Progress towards scalable QC algorithms for HEP

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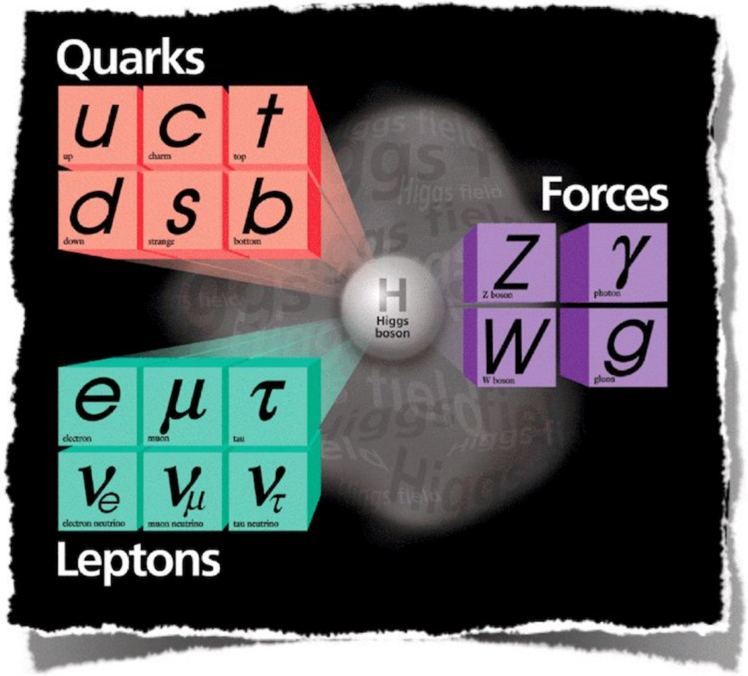
LHCb

The Standard Model of Particle Physics

A **successful** theory that describes the interactions among particles ...



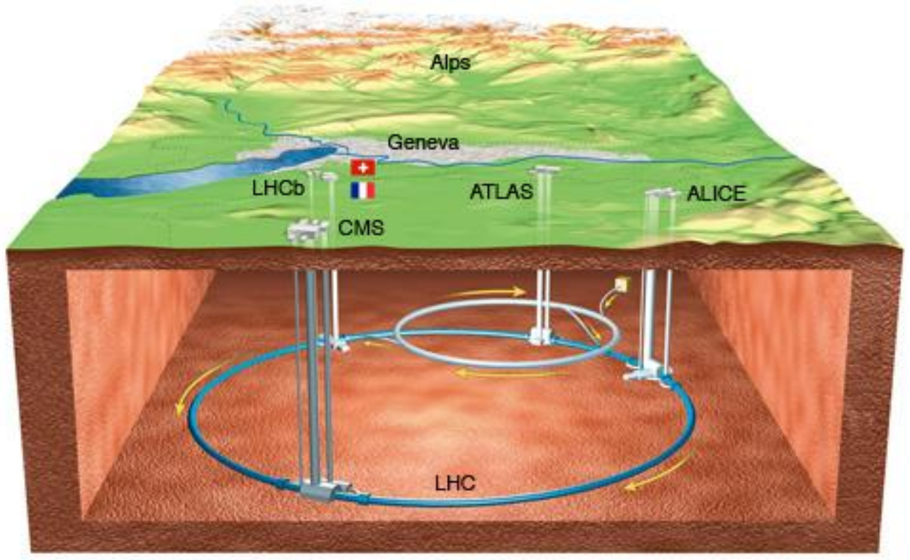
... **but** fails to explain several phenomena observed in the Universe:

- Neutrinos masses
- Origin of Dark Matter & Dark Energy
- etc

⇒ need of Beyond the Standard Model physics!!

