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Quantum Computing for HEP

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Summary:

- The classical and quantum representations
- Particle tracking
- Jet clustering

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Important information:

What is in this lecture:

- QC Algorithms for experimental event reconstruction
- Examples of QC for experimental data analysis

What is not in this lecture:

- QC and QFT aspects
- QC and LTG applications

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Classical computation is based on the idea of *binary digit* or *bit* as the basic unit of information. The bit represents a logical state with *only one* of two possible values of a physical system which we denote as *true* or *false*, "0" or "1".

Let us start with a very simple such system, a coin:

$$\mathbf{0} \equiv \mathbf{HEADS};\ \mathbf{1} \equiv \mathbf{TAILS}$$

With this very simple system we can already do the logical operation **NOT** (or $\neg$):

$$\neg \text{HEADS} \equiv \text{TAILS}$$

$$\neg \text{TAILS} \equiv \text{HEADS}$$

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Let us introduce randomness in our description: a bit can have probability p of being HEADS and probability $(1-p)$ of being TAILS with $p \in \mathbb{R}$, $0 \leqslant p \leqslant 1$.
Let us borrow Dirac's notation ($|0\rangle \equiv$ HEADS, $|1\rangle \equiv$ TAILS) and write the state of the coin at a given moment by

$$|coin\rangle = p\,|0\rangle + (1-p)\,|1\rangle \ .$$

Using (*a bit forcing*...) the notation we say that the coin is the (classical) superposition of the two outcomes $|0\rangle$ and $|1\rangle$.
If it is a fair coin we know that after tossing many times the state of the system, **before the next tossing**, is

$$|coin\rangle = \frac{1}{2}\,|0\rangle + \frac{1}{2}\,|1\rangle \ .$$

This conveys **all of our knowledge** about the system at that moment.

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We then throw the coin and (classically) **observe the result**. The coin will be either in the state $|0\rangle \equiv$HEADS or in the state $|1\rangle \equiv$TAILS.

We say (*somewhat abusively...*) that our observation (or **measurement**) has **collapsed the state of the coin into one of the basis states $|0\rangle$ or $|1\rangle$**.

But what happens **if we do not observe the result**? Since it is a 2-state system, all we know is that the possible outcomes are $|coin\rangle$ and $\neg\,|coin\rangle$. But $\neg\,|coin\rangle = |coin\rangle$ and therefore the state after the tossing is

$$|coin\rangle' = \frac{1}{2}\left(\frac{1}{2}|0\rangle + \frac{1}{2}|1\rangle\right) + \frac{1}{2}\left(\frac{1}{2}|0\rangle + \frac{1}{2}|1\rangle\right) = |coin\rangle \ .$$

The system remains in the superposition state, in agreement with classical probability theory.

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Any physical operation on the coin must preserve the observation of either $|0\rangle$ or $|1\rangle$ preserving at all times the "unit norm" of the bit state, that is, $p_0 + p_1 = 1$.

Exercise: *Prove that the most general linear transformations that keep the unit norm are stochastic matrices, that is, matrices of non-negative real entries where every column adds to unity.*

For example, the stochastic matrix corresponding to the coin toss is

$$\text{TOSS} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \Rightarrow \text{TOSS}\,|0\rangle = \text{TOSS}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{2}\Big(|0\rangle + |1\rangle\Big)$$

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We can also throw 2 coins at the same time. The possible outcomes are $|00\rangle$, $|10\rangle$, $|01\rangle$ and $|11\rangle$, where the first position corresponds to coin 1, while the second corresponds to coin 2. The general 2-bit state is

$$|2\ coins\rangle = p_{00}\,|00\rangle + p_{01}\,|01\rangle + p_{10}\,|10\rangle + p_{11}\,|11\rangle\ ,$$

where all $p_{ij} \in \mathbb{R}$ and

$$p_{00} + p_{01} + p_{10} + p_{11} = 1\ .$$

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If the two bits are independent the probability $P(x, y)$ of observing x in the first bit and y in the second bit is equal to the product of probability $P(x)$ of observing outcome x in the first bit and probability $P(y)$ of observing y in the second bit (*tensor product rule for composite systems*):

$$P(x, y) = P(x) \times P(y) \ .$$

This implies that if $|coin_1\rangle = p\,|0\rangle + (1-p)\,|1\rangle$ and $|coin_2\rangle = q\,|0\rangle + (1-q)\,|1\rangle$, then

$$|2\ coins\rangle = \Big(p\,|0\rangle + (1-p)\,|1\rangle\Big)\Big(q\,|0\rangle + (1-q)\,|1\rangle\Big) =$$

$$= pq\,|00\rangle + p(1-q)\,|01\rangle + (1-p)q\,|10\rangle + (1-p)(1-q)\,|11\rangle \ .$$

Exercise: *Verify that probabilities add to unity.*

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At the quantum level information is coded in **qubits**. Again the (quantum) state of the coin is of the form

$$|coin\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \ ,$$

but now $\alpha, \beta \in \mathbb{C}$ and the probabilities of the outcomes are

$$P(|0\rangle) = |\alpha|^2 \ ,$$
$$P(|1\rangle) = |\beta|^2 \ .$$

Thus

$$|\alpha|^2 + |\beta|^2 = 1 \ .$$

Therefore, any physical operation must preserve the 2-norm of the state.

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The most general linear transformations compatible with this rule are no longer stochastic matrices, but **unitary matrices**. One example is the so-called **Hadamard gate**:

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{2}} (\sigma_x + \sigma_z)$$

where σ_x and σ_z are Pauli matrices.

Physically it is easy to visualize the action of the Hadamard gate. Consider, in a given light (polarization) reference frame, two states of vertical and horizontal polarization

$$|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \; |\rightarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}; \; H|\uparrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{1}{\sqrt{2}}|\rightarrow\rangle = |\nwarrow\rangle$$

The Hadamard gate is equivalent to a rotation by 45°.

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Let us now see the result of successive applications of the Hadamard gate to the initial state $|0\rangle$. Again we can use the representation

$$|0\rangle := \begin{bmatrix} 1 \\ 0 \end{bmatrix} \; ; \; |1\rangle := \begin{bmatrix} 0 \\ 1 \end{bmatrix} \; .$$

Now:

$$H\,|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \; .$$

So far this is equivalent to the TOSS operator on a classical bit. The outcomes 0 and 1 occur with a probability $(1/\sqrt{2})^2 = 50\%$ each.

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But:

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \; ; \; H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \; ;$$

$$H(H|0\rangle) = \frac{1}{\sqrt{2}}(H|0\rangle + H|1\rangle) = \frac{1}{2}(|0\rangle + |1\rangle) + \frac{1}{2}(|0\rangle - |1\rangle) =$$

$$= |0\rangle \; .$$

$$H(H|1\rangle) = \frac{1}{\sqrt{2}}(H|0\rangle - H|1\rangle) = \frac{1}{2}(|0\rangle + |1\rangle) - \frac{1}{2}(|0\rangle - |1\rangle) =$$

$$= |1\rangle \; .$$

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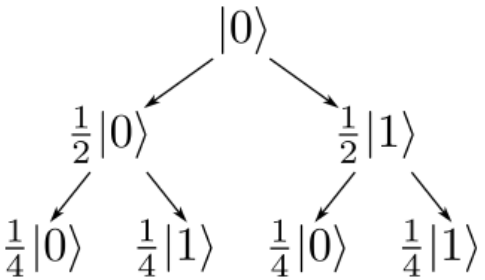
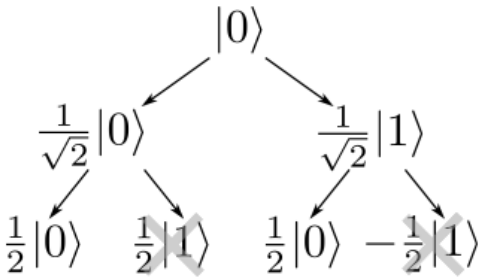
Classical



bits

Quantum



qbits

In the quantum case the paths leading to outcome 1 interfere **destructively**, while the paths leading to outcome 0 interfere **constructively**.

The fact that we have constructive and destructive interference is due to the nature itself of QM. We will now see the importance of this fact for Quantum Computing.

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Consider a function over the alphabet $\{0,1\}$ to itself, $f(x) : \{0,1\} \to \{0,1\}$. The function is defined as

constant: if $f(0) = f(1) = 0 \ \vee \ f(0) = f(1) = 1$;

balanced: if $f(x) = x \ \vee \ f(x) = \neg x$.

Problem: Using only this information determine whether a given function $f(x)$ is constant or balanced.

Notice that f can be very complicated and take a lot of time to compute!

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Classical solution:

```
if f(0) = 0:
  if f(1) = 0:
    print("Constant")
  else:
    print("Balanced")
else:
  if f(1) = 0:
    print("Balanced")
  else:
    print("Constant")
```

Function f must be evaluated **twice.**

The Deutsch-Josza algorithm

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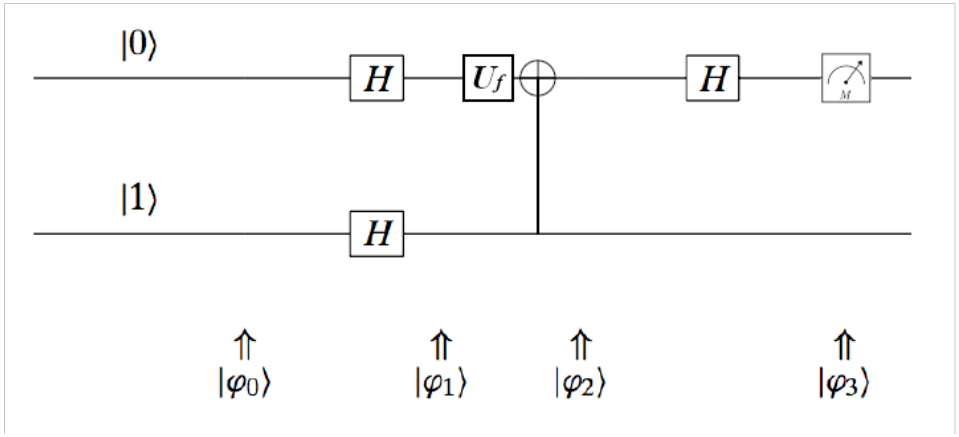
Quantum solution (Deutsch-Josza algorithm):



Let's go step by step:

Step1 - Input: $|x\rangle = |0\rangle$; *ancilla qubit* $|1\rangle$. Initial 2-qubit state $|01\rangle$:

$$|\varphi_0\rangle = |01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{matrix} \text{“00”} \\ \text{“01”} \\ \text{“10”} \\ \text{“11”} \end{matrix}$$

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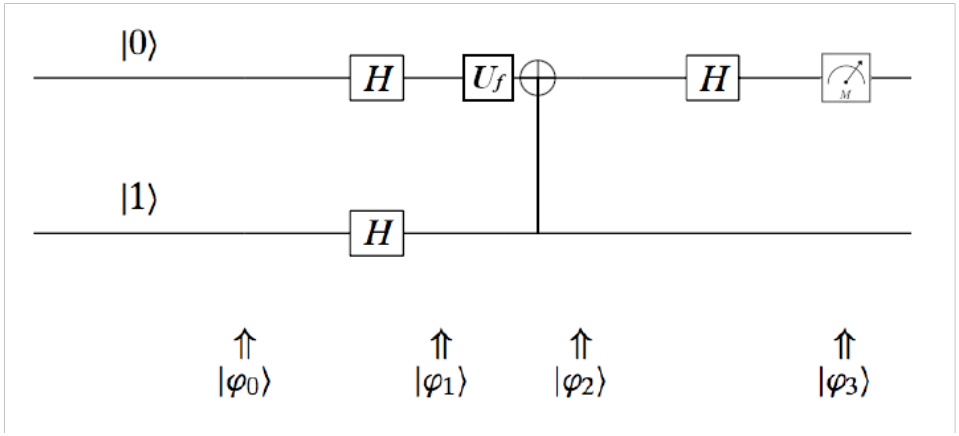

Step 2 - Hadamard 1: Apply a Hadamard gate to both qubits:

$$|\varphi_1\rangle = |H.0, H.1\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

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Quantum solution (Deutsch-Josza algorithm):

Step 3: Tricks of the trade

Before we embark on the rest of the algorithm, let us look at one crucial part: the application of the function f through the operator U_f and the XOR operation $\oplus$ between the 2 qubits.

