Quantum Computing in High Energy Physics

Examples from CERN



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Outline

- Introduction
 - Bell Inequalities & Quantum Technologies
- Quantum Computing
 - Qubits and Quantum Computers architectures
 - Quantum algorithms
- The CERN Quantum Technology Initiative
- Quantum Machine Learning and Applications at CERN
 - Anomaly Detection
 - Beam Optimisation in linear accelerators
- Summary & Outlook

Hype and Potential...

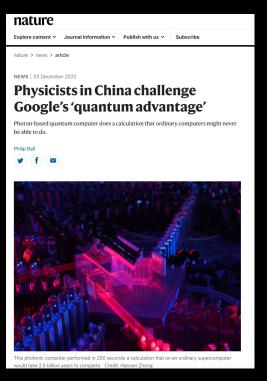
2019: Google

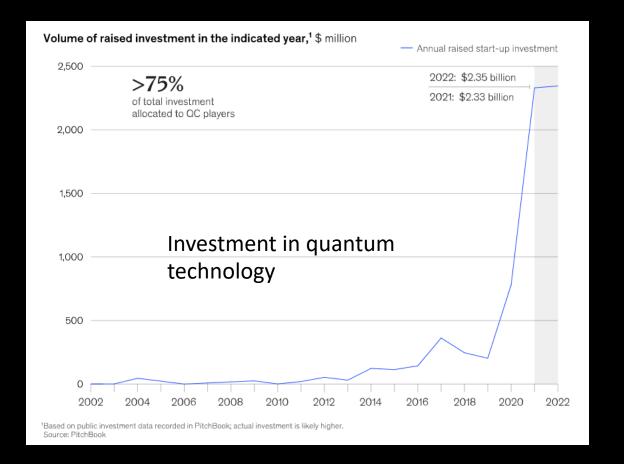


https://www.nature.com/articles/s41586 -019-1666-5

https://www.nature.com/articles/d4 1586-020-03434-7

2020: Hefei National Lab





Source: McKinsey 2023

https://www.mckinsey.com/capabilities/mckinsey-digital/our-insights/quantum-technology-sees-record-investments-progress-on-talent-gap

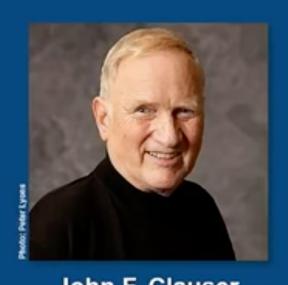


NOBELPRISET I FYSIK 2022 THE NOBEL PRIZE IN PHYSICS 2022





Alain Aspect
Université Paris-Saclay &
École Polytechnique, France



John F. Clauser

J.F. Clauser & Assoc.,

USA



Anton Zeilinger
University of Vienna,
Austria

"för experiment med sammanflätade fotoner som påvisat brott mot Bell-olikheter och banat väg för kvantinformationsvetenskap"

"for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

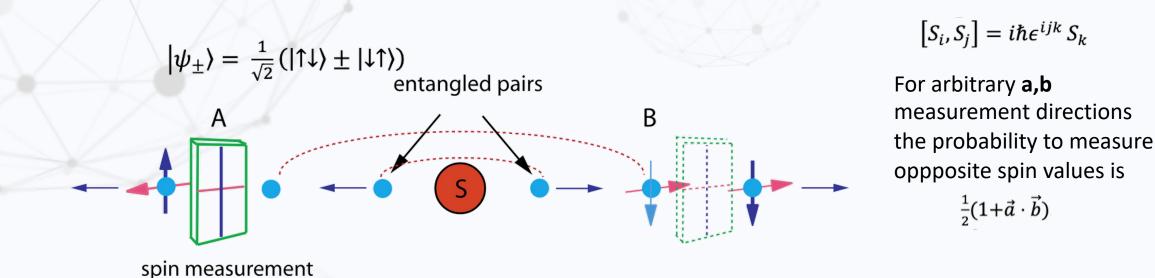
https://youtu.be/mtgYG2zsbbQ



#nobelprize

MORE VIDEOS

Einstein Podolsky Rosen Paradox



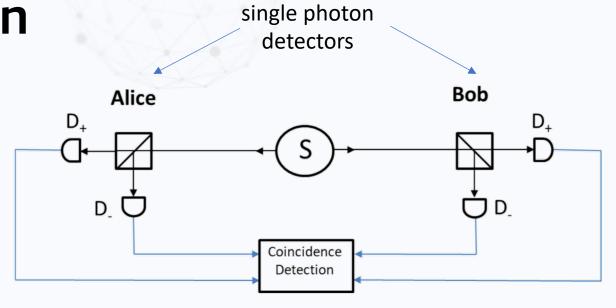
• 1935: EPR paradox questions completeness of Quantum Mechanics

'From this follows that either (1) the quantum-mechanical description of reality given by the wave function is not complete or (2) when the operators corresponding to two physical quantities do not commute the two quantities cannot have simultaneous reality'

Bell Inequalities and the second quantum revolution

• 1964: Bell inequality are a mathematical proof that no theory based on local hidden variables (realism) can reproduce QM results

- 1969: Clauser, Horne, Shimony (CHSH) formulation
- 1972 Freedman & Clauser experiment
- 1976-1982 Aspects experiments
- Measure the correlation across the possible outcomes of multiple measurements in A and B
- «Classical» (local realist) theory predicts bound correlation
- It is possible to design experimental conditions in which QM violates the bound



Second Quantum Revolution
Use distant entangled photons as a
quantum reource

- No clone theorem
- Quantum networks and teleportation

Many particles entanglement

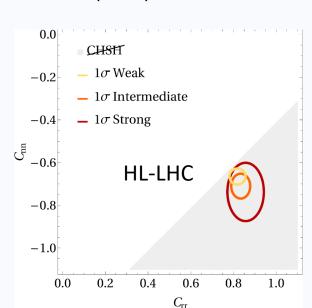
Computing and criptography

Bell Inequalities tests at colliders

- Multiple tests at colliders over the years at different energy scales
- Recent proposals at the LHC / HL-LHC:
 - Fabbrichesi et al. "Testing Bell inequalities at the LHC with top-quark pairs." Physical Review Letters 127.16 (2021): 161801.
 - Severi et al. "Quantum tops at the LHC: from entanglement to Bell inequalities." The European Physical Journal C 82.4 (2022): 285
 - Aguilar-Saavedra and Casas. "Improved tests of entanglement and Bell inequalities with LHC tops." *The European Physical Journal C* 82.8 (2022): 666
 - Aguilar-Saavedra et al. "Testing entanglement and Bell inequalities in H→ Z Z." Physical Review D 107.1 (2023): 016012
 - Barr, Alan J. "Testing Bell inequalities in Higgs boson decays." Physics Letters B 825 (2022): 136866

tt production at hadron colliders:

- Leading mechanism generates top spins that are highly correlated
- Tops decay semi-weakly before spin is randomised
- Charged lepton from $t \rightarrow Wb$, $W \rightarrow \ell \nu$ is 100% correlated with top spin



Severi, Claudio, et al. "Quantum tops at the LHC: from entanglement to Bell inequalities." *The European Physical Journal C* 82.4 (2022): 285

Quantum Technology

Second quantum revolution

Use quantum mechanics principles to develop new technology

"Artificial" quantum states

First Quantum Revolution

Max Planck black-body radiation

Transistor, laser, atomic clock, computers, optical fibre communication, ...

1900

Dowling & Milburn. "Quantum technology: the second quantum revolution." Philosophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences 361.1809 (2003): 1655-1674.