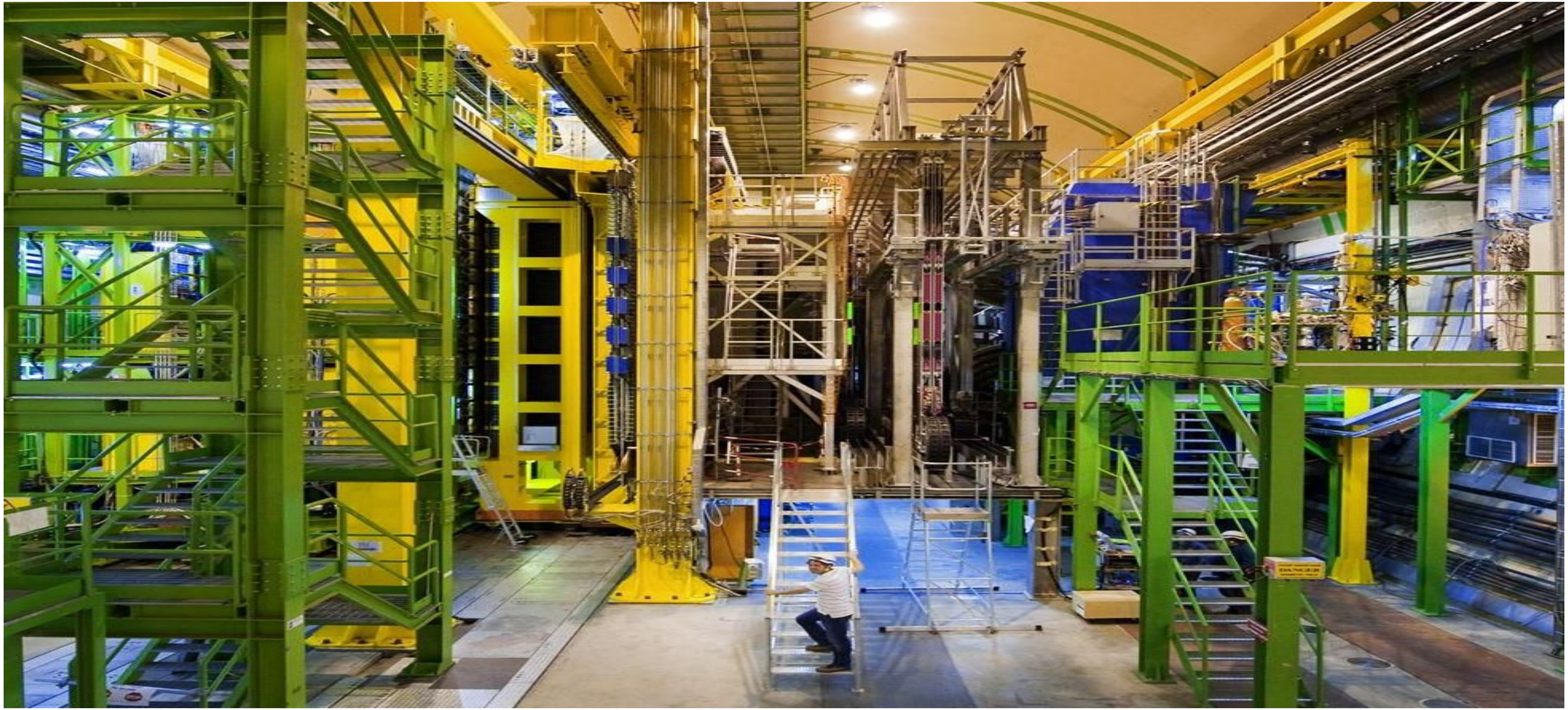
The LHCb detector

One of the 4 main experiments @ **L**arge **H**adron **C**ollider at CERN



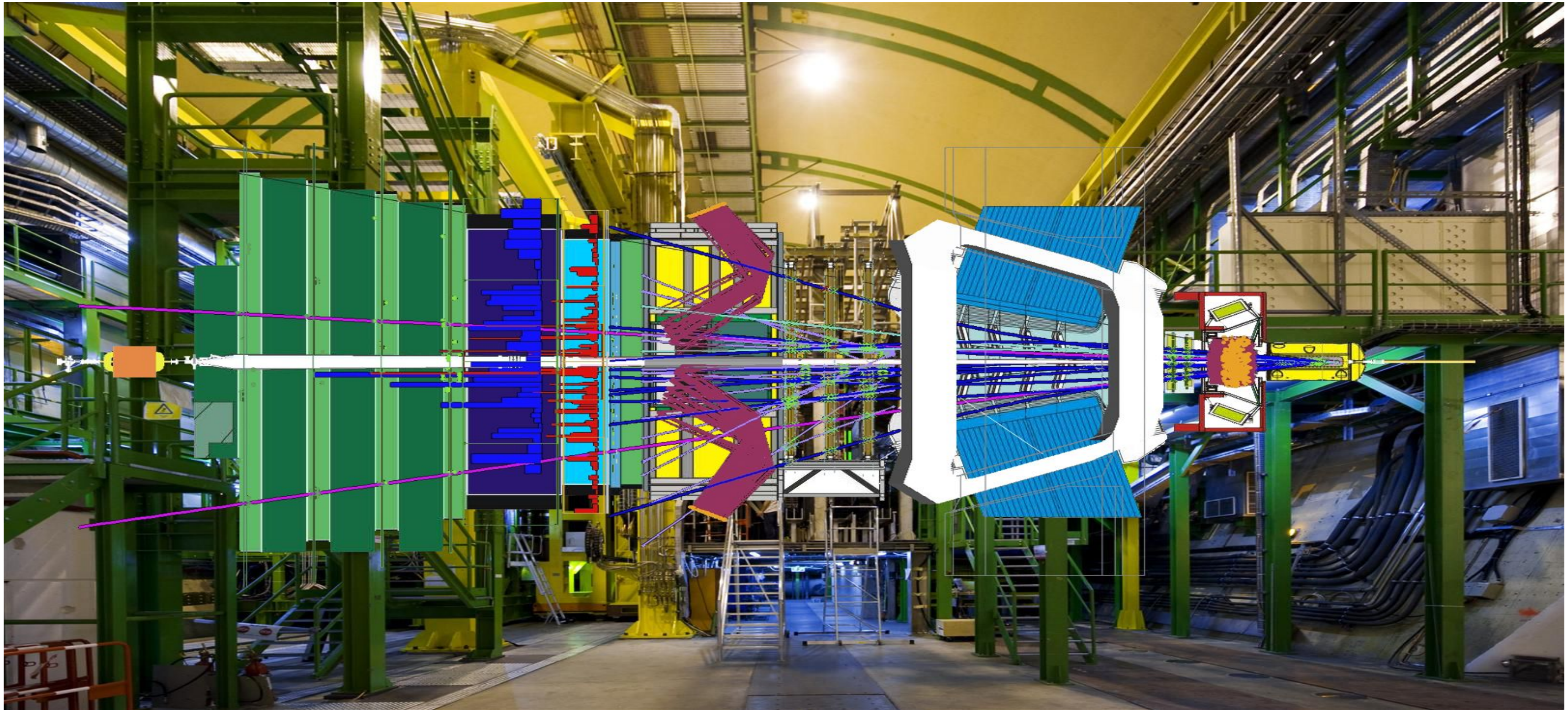
- Initially designed for the study of the **b,c-quarks**
- Now evolved into a general purpose spectrometer in the forward region
- Look for hints of BSM physics

How does an event look like?



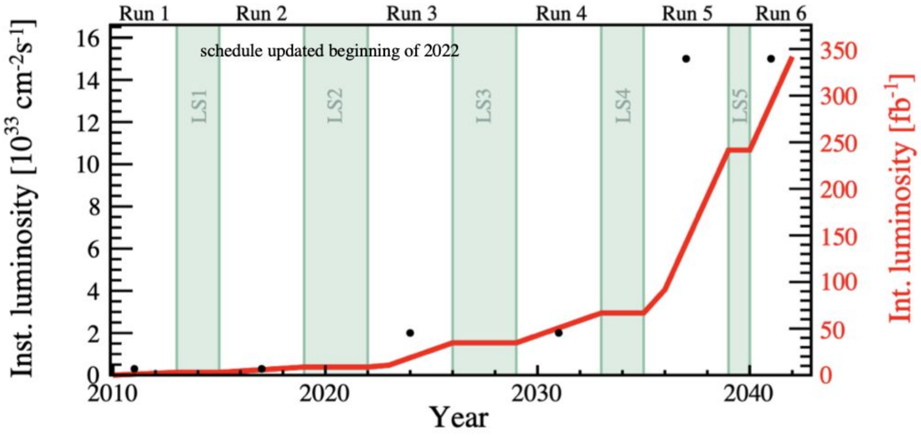
How does an event look like?

Reconstruct events **40 Million times per second**.

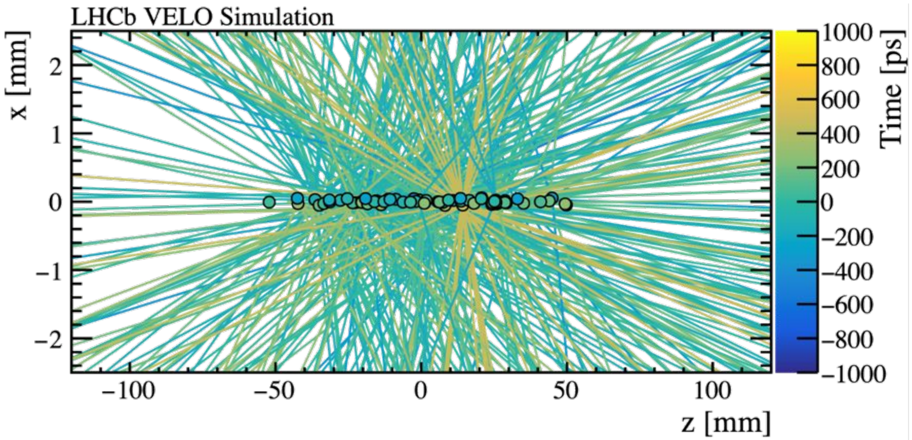


Motivation for QC

- New algorithms and architectures needed to deal with the increased luminosity & limited bandwidth @ **HL-LHC**



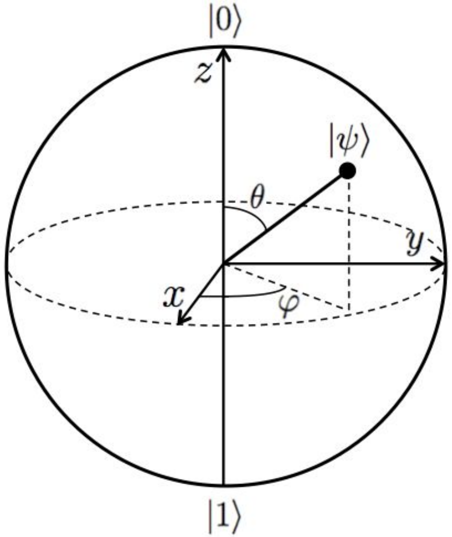
ECFA



Courtesy of Robbert Geertsema

Quantum Computing in a nutshell

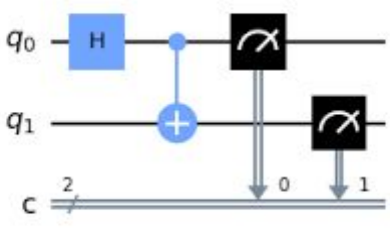
- Instead of **bits** we use qubits, the fundamental units of quantum information
  - Not 0 **or** 1, but a two-state quantum system → coherent superposition of both
  - They can be **measured** → probabilistic results
- There are quantum logic gates that operate on these qubits
  - Unitary transformations
  - Quantum gates can be **single** or **multiple**



$$|0\rangle = \binom{1}{0},\ |1\rangle = \binom{0}{1}$$
$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

Quantum Computing in a nutshell

A sequence of gates acting on a register of qubits is called a quantum circuit



Some computational problems can profit from Quantum Computing using the principles of superposition and interference.

https://quantumalgorithmzoo.org/

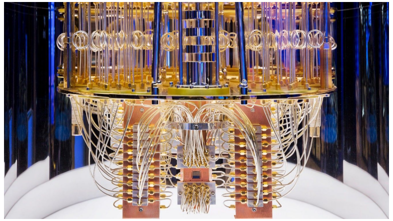
Quantum Computing - Hardware

Several technologies are being explored as physical qubits:

