Quantum Technology and Artificial Intelligence

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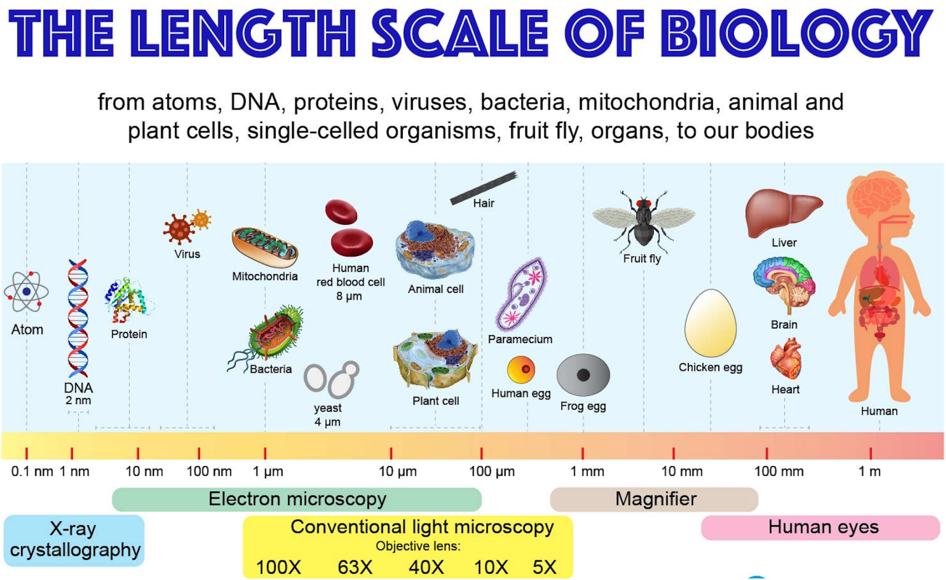
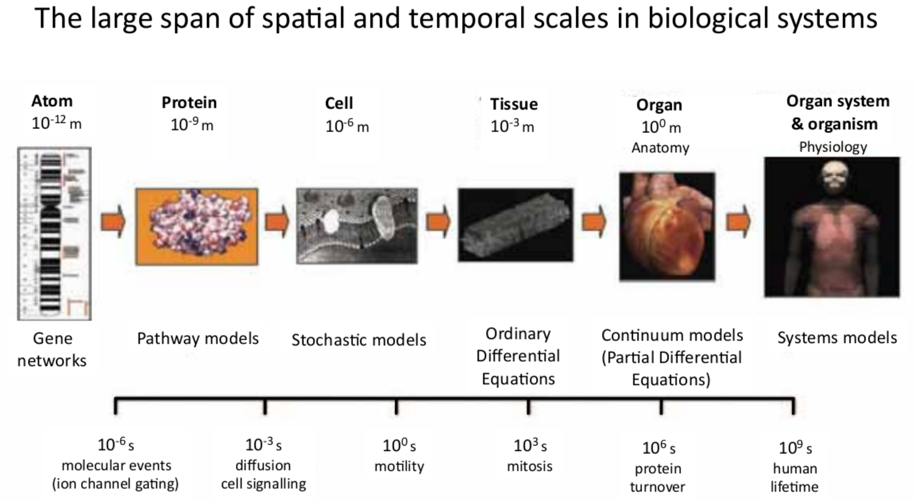
What is this talk about?

The main emphasis is to give you a short and hopefully pedestrian overview to the whys and hows of machine learning and quantum technologies, why this could (or should) be of interest and where to find info about courses and study programs at UiO.

