Quantum Machine Learning at CERN

QUANTUM
TECHNOLOGY
INITIATIVE

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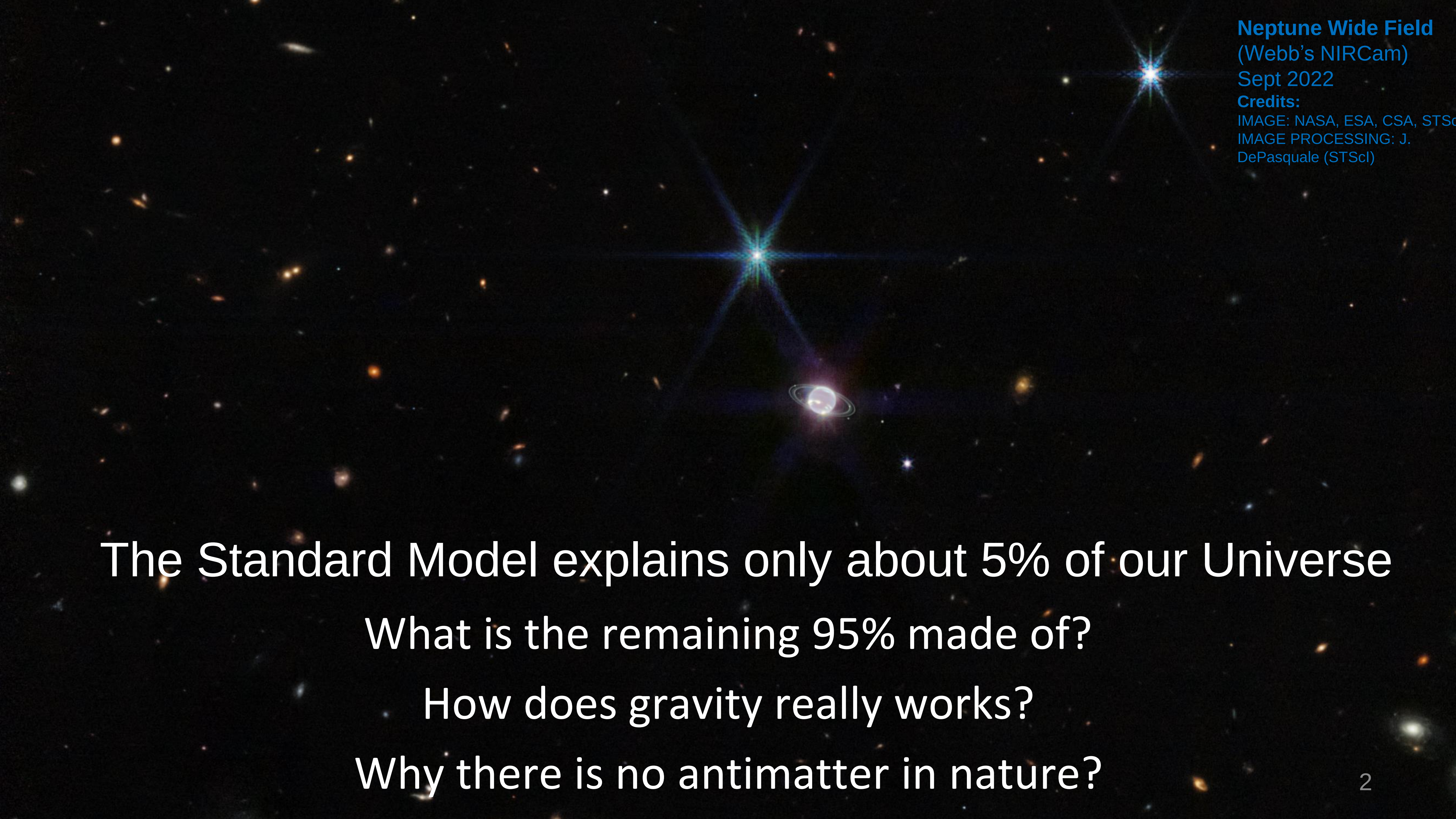
AI and Quantum Research Lead

CERN



Neptune Wide Field
(Webb's NIRCam)
Sept 2022
Credits:
IMAGE: NASA, ESA, CSA, STSc
IMAGE PROCESSING: J. DePasquale (STScI)

The Standard Model explains only about 5% of our Universe

What is the remaining 95% made of?