2000 Worldwide Initiatives and Investments

Now



Quantum Computing:

From Quantum Mechanics to Computer Science

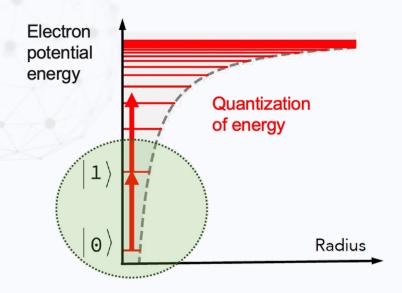
Qubit: Quantum Bit

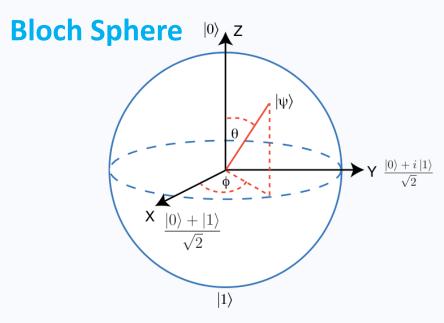
- Basic Unit of Quantum Computation representation
 - Classical bits are binary "0 or 1"
- Quantum Mechanics predicts superposition states (exponential storage information)
- Dirac notation is used to describe quantum states

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$$

 $\alpha, \beta \in C^2$ $|\alpha|^2 + |\beta|^2 = 1$

Interest in multi level representations: qutrits...





$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$
 10

Quantum Computing

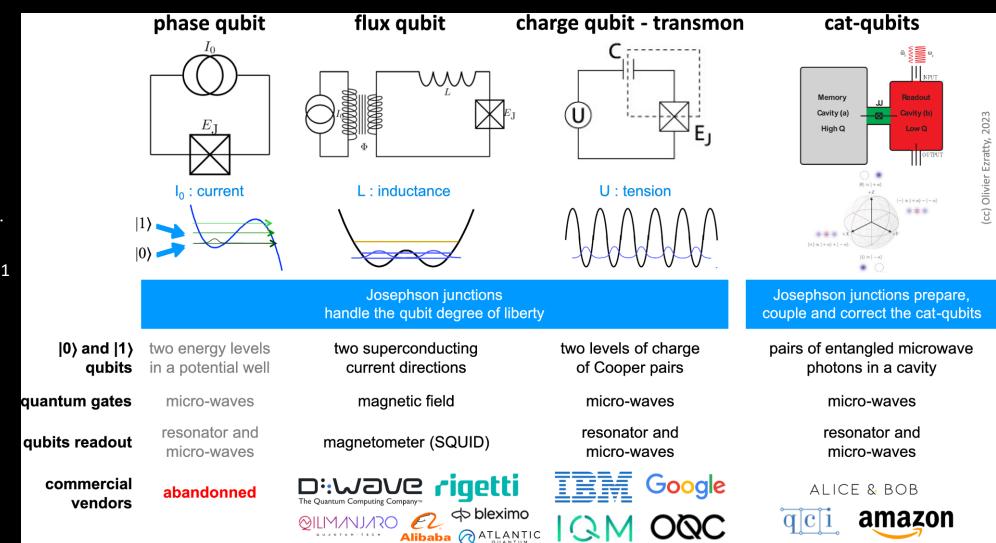
Principles of quantum mechanics enhance computations

- **Superposition** leads to parallelism → **exponential speedup?**
- Entanglement → non linear correlation and classical simulability?
- Operations (gates) are unitary transformations -> reversible computing?
- Output is the result of a quantum state measurement according to Born rule → stochastic computation?
- No-cloning theorem → information security
- Quantum state coherence and isolation

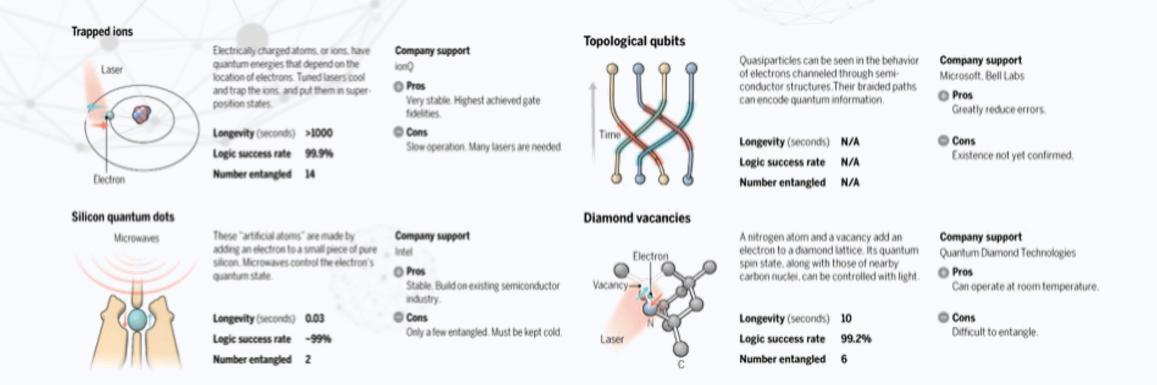
 computation stability and errors
- Qubit state collapses → reproducibility?

Superconducting Qubits

Ezratty, O. Perspective on superconducting qubit quantum computing. Eur. Phys. J. A 59, 94 (2023). https://doi.org/10.1140/epja/s1 0050-023-01006-7

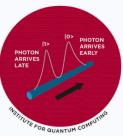


Multiple technologies





Polarization States



Time qubits



Path Qubits:

See Institute of Quantum Computing, U. of Waterloo, https://uwaterloo.ca/institute-for-quantum-computing/quantum-101/quantum-information-science-and-technology/what-qubit#Spin

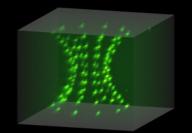
D. Barredo *et al.*, "Synthetic three-dimensional atomic structures assembled atom by atom." <u>arXiv:1712.02727</u>, 2017.

Neutral atom arrays

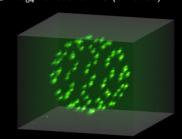
- Configurable arrays of single neutral atoms
- 2 energy levels represent the qubit states
- Use lasers to control position and the state of the atom
 - assemble and read-out registers made of hundreds of qubits
 - fully programmable quantum processing
- High connectivity
- Specific computation cycle because the register is not permanently built
 - register preparation
 - quantum processing
 - register readout



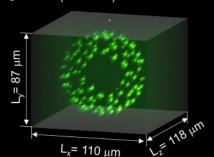




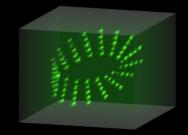
c C₈₄ fullerene-like (84 sites)



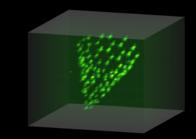
e Torus (120 sites)



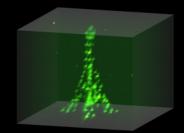
b Möbius strip (85 sites)



d Cone (100 sites)

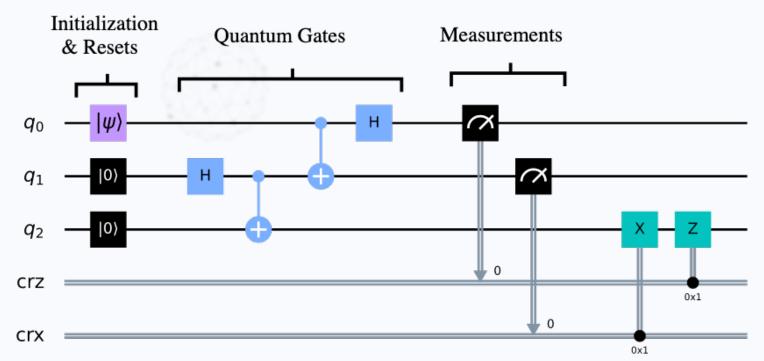


f Eiffel tower (126 sites)



Gates and circuits

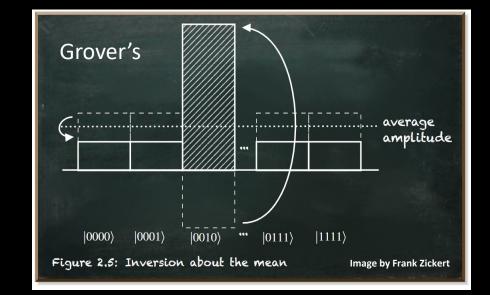
- Operations on qubits are unitary matrices describing Schrodinger state evolution
 - Reversible operations
 - Input and output states have the same dimension
 - Some classical gates (or , and, nand, xor...) cannot be implemented directly
 - Can simulate any classical computation with small overhead