Let us look again at $|\varphi_1\rangle$. The application of the operations to one of the terms in the direct product yields, for instance,

$$|0\rangle \otimes \frac{|0 \oplus f(0)\rangle - |1 \oplus f(0)\rangle}{\sqrt{2}} = \begin{cases} |0\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} & \Leftarrow f(0) = 0 \ , \\ |0\rangle \otimes \frac{|1\rangle - |0\rangle}{\sqrt{2}} & \Leftarrow f(0) = 1 \ . \end{cases}$$

This can be written, for all terms

$$(-1)^{f(x)} |x\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \ .$$

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Quantum solution (Deutsch-Josza algorithm):

Step 3: Tricks of the trade

So, after this operations we get the full state

$$|\varphi_2\rangle = \frac{(-1)^{f(0)}\,|0 \oplus f(0)\rangle - (-1)^{f(1)}\,|1 \oplus f(0)\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

Taking into account all possibilities for function $f(x)$ (constant or balanced), we get:

$$|\varphi_2\rangle = \begin{cases} (\pm 1)\frac{|0\rangle+|1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle-|1\rangle}{\sqrt{2}} \Leftarrow f \text{ is constant} \\ (\pm 1)\frac{|0\rangle-|1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle-|1\rangle}{\sqrt{2}} \Leftarrow f \text{ is balanced} \end{cases}$$

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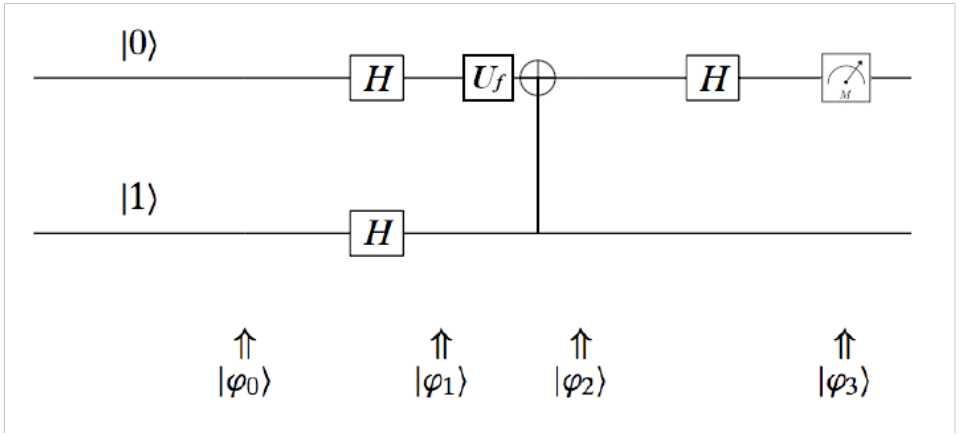
Quantum solution (Deutsch-Josza algorithm):



Step 4 - Hadamard 2: Apply a Hadamard gate again to the first qubit:

$$|\varphi_3\rangle = \begin{cases} (\pm 1)\,|0\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \Leftarrow f \text{ is constant} \\ (\pm 1)\,|1\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \Leftarrow f \text{ is balanced} \end{cases}$$

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Quantum solution (Deutsch-Josza algorithm):

Step 5 - Final result (& surprise!): Let us look closely at our result:

$$|\varphi_3\rangle = \begin{cases} (\pm 1)\,|0\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \Leftarrow f \text{ is constant} \\ (\pm 1)\,|1\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \Leftarrow f \text{ is balanced} \end{cases}$$

1. If we now **measure the first qubit only** this is what happens:
   - if the outcome is $|0\rangle$ the function f is constant;
   - if the outcome is $|1\rangle$ the function f is balanced;
2. The function f has been evaluated **only once** in the whole process. Since this can be the major time/resources overhead in the calculation we can achieve a **major speedup compared to the classical case**

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In the Deutsch-Josza algorithm we have used a universal **quantum gate-based model** similar to the classical computing model. However this is not the only possible approach for QC. We have also the **adiabatic quantum computing model**

Quantum Adiabatic Theorem:

Given a time-varying Hamiltonian, $H(t)$, which is equal to H_i at $t = t_i$, and subsequently H_f at some later time, $t = t_f$, then if the system is initially in the ground-state of H_i , and as long as the time-evolution of the Hamiltonian is sufficiently slow, the state is likely to remain in the ground-state throughout the evolution, therefore being in the ground-state of H_f at $t = t_f$.

If a quantum system starts in a ground-state, provided we evolve the state slowly, it is likely to remain in a ground-state.

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Adiabatic quantum computing (AQC) is also a universal computational model, and in terms of computational complexity is polynomially equivalent to gate-based quantum computing.

To use the AQC we need to specify:

- An **initial Hamiltonian**, H_i, whose ground-state is easy to prepare.
- A **final Hamiltonian**, H_f, whose ground-state encodes the solution to the problem of interest.
- An **adiabatic evolution path**, $s(t)$ where $s(0) = 1$ and $s(t_f) = 0$, which defines the Hamiltonian evolution:

$$H(t) = s(t)H_i + \Big(1 - s(t)\Big)H_f \ .$$

Example, $s(t) = 1 - t/t_f$**:** $H(t) = (1 - t/t_f)H_i + t/t_f H_f$.

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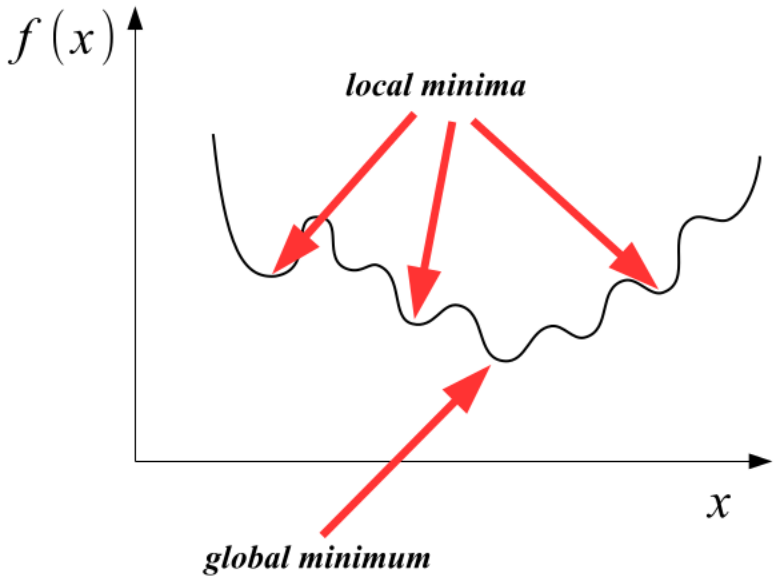
AQC is often used in **optimization** problems in which we try to find an x such that a given function $f(x) : \mathbb{R}^n \mapsto \mathbb{R}$ is minimised.

The optimisation can be constrained by inequality and/or equality constraints, *i.e.*, finding x in the range $0 \leqslant x \leqslant 0$ s.t. $f(x)$ is minimised.

The minimum can be unique (**convex optimization**), but often there are several minima and we look for the **global** minimum.



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Finding the right path $s(t)$ can be achieved using a **metaheuristic**.

A metaheuristic is a search policy that explores the optimisation function, $f(x)$, by evaluating it at certain values of x.

There are many metaheuristic algorithms which decide at which value of x we should evaluate $f(x)$ given the history of function evaluations.

All are based on the same principle: **good solutions are likely to be near other good solutions**.

This implies that the function is **smooth**.

A well-known (and widely used) metaheuristic is the the **Markov chain Monte Carlo** (**MCMC**) of which the Metropolis algorithm is one example.

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Quantum annealing is set-up in the following way:

- We have a "final" Hamiltonian, H_f , whose ground-state encodes the solution of an optimisation problem.
- We have a **transverse field Hamiltonian**, H_T, that does not commute with H_f.
- Starting in an arbitrary initial state, we evolve the system according to

$$H(t) = H_f + \Gamma(t) H_T$$

  where $\Gamma(t)$ is the transverse field coefficient, which is initially very high, and reduces to zero over time.

Quantum annealing is a metaheuristic, which starts in an **arbitrary** initial state. The transverse Hamiltonian explores the optimisation surface until the final Hamiltonian is reached. (This is the method used by **D-Wave**)

How a typical HEP detector looks like

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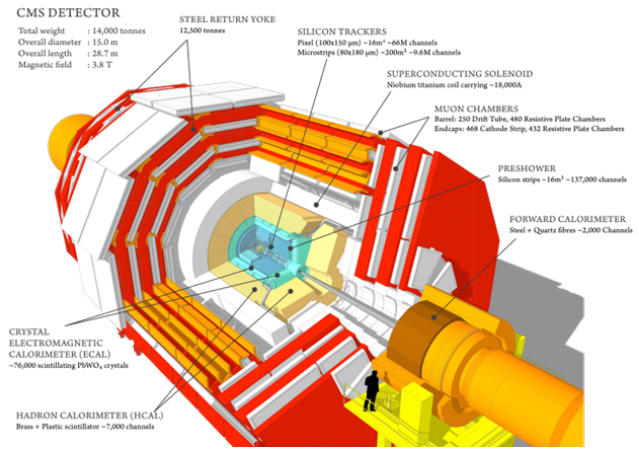
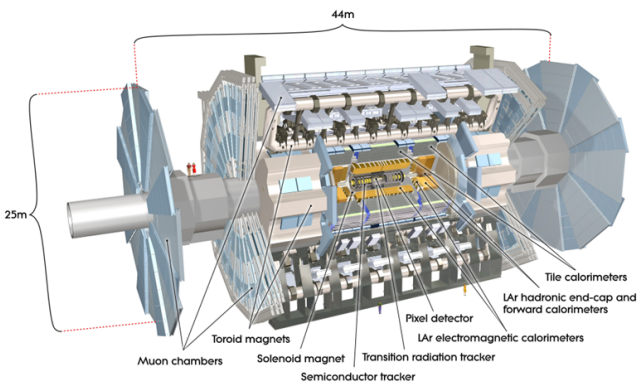
- A HEP detector is a multi-layered device designed to detect different objects
- One needs to detect both charged and neutral particles, which requires different technologies
- "Particles" leave signals on a given position at a given time and from these signals one must reconstruct their trajectories.
- The presence of a magnetic field is extremely important for reconstruction.





Types of objects

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- Leptons (electrons, muons, taus)
- Photons, W, Z, Higgs
- Neutral hadronic particles (e.g. neutrons, neutral pions, quarkonia)
- Charged hadrons
- **Jets**
- ...

