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

2020: Hefei National Lab

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

https://www.nature.com/articles/d41586-020-03434-7

Source: McKinsey 2023
Announcement of the 2022 Nobel Prize in Physics

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

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

https://youtu.be/mtgYG2zsbbQ
The Einstein Podolsky Rosen (EPR) Paradox

\[ |\psi_{\pm}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle) \]

extinguished pairs

- 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’


For arbitrary \(a, b\) measurement directions the probability to measure opposite spin values is

\[ \frac{1}{2} (1 + a \cdot b) \]
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 resource
- 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:
  • Aguilar-Saavedra and Casas. "Improved tests of entanglement and Bell inequalities with LHC tops." *The European Physical Journal C* 82.8 (2022): 666

$t\bar{t}$ production at hadron colliders:
• Leading mechanism generates top spins that are highly correlated
• Tops decay semi-weakly before spin is randomised
• Charged lepton from $t\rightarrow Wb, W\rightarrow \ell v$ is 100% correlated with top spin

Quantum Technology

First Quantum Revolution
Max Planck black-body radiation
Transistor, laser, atomic clock, computers, optical fibre communication, ...

Second quantum revolution
Use quantum mechanics principles to develop new technology
“Artificial” quantum states

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

\[ |\psi\rangle = \alpha |0\rangle + \beta |1\rangle \]
\[ \alpha, \beta \in \mathbb{C} \quad |\alpha|^2 + |\beta|^2 = 1 \]

Interest in multi level representations: qutrits..
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

Multiple technologies

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

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](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.

\[ H(t) = A(t)H_0 + B(t)H_p \]

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 quantum-classical infrastructure**
  - Engineering, cooling, I/O
  - Hybrid algorithms, QPU as accelerators

What the future brings

An example quantum roadmap from IBM
Prototype quantum software applications ➔ Quantum software applications

Quantum algorithm and application modules

Machine learning | Natural science | Optimization

Quantum Serverless
Intelligent orchestration | Circuit Knitting Toolbox | Circuit libraries

Circuits

Dynamic circuits ➔ Threaded primitives ➔ Error suppression and mitigation ➔ Error correction

Falcon 27 qubits
Hummingbird 65 qubits
Eagle 127 qubits
Osprey 433 qubits
Condor 1,121 qubits
Flamingo 1,386+ qubits
Kookaburra 4,158+ qubits
Heron 133 qubits x p
Crossbill 408 qubits

https://www.ibm.com/quantum/roadmap
• 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

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

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

Quantum Algorithms for:
Sampling, searches
Linear algebra
Cryptography and communication

Re-think algorithms design
Define fair benchmarking

Potential applications:
• Monte Carlo and Event Generation
• Quantum Simulation
• Pattern Recognition
• Quantum Machine Learning
QC @CERN


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

Quantum Machine Learning: Some basic concepts
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

The advantage of many known QML algorithms is impeded today by I/O bottleneck.
**Variational algorithms (ex. QNN)**

- Gradient-free or gradient-based optimization
- Data Embedding can be learned
- Ansatz design can leverage data symmetries

**Kernel methods (ex. QSVM)**

- Feature maps as quantum kernels
- Classical kernel-based training (convex losses)
- Identify classes of kernels that relate to specific data structures

**Energy-based ML (ex. QBM)**

- Build network of stochastic binary units and optimise their energy
- QBM has quadratic energy function that follows the Boltzmann distribution (Ising Hamiltonian)

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**Models**

Quantum Machine Learning examples:

Anomaly Detection
**New Physics at the LHC**

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

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**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 AutoEncoder learns the jet internal structure

\[ \mathbb{R}^{300} \rightarrow \mathbb{R}^\ell, \ell = 4, 8, 16 \]
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)
Results

Is this an «advantage» we can use?

Quantum anomaly detection in the latent space of proton collision events at the LHC
Quantum anomaly detection in the latent space of proton collision events at the LHC


In reality....

Higher is better

Classical is better

Increasing entanglement & expressivity
Quantum Machine Learning examples:

Reinforcement Learning
Reinforcement learning

... in a nutshell

Trial-and-error learning

- Agent takes actions in environment and collects rewards

Q-learning

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

Example: Pacman

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)
Developing a hybrid actor-critic scheme

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

- QBM replaces classical critic net

Q-learning

![Q-learning diagram]

Discrete set of $m$ actions

**DDPG family**

Actor

Classical

$\pi(s|\chi) = a \in \mathbb{R}^n$

Critic

QBM

$Q(s, a|\theta)$

Policy gradient: $\nabla_{\chi} \pi(s|\chi)$
2\textsuperscript{nd} study: 10D continuous beam steering

**Environment:** e\textsuperscript{-} 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)

**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)
  ➡ Move towards more complex RL benchmarks
3rd study: Cartpole-v1

Discrete action problem, non-linear dynamics

- **Cartpole-v1**: official OpenAI 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

**DQN**

**FERL (simulated QA)**

**FERL (trained on D-Wave)**

![Graphs showing performance improvements for DQN and FERL](image-url)
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?

QML is the right solution

M. Grossi, CERN
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!

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@CERN

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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 \( E(a_1, b_1) = -a_1 \cdot b_1 \) for \( |\psi_\pm\rangle \)

and experiment directions can be chosen so that:

\[
a_1 \cdot b_1 = a_1 \cdot b_2 = a_2 \cdot b_1 = -a_2 \cdot b_2 = 1/\sqrt{2}
\]