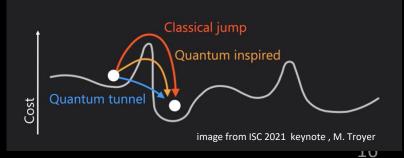


Quantum Algorithms

A collection on http://quantumalgorithmzoo.org

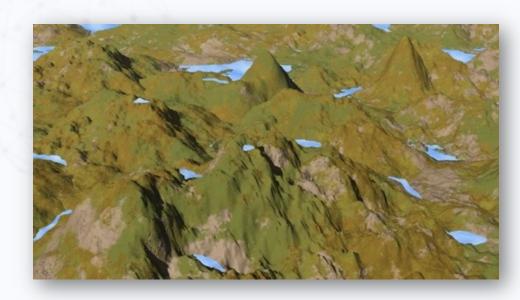
- Multiple algorithms have been studied
 - Shor algorithm for **prime factorization**
 - Grover algorithm for unsorted DB searches
 - Quantum Fourier Transform
- Quantum-inspired algorithms (emulate quantum effects on classical hardware)
- **Quantum Machine Learning**
- Challenge is re-thinking algorithms design and define fair benchmarking and comparison to classical algorithms

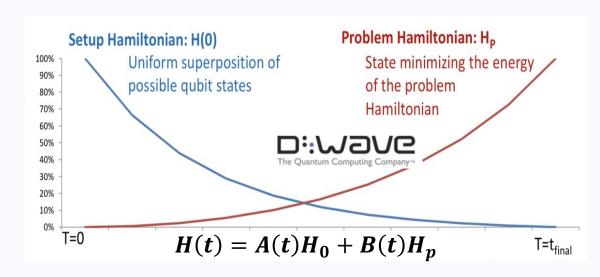




Quantum Annealing

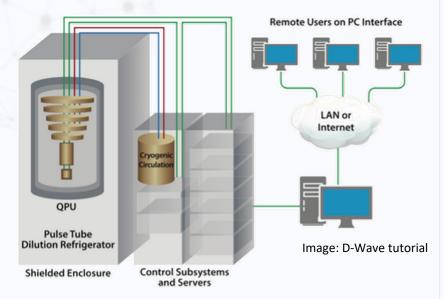
- Annealing for optimization problems
 - Smoothly evolve probability of being at any given coordinate with time.
 - Probability increases around the coordinates of deep valleys
- Quantum systems based on superconducting qubits
- D-Wave Advantage: 5436 qubits 15 connection (Pegasus)
 - Quantum superposition: scan simultaneously multiple coordinates
 - Quantum tunneling: reduces risk of local minima (tunnel through hills)
 - Quantum entanglement: discover correlations between the coordinates that lead to deep valleys.



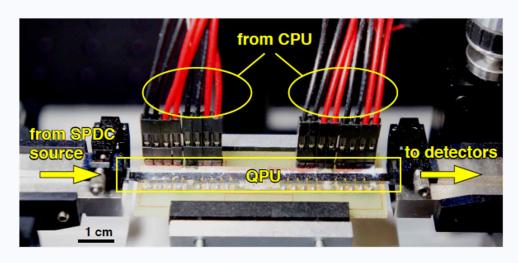


Today's challenges

- Noisy Intermediate-Scale Quantum devices
 - Limitations in terms of stability and connectivity
 - De-coherence, measurement errors or gate level errors
 - Specific error mitigation techniques
 - Circuit optimisation
 - Prefer algorithms robust against noise
- Quantum computers initially integrated in hybrid quantumclassical infrastructure
 - Engineering, cooling, I/O
 - Hybrid algorithms, QPU as accelerators

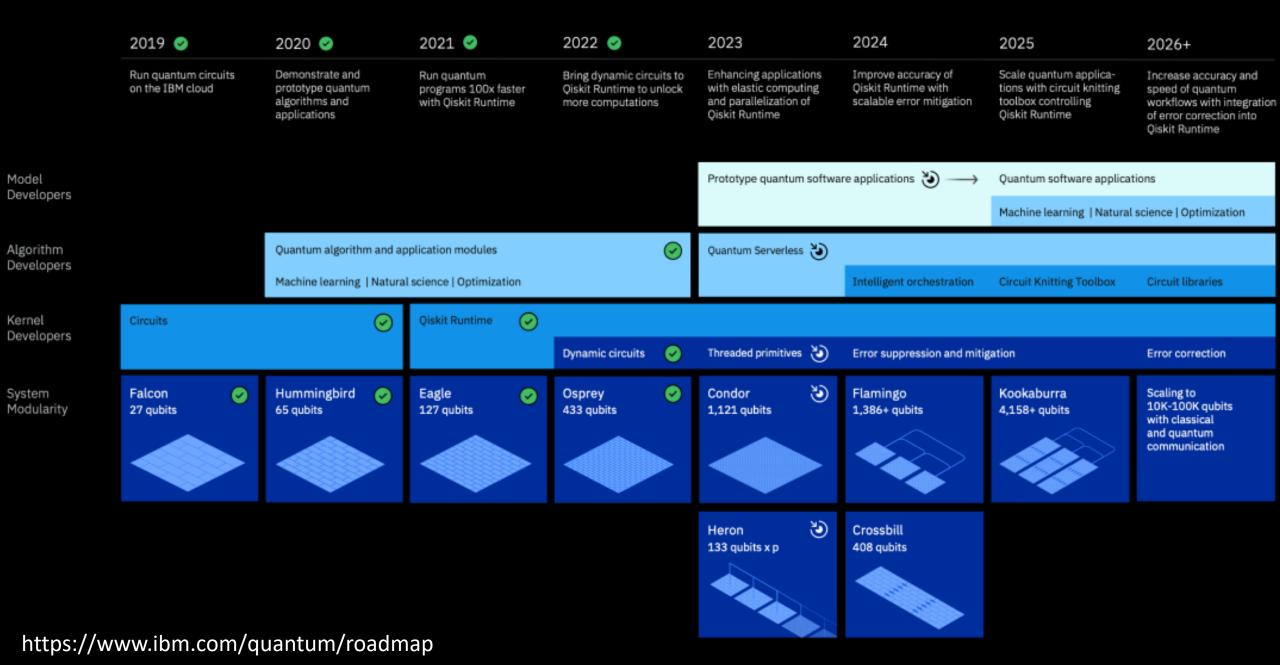


Peruzzo, A. "A variational eigenvalue solver on a quantum processor." arXiv preprint arXiv:1304.3061 (2013).



What the future brings

An example quantum roadmap from IBM



- How do we define advantage?
 - Speed-up and complexity
 - Sample efficiency
 - Representational power
 - Energy efficiency???

Evaluate performance on realistic use cases

The CERN Quantum Technology Initiative:

Understanding the impact of quantum technologies in HEP

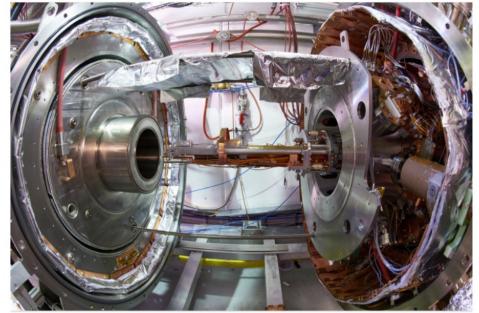
The CERN QTI launched in 2020

Voir en français

CERN meets quantum technology

The CERN Quantum Technology Initiative will explore the potential of devices harnessing perplexing quantum phenomena such as entanglement to enrich and expand its challenging research programme

30 SEPTEMBER, 2020 | By Matthew Chalmers



The AEgIS 1T antimatter trap stack. CERN's AEgIS experiment is able to explore the multi-particle entangled nature of photons from positronium annihilation, and is one of several examples of existing CERN research with relevance to quantum technologies. (Image: CERN)