Problems in data reconstruction

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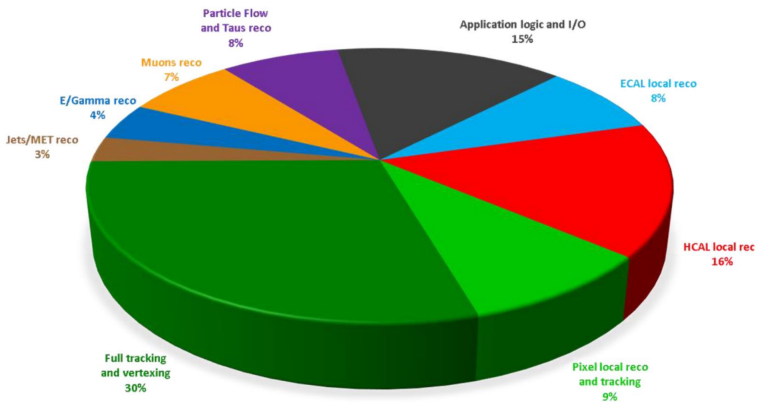
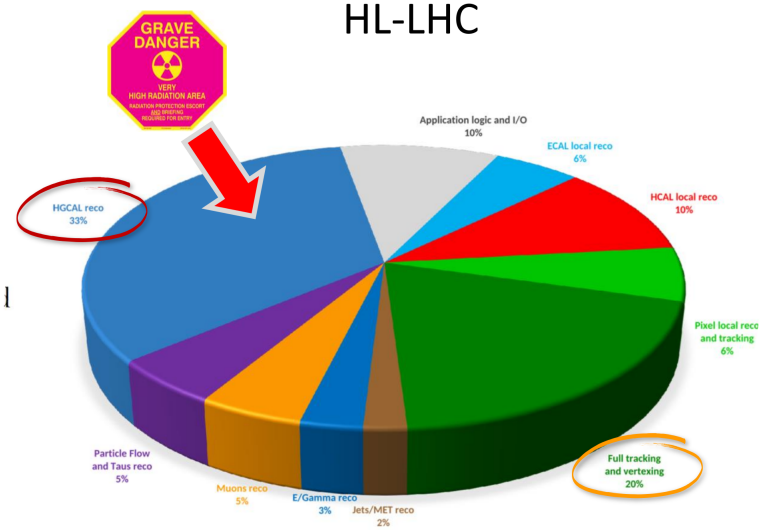
Now



HL-LHC



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The goal of tracking is to reconstruct the particles' tracks from the event record.
Given that in real experiments an event can contain several thousand hits, most combinations of hits (track candidates) will not correspond to an actual particle. Therefore, we need efficient algorithms to be able to reconstruct the tracks in a reasonable time.

First question that comes to mind:

Is it useful, in the present technological status, to use a quantum computer at all stages of track reconstruction?

It is possible to answer this question using a **complexity analysis**.

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The current tracking methods can be broadly classified into 2 classes:

Global methods treat all hit information in an equal and unbiased way and are essentially clustering algorithms in some feature space. All the quantum approaches so far were based on global methods.

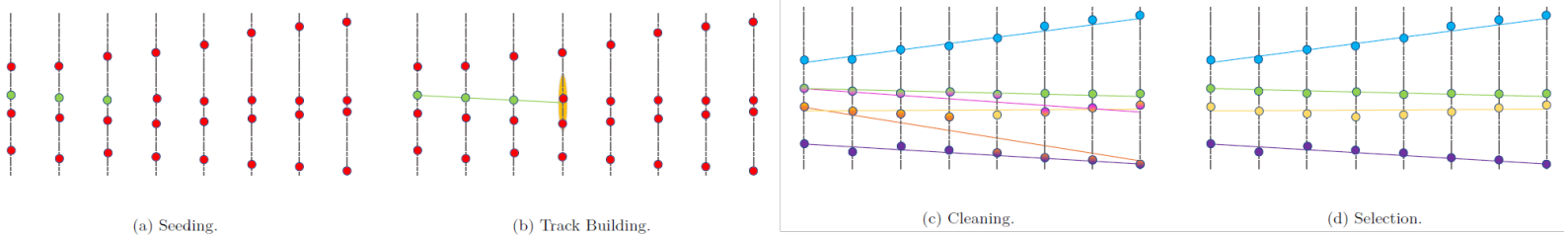
Local methods use information from close hits to create a track proposal.

Because global methods can be very inefficient in terms of speed, local methods are still the standard at several reconstruction programmes in high-energy physics. We will focus here on local methods.

What is tracking

There are four fundamental computational routines in every local tracking method:

1. **seeding**: form initial rudimentary track candidates, called seeds, using just a few hits
2. **track building**:extrapolate seeds' trajectories along the expected path and build track candidates by adding compatible hits from successive detector layers.
3. **cleaning**: removes track candidates that are too similar (too many common hits)
4. **selection**: only the track candidates that respect some quality criteria are accepted



(a) Seeding. (b) Track Building. (c) Cleaning. (d) Selection.

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The tracking problem

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Definition: For two functions $f, g : \mathbb{N} \mapsto \mathbb{R}$ we say that $f = O(g)$ if $\exists C, x_0 > 0 : \forall x, (x > x_0 \Leftarrow f(x) < C.g(x))$. We write $f = \Omega(g)$ if $g = O(f)$. We say that $f = \Theta(g)$ if $f = O(g)$ and $g = O(f)$. By "constant time", we mean $O(1)$.

For complexity analysis we only consider the dependence on the variable n, the number of particles.

The data in the event record also depends on quantities like the number of layers of the detector, the granularity of the sensors, or the efficiency of the detectors. But these are fixed from the experimental hardware and do not vary from event to event.

On the other hand, we expect the average n to grow as we increase the beam's instantaneous luminosity.

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We require the granularity of the sensors to be high enough such that each detected hit can always be differentiated from others. At every layer, we identify the hits with labels from $\{0, \ldots, n-1\}$, using the notation $\mathbf{m}_{l,j}$ for the coordinates of j-th hit in layer l. It is possible that some hits are not measured at all due to sensor inefficiencies, that is, we do not necessarily have a hit $\mathbf{m}_{l,j}$ for every pair (l, j).

We will focus on the **Combinatorial Track Finder algorithm (CTF)**.

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Recommended reading: D. Magano, A. Kumar, M. Kālis, A. Locāns, A. Glos, S. Pratapsi, G. Quinta, M. Dimitrijevs, A. Rivošs, P. Bargassa, J. Seixas, A. Ambainis, and Y. Omar, *Quantum speedup for track reconstruction in particle accelerators*, Physical Review D 105, 076012 (2022).

Tracking stages	Input size	Output size	Classical complexity	Quantum complexity
Seeding	$O(n)$	k_{seed}	$O\left(n^c\right)$ (Theorem 2.4.2)	$\tilde{O}\left(\sqrt{k_{\text{seed}} \cdot n^c}\right)$ (Theorem 2.4.3)
Track Building	$k_{\text{seed}} + O(n)$	k_{cand}	$O(k_{\text{seed}} \cdot n)$ (Theorem 2.4.4)	$\tilde{O}\left(k_{\text{seed}} \cdot \sqrt{n}\right)$ (Theorem 2.4.5)
Cleaning (original)	k_{cand}	$O(k_{\text{cand}})$	$O(k_{\text{cand}}^2)$ (Theorem 2.4.6)	–
Cleaning (improved)	k_{cand}	$O(k_{\text{cand}})$	$\tilde{O}(k_{\text{cand}})$ (Theorem 2.4.7)	–
Selection	$O(k_{\text{cand}})$	$O(k_{\text{cand}})$	$O(k_{\text{cand}})$ (Theorem 2.4.8)	–
Full Reconstruction	n	$O(n^c)$	$O\left(n^{c+1}\right)$ (Theorems 2.4.2, 2.4.4, 2.4.7, 2.4.8)	$\tilde{O}\left(n^{c+0.5}\right)$ (Theorems 2.4.3, 2.4.5, 2.4.7, 2.4.8)
Full Reconstruction with $O(n)$ reconstructed tracks	n	$O(n)$	$O\left(n^{c+1}\right)$ (Theorems 2.4.2, 2.4.4, 2.4.7, 2.4.8)	$\tilde{O}\left(n^{(c+3)/2}\right)$ (Theorem 2.5.1)

The tracking problem: conclusions

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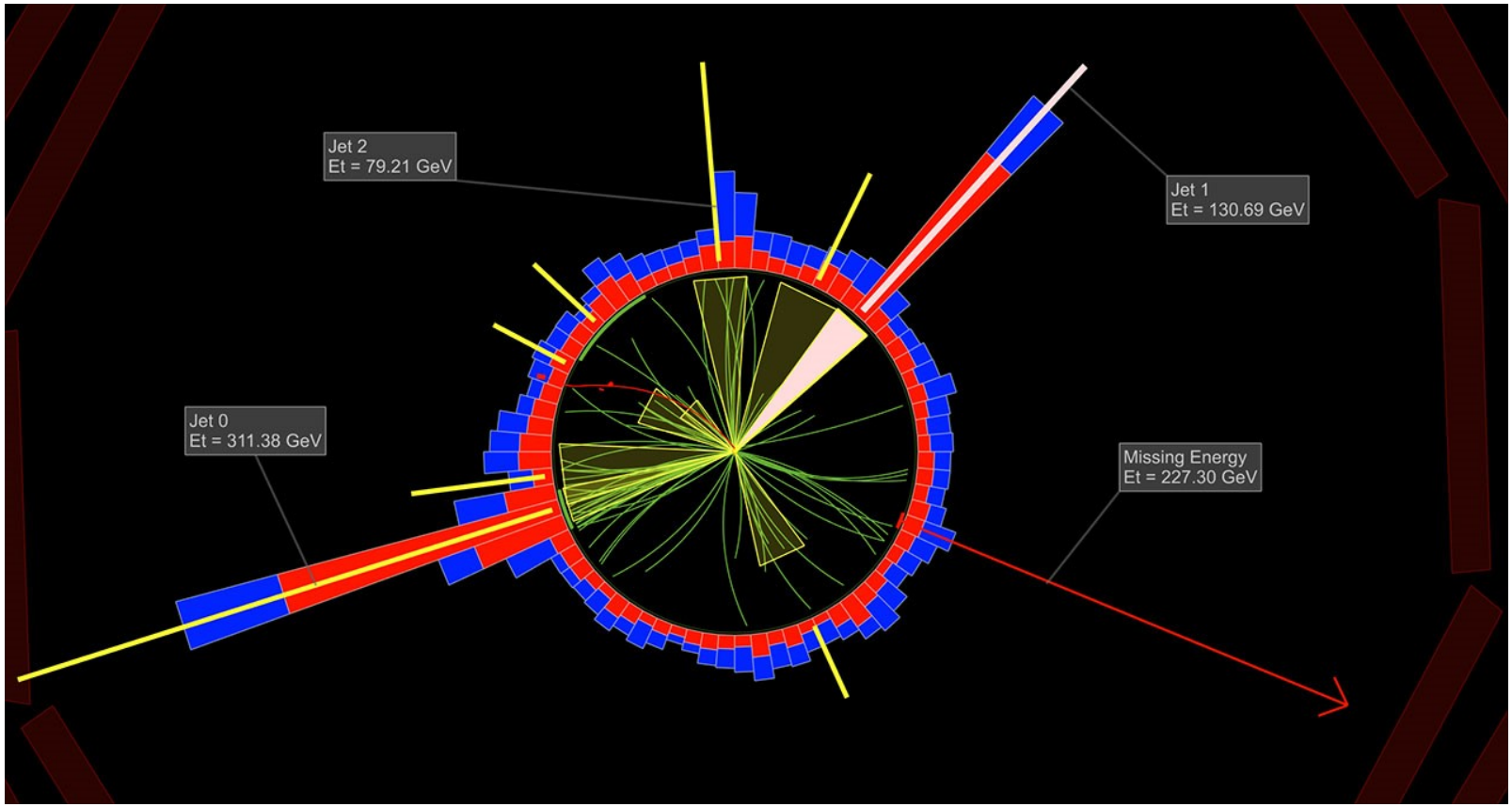
The reached quantum speedups are evidently mild. We conjecture that they are the best possible while constrained to matching the exact output of the corresponding classical algorithm (up to bounded-error probability) at arbitrarily fine scales. In other words, the direct quantization of (local) tracking methods may not be the best path to establish a significant advantage in quantum computing for HEP problems. **Instead, one may find more success by breaking the direct correspondence with the classical setting and designing completely new tracking algorithms that inherently take advantage of the features of quantum processors.**

Moreover, our comprehensive analysis of the CTF algorithm reveals that classical improvements to the computational complexity are also possible.