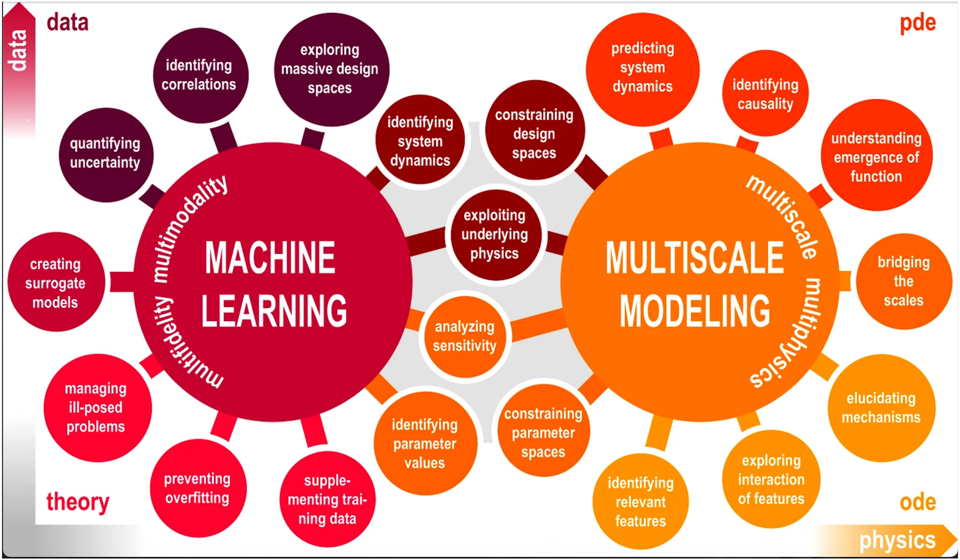
Multiscale scientific problem, life science example



Multiscale scientific problem, life science example, with mathematical methods



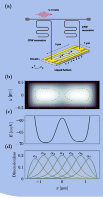
Multiscale scientific problem, life science example with Machine learning



Quantum technology and machine learning/AI

Quantum Hardware

- Quantum control and sensors
- Quantum computers
- Catalysis



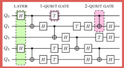
AI for Quantum Technology

- Quantum mechanical many-body theories
- Molecular dynamics
- Density functional theory

Quantum Technology and AI

Quantum Algorithms for AI

- Quantum computing
- Quantum algorithms
- Quantum machine learning
- Quantum inspired classical computing

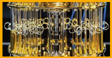


Societal impact and products

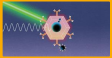
New medicines

Better shipping

Financial innovation



Quantum readiness



Quantum sensors and computers

- Drug discovery
- Quantum sensing
- Supply chain optimization
- Financial market modelling and risk analysis
- Material discovery

What is Machine Learning?

Machine Learning (ML) is the study of algorithms that improve through data experience.

Types of Machine Learning:

- **Supervised Learning:** Labeled data for classification or regression.
- **Unsupervised Learning:** No labels; discover hidden patterns.
- **Reinforcement Learning:** Learning through interaction with the environment.

ML Workflow:

$$\text{Data} \rightarrow \text{Model Training} \rightarrow \text{Prediction}$$

What is Quantum Computing?

Quantum computing leverages principles of quantum mechanics to perform computations beyond classical capabilities.

Key Concepts:

- **Superposition:** Qubits can exist in a combination of states.
- **Entanglement:** Correlation between qubits regardless of distance.
- **Quantum Interference:** Probability amplitudes interfere to solve problems.

Qubit Representation:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1$$

What is Quantum Machine Learning?

Quantum Machine Learning (QML) integrates quantum computing with machine learning algorithms to exploit quantum advantages.

Motivation:

- High-dimensional Hilbert spaces for better feature representation.
- Quantum parallelism for faster computation.
- Quantum entanglement for richer data encoding.

Quantum Speedups in ML

Why Quantum?

- **Quantum Parallelism:** Process multiple states simultaneously.
- **Quantum Entanglement:** Correlated states for richer information.
- **Quantum Interference:** Constructive and destructive interference to enhance solutions.

Example - Grover's Algorithm:

$$\text{Quantum Search Complexity: } O(\sqrt{N}) \text{ vs. } O(N)$$

Advantage: - Speedups in high-dimensional optimization and linear algebra problems.

Challenges and Limitations

1. **Quantum Hardware Limitations:**
   - Noisy Intermediate-Scale Quantum (NISQ) devices.
   - Decoherence and limited qubit coherence times.
2. **Data Encoding:**
   - Efficient embedding of classical data into quantum states.
3. **Scalability:**
   - Difficult to scale circuits to large datasets.