Quantum simulation and HEP theory applications

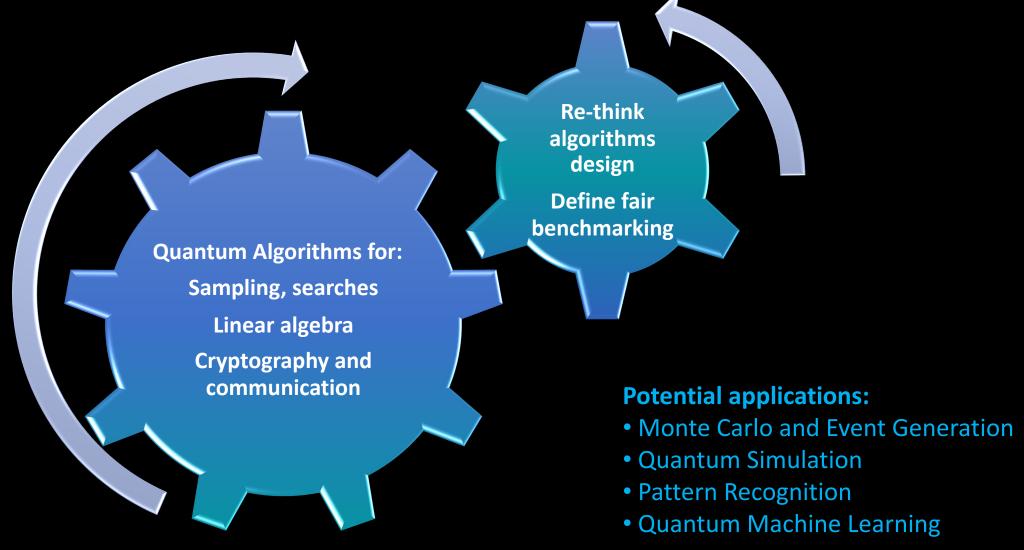
Quantum Computing

Quantum Sensing

Quantum Communication

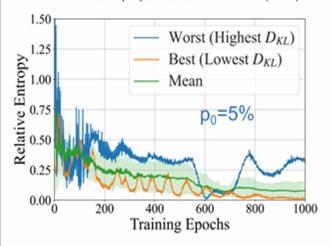
QTI Roadmap: https://doi.org/10.5281/zenodo.5553774

Quantum Algorithms for HEP

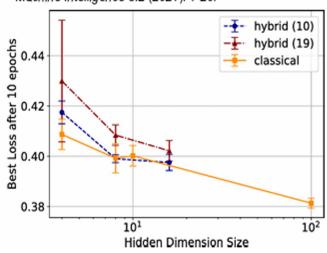


QC @CERN

Borras, Kerstin, et al. "Impact of quantum noise on the training of quantum Generative Adversarial Networks." arXiv preprint arXiv:2203.01007 (2022).



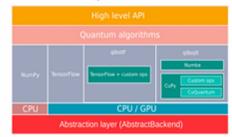
Tüysüz, Cenk, et al. "Hybrid quantum classical graph neural networks for particle track reconstruction." Quantum Machine Intelligence 3.2 (2021): 1-20.

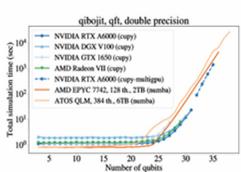


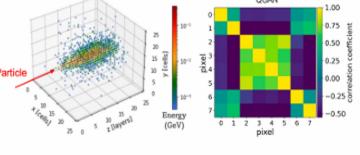
F.Rehm, Full Quantum GAN Model for HEP Detector Simulations, ACAT22

E.Stavros et all., Quantum simulation with just-in-time compilation, Quantum 2022

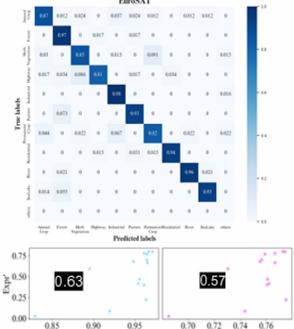
Oibo stack





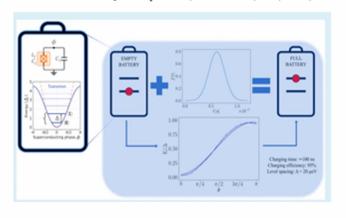


S.Chang, et all, Hybrid Quantum-Classical Networks for Reconstruction and Classification of Earth Observation Images, ACAT22



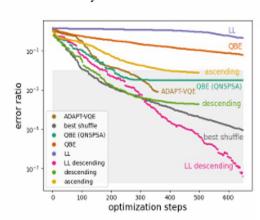
Training Accuracy

G. Gemme, M. Grossi et al, IBM Quantum Platforms: A Quantum Battery Perspective, Batteries 8, 43 (2022)



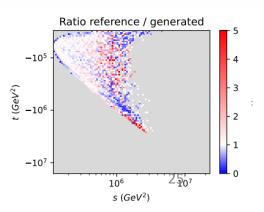
O. Kiss, Quantum computing of the 6Li nucleus via ordered unitary coupled cluster,

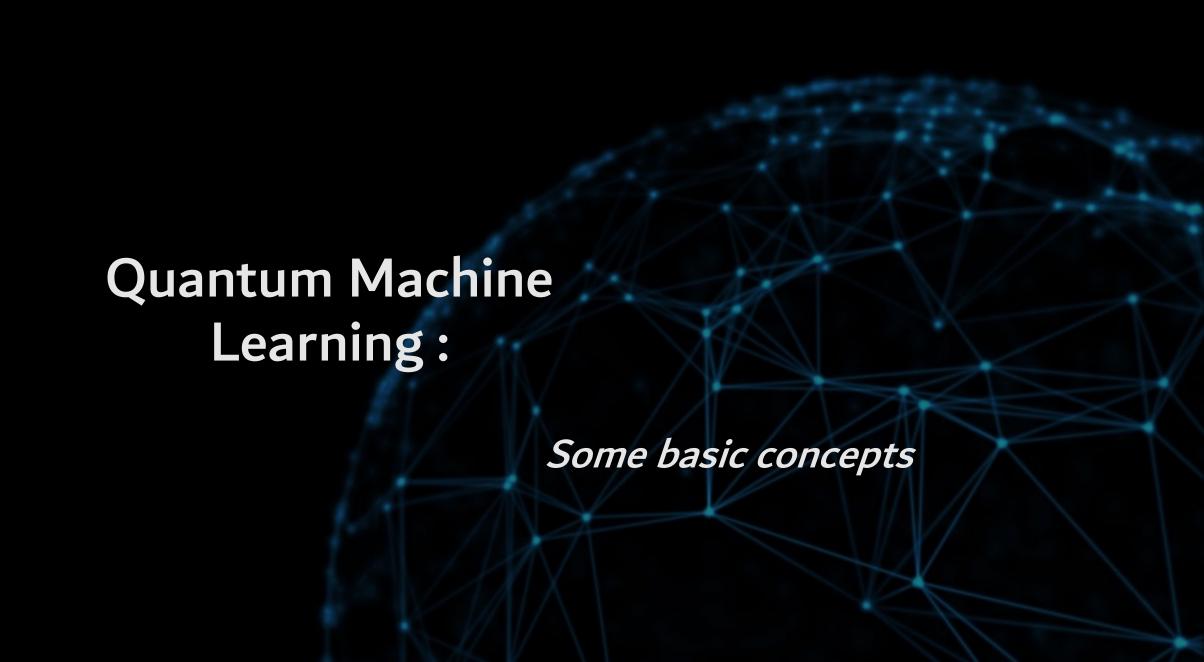
10.1103/PhysRevC.106.034325



Bravo-Prieto, Carlos, et al. "Style-based quantum generative adversarial networks for Monte Carlo events." Quantum 2022

Test Accuracy



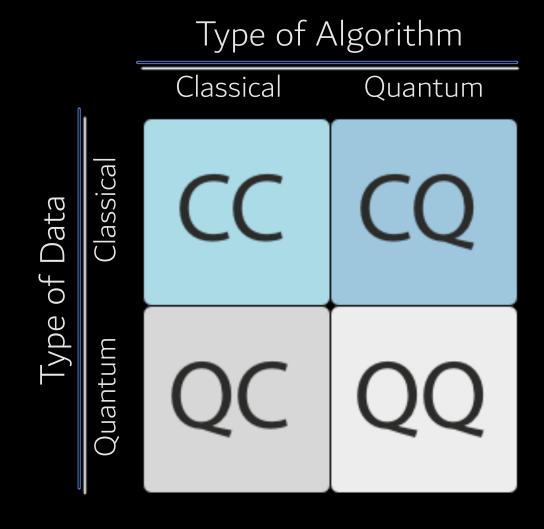


QML in HEP

- Does it make sense to use QML in HEP?
- How do we understand when it is useful?
- Which are the QML models we can leverage?

