**DOCTORAL (PHD) STUDIES**

# COURSE UNIT DESCRIPTION

| Course unit title | Scientific areas | Faculty | Institute, department |
|---|---|---|---|
| **Quantum Computing** | 07T | Mathematics and Informatics faculty | Institute of Data Science and Digital Technologies |

| Study method | Number of credits | Study method | Number of credits |
|---|---|---|---|
| Lectures | 1 | Consultations | 1 |
| Individual works | 4 | Seminars | 1 |

| Summary |
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**Annotation**: The course is designed to develop PhD students’ competencies in the rapidly expanding and still emerging field of quantum computing, covering fundamental principles of quantum information as well as modern applied algorithms. The primary focus is on *Quantum Advantage* and Hybrid Computational schemes under current conditions of noisy intermediate-scale quantum (NISQ) devices.
PhD students will critically analyze quantum circuit models, complexity classes (including BQP), and specialize in quantum optimization (QUBO/Ising formulations) and quantum machine learning (QML). The core of the course is hands-on research activity that spans the full development cycle: from mathematical problem modeling to validation using quantum simulators and high-performance cloud infrastructures (IBM Quantum, PennyLane, D-Wave), while assessing the competitiveness of the obtained solutions against classical state-of-the-art results.

**Requirements:** Participants are expected to have a mathematical background that includes linear algebra, complex numbers, basic probability theory, and statistical analysis. Familiarity with the fundamentals of algorithm theory and computational complexity, as well as basic knowledge of optimization methods and machine learning paradigms, is desirable. Programming skills in Python are also required, with the ability to work with specialized quantum-computing libraries and data-science packages.

**Content:**

1) Fundamentals of Quantum Computing
   a) Fundamentals of Quantum Information
      - Introduction to bits and qubits; Dirac notation.
      - Postulates of quantum mechanics; entanglement; no-cloning and no-deleting theorems.
      - Examples of quantum communication protocols: quantum teleportation, superdense coding.
   b) Quantum Circuit (Gate) Model
      - Quantum gates and circuit construction; reversibility and its role in computation.
      - Universal gate set (the idea of universality); introduction to computational complexity classes, including Bounded-Error Quantum Polynomial Time (BQP).
   c) Core Quantum algorithms and Limitations
      - Quantum Fourier Transform (QFT) and Quantum Phase Estimation.
      - Representative algorithms: Grover’s, Shor’s, etc.
      - Capabilities and limitations of quantum computing, including the Noisy Intermediate-Scale Quantum (NISQ) context.
2) Quantum Optimization
   a) Formulation of Optimization Problems
      - Combinatorial problems: objective function, constraints, and penalties.
      - Transformation into Quadratic Unconstrained Binary Optimization (QUBO) and Ising form; solution decoding and feasibility checking.
   b) Annealing Methods and (D-Wave-Type) Solutions

- Simulated annealing.
- Quantum annealing and hybrid schemes.

c) Optimization with Quantum Circuits
- Variational optimization methods in the gate model.
- Comparison with classical methods: solution quality, resources, reliability, and reproducibility; reference solvers, e.g., Mixed-Integer Linear Programming (MILP) and Constraint Programming (CP-SAT).

3) Quantum Machine Learning

a) Data Encoding and Feature Representation
- Main approaches to encoding data into quantum states (angle, basis, amplitude).
- Feature Maps including periodic and entanglement-based maps.
- Data preparation and scaling considerations (number of features, number of qubits).

b) Quantum and Hybrid Models
- Quantum Kernel Methods.
- Variational discriminative models: Variational Quantum Classifier (VQC), Quantum Neural Networks (QNN), and hybrid models.
- Unsupervised learning / dimensionality reduction: Quantum PCA (qPCA) and quantum autoencoders.
- Other methods: generative models (quantum Born machines, Quantum GAN (QGAN)), reinforcement learning, quantum graph models.

c) Training and Evaluation
- Training strategies under NISQ conditions: impact of noise and the number of measurements (shots), parameter optimization.
- Risk of Barren Plateaus and practical mitigation strategies (ansatz design, circuit depth).
- Evaluation methodology: metrics, reproducibility, comparison with baseline models, ablation studies.