How a (multi-)jet event looks like



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Let us look at the next-to-leading process $e^+e^- \to q\bar{q}g$. The cross section is

$$\frac{1}{\sigma}\frac{\partial^2\sigma}{\partial x_1 \partial x_2} = C_F \frac{\alpha_s}{2\pi}\frac{x_1^2 + x_2^2}{(1-x_1)(1-x_2)}$$

where x_1, x_2 are the quark momentum fractions, C_F is a constant associated with the group structure and α_s is the strong coupling constant.
It explodes as $x_i \to 1$ corresponding to a soft gluon (collinear with one of the quarks).
If we assume that quarks and gluons fragment collinearly into hadrons then the preference for the gluon to be soft implies that the two-jet-like structure of the lowest order is maintained at $\mathcal{O}(\alpha_s)$.

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If, on the other hand we **require** that the gluon is well separated in phase space from the quarks (3-jet event), then the singular regions of the matrix element are avoided and the cross section is suppressed relative to the lowest order by one power of α_s. This qualitative result is valid to **all orders** in perturbation theory.
The amplitudes for multiple gluon emission contain the same type of singularities as those that appear at first order, which leads to a final state which is predominantly 2-jet-like with a smaller probability (determined by α_s) for 3 or more distinguishable jets. This justifies some choices in the following.

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To make this quantitative we need to define a **jet measure**, that is, a procedure to classify a (experimental, hadron) final state according to the number of (theoretical quark or gluon) jets it contains.
In order to be useful, this procedure must yield total cross sections free of soft and collinear singularities when calculated in perturbation theory and should be insensitive (as much as possible) to the non perturbative fragmentation of quarks and gluons into hadrons.
One of the first attempts was done by Sterman and Weinberg in 1977. In their picture a final state is defined as 2-jet like if **all but a fraction ε of the total available energy is contained in a pair of cones of (fixed) half angle δ**.
This procedure is not suited to analyse multi-jet final states.
One reason is that **fixed-angle cones provide an inefficient tiling of the phase space 4π angle**.

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In the k_t and anti-k_t algorithms (M. Cacciari et al JHEP04(2008)063) one introduces distances d_{ij} between entities (particles, pseudojets) i and j and d_{iB} between entity i and the beam (B).

- if d_{ij} is the smallest distance $\Rightarrow$ recombine entities;
- if d_{iB} is the smallest distance $\Rightarrow$ entity is a jet $\Rightarrow$ remove from list of entities;
- repeat until no entities are left.

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The difference between k_t, anti-k_t & Cambridge/Aachen algorithms lays in the definition of distance:

$$
\begin{aligned}
d_{ij} &= \min(k_{ti}^{2p}, k_{ti}^{2p}) \frac{\Delta_{ij}^2}{R^2} \ , \\
d_{iB} &= k_{ti}^{2p} \ , \\
\Delta_{ij}^2 &= (y_i - y_j)^2 + (\phi_i - \phi_j)^2 \ ,
\end{aligned}
$$

y_i, ϕ_i, k_{ti} rapidity, azimuthal angle and transverse momentum of particle i. R is the radius parameter and the parameter p governs the relative power of the energy versus geometrical (Δ_{ij}) scales.

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$p = 0$: Cambridge/Aachen algorithm;

$p = 1$: Inclusive k_t algorithm. What matters is the ordering between particles and for finite Δ this is maintained $\forall p > 0$.

$p < 0$: The behaviour with respect to soft radiation will be similar for all $p < 0$. The algorithm with $p = -1$ corresponds to the anti-k_t jet-clustering algorithm.

The anti-k_t algorithm is known to be computationally very efficient.

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As the center of mass energy and/or luminosity increases in future high-energy particle accelerators, the computational resources demand is set to increase drastically, resulting in the near future in a predicted $\sim$ 10X increase in both pile-up, from $< \mu > \sim 20$ to $< \mu > \sim 200$, and subsequent produced particle multiplicity. As a consequence, event reconstruction, and in particular jet clustering, is bound to become an even more complex combinatorial problem, with a significant increase in final-state number of particles N to be clustered. The amount of clustering possibilities will increase thus challenging present day computing resources.

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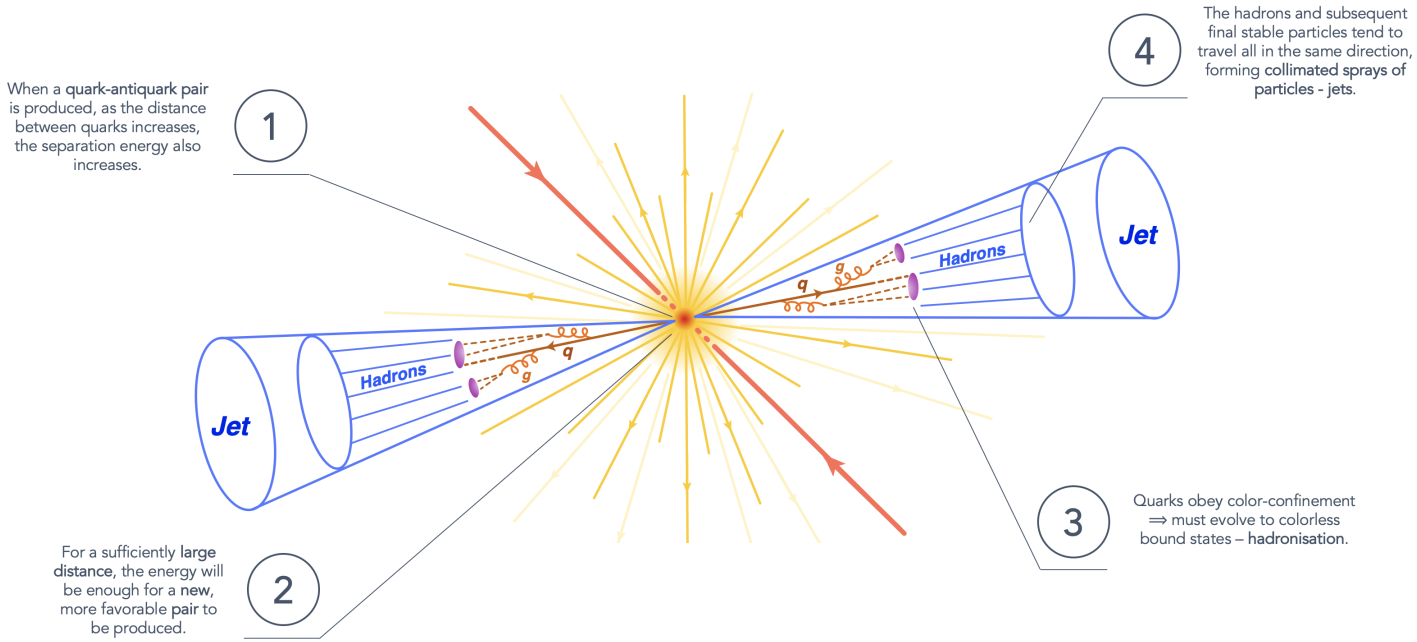

As an example, take the case of a 2-jet event in a e^+e^- collision. The e^+e^- annihilate (given that they possess opposite momenta, charge, and the same energy), and end up emitting a $q\bar{q}$ pair, through either a virtual Z^0 gauge boson or a virtual photon.

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Our goal is to map a collection of N particles' momentum vectors $\{\vec{p}_i\}$, corresponding to N final-state particles, onto a set of output final jets, $\{\vec{j}_k\}$ (here with $k \in \{1, 2\}$). All these particles are assumed to originate from the same point in space, and should be sorted into the relevant jet clusters, adequately recombined into the jet's final total momenta, $\vec{j}_k$. Starting from the assumption that N particles are to be assigned to $K = 2$ jets, it is conceptually more intuitive to express the objective function in terms of Ising variables $s_i = \pm 1$:

$s_i = +1$ particle $i \in j_1$;

$s_i = -1$ particle $i \notin j_1 \Rightarrow i \in j_2$;

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We start by writing a (Ising) general objective function *ansatz*:

$$H = \frac{1}{2} \sum_{i,j=1}^{N} d(\vec{p}_i, \vec{p}_j) s_i s_j \ , \tag{1}$$

where $d(\vec{p}_i, \vec{p}_j)$ represents a dissimilarity metric.

- If the dissimilarity $d(\vec{p}_i, \vec{p}_j)$ between two particles $\vec{p}_i$ and $\vec{p}_j$ is large, s_i and s_j tend to take opposite signs $\Rightarrow$ assigned to different clusters.
- If $d(\vec{p}_i, \vec{p}_j)$ is small, s_i and s_j take the same value and are assigned to the same cluster. Since s_i can never be set to zero there is only one s_i per particle for the N particles.

Each particle is thus assigned to one and only one cluster.

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The factor $1/2$ accounts for the symmetric nature of the dissimilarity metric $d(\vec{p}_i, \vec{p}_j) = d(\vec{p}_j, \vec{p}_i)$ in the sum.
Since we have an s_i variable, and thus a qubit per particle, we end up with a qubit usage $O(N)$, representative of the N final-state particles being clustered.
When choosing $d(\vec{p}_i, \vec{p}_j)$, a standard Euclidean distance metric is not the best choice:

- Take two soft particles with momenta $\vec{p}_i$ and $\vec{p}_j$ belonging to different jets. These are registered as being closer to the vertex than their hard companions, that is, they possess a smaller momentum norm relative to the others.
- In the cases where the energy gap is sufficiently large, the minimization process will be harmed since $d(\vec{p}_i, \vec{p}_j)$ is smaller relative to the average $\overline{d}$, thus erroneously grouping $\vec{p}_i$ and $\vec{p}_j$ together.

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Goal for the dissimilarity function:
as $d(\vec{p}_i, \vec{p}_j)$ increases/decreases the larger/smaller the output energy of the corresponding Ising hamiltonian should be.

Given the high energy of the initial outgoing quark-antiquark pair, the final jets tend to be highly collimated. One can use the angle θ between particles as a starting point to build an appropriate dissimilarity metric.

$$H = \frac{1}{2}\sum_{i,j=1}^{N} -\cos\left[\theta(\vec{p}_i, \vec{p}_j)\right] s_i s_j = \frac{1}{2}\sum_{i,j=1}^{N} -\frac{\vec{p}_i \cdot \vec{p}_j}{|\vec{p}_i| \cdot |\vec{p}_j|} s_i s_j \ ,$$

where $d_{ij} = -\cos\left(\theta_{ij}\right)$.