Superconducting

OQC IBM Google

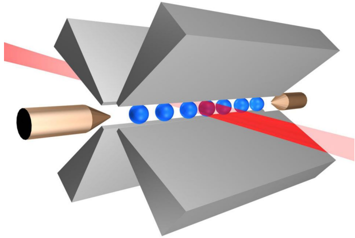
Superconducting electric circuits at 10mK behave as quantum systems with discrete energy levels



Trapped ions

IONQ QUANTINUUM

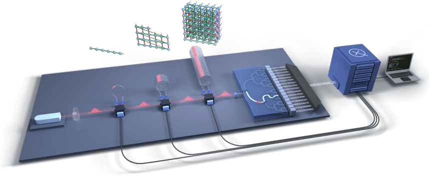
Charged atoms constrained in electromagnetic traps and manipulated with laser



Optical

XANADU

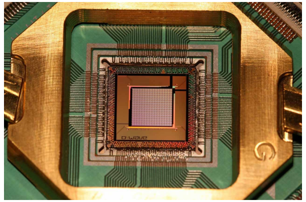
Linear optics devices using photons as information carriers



Annealing

D-Wave The Quantum Computing Company™

Ising-chain qubits interacting with a customizable Hamiltonian

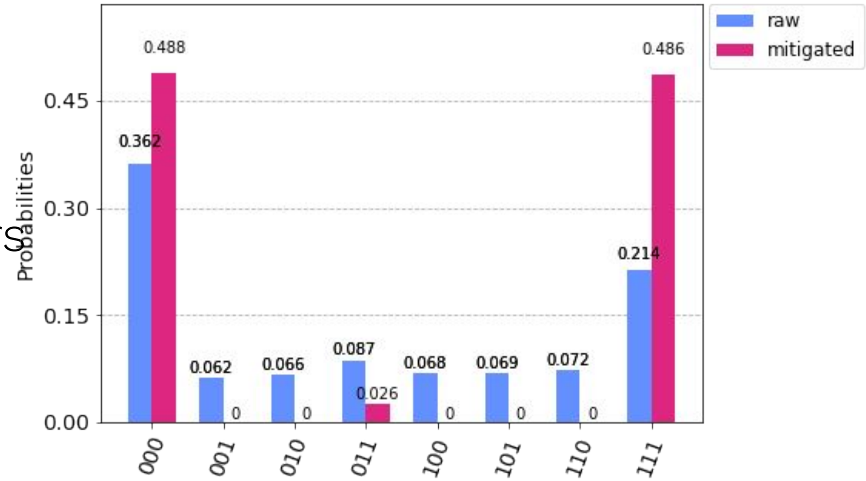


Quantum Computing - Noise

All the previous technologies are far from being perfect. Current qubits are **noisy**:

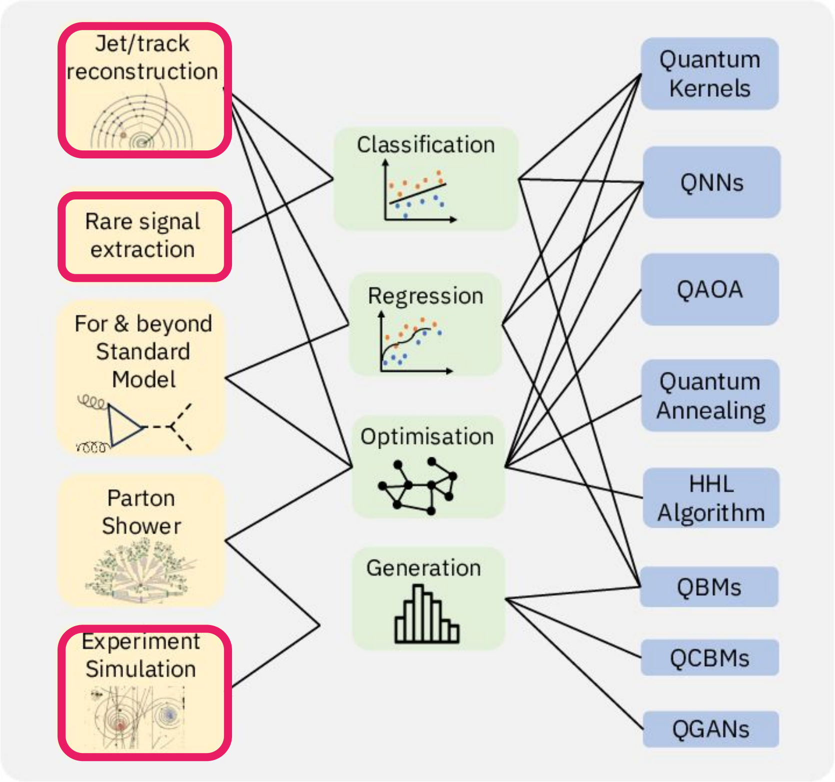
- Measurement errors
- 1-qubit and 2-qubit gates fidelities
- T1 and T2 decoherence time
- Calibration errors

→ *Noise Error Mitigation*



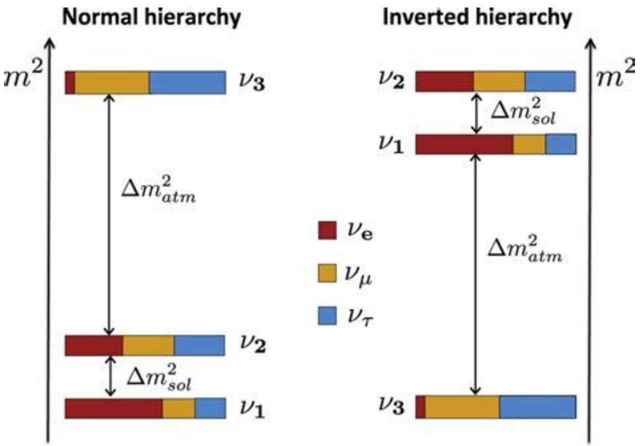
HEP use-cases

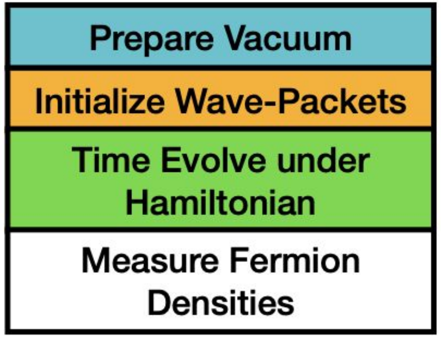
- [Summary of the QC4HEP WG]
- Focused mostly in projects concerning experimental particle physics at LHC
- Datasets are **quantum** in nature, but measurements are **classical**
- Quantum sensing not covered in this talk

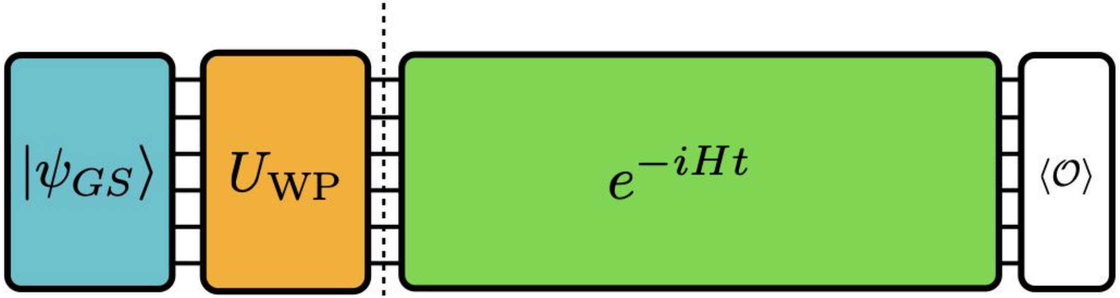


HEP use-cases

- QC for Lattice QCD [arXiv:2302.00467]
- QC and Neutrino oscillations
  - also using qutrits [arXiv:2503.00607]
- Fermionic Wave Packet Scattering [arXiv:2312.02272]