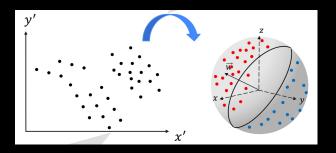
Classical Intractability:

- No established recipe for classical data
- Compromise between algorithm expressivity vs trainability and generalization



(Quantum) ML Lifecycle

Data Preparation



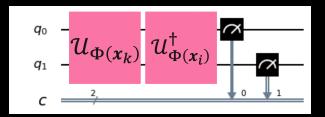
Data Embedding



Model Interpretation

Adapt classical learning models to quantum space

Model Definition



measurement "shots"

Readout and





Model Testing

Model Training

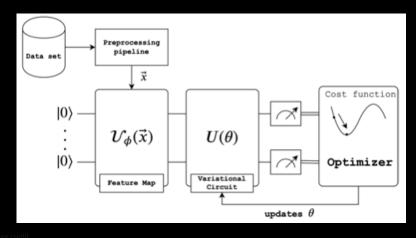
Models

Variational algorithms (ex. QNN)

Gradient-free or **gradient-based** optimization

Data Embedding can be learned

Ansatz design can leverage data symmetries¹



Representer theorem:

Implicit models achieve better accuracy³

Explicit models exhibit better generalization performance

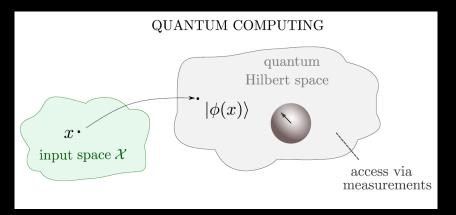
Kernel methods (ex. QSVM)

Feature maps as quantum kernels

Classical **kernel-based training (convex** losses)

Identify classes of kernels that relate to specific data

structures²



Energy-based ML (ex. QBM)

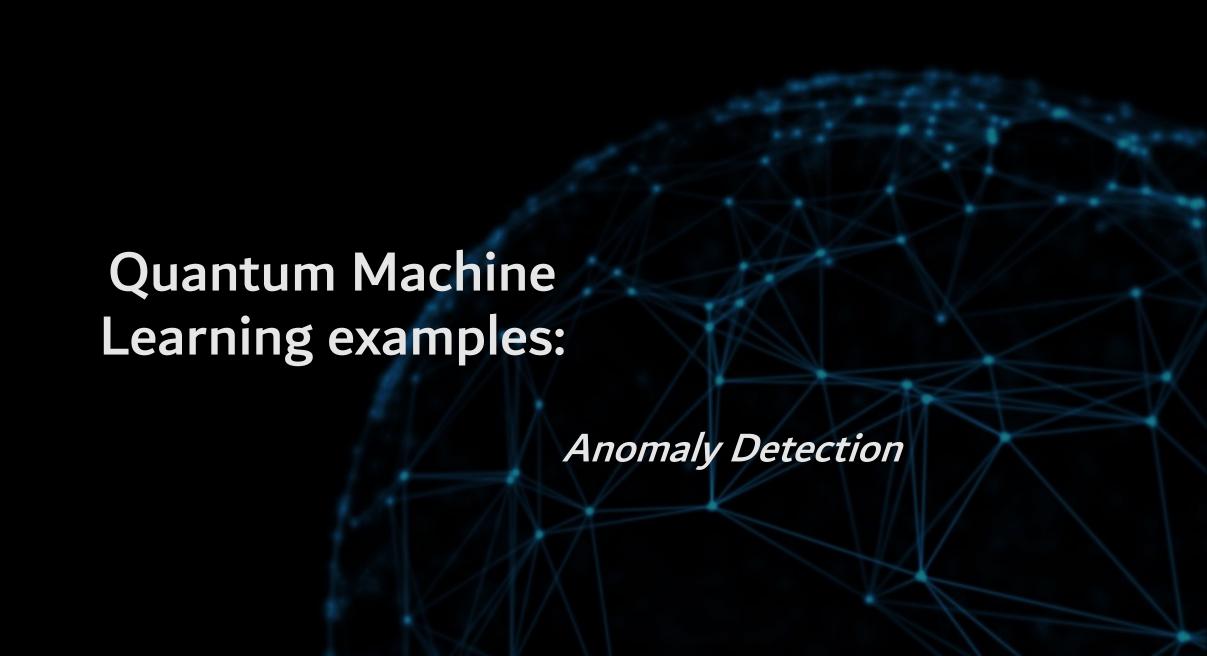
Build network of stochastic binary units and optimise their energy.

QBM has quadratic energy function that follows the Boltzman distribution (Ising Hamiltonian)

¹ Bogatskiy, Alexander, et al. "Lorentz group equivariant neural network for particle physics." PMLR, 2020.

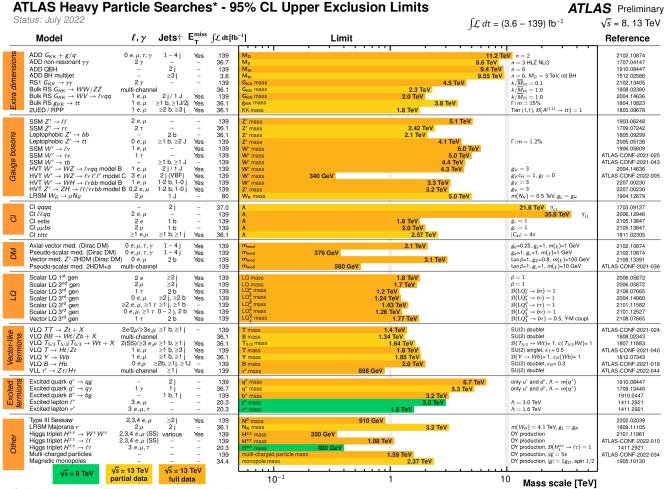
² Glick, Jennifer R., et al. "Covariant quantum kernels for data with group structure." arXiv:2129.03406 (2021).

3 Jerbi, Sofiene, et al. "Quantum machine learning beyond kernel methods." arXiv preprint arXiv:2110.13162 (2021).



New Physics at the LHC

So far only **negative results** in **direct** (model dependent) searches

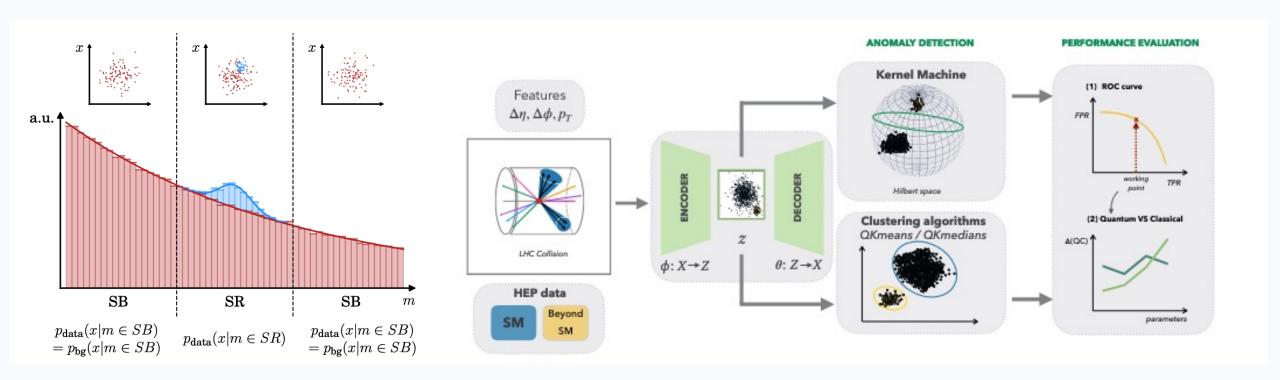


How to insure we do not miss potential discoveries?

We can design model agnostic searches!