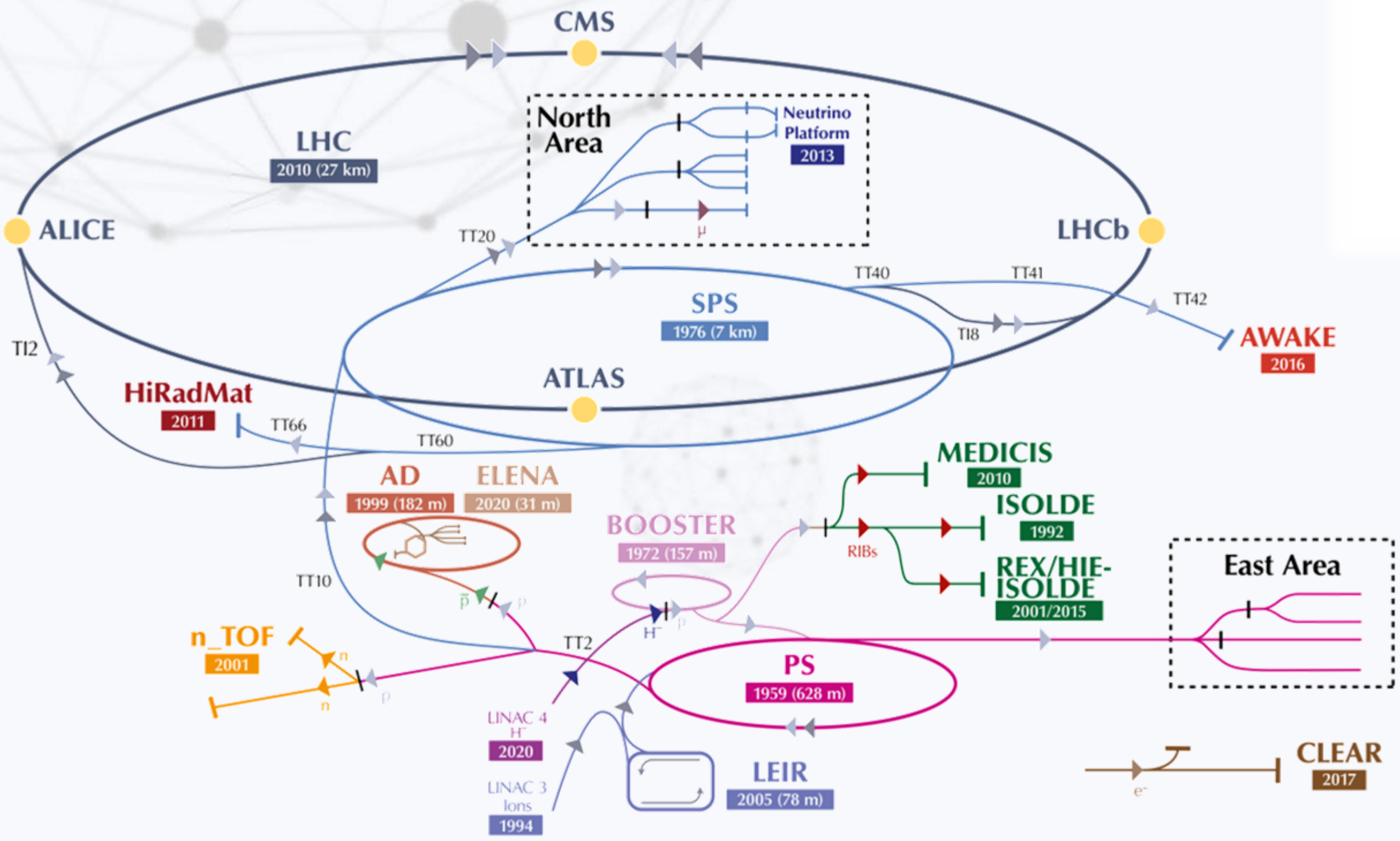
How does gravity really works?

Why there is no antimatter in nature?