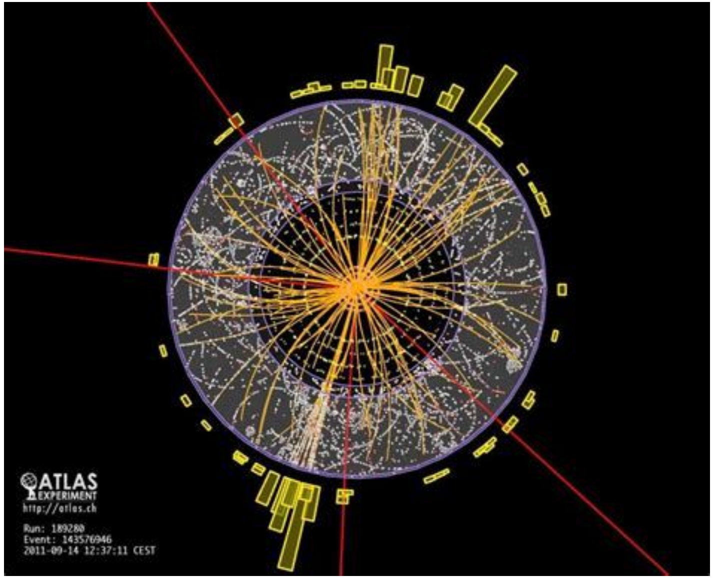




Quantum Computing & Track Reconstruction

Track reconstruction

- Recover the original trajectories from signals left by charged particles
  - signals → 3D points or hits
  - need efficient distinction between the combinations of hits that are of interest and those that aren't
- Typical event: large number of tracks, modelled by a collection of segments

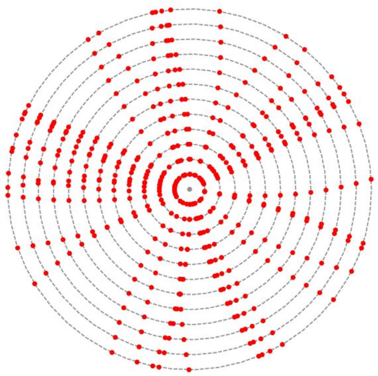


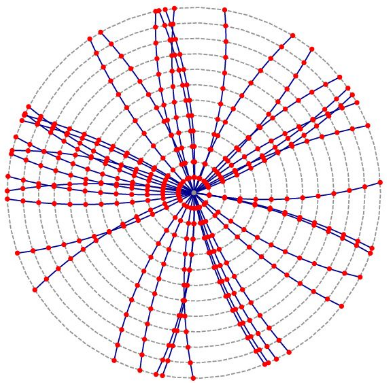
Track Reconstruction

- **Local tracking methods:** steps are performed sequentially. Some studies exist on QC for local tracking methods [arXiv:2104.11583]
- **Global tracking methods:** all hits are processed by the algorithm in the same way. Global algorithms are **clustering** algorithms. E.g.: QAOA, quantum annealing, Hopfield Networks, Hough transform

→ LHCb's current method of search by triplet

→ Focus of this talk: *global* algorithms





QC for Track Reconstruction

- QC has very interesting prospects of improvements in algorithm **complexity/timing**
- This talk: two track reconstruction algorithms
- Define **Ising-like** $H^{TrackReco}$(hits):

$$H = -\frac{1}{2}\sum_{ij}\omega_{ij}\sigma_z^i\sigma_z^j - \sum_i \omega_i\sigma_z^i$$

→ $\mathbf{H_{min}^{TrackReco}}$ == solution with the correct reconstructed tracks

HHL for Track Reconstruction [*JINST* 18 (2023) 11, P11028]

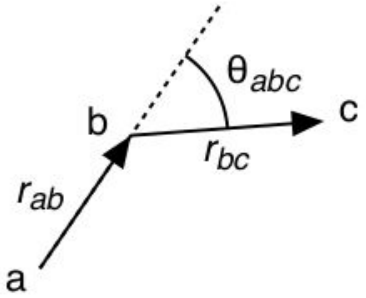
Differentiable Hamiltonian:

$$\nabla\mathcal{H} = 0 \Rightarrow A\mathbf{S} = \mathbf{b}$$

HHL: QC algorithm to solve the **system of linear equations**

Segment [S_{ab}]: combination of hit *a* and hit *b*
→ in consecutive layers - for now

Hamiltonian accounts for **all** possible segments



HHL for Track Reconstruction [JINST 18 (2023) 11, P11028]

$$\mathcal{H}(\mathbf{S}) = -\frac{1}{2}\left[\sum_{abc} f(\theta_{abc}, \varepsilon) S_{ab} S_{bc} + \gamma \sum_{ab} S_{ab}^2 + \delta \sum_{ab} (1 - 2S_{ab})^2\right]$$

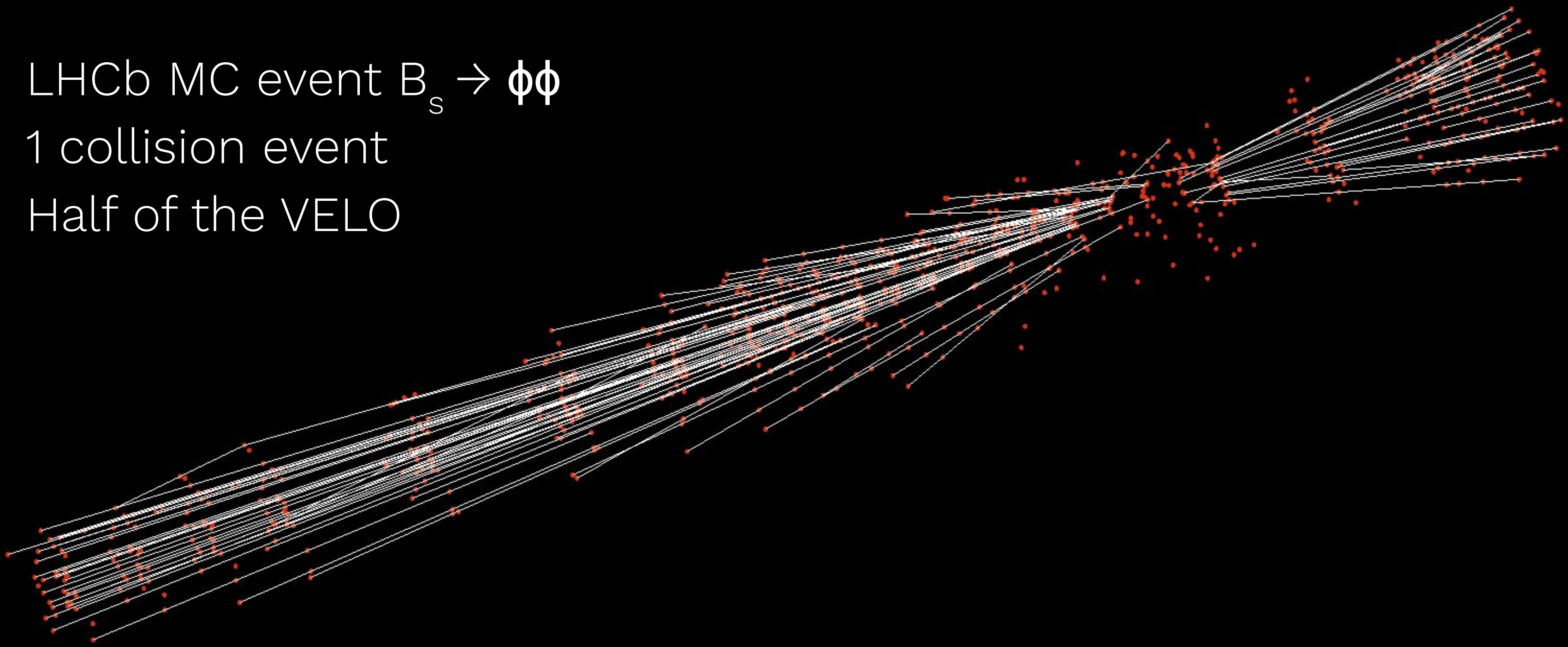
angular term (a) (b)

$$f(\theta_{abc}, \varepsilon) = \begin{cases} 1 & \text{if } \cos\theta_{abc} \geq 1 - \varepsilon \\ 0 & \text{otherwise} \end{cases}$$