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- When particles $\vec{p}_i$ and $\vec{p}_j$ belong to the same jet, we measure $\theta_{ij} \ll \frac{\pi}{2} \Rightarrow \cos\left(\theta_{ij}\right) \approx 1$.
- When two particles $\vec{p}_i$ and $\vec{p}_j$ belong to opposite jets), we measure $\theta_{ij} \sim \pi \Rightarrow \cos(\theta_{ij}) \approx -1$.
- Because our goal is to minimize H and not to maximize it, we introduce a minus sign in the definition of H. As a result, the minimization of H will favor the clustering of particles closer in angular distance, that is, with smaller $\theta(\vec{p}_i, \vec{p}_j)$ relative to one another.

Even though H refers to simpler cases of dijet events, the dissimilarity metric used is much more versatile and can be generalized to more complex events. As such, opposed to the *Thrust* concept discussed in Wei *et al.* Phys. Rev. D 101(2020)9, we are therefore safe while carrying this concept to more elaborate, K-jet generalizations.

Extension to $K > 2$ jets

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For $K > 2$ the previous approach does not work.

- We use binary variables x_i^k and x_j^k to denote whether or not two given particles $\vec{p}_i$ and $\vec{p}_j$ belong to the same jet j_k. If particle $\vec{p}_i \in$ jet $j_k \Rightarrow x_i^k = 1$. If not, it would have $x_i^k = 0$. This type of formulation where we have one qubit per particle per jet, we call **One-Hot Encoding**. It comes at the cost of a more intensive qubit usage of the order of $O(KN)$.
- First term of our K-jet objective function:

$$H'_K = \frac{1}{2} \sum_{k=1}^{K} \sum_{i,j=1}^{N} -\cos\left[\theta(\vec{p}_i, \vec{p}_j)\right] x_i^k x_j^k \ .$$

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For $K > 2$ the previous approach does not work.

- Now the lowest energy possible for a given configuration is **zero**! We know that the minimization process of the objective function favors the scenario in which all particles are assigned to zero jets, such that we have $x_i^k = 0$ either for a given particle $\vec{p}_i$ and all jets j_k with $k \in \{1, \ldots, K\}$, or for a given jet j_k and all particles $\vec{p}_i$ with $i \in \{1, \ldots, N\}$.
- W must not allow for any given particle to be assigned to more than one jet!

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Both of these issues can be solved by adding a constraining term. Again, one needs to guarantee that for each particle $\vec{p}_i$, there is one and only one $x_i^k = 1$ for some jet j_k, with the rest of $x_i^{k' \neq k} = 0$. Introduce

$$\phi_i = \left(1 - \sum_{k=1}^{K} x_i^k\right)^2 , \tag{2}$$

and add it with a tunable parameter λ in order to obtain the complete hamiltonian:

$$H_K := H'_K + \lambda \sum_{i=1}^{N} \phi_i = \frac{1}{2} \sum_{k=1}^{K} \sum_{i,j=1}^{N} -\cos\left[\theta(\vec{p}_i, \vec{p}_j)\right] x_i^k x_j^k$$

$$+ \lambda \sum_{i=1}^{N} \left(1 - \sum_{k=1}^{K} x_i^k\right)^2 .$$

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- If a particle is assigned to more than one jet, the constraining term grows with each additional jet the particle is assigned to. Consequently H'_K will never energetically favor this possibility, since it will always result in an increase of its energy.
- In the remaining case in which a given number of particles are assigned to zero jets, the corresponding first terms of the hamiltonian will be set to zero and reduce the value of H_K, thus being energetically favored.
- The goal to be achieved with the addition of the constraint, is simply to offset the largest possible "incorrect"energy reduction in H'_K. When a particle $\vec{p}_i$ is assigned to zero jets, it can, in a worst case scenario basis, result in $N - K$ pairwise dissimilarity metrics set to zero.

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We are now in conditions to conclude that the approximate order of magnitude for λ should be

$$\lambda \sim (N - K) \cdot \max\left(- \cos\left[\theta(\vec{p}_i, \vec{p}_j)\right]\right), \quad \forall \vec{p}_i, \vec{p}_j \ . \tag{3}$$

In practice λ cannot be made arbitrarily large due to the current hardware state of the art inherent limitations mainly related to the allowed range of the qubit couplings.
When compared to the $K = 2$ jet event, the K-jet one-hot encoding formulation is considerably harder to implement on current quantum annealing hardware. Previous numerical studies have shown that clustering problems making use of multiple qubits to implement one-hot encoding are prone to errors, thus widening the performance gap between dijet and multijet events.

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- The *PYTHIA* Monte-Carlo event generator (version 8.3) was used to as realistically as possible simulate real data. Given the $K = 2$ binary nature of the jet events being studied, we generated $e^+e^- \rightarrow Z^0 \rightarrow q\bar{q}$, with all Z^0 decays switched off except those to quarks which have been manually switched on.
- We measure the algorithms' performance against that of the classical state-of-the-art k_t clustering algorithm.
- The k_t clustering algorithm implemented and used through the *FastJet* software package. By using the Jet Definition *jet_def(kt_algorithm, R)*, the k_t clustering algorithm has been chosen to run with an R parameter of $R = 0.8$.

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The output was then a list of the final jets' total transverse momenta $||\vec{j}_{T_k}||$, its pseudorapidity η_k and the corresponding azimuthal angle ϕ_k. In addition, the list of the regrouped final-state particles for each final jet was also produced, so that it could be used to compare the classical benchmark's results with those of the developed quantum algorithm.
PYTHIA generated e^+e^- events are not bound to $K = 2$ despite being the most common. As such, given that the developed algorithm is meant to be applied to binary clustering dijet events where $K = 2$, we have made the choice of always considering only the two highest p_T jets obtained by the k_t benchmark for comparison with the (always) binary results obtained by the quantum annealing algorithms.

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Efficiency metric to evaluate the obtained results for a given event n:

$$\epsilon^{(n)} = \frac{\#\text{ of particles grouped in the same way as } k_t}{\#\text{ of particles in the two highest-}p_T\text{ jets } (k_t)} \ .$$

We have, ϵ_{QBC} and ϵ_{Thr}, which reflect the efficiencies of the proposed quantum binary clustering algorithm and of the Thrust-based quantum annealing of Wei *et al.*:

$$\epsilon_{\text{QBC}} = \frac{1}{n}\sum_{n} \varepsilon^{(n)}_{\text{QBC}} \ , \qquad \epsilon_{\text{Thr}} = \frac{1}{n}\sum_{n} \varepsilon^{(n)}_{\text{Thr}} \ .$$

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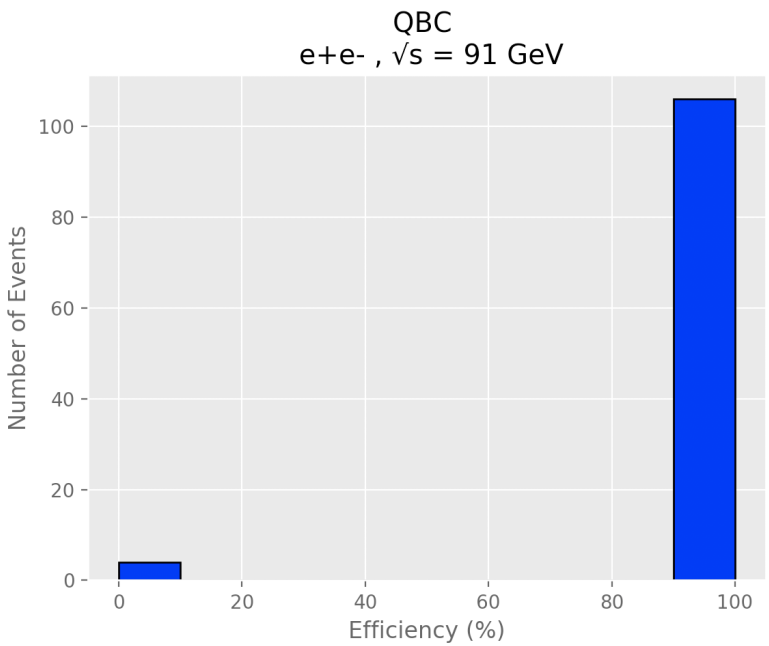

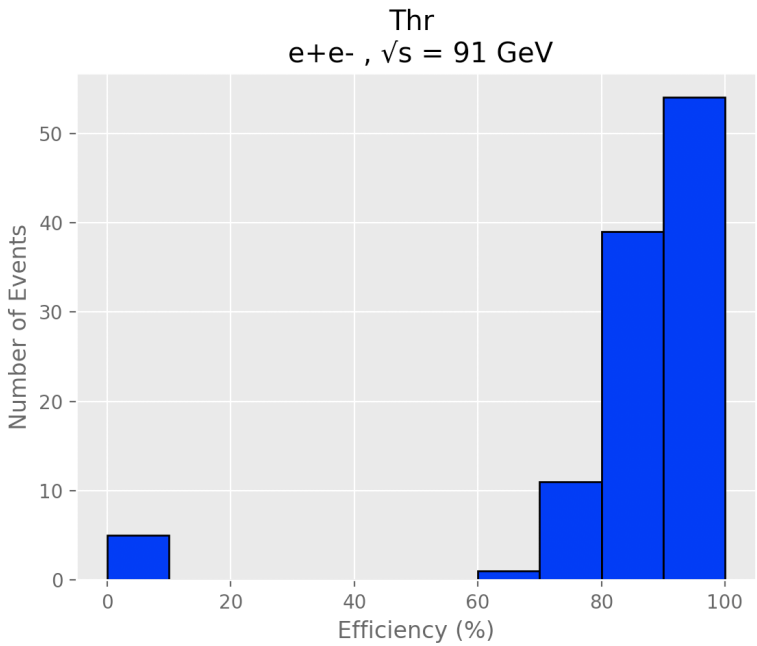

Quantum digital approach: *k-means* algorithm

arXiv:2101.05618v1 [physics.data-an]

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The classical *k-means* algorithm (S. Lloyd, doi:10.1109/TIT.1982.1056489), applied to jet clustering for the first time in 2006 and subsequently in 2012 (J. Thaler jhep02(2012)093) and 2015 (I. Stewart jhep11(2015)072)
It receives as input a set of N, D-dimensional data points and outputs K centroids, calculated through the mean of each group of data points, thus defining K clusters.
To be assigned to any particular cluster, a data point needs to be closer to that cluster's centroid than to any other centroid in the data set. In order to successfully converge to the final set of centroids, the algorithm iteratively alternates between assigning the data points to K clusters based on the current centroids and choosing the centroids based on the current assignment of the data points to clusters.

k-means algorithm - *Swap test* routine

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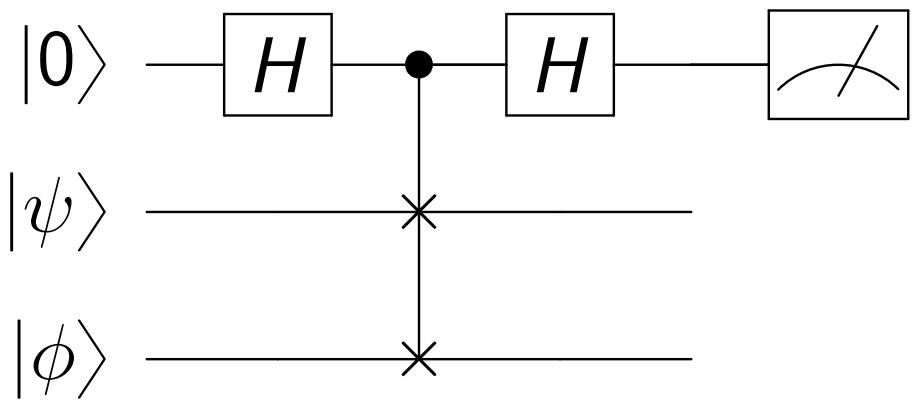
The algorithm presents a scaling complexity of $O(KND)$, which corresponds to the dominating step where the KN distances between all the N data points and the K centroids are calculated.
In order to compute the distances on a quantum circuit, we use the **SwapTest** quantum sub-routine:



k-means algorithm - *Swap test* routine

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Measure the overlap between two quantum states $|\psi\rangle$ and $|\phi\rangle$, $\langle\psi|\phi\rangle$, based on the measurement probability of the control qubit being in state $|0\rangle$, $P(|0\rangle) = \frac{1}{2} + \frac{1}{2}|\langle\psi|\phi\rangle|^2$:

1. **State Preparation:** Prepare two quantum states, particle's momentum vector $\vec{p}_i$ and a given jet cluster's centroid μ_k

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|0, \vec{p}_i\rangle + |1, \mu_k\rangle\big),$$

$$|\phi\rangle = \frac{1}{\sqrt{Z}}\big(||\vec{p}_i||\,|0\rangle - ||\mu_k||\,|1\rangle\big),$$

2. **Find Overlap:** Compute overlap $|\langle\psi|\phi\rangle|^2$ through the *SwapTest* sub-routine.
3. **Compute Squared Euclidean Distance:** Get the desired squared Euclidean distance through the following equation,

$$||\vec{p}_i - \mu_k||^2 = 2Z|\langle\psi|\phi\rangle|^2,$$

k-means algorithm - *Silhouette* index

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The number K of jets produced is not known *a priori*. Nevertheless, one does know the expected range of K values as a function of the center-of-mass energy $\sqrt{s}$ and which particles are being collided. To avoid any bias in the present algorithm the number of jets K is chosen after a range sweep is performed for a reasonably expected range of values of K. We ran the algorithm a small number of times over the expected range of K, so that the most adequate number of jets can be inferred. We chose the value of K which produces the highest quality clustering. We chose the **Silhouette Index** (P. Rousseeuw, doi: 10.1016/0377-0427(87)90125-7) as a figure of merit for clustering quality.

k-means algorithm - *Silhouette* index

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A quick complexity analysis yields a computational cost is of the order of $O(N^2 D)$, thus surpassing that of the algorithm itself. For this reason, a simplified *Silhouette* figure of merit is used, composed of the similarity measure $a(\vec{p}_i)$, dissimilarity measure $b(\vec{p}_i)$, and *Silhouette* index $s(\vec{p}_i)$ for each of the clustered particles:

$$
\begin{aligned}
a(\vec{p}_i) &= d(\vec{p}_i, \mu_i) \ , \\
b(\vec{p}_i) &= \min_{C_k \neq C_i} d(\vec{p}_i, \mu_k) \ , \\
s(\vec{p}_i) &= \begin{cases} \frac{b(\vec{p}_i) - a(\vec{p}_i)}{\max\left\{a(\vec{p}_i), b(\vec{p}_i)\right\}}, & \text{if } |C_i| > 1 \ , \\ 0, & \text{if } |C_i| = 1 \ . \end{cases}
\end{aligned}
$$

where C_i represents the jet cluster to which particle $\vec{p}_i$ belongs.

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This way we have managed to reduce its computational cost to $O\big(N(K-1)\big)$, which scales slower than the overall algorithm.
The overall clustering's *Silhouette* is then obtained by computing the mean of all N particles' *Silhouette* values:

$$S_K = \frac{1}{N}\sum_i s(\vec{p}_i) \ .$$

Only the information about final-state particles has been used as input for the algorithm, in order to follow the same procedure as for real data.
Any information prior to the final-state particles is disregarded, as it is the case in any jet reconstruction using real data. The observables used in the clustering process are the 3-momentum vectors of the particles.

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- The dimensionality of the problem is thus constant with $D = 3$. Since D is constant, so is $\log D$ and this factor drops out in the calculation of the algorithmic complexity. The computational cost of the algorithm is thus simply $O(KN)$.
- Despite the possible naive $O(N^2)$ or even $O(N^3)$ implementations, the classical k_t can be cleverly implemented in $O(N \log N)$ by exploiting some of its geometrical and minimum-finding aspects. The new proposed method becomes of interest only in the regime where the number of reconstructed jets $K \leqslant \log N$.
- It is important to notice that the $D = 3$ dimensionality affects not only the scaling of the proposed quantum *k-means* algorithm, but also its classical counterpart. Dropping the D factor, we obtain a complexity of $O(KN)$ for the classical *k-means* algorithm.

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- Since this is equivalent to that of its quantum analog, it can be said that the use of this quantum algorithm for real day-to-day jet clustering analysis becomes only relevant if one is able to exploit the advantage of $\log D$ versus D relative to the classical version. Use of the dimensionality D may be possible considering synergies with other stages of the jet clustering process (i.e. pile-up).
- When measuring the algorithm's jet clustering efficiency, the ideal would be to compare it to the true jet regrouping for any given generated event, giving us information on the parenthood of each final-state particle and enabling us to know which particles should be clustered together. **Unfortunately such Monte-Carlo truth is not available by design**.

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- Consequently, as mentioned above, we have chosen to measure the algorithm's performance against that of the classical k_t algorithm. For a given clustering output, where the N final-state particles have been sorted into K jets, we compare both algorithm's clustering results on a particle-by-particle basis according to the following efficiency metric, ϵ:

$$\epsilon = \frac{\#\text{ of particles grouped in the same way as } k_t}{\#\text{ of particles in meaningful jets found by } k_t}.$$

To identify the physically meaningful jets out of all the jets found by the k_t algorithm, we apply a minimum transverse momentum p_T jet cutoff, such that any given jet with transverse momentum lower than the set cutoff p_T is discarded.

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We have again used *PYTHIA* (version 8.3) to generate the events on which the clustering should be performed (see Appendix for more details on event generation). To study the events' scaling of K versus $\log N$, we have generated both $e^+e^- \rightarrow Z^0 \rightarrow q\bar{q}$ collision events at a center-of-mass energy of $\sqrt{s} = m_Z = 91.1876 \pm 0.0021\ GeV/c^2$, (PDG value) as well as pp collision events at center-of-mass energies of $\sqrt{s} = 7\ TeV$ and $\sqrt{s} = 14\ TeV$. We have also explored pp collision events involving t-quarks given its high jet multiplicity. As such we have performed clustering on 1000 generated events of each kind, storing both the number of found meaningful jets K, as well as the corresponding event's logarithm of the number of final-state particles, $\log N$.

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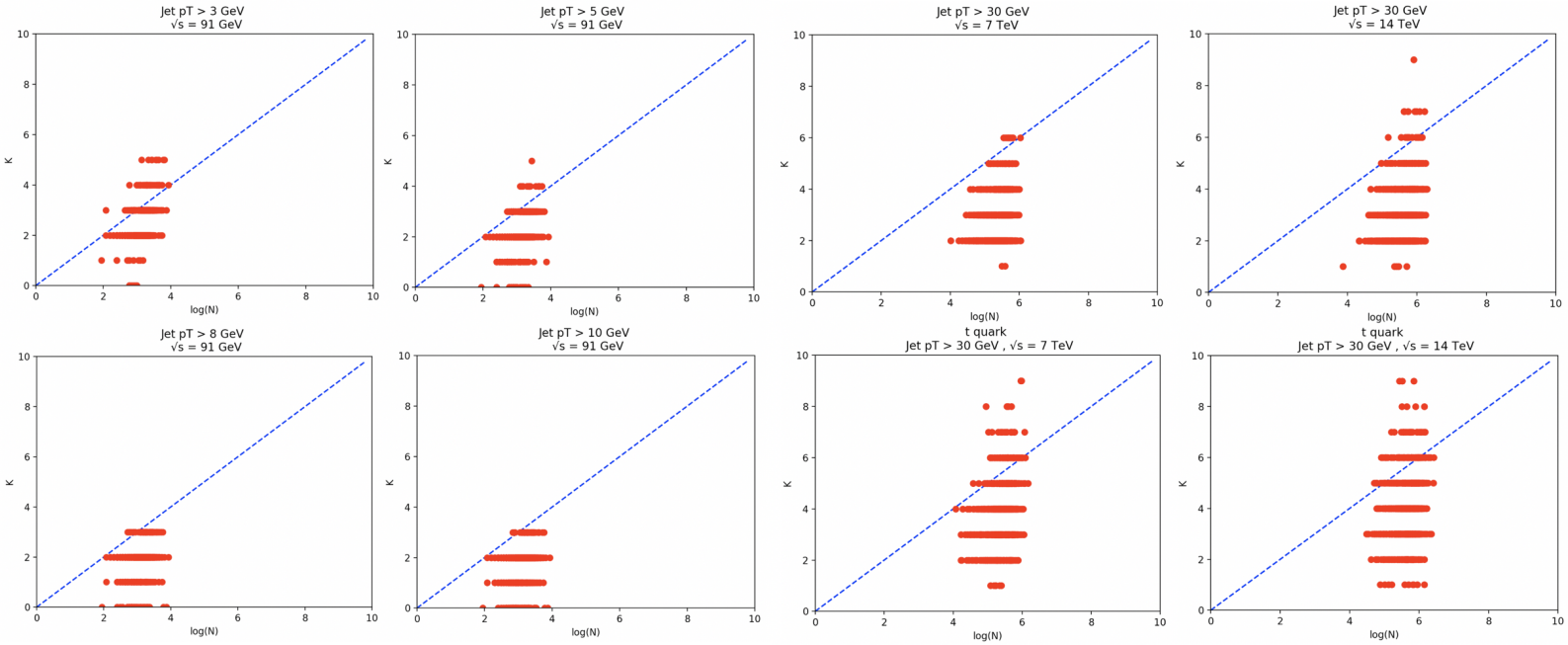

Plots of K *vs* $\log N$ for four different jet p_T cutoff scenarios in e^+e^- collision generated events (four left plots), and two different center-of-mass energies in pp collision generated events (four right plots). Each red point represents a generated event, where K jets have been found for $\log N$ particles.

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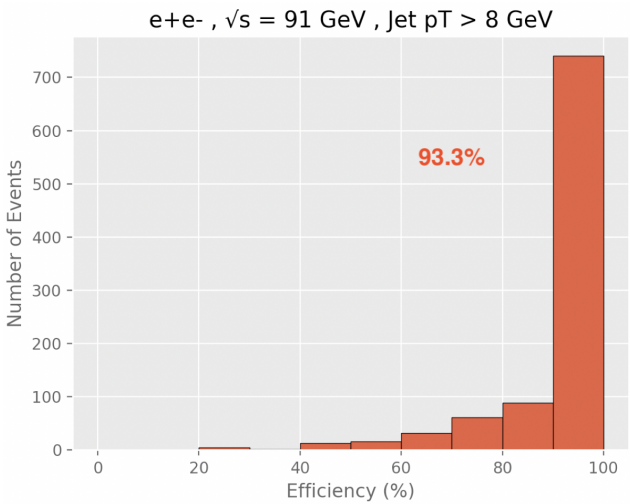
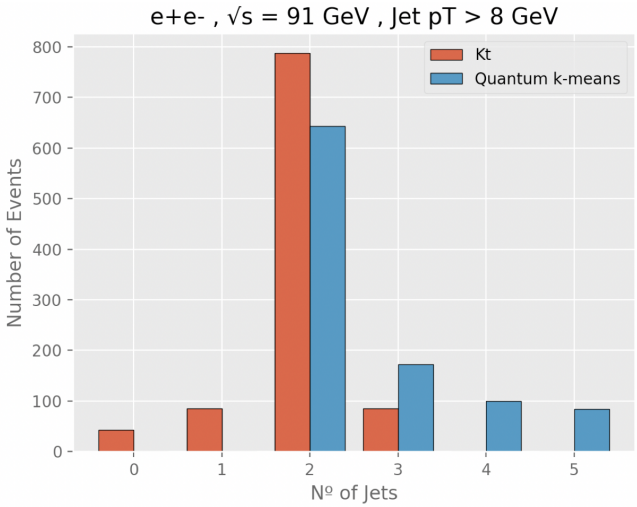
We ran the algorithm on the same 1000 events, checking its clustering efficiency and its jet finding distribution, comparing it with the k_t algorithm.