CERN

Engineering and technological challenges

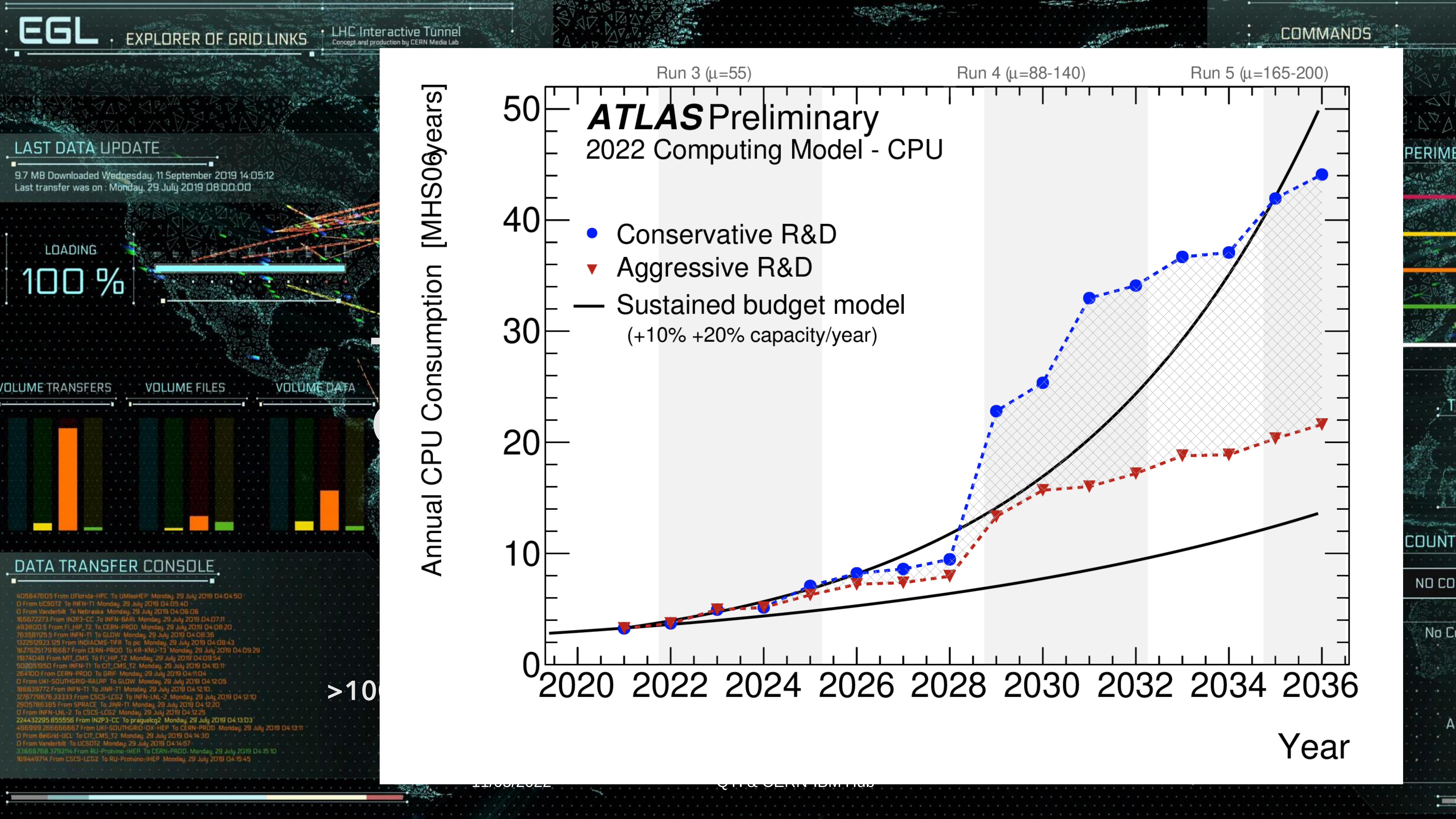
... in a nutshell



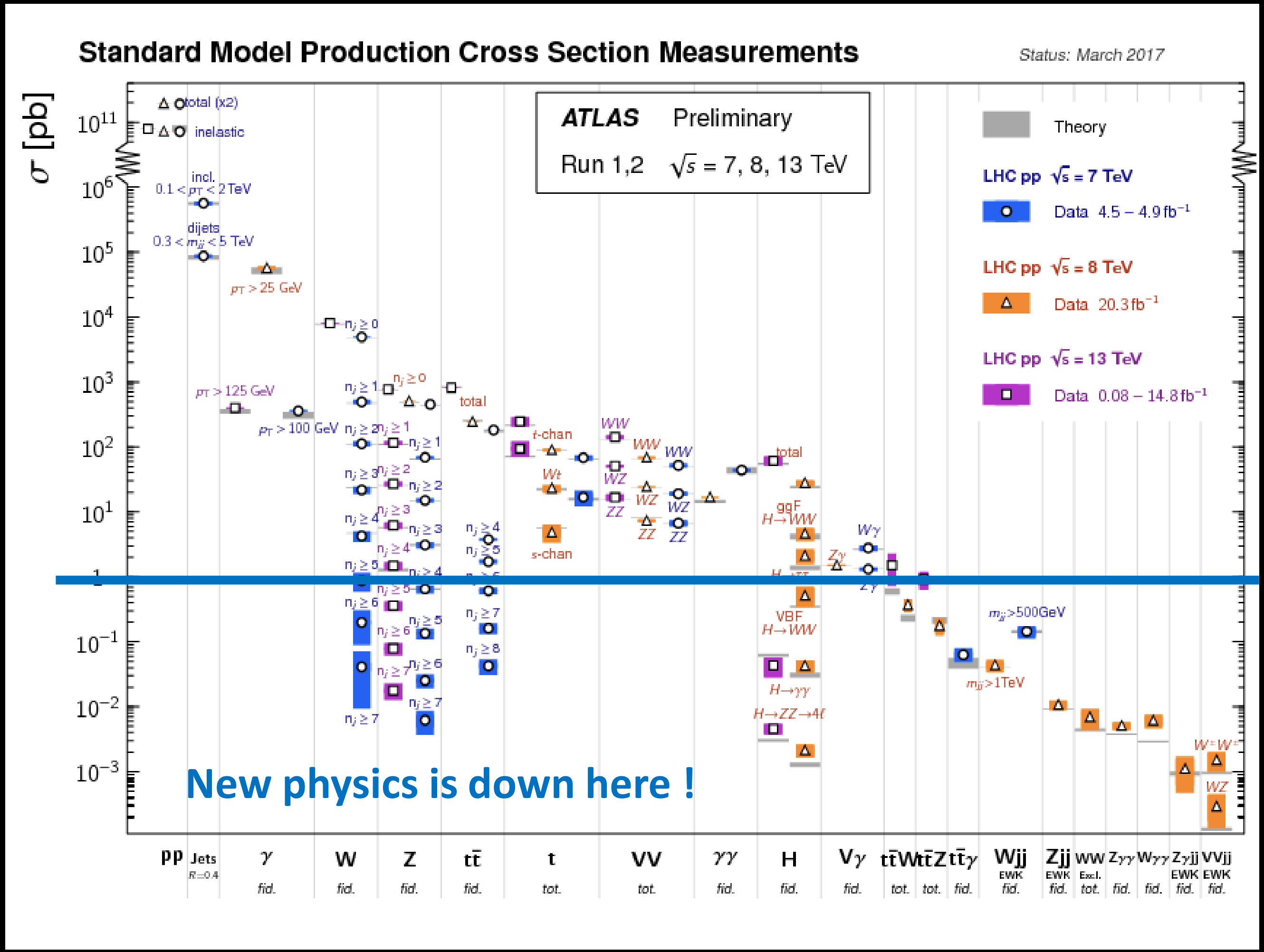
Accelerators infrastructure

~10000 magnets for beam control

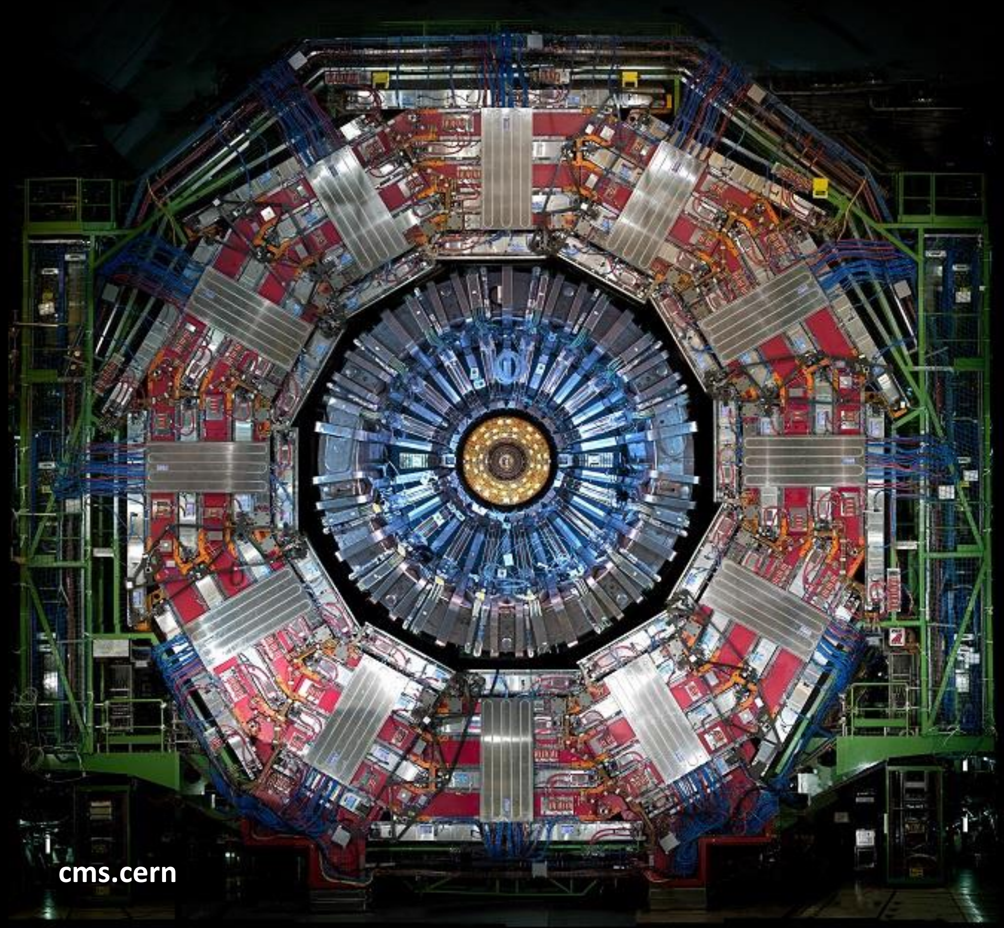
>1000 superconducting dipoles for bending


EGL
EXPLORER OF GRID LINKS
LHC Interactive Tunnel
Concept and production by CERN Media Lab
COMMANDS
LAST DATA UPDATE
9.7 MB Downloaded Wednesday, 11 September 2019 14:05:12
Last transfer was on : Monday, 29 July 2019 08:00:00
LOADING
100 %
VOLUME FILES
VOLUME DATA
DATA TRANSFER CONSOLE
Run 3 (μ=55)
Run 4 (μ=88-140)
Run 5 (μ=165-200)
ATLAS Preliminary
2022 Computing Model - CPU
Conservative R&D
Aggressive R&D
Sustained budget model
(+10% +20% capacity/year)
Annual CPU Consumption [MHS06years]
0
10
20
30
40
50
2020
2022
2024
2026
2028
2030
2032
2034
2036
Year

