluate the circuit is given by $O(2n/2 \text{ poly}(n))$. The method is represented as $f : \{0, 1\}n \rightarrow \{0, 1\}$, for output to match $f(x) = 1$. The $N$-dimensional quantum state is stored in O(log N) qubits [39]. Numerous gates are combined together to create a quantum circuit in order for performing required operations on single qubits. The qubits are flipped to the equator for producing superposition. All quantum gates are reversible since quantum mechanics is reversible. CNOT is an analog to the classical XOR gate but unitary.

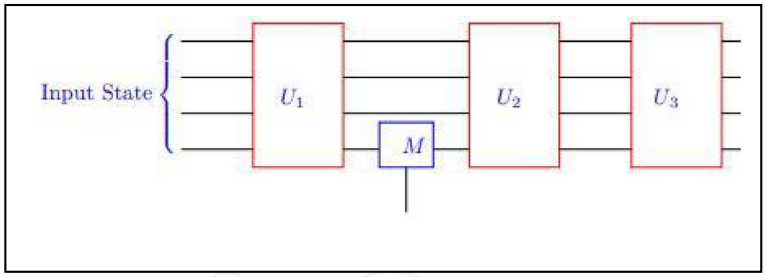


*Figure 3.* The figure represents the quantum circuit as a unitary operation and is in sequence in the $n$-qubit state.

Quantum annealing is a method to implement optimization algorithms on a quantum computer which is referred to as adiabatic quantum computation. In this case the gas turbine overall efficiency has to be optimized for a set of input variables. The input variables chosen are turbine inlet temperature, mass flow rate of the working fluid, pressure ratio and power output of the gas turbine. The fuel used was considered to be jet engine kerosene. The mathematical problem is converted to the ground state of the Hamiltonian problem $H_0$ [40]. The value is adiabatically transformed to the $H_i$ over the time series. As long as the energy is less the parameter would be near the ground state as stated by the adiabatic theorem, thus the minimum energy difference ($\Delta$) when measured would be the optimized value. This process has been adopted as the universal model of quantum computation. Quantum annealing helps in stimulating adiabatic quantum computation and has features to add intermediate Hamiltonian states. The energy state jumps are performed using quantum tunneling events which is an approximation of adiabatic computing [41].

Figure 3 shows how one bit of data is extracted to measure the state with certain probability. They could be represented in the form of $|\varphi\rangle$ which is known as ket, Dirac notation for vectors. The figure 3 represents the quantum circuit as a unitary operation and is in sequence in the $n$-qubit state. The $U_i$ is a representation of the $2n \times 2n$ matrix sequence in the $n$-qubit state. The $U_i$ is a representation of the $2n \times 2n$ matrix. The unitary matrices operate on $2\,n$-dimensional vectors as the quantum gates.

An alternate method to quantum annealing would be the feed-forward neural networks. The neural network consists of layers of neurons and each layer is initialized by the input function. The nodes are updated and the output is presented at the last layer [42, 43]. A Feed-forward neural network activates the node using a sigmoid function. The figure 4 represents a proposed model of a hybrid gas turbine design optimizer using a quantum circuit that has been integrated with neural networks. In the quantum world, fuzzy based neurons are easy to integrate as a quantum dot. The forward neural network layers also known as perceptron should be able to satisfy linear and nonlinear problems. This is obtained by using the