Unsupervised learning for Anomaly Detection

Anomaly detection can point to new physics at the LHC



Standard Model jets

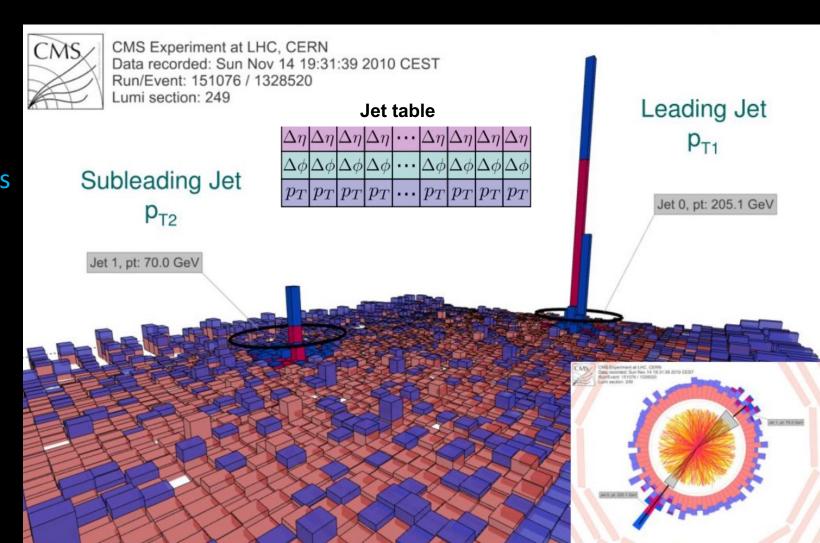
Simulate QCD multi-jets at the LHC

Build jet from 100 highest pt particles

Apply realistic event selection

Convolutional AutoEncoderlearns the jet internal structure

 $\mathbb{R}^{300}
ightarrow \mathbb{R}^{\ell}$, $\ell=4,8,16$

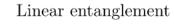


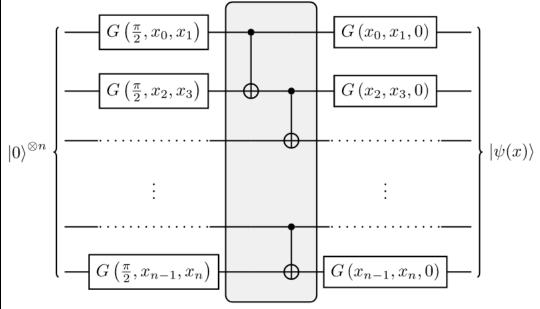
Unsupervised kernel machine

Find the hyperplane that maximizes the distance of the data from the origin of the feature vector space

Upper bound on fraction of anomalies in training data at 0.01 (at most 1% QCD training data are falsely flagged)

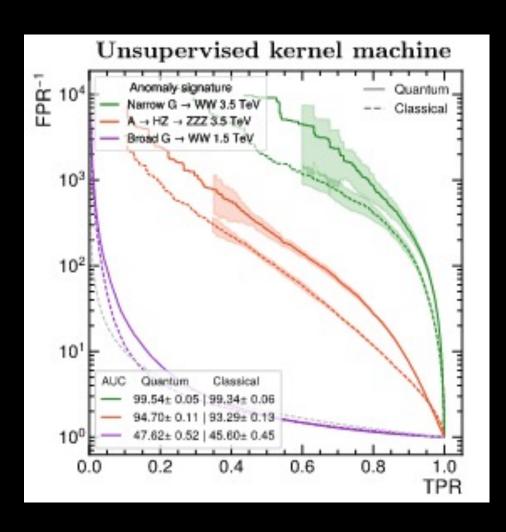
$$k(x_i, x_j) \coloneqq \operatorname{tr}[\rho(x_i)\rho(x_j)] = \left| \langle 0|U^{\dagger}(x_i)U(x_j)|0\rangle \right|^2$$
$$\rho(x_i) \coloneqq U(x_i) \left| 0 \right\rangle \langle 0|U^{\dagger}(x_i)$$





$$\min_{w \in \mathcal{F}, \, \xi \in \mathbb{R}^{\ell}, \, \rho \in \mathbb{R}} \quad \frac{1}{2} ||w||^2 + \frac{1}{\nu \ell} \sum_i \xi_i - \rho$$
subject to $w \cdot \Phi(x_i) \ge \rho - \xi_i, \, \xi_i \ge 0, \, \forall i \quad \nu \in (0, 1)$

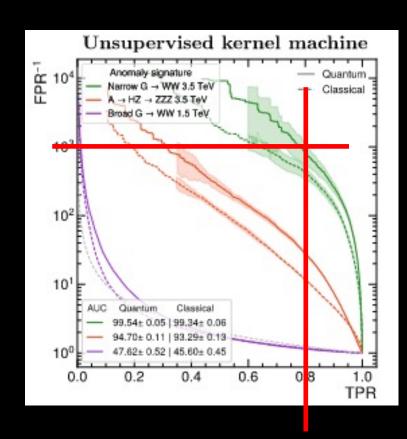
Results



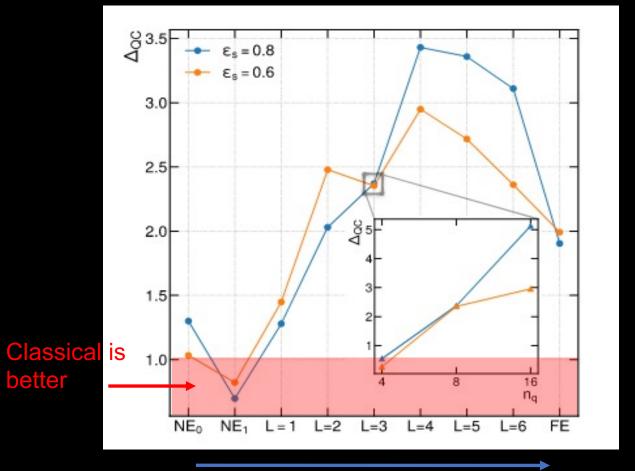
Is this an «advantage» we can use?

Quantum anomaly detection in the latent space of proton collision events at the LHC Vasileios Belis *et al.*, *arXiv:2301.10780*.

In reality....



better



Increasing entanglement & expressivity

Quantum anomaly detection in the latent space of proton collision events at the LHC Vasileios Belis et al., arXiv:2301.10780.

Higher

is better

Quantum Machine Learning examples:

Reinforcement Learning

Reinforcement learning

Trial-and-error learning

• Agent takes actions in environment and collects rewards

state reward r_{t} r_{t+1} r

RL book: Sutton & Barto

Q-learning

- Estimate return using Q-function Q(s, a)
- Learn iteratively using collected interactions
- Once trained, select action greedily

$$a = \arg \max_{a} Q(s, a)$$

State where am I? Where are ghosts, snacks, cookies? Actions up, down, left, right Reward food (+), ghosts (-) Return how much food am I going to eat over time

Free-energy based RL (FERL)

RL performance depends on type of Q-function approximator

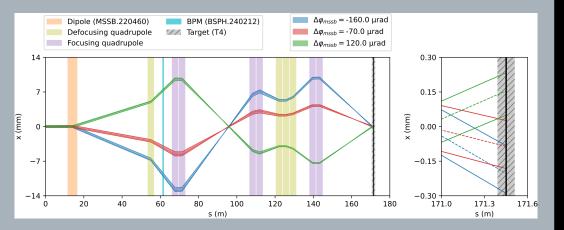
- Classical Deep Q-learning (DQN)
 Feed-forward neural net
- Free-energy based RL (FERL)Quantum Boltzmann machine (QBM)

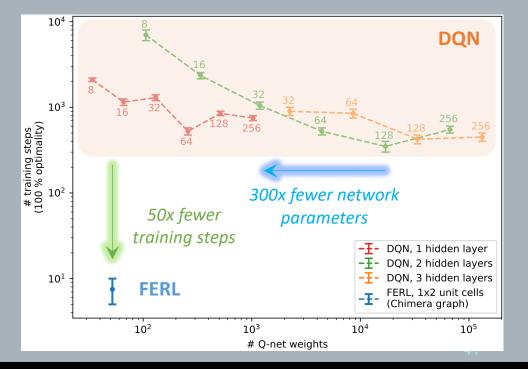
Key concept: sample-efficiency

Relevant for particle accelerator control given cost of beam time (online training)

1st study: 1D beam steering

CERN North Area transfer line (discrete action space)