- **(a) regularization term**: makes the spectrum of A positive
- **(b) gap term**: ensures gap in the solution spectrum

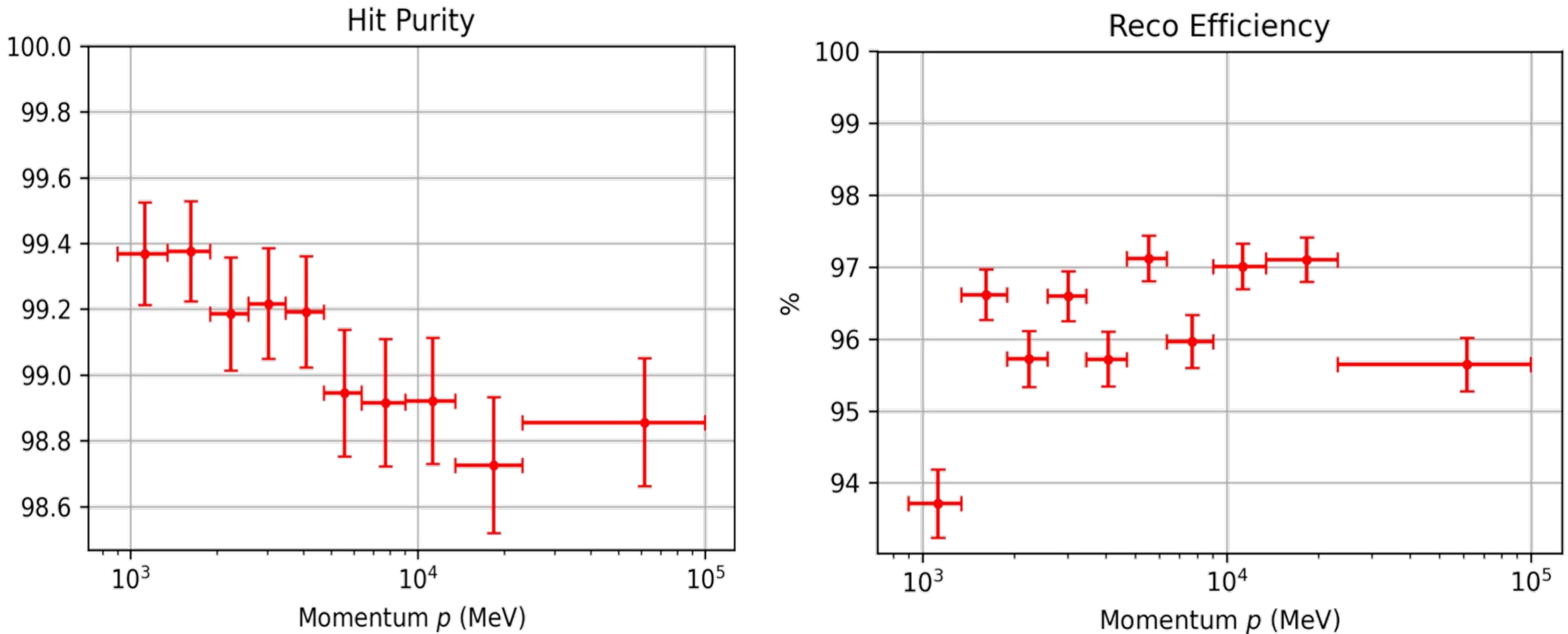
Validation with a classical linear solver

LHCb MC event $B_s \rightarrow \phi\phi$
1 collision event
Half of the VELO



Tracking performances with classical solver

- Very good performance **with LHCb MC**. Integrated fake rate: 4.3%

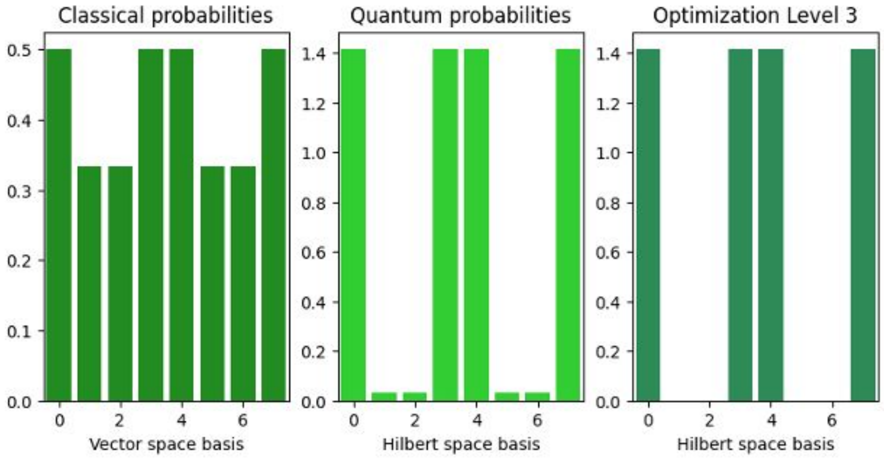


Updates since publication

Significant amount of progress ongoing to improve circuit depth

- E.g. 1-bit phase estimation
+ Work ongoing on optimal output retrieval

→ talk with current results at **CHEP**



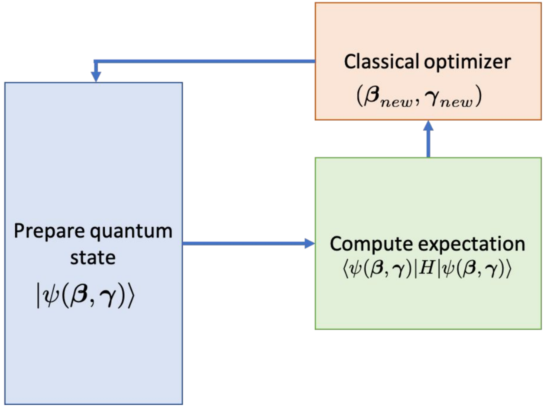
QAOA for Track Reconstruction

- Quantum Approximate Optimization Algorithm [arXiv:1411.4028]
- A variational algorithm ideal to solve combinatorial optimization problems, e.g. Max-Cut problem
    - *'Finding an optimal object out of a finite set of objects'*

$$|\psi(\beta,\gamma)\rangle = U(\beta)U(\gamma)...U(\beta)U(\gamma)\,|\psi_0\rangle$$

$$U(\beta) = e^{-i\beta H_B},\ U(\gamma) = e^{-i\gamma H_P}$$

- H_B: mixing Hamiltonian, H_P: **problem** Hamiltonian
- **Goal:** find optimal parameters **$(\square_{opt}, \gamma_{opt})$** such that the quantum state encodes the solution to the problem



QAOA implementation

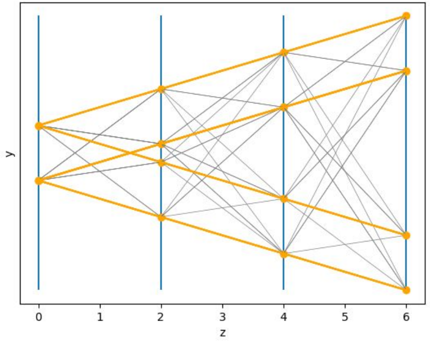
$$\mathcal{H} = -\frac{1}{2}\left[\left(\sum_{a,b,c}\frac{\cos^{\lambda}(\theta_{abc})}{r_{ab}+r_{bc}}s_{ab}s_{bc}\right) - \alpha\left(\sum_{b\neq c}s_{ab}s_{ac}+\sum_{a\neq c}s_{ab}s_{cb}\right) - \beta\left(\sum_{a,b}s_{ab}-N\right)^2\right]$$

(1) (2) (3)

(1) main term: favours aligned, short segments
(2) 1st penalty term: forbids segments that share head/tail from belonging to the same track
(3) 2nd penalty term: keeps the number of active segments equal to #hits

Results and ongoing work

- Irreducible memory issues
- Triplets instead of doublets don't help → worse scalability
- Rydberg atoms - ToDo
- Distributed QAOA (OakRidge)
- Modified QAOA
- sub-QUBO approach?