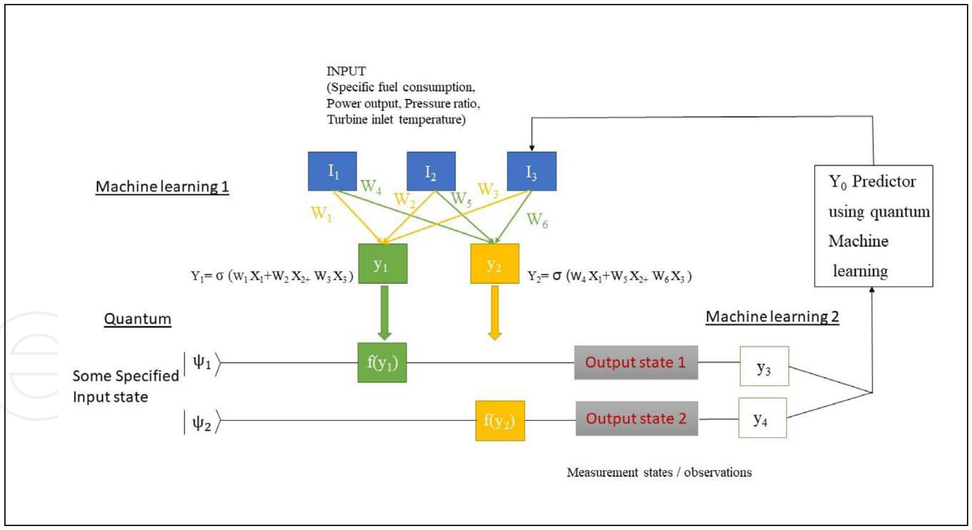


*Figure 4.* Illustration of a proposed quantum machine learning model using a feed-forward neural network. Integration of neural networks with quantum circuits.

carrying by phase estimation algorithm known as the quantum perceptron [44–46]. The machine learning 2 in the model acts as a filter to reduce the noise in the system.

## 6.1. Model evaluation and validation

To evaluate and validate the proposed model, different statistical measures are available such as mean squared error (MSE), root mean squared error (RMSE), mean absolute error (MAE), and $R^2$ error [47]. Mean squared error is defined as the quality of predicted data line points closer to the data points. A measure of data fit as accurately as possible. The lower the value of the estimator the higher is the accuracy of the model whereas the RMSE uses the average Euclidean distance of the predicted line to the data points. The MAE measures difference between the predicted results to the actual observations and $R^2$ error is a measure of variance and also known as coefficient of determination [48].

## 6.2. Quantum software and simulators

Recent growth in technology has paved the way for interest in quantum computing. There are currently numerous quantum simulators and tools available to compute and validate quantum algorithm models. In order to perform research on quantum based optimization and design of gas turbines quantum computers and quantum simulators are the two technologies required. Quantum computers help in computing models faster. The development and operation cost of quantum computers are extremely high and thus a need for quantum simulators is necessary. The quantum sensors would allow researchers to measure data with higher accuracy and precision. Optimization and computational problems could be solved efficiently using quantum simulators [49].

The quantum simulators available for various methods of computing such as Discrete variable gate-model quantum computing, Continuous variable gate-model quantum computing, Adiabatic quantum computation and Quantum simulators [50].

Due to the high cost of operating a quantum computer few simulators are recommended. QISKit, an open-source quantum computing framework for conducting research on quantum processors. Qubit Workbench, a simulator with drag and drop circuit gate builder and QC Simulator, universal computation simulator.

Quantum cloud computers provide access to quantum technology over the internet and are offered freely for research purposes and students who would like to run their algorithm with less than 5 qubits. IBM, Microsoft, Google and Huawei are providers of quantum cloud services.

### 6.3. Problems in quantum computing

Quantum computing presently faces challenges due to engineering capabilities. The qubits, as mentioned earlier, have errors due to external interference. Any perturbations would lead to calculating errors causing imperfect physical models. The errors in qubits are exponentially related to each qubit and modern systems would need millions of qubits to be operational and productive. Error compensation is an interesting research area for the future. In this article, a machine learning based quantum computing model would potentially be the future for error corrections [51]. Quantum computers require cryogenics operating temperatures. Thus, only a few companies provide cloud services. The ambient disturbances and noises, often thermal signatures, produce errors on the quantum states resulting in loss of coherence. A proposal of a quantum repeater would solve this problem in the future.

## 7. Conclusion

Quantum machine learning algorithms are needed to be designed and implemented for gas turbine designs and optimization problems. They could be used for fault diagnostics and maintenance using data classification models by training deep learning networks. In the future, quantum sensors and quantum communication networks will play a huge role in aerospace industries. Parametric optimization has not been fully developed in the quantum perspective. Various approaches to quantum computing have been proposed using the unitary quantum gates and quantum machine learning has been able to solve optimization problems at a faster rate.

## Conflict of interest

The authors declare no conflicts of interest.

## Acknowledgement

The Ministry of education and science of the Russian Federation in the framework for implementation of the Program for increasing the competitiveness of Samara University among the world's leading scientific and educational centers for 2013–2020 years supported this work.

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