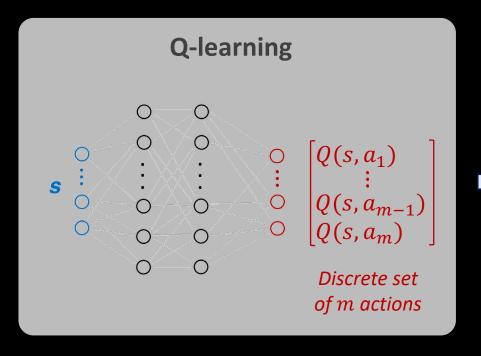


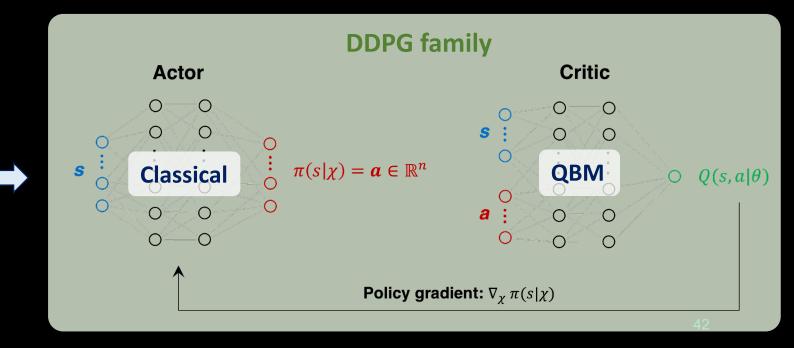


Developing a hybrid actor-critic scheme

Accelerator optimization requires **continuous action space** \Rightarrow **develop hybrid actor-critic algorithm**

QBM replaces classical critic net



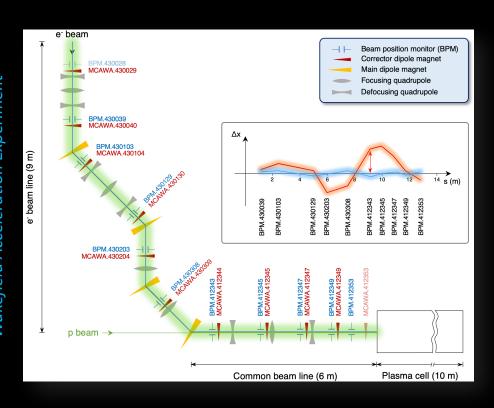


AWAKE: Advanced Proton Driven Plasma Wakefield Acceleration Experiment

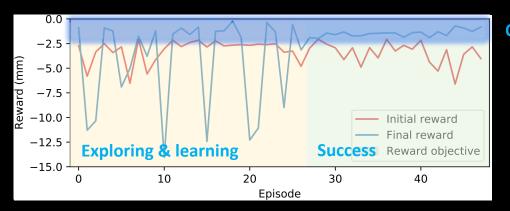
2nd study: 10D continuous beam steering

Environment: e⁻ beam line of AWAKE

- > **Action:** deflection angles at 10 correctors
- > **State:** beam positions at 10 BPMs
- Objective: minimize beam trajectory rms
 - reward: negative rms from 10 BPMs



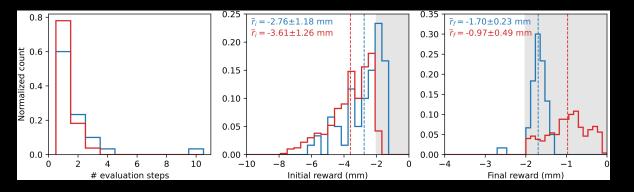
Training: on D-Wave Advantage quantum annealer (QA)



Objective

Evaluation: on actual beam line

Real vs. simulated QA



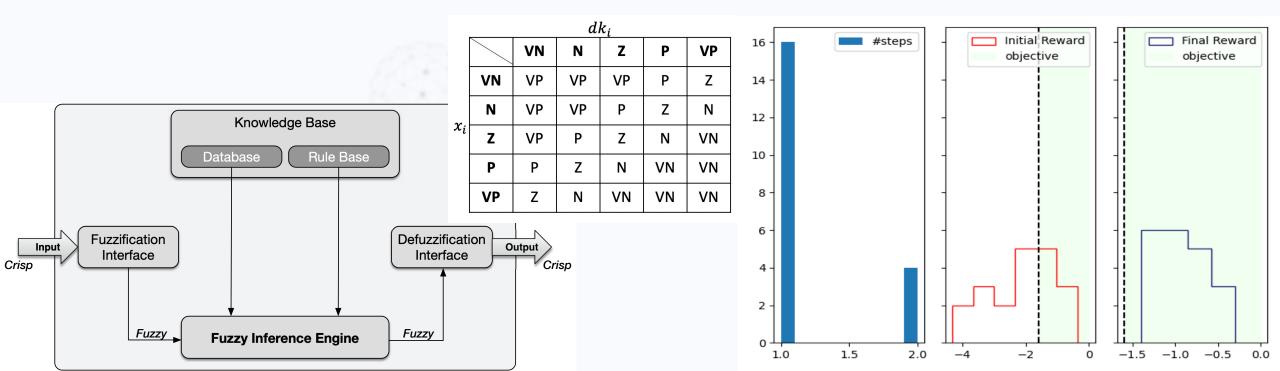
- Agent minimizes rms in 1 step in 60 % cases
- Hyperparameter tuning with simulated QA

1-slide excursion: quantum fuzzy logic controller

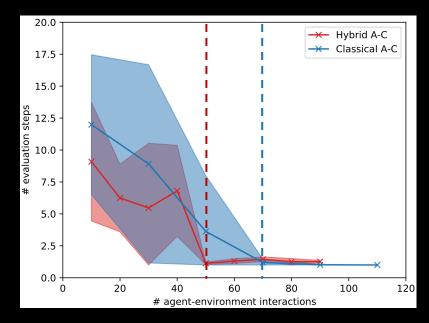
- Alternative control algorithm to RL
- Fuzzy Logic is used to develop control systems based on linguistic rules

 highly interpretable
- Quantum Fuzzy Control System (G. Acampora, R. Schiattarella, A. Vitiello)
 Exploit exponential advantage in computing fuzzy rules on quantum computers
- Successfully evaluated on AWAKE beam line, no training required

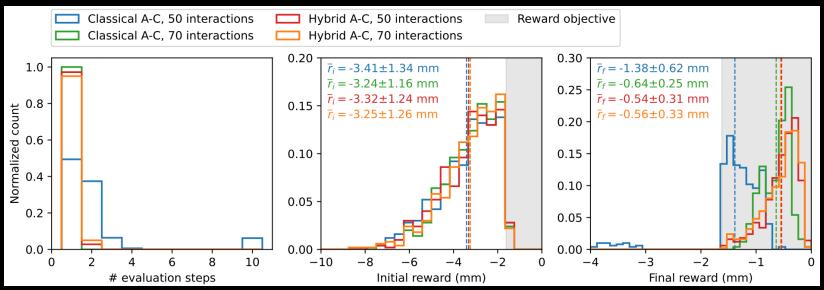
Evaluation: on AWAKE beam line *Objective reached typically in 1 step*



2nd study: 10D continuous beam steering



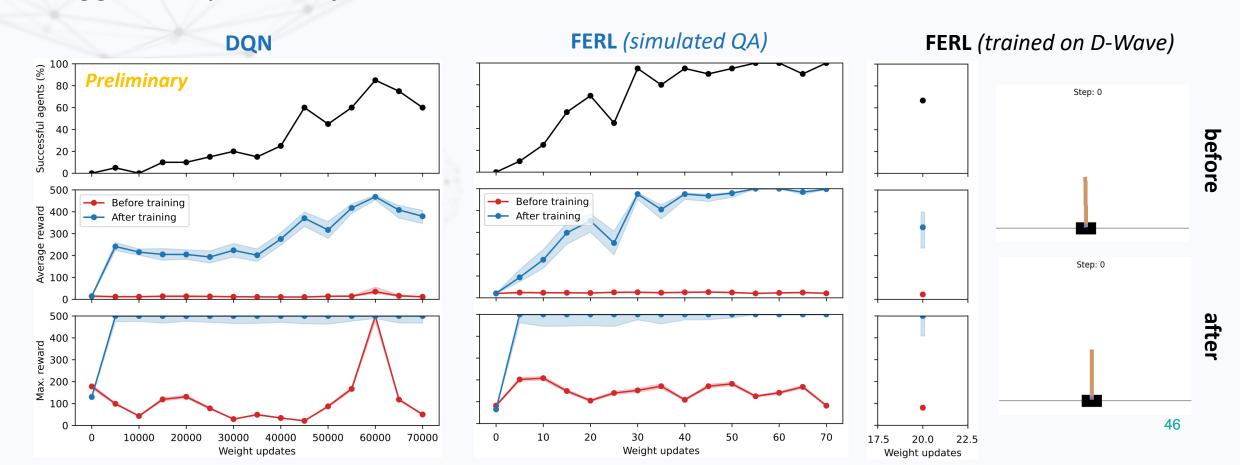
- Hybrid actor-critic (A-C) works
- Minor improvement in terms of sample efficiency 50 vs 70 interactions
- Very few interactions sufficient for both approaches
- Dynamics potentially too simple (linear)