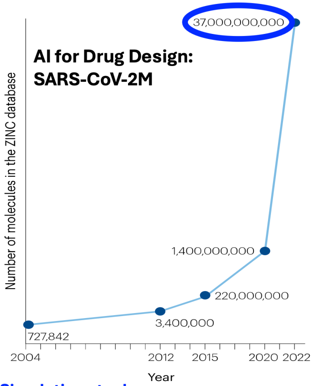
AI/ML and some statements you may have heard (and what do they mean?)

1. Fei-Fei Li on ImageNet: **map out the entire world of objects** (The data that transformed AI research)
2. Russell and Norvig in their popular textbook: **relevant to any intellectual task; it is truly a universal field** (Artificial Intelligence, A modern approach)
3. Woody Bledsoe puts it more bluntly: **in the long run, AI is the only science** (quoted in Pamilla McCorduck, Machines who think)

If you wish to have a critical read on AI/ML from a societal point of view, see Kate Crawford's recent text Atlas of AI.

Here: with AI/ML we normally intend a collection of machine learning methods with an emphasis on statistical learning and data analysis

Machine learning and AI models are computationally expensive



Simulations took:

90 days on **250 GPUs & 640 cpu-core**
1 day on **27000 GPU** Summit supercomputer

Nature Reviews Drug Discovery **23**, 141–155 (2024)

TOP4 Powerful Supercomputers as of Nov 2024

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,039,616	1,742.00	2,746.38	29,581
		76	1,353.00	2,055.72	24,607
	Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States				
4	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	

Advance nuclear weapon science and scientific discovery.

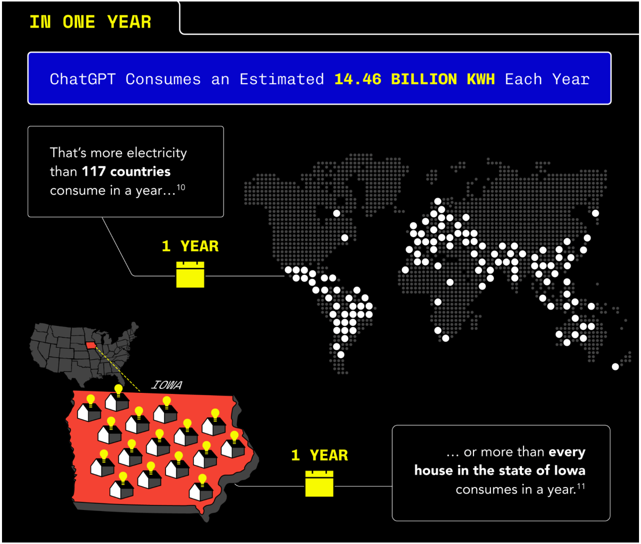
US$600 million

nature reviews drug discovery

Perspective | Published: 08 December 2023

Integrating QSAR modelling and deep learning in drug discovery: the emergence of deep QSAR

And power greedy, perhaps quantum computers can reduce the impact?