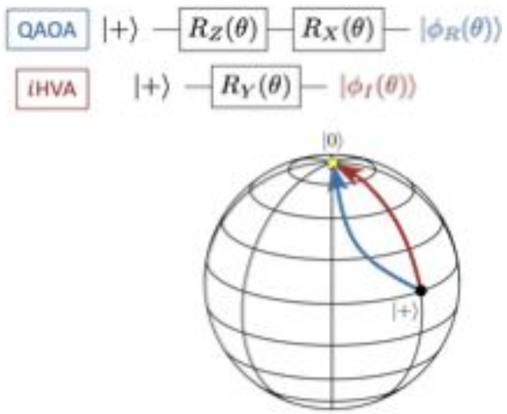
# tracks	# layers	#qubits (segments)	Circuit depth
2	3	8	103
2	4	12	223
3	3	18	497
3	4	27	1105
4	3	32	1553
4	4	48	3473
5	3	50	3775
5	4	75	8463

iHVA (C. Tüysüz et al., DESY)

- QITE-inspired
- Avoid Barren Plateaus from QAOA
- Not unique set of gates possible
- Geodesics for parametrized quantum circuits also considered by people at IFIC

[arXiv:2408.09083, Presentation at QC4HEP]

Target Hamiltonian: -Z



The iHVA follows the geodesic.
This leads to faster convergence.

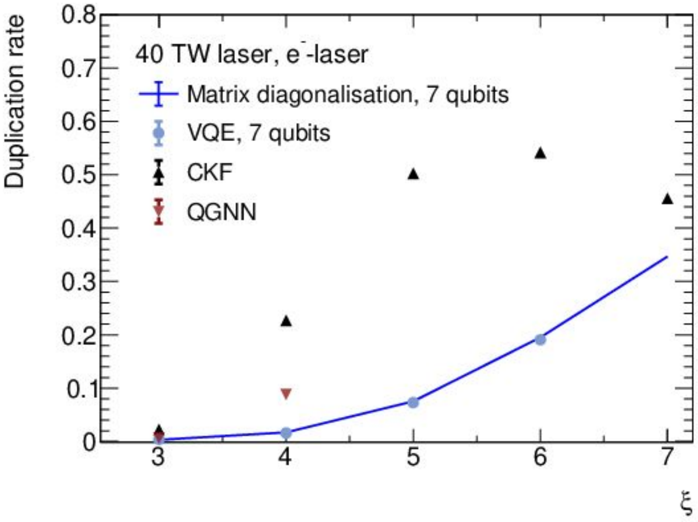
LUXE [arXiv:2304.01690]

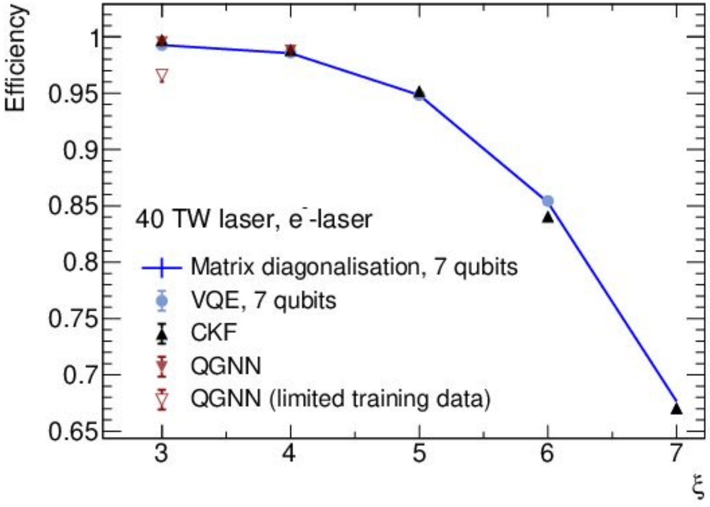
- Tracking of positrons traversing 4 layers of tracking detectors
- Several methods:
  - VQE
  - Combinatorial Kalman Filter using triplets of hits
  - (q)GNN where each hit is a node

$$O = \sum_{i}^{N} \sum_{j<i} b_{ij} T_i T_j + \sum_{i=1}^{N} a_i T_i \quad T_i, T_j \in \{0, 1\}$$

LUXE [arXiv:2304.01690]

Variational Quantum Eigensolver: hybrid quantum-classical algorithm

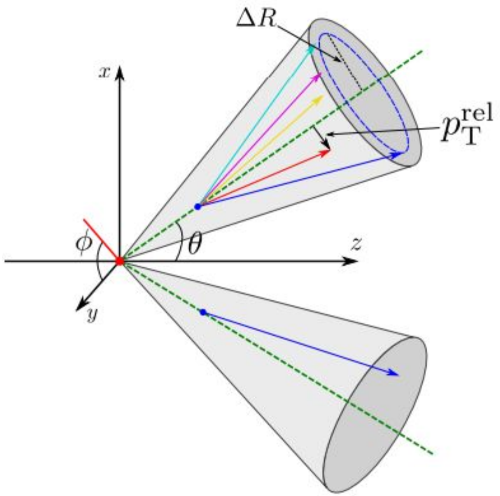


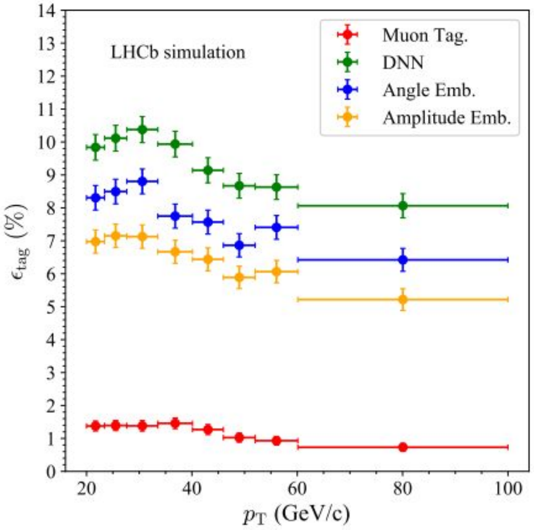


QML for b-jet flavour tagging

b-jet flavour tagging [JHEP 08 (2022) 014]

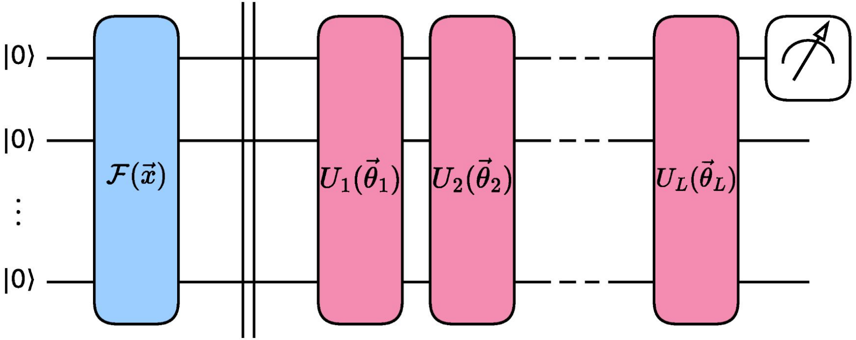
- Identify if a jet contains a hadron formed by a **b** or **anti-b** quark at the moment of production
  - (Q)ML algorithm that uses variables from the particles of the jets to do so
- Deep Neural Network vs 16-qubit **Variational Quantum Classifier**





Entropy studies

Study of the Entropy production within a Variational Quantum Circuit during its training phase:
Goal: Use the information of the entropy values to enhance the training performance for the task of jet-tagging (b vs c)



