Quantum Computing in Energy Systems

Course Code:	46394
Course Type:	Theoretical
Credits:	3
Course Status:	Elective specialized
Prerequisite:	Advisor approval

Aim/Scope/Objectives: This course is designed to provide graduate students with the knowledge needed to apply quantum computing to engineering calculations. This course covers all the required theoretical bases in linear algebra and quantum mechanics. The students would learn to run the homework and projects on real quantum computers. This course has an extensive application in mechanical engineering, chemical engineering, energy engineering, and machine learning calculations.

Course Outline:

1- **Dirac's Bra-ket Notation and Hermitian Operators**
Vectors Product, Different Matrices and their Properties, Linear Vector Spaces, Using Dirac's Bra-Ket Notation, Expectation Values and Variances, Eigenvalues and Eigen Functions, Tensor Product.

2- **The Quantum Superposition Principle and Bloch Sphere Representation**
Hilbert Space, Schrodinger Equation, Postulates of Quantum Mechanics, Quantum Tunneling, Stern and Gerlach Experiment, Bloch Sphere Representation, Projective Measurements, Measuring Multi-Qubit Systems, Qudits, Quantum Computing using Photons.

3- **Quantum Circuits**
Noisy Intermediate Scale Quantum Technology, Quantum Frameworks and Programming Languages, Introducing Quantum Circuits, Single Qubit Gates, Physical Gates, Multi Qubit Gates, Extended Quantum Gates, Universality of Quantum Gates, Quantum Circuits Optimization, The Compute Stage, Quantum Entanglement, Density Matrix Formalism, No-Cloning Theorem, Greenberger–Horne–Zeilinger (GHZ) State, Walsh–Hadamard Transform, Quantum Interference, Phase Kickback, DiVincenzo's Criteria for Quantum Computation.

4- **Quantum Algorithms**
Quantum Ripple Adder Circuit, Quantum Fourier Transformation, Quantum Phase Estimation (QPE), Quantum Arithmetic Using QFT, Grover's Search Algorithm, Quantum Distance Estimation, A Quantum Algorithm for K-Means, HHL Algorithm for Solving Linear Equations.

5- **Quantum Optimization**
Quadratic Unconstrained Binary Optimization (QUBO) problems, Ising Model, Adiabatic Quantum Computing (AQC), Quantum Annealing (QA), Quantum Approximate

Operation Algorithm (QAOA), Quantum Circuits for QAOA, Variational Quantum Eigensolver (VQE)

6- Quantum Neural Networks
Quantum-Classical Models, Feature Maps, Different Quantum Neural Networks Structure, Gradient Computation and Training, Practical notes in Quantum Neural Networks.

7- Quantum Algorithms for Solving Partial Differential Equations
Introduction to Partial Differential Equations (PDEs), Classical Methods for Solving PDEs, Different Quantum Methods for Solving PDEs, Discretization of PDEs, Vibrational Quantum Algorithms, Chebyshev Feature Map and Anstaz, Derivative Quantum Circuits, Loss Functions and Boundary Handling.

8- Quantum Machine Learning
Quantum Deep Neural Networks, Quantum Genetic Algorithm, Quantum Generative Adversarial Networks, Quantum Reinforcement Learning.

Grading: 35% Final exam, 35% Homework, 30% Final Research Project

References:

1. Venkateswaran Kasirajan, "Fundamentals of Quantum Computing, Theory and Practice", Springer, 2021.
2. Elias F. Combaro, "A Practical Guide to Quantum Machine Learning and Quantum Optimization", Packt Publishing, 2023.
3. Anna Sallés Rius, "Solving and Development of Quantum Algorithms for Solving and Estimating Parameters of Partial Differential Equations", Leiden University Thesis, 2022.
4. Andreas Wichert, "Quantum Artificial Intelligence with Qiskit", Taylor & Francis, 2024.
5. Xavier Vasques, "Machine Learning Theory and Applications Hands-on Use Cases with Python on Classical and Quantum Machines", John Wiley, 2024.
6. Maria Schuld, "Machine Learning with Quantum Computers", Springer, 2021
7. Alex Khan, "Quantum Computing Experimentation with Amazon Braket", Packt Publishing, 2022.