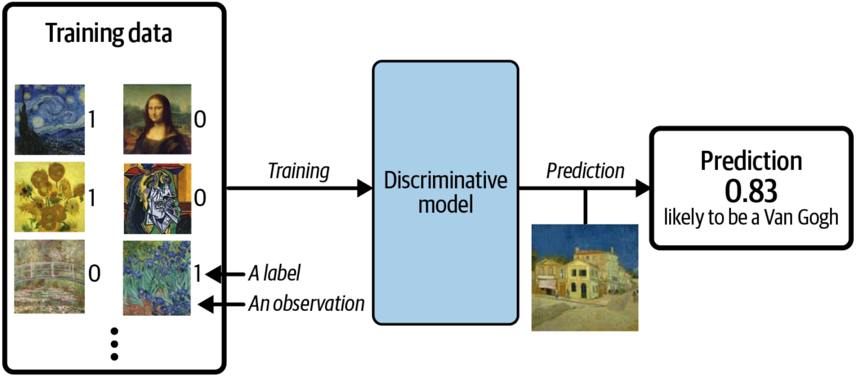


Taken from https://www.businessenergyuk.com/knowledge-hub/

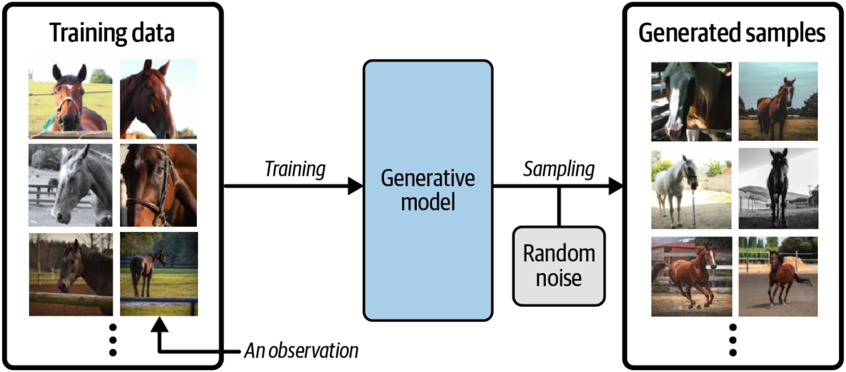
The plethora of machine learning algorithms/methods

1. Deep learning: Neural Networks (NN), Convolutional NN, Recurrent NN, Boltzmann machines, autoencoders and variational autoencoders and generative adversarial networks, stable diffusion and many more generative models
2. Bayesian statistics and Bayesian Machine Learning, Bayesian experimental design, Bayesian Regression models, Bayesian neural networks, Gaussian processes and much more
3. Dimensionality reduction (Principal component analysis), Clustering Methods and more
4. Ensemble Methods, Random forests, bagging and voting methods, gradient boosting approaches
5. Linear and logistic regression, Kernel methods, support vector machines and more
6. Reinforcement Learning; Transfer Learning and more

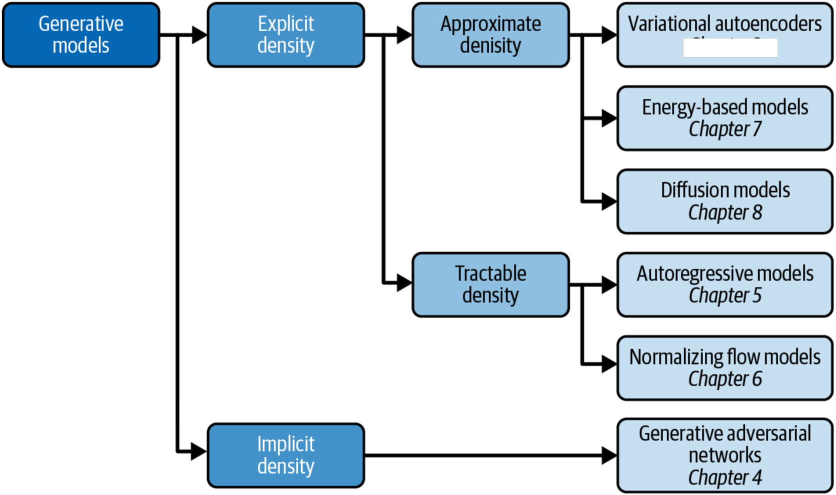
Example of discriminative modeling, taken from Generative Deep Learning by David Foster



Example of generative modeling, taken from Generative Deep Learning by David Foster



Taxonomy of generative deep learning, taken from Generative Deep Learning by David Foster



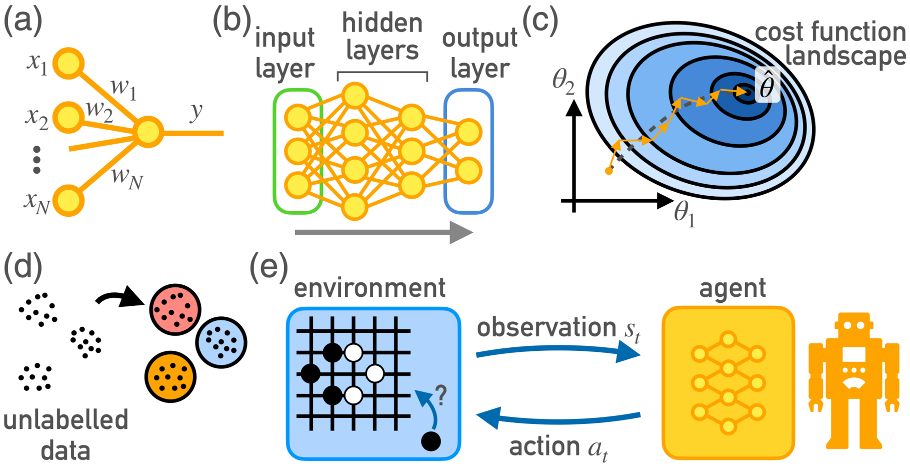
What are the basic Machine Learning ingredients?