Values of Entropy were inspected

- For each training step “t”
  - At each “depth” of the circuit:
    - depth 0 : $\mathcal{F}(\vec{x})\left|0^{\otimes N}\right\rangle$
    - depth 1 : $U_1(\vec{\theta}_1)\mathcal{F}(\vec{x})\left|0^{\otimes N}\right\rangle$
    - depth L : $U_L(\vec{\theta}_L)...U_1(\vec{\theta}_1)\mathcal{F}(\vec{x})\left|0^{\otimes N}\right\rangle$ (output state)

Ongoing/future work

- Hybrid HPC-QC approach to HEP-ex usecases
- Sustainability & Quantum
- Apply a hybrid HPC-QCReco approach to smaller scale experiments (e.g. ALADDIN @ LHC)
- QML for experiment simulation, promising preliminary results from LHCb
- Further applications of QAOA for HEP with better scalability

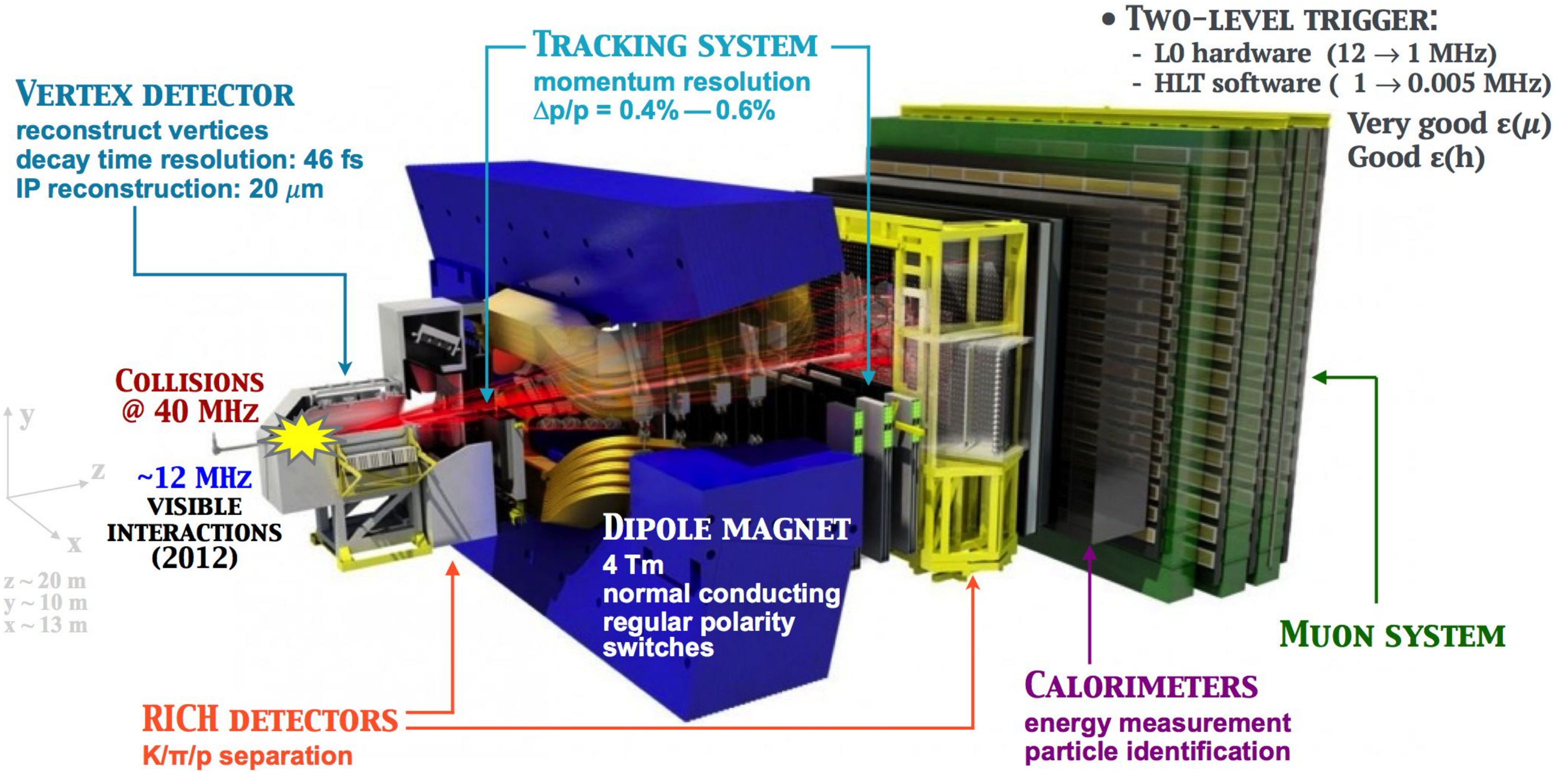
Conclusions

- Quantum Computing has great potential in solving HEP most common challenges
- Careful thinking is required on how to deal with data encoding and data retrieval
- Considerable progress has been made towards building blocks for the future of quantum computers
- **QC4HEP Working Group** is open to new members: feel free to contact me, miriam.lucio.martinez@cern.ch, to get you in touch with the Steering Committee

Thanks for your attention!

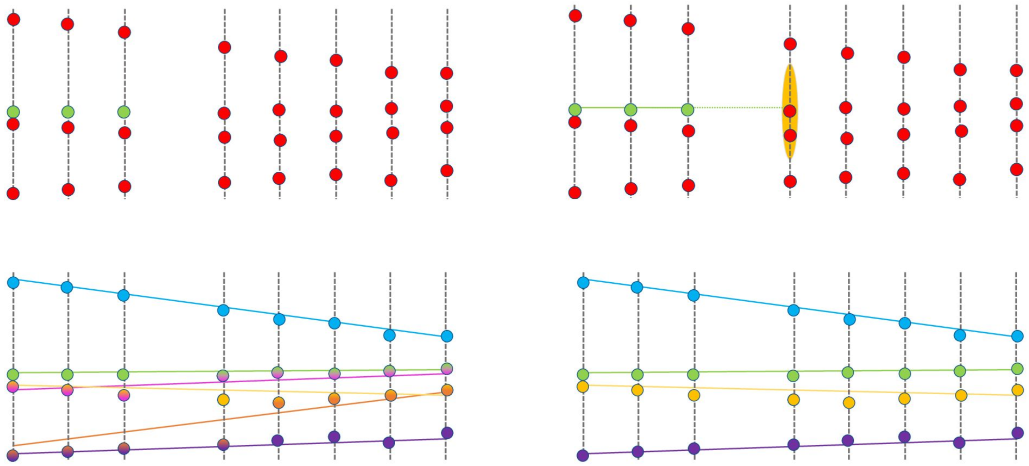
The LHCb detector

<u>Single forward-arm spectrometer</u>



Local tracking methods [arXiv:2104.11583]