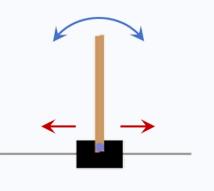


3rd study: Cartpole-v1

Discrete action problem, non-linear dynamics

- Cartpole-v1: official OpenAl gym env from classic control problems domain
- Continuous state (4D), discrete action (right, left) problem with non-linear dynamics
- Terminate episodes after max. 500 steps
- Big gain in sample-efficiency and robustness for FERL vs DQN

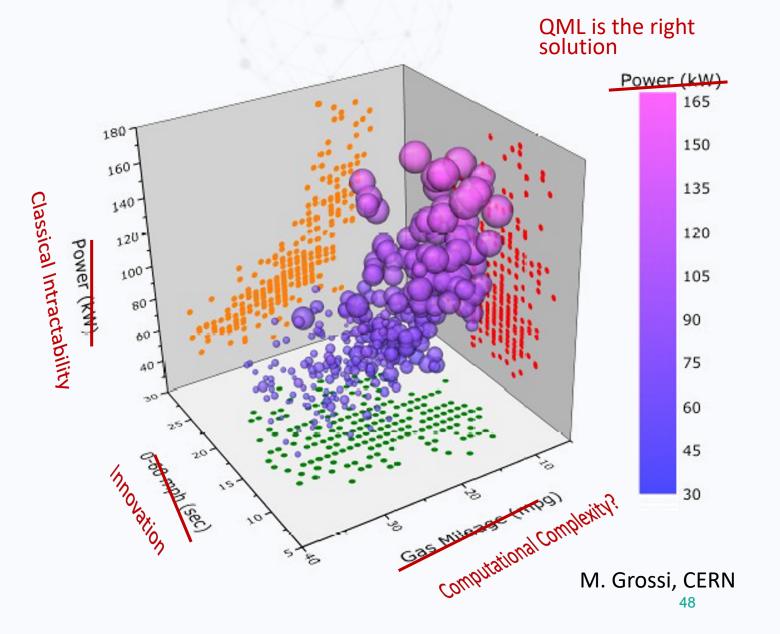




Outlook and open questions

- Quantum technologies could be revolutionary in terms of computing
- HEP provides challenges to Quantum Computing
 - What are the most promising applications?
 - How do we define performance and validate results on realistic use cases?
- Experimental data has high dimensionality
 - Can we train Quantum Machine Learning algorithms effectively?
 - Can we reduce the impact of data reduction techniques?
- Experimental data is shaped by physics laws
 - Can we leverage them to build better algorithms?

QML Exclusion Region in HEP?



Lectures and Hands-On at CERN

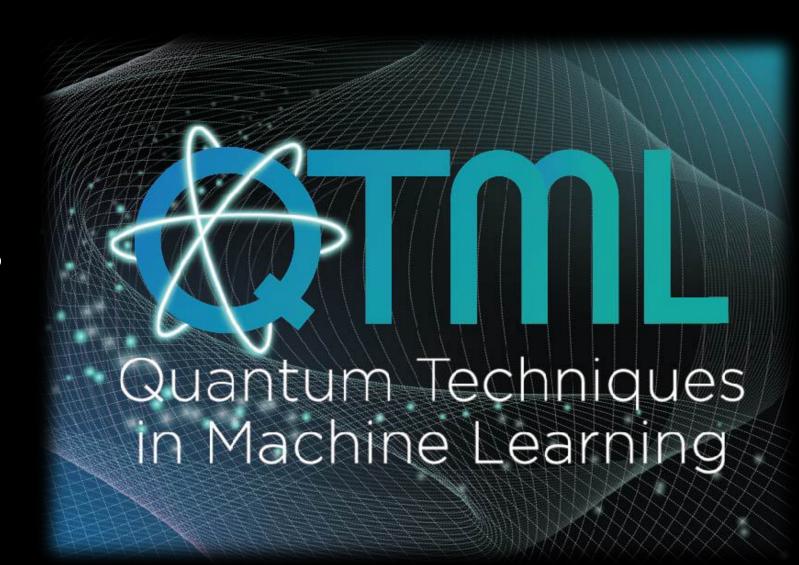
- «A practical Introduction to quantum computing», Elias Combarro https://indico.cern.ch/event/970903/
- «Introduction to quantum computing », Heather Grey https://indico.cern.ch/event/870515/
- A set of two hands-on (introduction) sessions for summer students (2023 openlab summer student lectures)

https://indico.cern.ch/event/1293871/

https://indico.cern.ch/event/1293874/

Thank you!

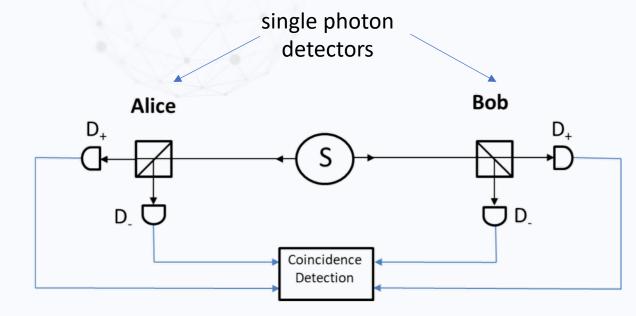
November 20th-24th, 2023 @CERN



Sofia.Vallecorsa@cern.ch

Bell Inequalities

- 1964: Bell inequality are a mathematical proof that no theory based on local hidden variables (realism) can reproduce QM results
- 1969: Clauser, Horne, Shimony (CHSH) formulation



- Measure the correlation $E(a, b) = (N_{++} N_{+-} N_{-+} + N_{--})/(N_{++} + N_{+-} + N_{-+} + N_{--})$
- Where N_{++} , N_{+-} , N_{-+} , and N_{--} are the number of coincidence events corresponding to the simultaneous detection

NB in a realist theory the measurement outcome is «known» even if the measurement is not performed

Bell Inequalities

For experimental outputs of the form $A_1 = \pm 1$

$$A_1(B_1 + B_2) + A_2(B_1 - B_2) = \pm 2,$$

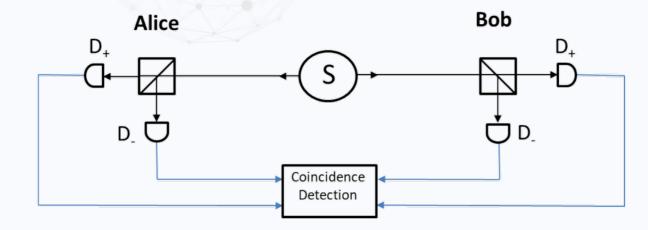
since
$$B_1 + B_2 = \pm 2$$
 and $B_1 - B_2 = 0$ or v.v.

Performing the experiment many times, the correlation is calculated using the ensemble average over the measurements

$$E(a_1, b_1) = \langle A_1, B_1 \rangle$$

 $S = |E(a_1, b_1) + E(a_1, b_2) + E(a_2, b_1) - E(a_2, b_2)|$

Classical theory: S < 2



Quantum mechanics: $S = 2\sqrt{2}$

since
$$E(a_1, b_1) = -\boldsymbol{a}_1.\boldsymbol{b}_1$$
 for $|\psi_-\rangle$

and experiment directions can be chosen so that:

$$a_1. b_1 = a_1. b_2 = a_2. b_1 = -a_2. b_2 = 1/\sqrt{2}$$