Almost every problem in ML and data science starts with the same ingredients:

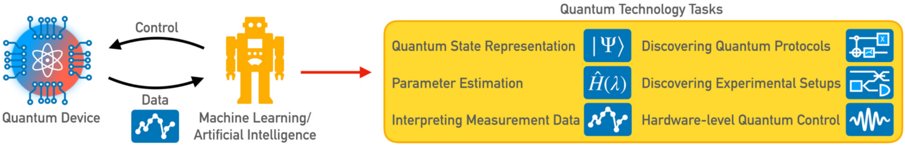
- The dataset $\boldsymbol{x}$ (could be some observable quantity of the system we are studying)
- A model which is a function of a set of parameters $\boldsymbol{\alpha}$ that relates to the dataset, say a likelihood function $p(\boldsymbol{x}|\boldsymbol{\alpha})$ or just a simple model $f(\boldsymbol{\alpha})$
- A so-called **loss/cost/risk** function $\mathcal{C}(\boldsymbol{x}, f(\boldsymbol{\alpha}))$ which allows us to decide how well our model represents the dataset.

We seek to minimize the function $\mathcal{C}(\boldsymbol{x}, f(\boldsymbol{\alpha}))$ by finding the parameter values which minimize $\mathcal{C}$. This leads to various minimization algorithms. It may surprise many, but at the heart of all machine learning algortihms there is an optimization problem.

Schematic view on Machine Learning approaches



Quantum technologies and ML/AI



What is Quantum Entanglement?

Quantum Entanglement is a quantum phenomenon where two or more particles become correlated in such a way that the state of one particle directly affects the state of the other, regardless of distance.

Key Features:

- Non-local correlations
- No classical analog
- Violates Bell's inequalities

Entangled State Example:

$$\left|\Phi^+\right\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Quantum Teleportation:

- Entanglement enables the transmission of quantum states using classical communication.
- No need to send the physical quantum particle.

Advantage:

- Instantaneous state transfer within quantum mechanics constraints.
- Quantum networks rely on entanglement for secure communication.

Quantum Key Distribution:

- Entanglement ensures secure communication.
- Eavesdropping disturbs quantum states, revealing interception attempts.
- Any measurement by a third party collapses the wavefunction.
- Ensures security based on quantum mechanics, not computational hardness.

Advantage: Unconditional security guaranteed by the laws of physics.

Speedup in Quantum Algorithms:

- Entanglement provides exponential state space.
- Quantum parallelism arises from entangled qubits.

Grover's Algorithm:

$$\mathcal{O}(\sqrt{N}) \text{ vs. } \mathcal{O}(N)$$

Shor's Algorithm:

$$\text{Factoring in } \mathcal{O}((\log N)^3)$$

4. Quantum Metrology

Quantum Metrology:

- Uses entangled states for ultra-precise measurements.
- Overcomes the classical shot-noise limit.

Heisenberg Limit:

$$\Delta\theta \geq \frac{1}{N},$$

where N is the number of entangled particles.

Advantage:

- Quantum entanglement improves sensitivity beyond classical limits.

Challenges of Quantum Entanglement

Decoherence:

- Entangled states are fragile.
- Interaction with the environment collapses the wavefunction.

Scalability:

- Difficult to entangle large numbers of qubits.
- Error correction requires complex protocols.

Measurement Problem:

- Measurement destroys entanglement.
- Trade-off between information gain and entanglement preservation.