1. Seeding
2. Track building
3. Cleaning
4. Selection

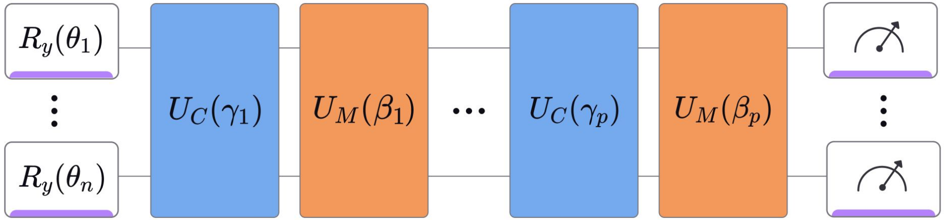


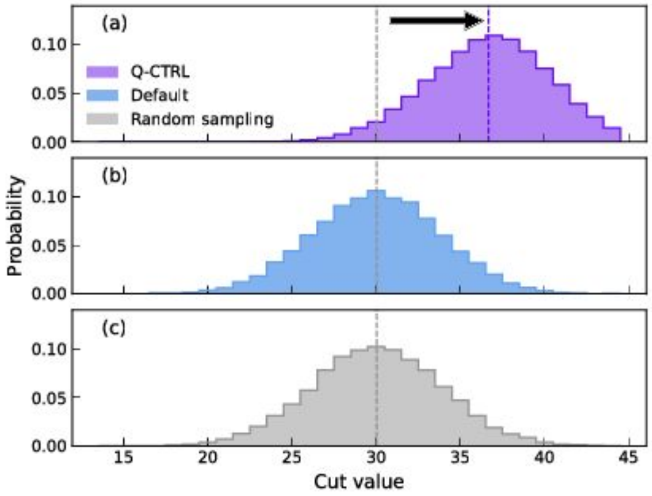
Tracking stages	Input size	Output size	Classical complexity	Quantum complexity
Seeding	$O(n)$	k_{seed}	$O(n^c)$ (Theorem 2)	$\tilde{O}(\sqrt{k_{\text{seed}} \cdot n^c})$ (Theorem 3)
Track Building	$k_{\text{seed}} + O(n)$	k_{cand}	$O(k_{\text{seed}} \cdot n)$ (Theorem 4)	$\tilde{O}(k_{\text{seed}} \cdot \sqrt{n})$ (Theorem 5)
Cleaning (original)	k_{cand}	$O(k_{\text{cand}})$	$O(k_{\text{cand}}^2)$ (Theorem 6)	–
Cleaning (improved)	k_{cand}	$O(k_{\text{cand}})$	$\tilde{O}(k_{\text{cand}})$ (Theorem 7)	–
Selection	$O(k_{\text{cand}})$	$O(k_{\text{cand}})$	$O(k_{\text{cand}})$ (Theorem 8)	–
Full Reconstruction	n	$O(n^c)$	$O(n^{c+1})$ (Theorems 2, 4, 7, 8)	$\tilde{O}(n^{c+0.5})$ (Theorems 3, 5, 7, 8)
Full Reconstruction with $O(n)$ reconstructed tracks	n	$O(n)$	$O(n^{c+1})$ (Theorems 2, 4, 7, 8)	$\tilde{O}(n^{(c+3)/2})$ (Theorem 9)

n: number of particles, c: number of hits, k_{seed}: total number of generated seeds, k_{cand}: number of track candidates

Modified QAOA (with P. Pariente, V. Chobanova, IFIC-UdC)

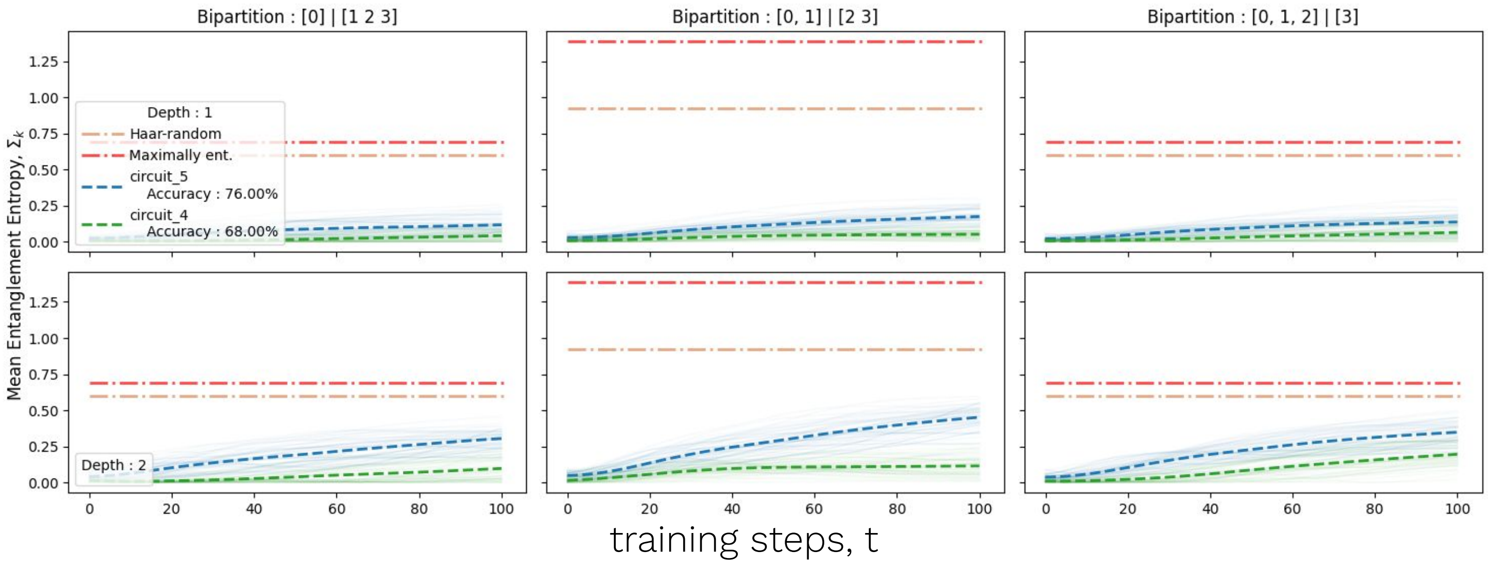
à la Q-CTRL [arXiv:2406.01743v1]





→ pdf of finding the correct solution seem to decrease, currently investigating why

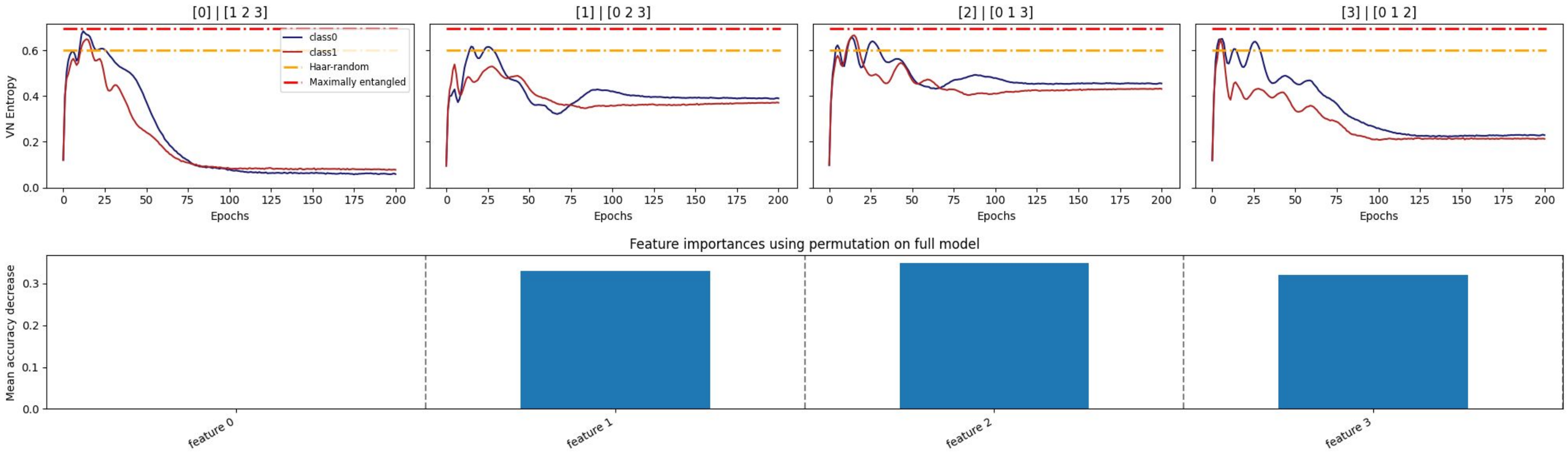
Study of the Entropy production within a Variational Quantum Circuit



- different circuits
- different datasets (b vs c jet-tagging and IRIS)
- different parameters initializations (Gaussian vs Uniform)
- different loss functions

Study of the Entropy production within a Variational Quantum Circuit

Feature importance from Entropy values



More results coming soon!

Another possible idea

'Quantum-probabilistic Hamiltonian learning for generative modelling & anomaly detection' [arXiv:2211.003803v2]

- Using LHC data & following a Quantum Hamiltonian-Based Models (QHBM) approach
- Generative modelling
- Anomaly detection