For a jet $p_T > 8\ GeV$ in the overwhelming majority of the clustered events, the quantum *k-means* algorithm found the same jet configurations as the k_t benchmark, with a decreasing fraction of events for lower clustering efficiencies. The overall jet finding efficiency with respect to the k_t algorithm is $\epsilon = 93.3\%$.

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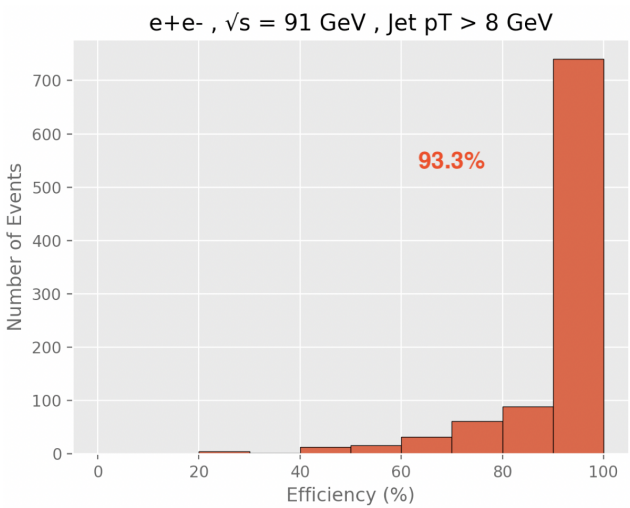
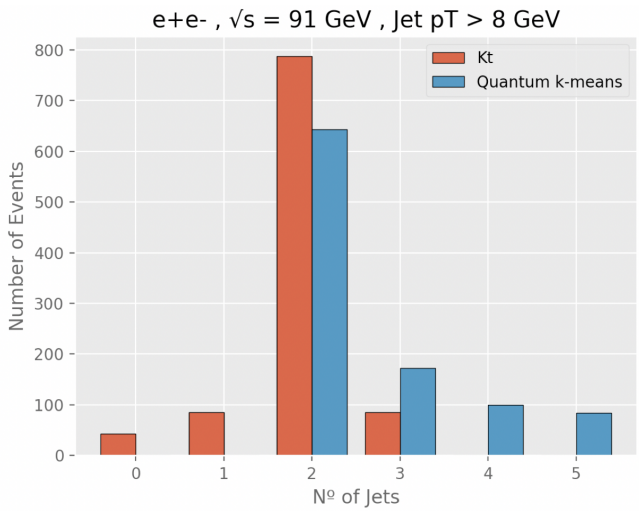
Moreover, it can be seen from the right plot that the number of jets found by the k_t algorithm is in the range from 0 to 3 while the proposed quantum *k-means* algorithm ranges between 2 and 5. This is expected given that the high transverse momentum jet cutoff of $p_T = 8\ GeV$ has been applied only to the k_t algorithm, thus resulting in a lower number of overall found jets .





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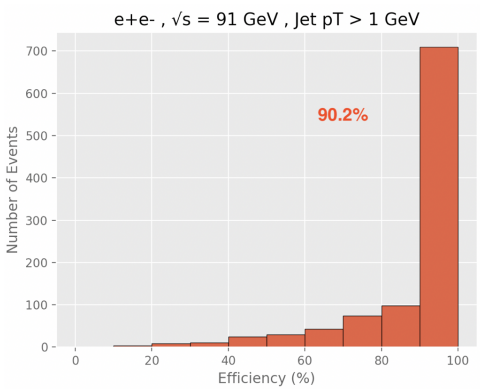

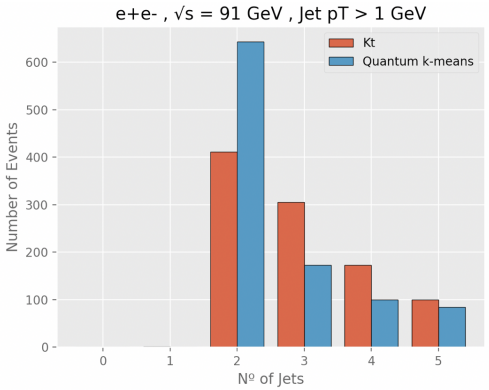

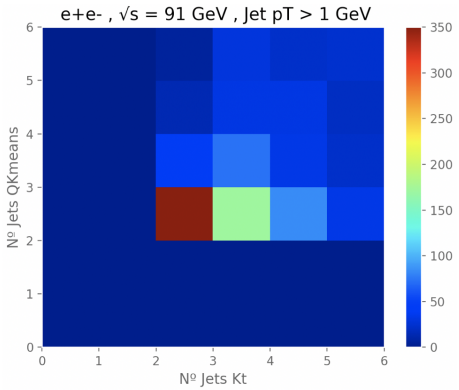

To better understand the relation between the two algorithms, the applied jet p_T cutoff was lowered to $p_T = 1\ GeV$, with the purpose of artificially imposing a near zero barrier to the number of meaningful jets found by the k_t algorithm. As before, a very high efficiency of $\epsilon = 90.2\%$ has been obtained: even for a significantly larger number of jets (see right plot) found by k_t, the clustering efficiency has remained similar. Regarding the distribution of the number of jets found, we can now see from both the right hand histogram and the heatmap plot, that there is a strong correlation between the number of jets found by both algorithms.

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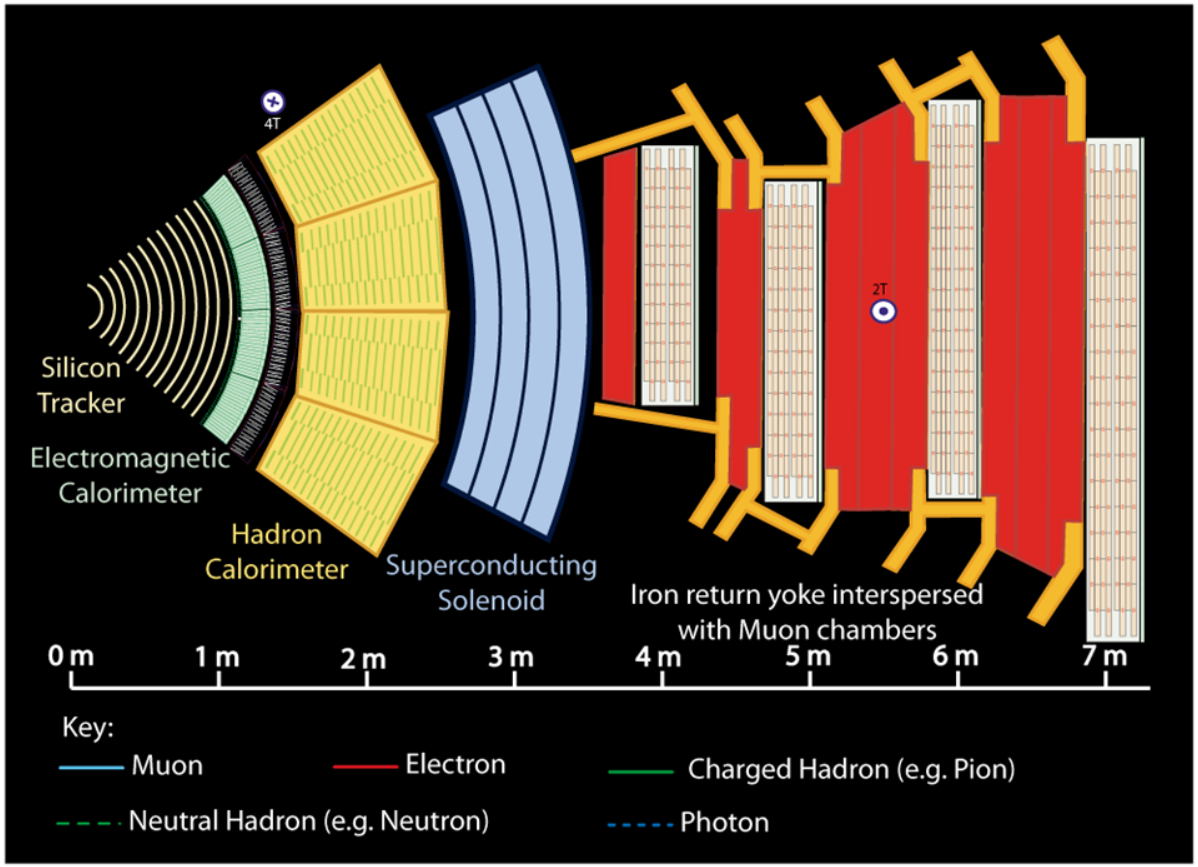

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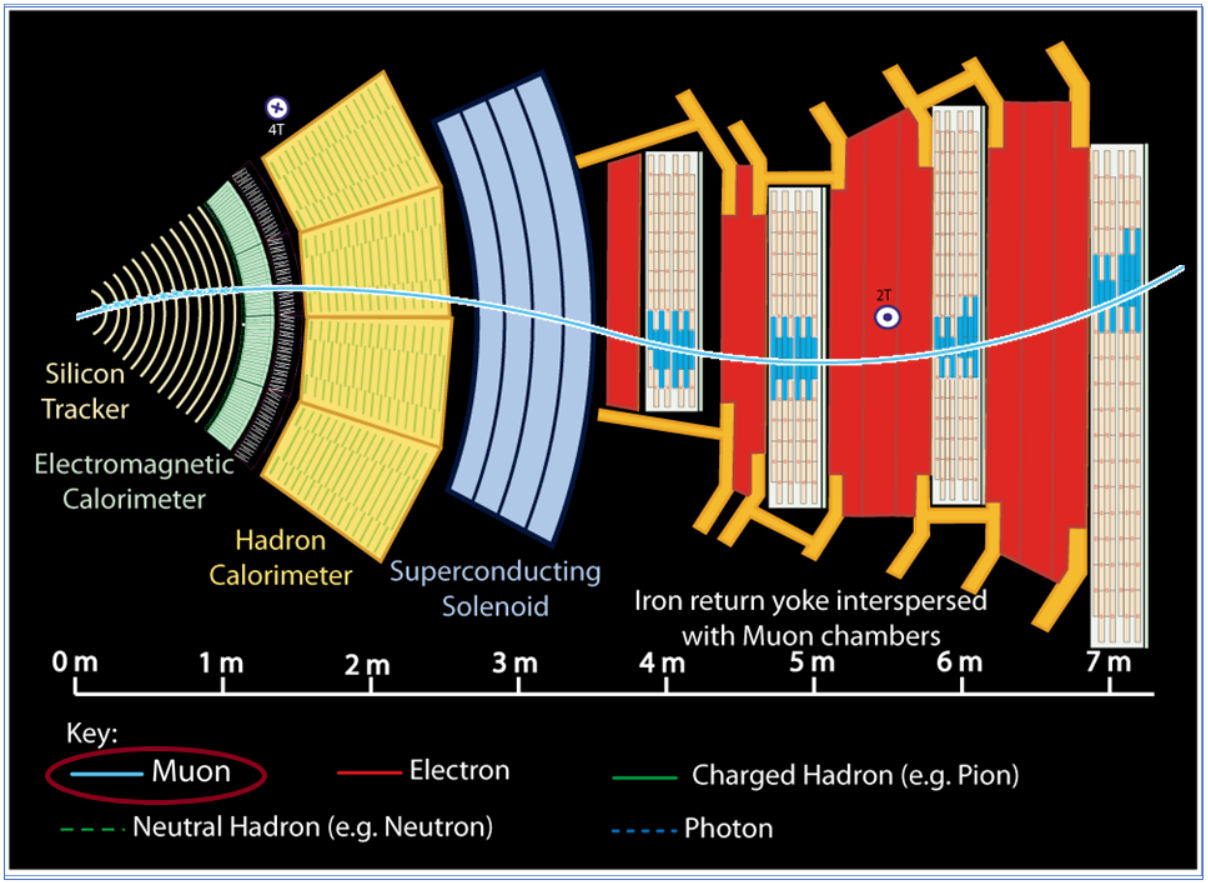