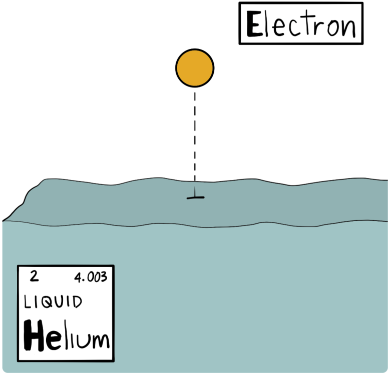
Di Vincenzo criteria

Quantum computing requirements

1. A scalable physical system with well-characterized qubit
2. The ability to initialize the state of the qubits to a simple fiducial state
3. Long relevant Quantum coherence times longer than the gate operation time
4. A **universal** set of quantum gates
5. A qubit-specific measurement capability

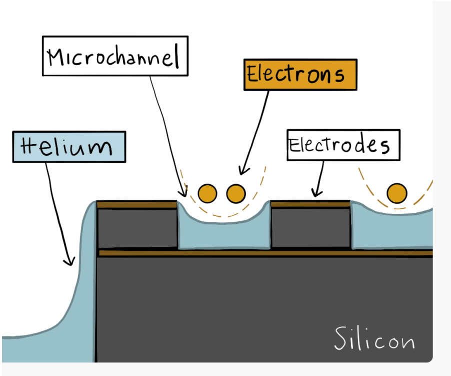
Single electrons can make great qubits

At the heart is the trapping and control of individual electrons floating above pools of superfluid helium. These electrons form the qubits of our quantum computer, and the purity of the superfluid helium protects the intrinsic quantum properties of each electron. The ultimate goal is to build a large-scale quantum computer based on quantum magnetic (spin) state of these trapped electrons.



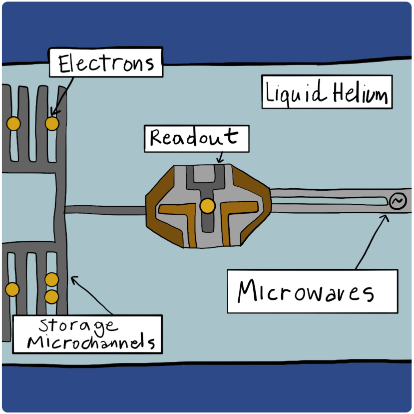
Trapping electrons in microchannels

Microchannels fabricated into silicon wafers are filled with superfluid helium and energized electrodes. Together with the natural electron trapping properties of superfluid helium, these allow for the precision trapping of individual or multiple electrons. The microchannels are only a few micrometers in size, or about five times smaller than the diameter of a human hair.



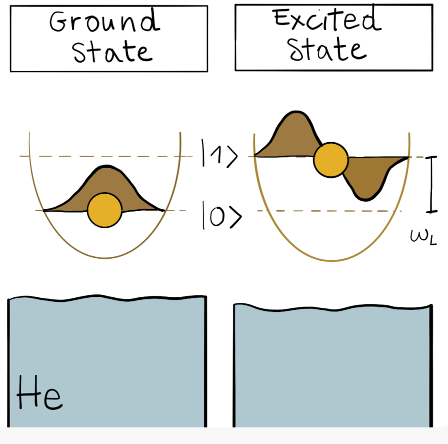
Control and readout

Microchannel regions can store thousands of electrons, from which one can be plucked and transported to the single electron control and readout area. In this region, microwave signals will interact with the electron to perform quantum logic gate operations, which will be readout via extremely fast electronics.



Operations for quantum computing

Quantum information can be encoded in a number of ways using single electrons. Currently, we are working with the side-to-side(lateral) quantum motion of the electron in the engineered trap. This motion can either be in its lowest energy state, the ground state, or in a number of higher-energy excited states. This electron motion also provides the readout capabilities for the ultimate goal of building a large-scale quantum computer based on the electron's magnetic moment (spin).



Can I study these topics at UiO?

- Several courses on Machine learning and AI at UiO, from bachelor level to PhD level, see https://github.com/CompPhysics/MachineLearning
- Quantum technologies, quantum information theory, quantum computing, quantum sensing and more. Study directions in Physics bachelor degree, Physics master degree and Computational Science master of science program
  1. Physics Bachelor of Science program https://www.uio.no/studier/program/fysikk-astronomi/studieretninger/kvanteteknologi/index.html
  2. Physics Master of Science program https://www.uio.no/english/studies/programmes/physics-master/programme-options/quantum-technology/index.html
  3. Computational Science Master of Science program https://www.uio.no/english/studies/programmes/computational-science-master/programme-options/quantum-technology/index.html