**Practical tasks**: For a selected applied problem (e.g., in logistics or finance), a QUBO/Ising model is formulated and implemented using a chosen quantum paradigm: either quantum or hybrid annealing (D-Wave Leap/Ocean) or gate-model variational optimization algorithms (e.g., QAOA) on a selected platform (IBM Quantum (Qiskit) or PennyLane), followed by a comparative analysis against classical optimization methods.
For a selected classification or regression problem (e.g., in medicine, cybersecurity, or chemistry), a quantum or hybrid solution is designed and implemented on a chosen platform (IBM Quantum (Qiskit) or PennyLane) using QML methods (e.g., quantum kernel methods, variational circuits, or generative models), selecting a data-encoding strategy consistent with the chosen methodology and conducting rigorous result verification (evaluating metrics and reproducibility) in comparison with classical models.

## Main literature

**Books**:


- Du, Y., Wang, X., Guo, N., Yu, Z., Qian, Y., Zhang, K., Hsieh, M.-H., Rebentrost, P., & Tao, D. (2025). *A Gentle Introduction to Quantum Machine Learning*. Springer Singapore. https://doi.org/10.1007/978-981-95-1284-3
- Schuld, M., & Petruccione, F. (2021). *Machine Learning with Quantum Computers* (2nd ed.). Springer Cham. https://doi.org/10.1007/978-3-030-83098-4
- Hidary, J. D. (2021). *Quantum Computing: An Applied Approach* (2nd ed.). Springer Cham. DOI: https://doi.org/10.1007/978-3-030-83274-2
- Combarro Fernández-Combarro Álvarez, E. F., & González-Castillo, S. (2023). *A Practical Guide to Quantum Machine Learning and Quantum Optimization: Hands-on Approach to Modern Quantum Algorithms*. Packt Publishing. ISBN: 9781804613832. https://www.packtpub.com/en-ID/product/a-practical-guide-to-quantum-machine-learning-and-quantum-optimization-9781804613832


**Papers**:

- Abbas, A., Ambainis, A., Augustino, B., et al. (2024). *Challenges and opportunities in quantum optimization*. *Nature Reviews Physics*, *6*, 718–735. https://doi.org/10.1038/s42254-024-00770-9
- Bharti, K., Cervera-Lierta, A., Kyaw, T. H., et al. (2022). *Noisy intermediate-scale quantum algorithms*. *Reviews of Modern Physics*, *94*(1), 015004. https://doi.org/10.1103/RevModPhys.94.015004
- Cerezo, M., et al. (2021). *Variational quantum algorithms*. *Nature Reviews Physics*, *3*, 625–644. https://doi.org/10.1038/s42254-021-00348-9
- Endo, S., Cai, Z., Benjamin, S. C., & Yuan, X. (2021). *Hybrid quantum-classical algorithms and quantum error mitigation*. *Journal of the Physical Society of Japan*, *90*(3), 032001. https://doi.org/10.7566/JPSJ.90.032001
- Larocca, M., Thanasilp, S., Wang, S., et al. (2025). *Barren plateaus in variational quantum computing*. *Nature Reviews Physics*, *7*, 174–189. https://doi.org/10.1038/s42254-025-00813-9
- Farhi, E., Goldstone, J., & Gutmann, S. (2014). *A Quantum Approximate Optimization Algorithm*. arXiv:1411.4028. https://doi.org/10.48550/arXiv.1411.4028


| Lecturer(s) (name, surname) | Science degree | Main publications |
|---|---|---|
| Ernestas Filatovas | PhD | http://www.elaba.mb.vu.lt/dmsti/?aut=Ernestas+Filatovas |
| Remigijus Paulavičius | PhD | http://www.elaba.mb.vu.lt/dmsti/?aut=Remigijus+Paulavi%C4%8Dius |
| Linas Petkevičius | PhD | https://elaba.mb.vu.lt/mif/?aut=Linas+Petkevi%C4%8Dius |

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| Doktorantūros komiteto teikimu patvirtinta fakulteto/instituto taryboje 20__ m.__ mėn.__d. , protokolo Nr. |
| Tarybos pirmininkas |

Pastaba: jei doktorantūros teisė bus suteikta kartu su kita institucija, tvirtinama ne fakulteto taryboje, o jungtinėje komisijoje.