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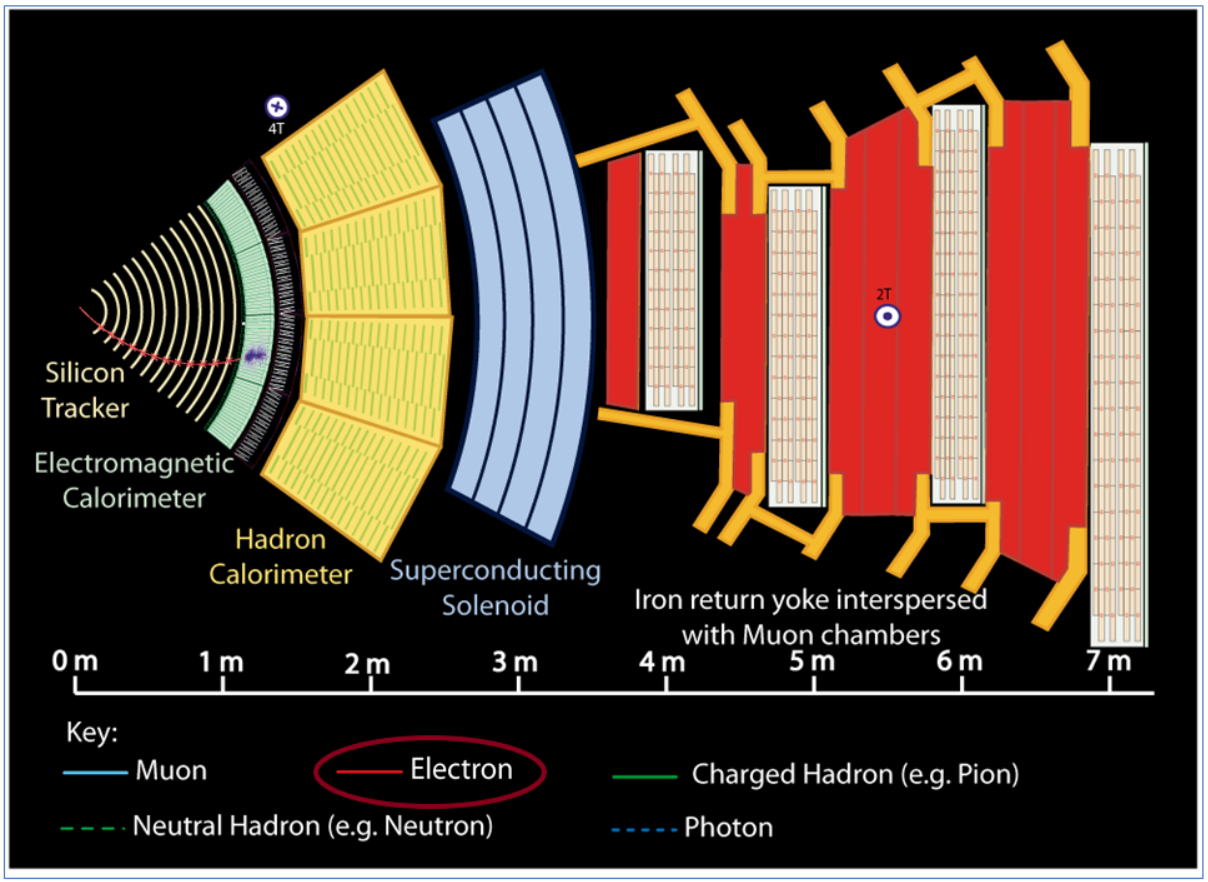

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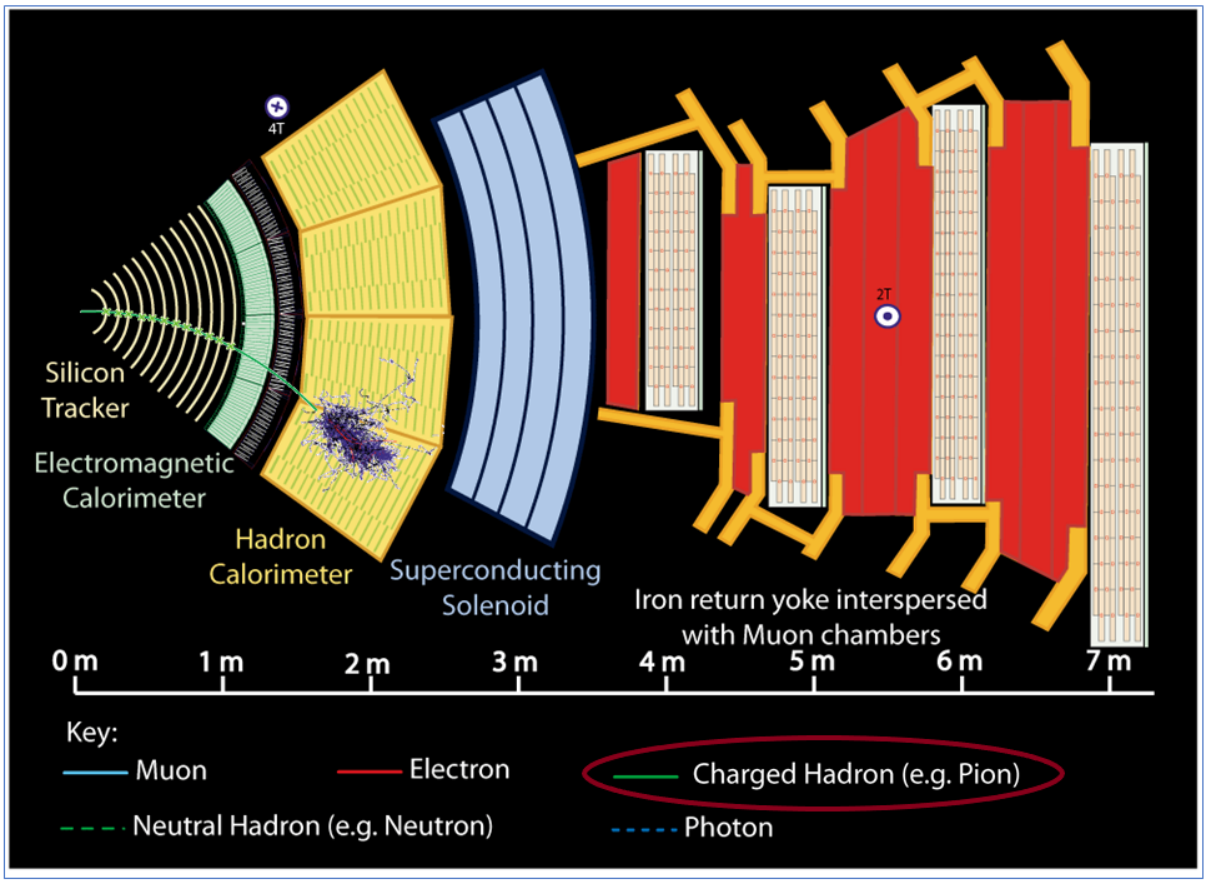

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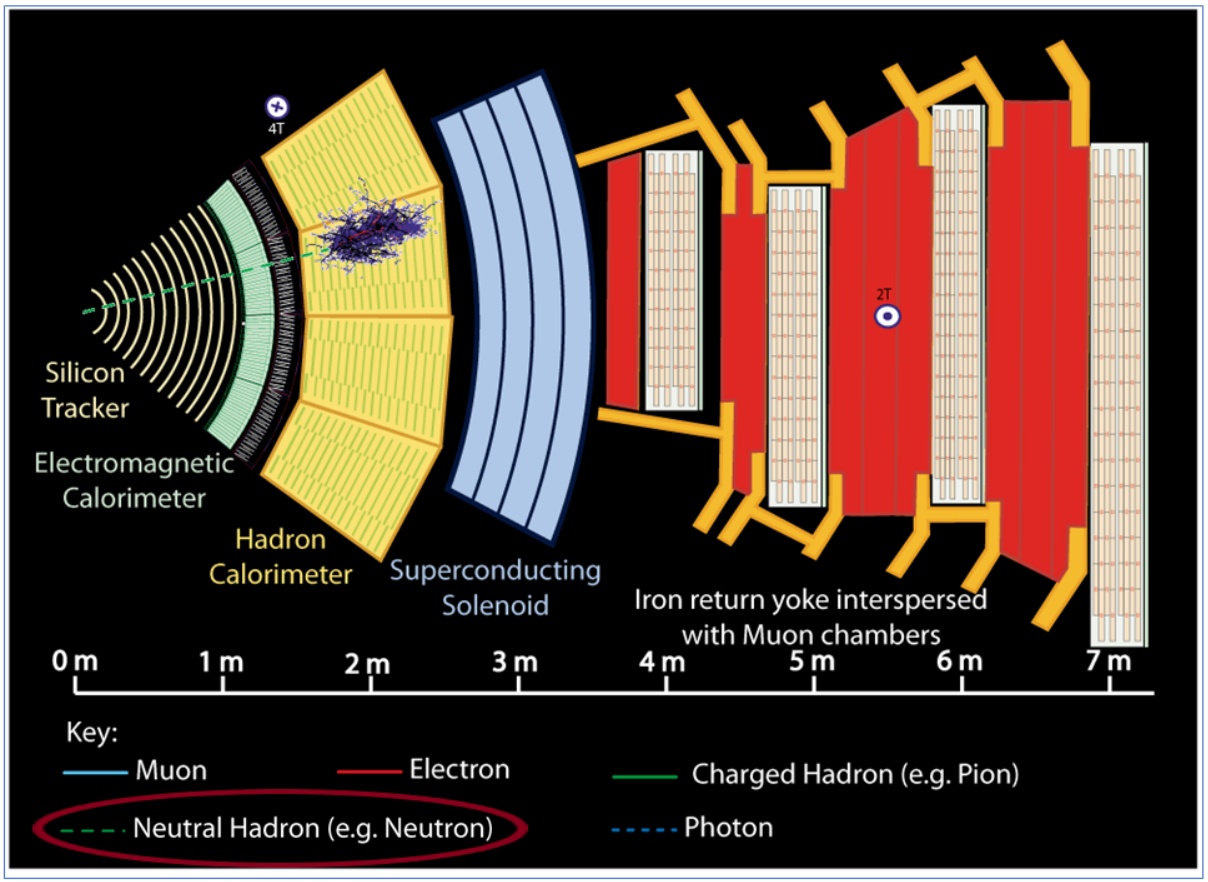

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