New Physics search as a Big Data problem

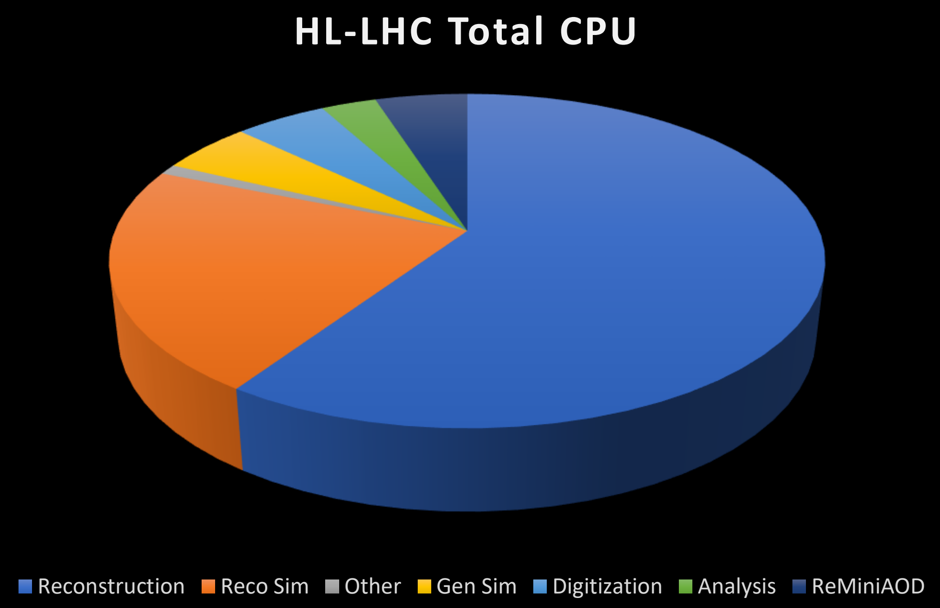


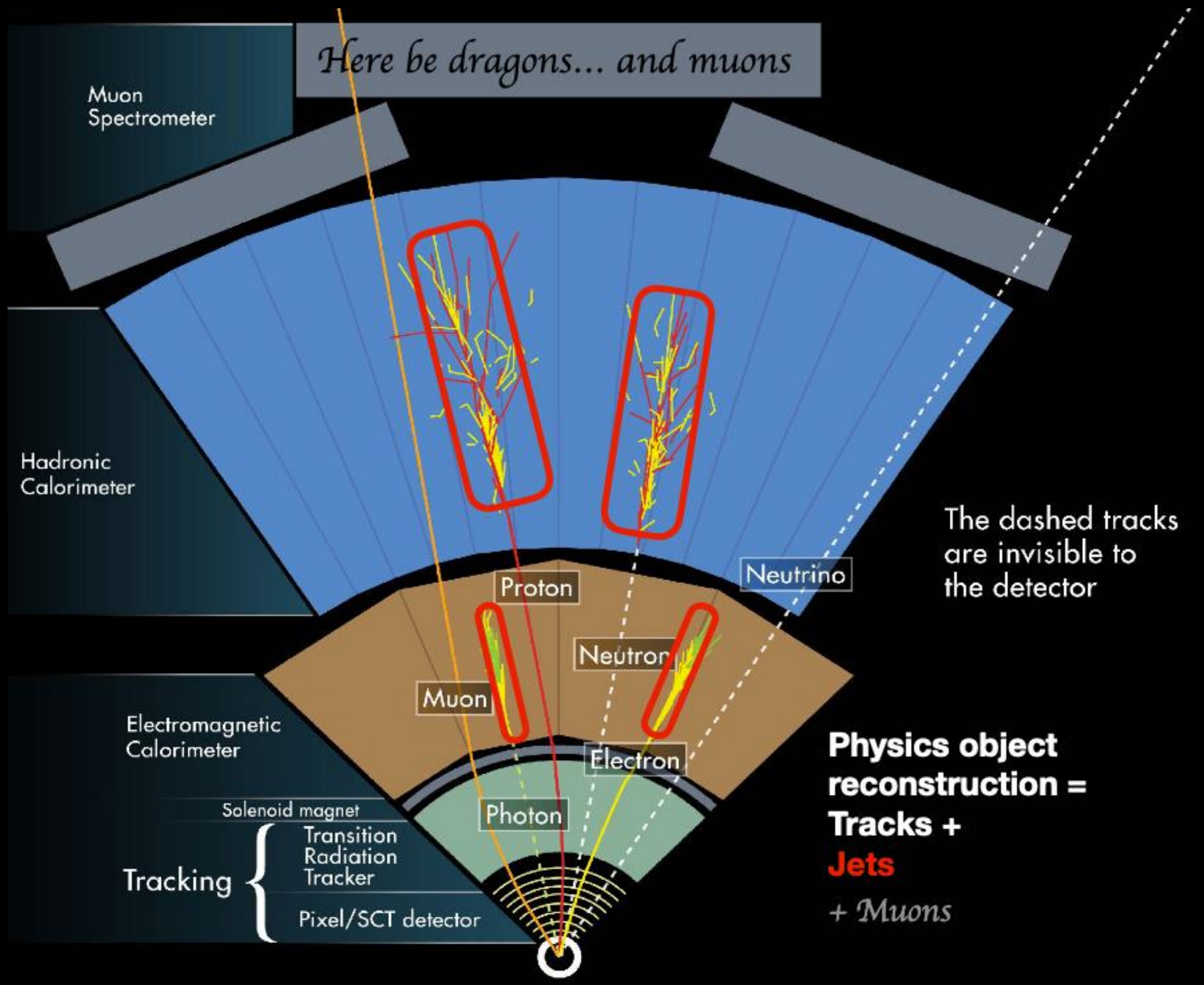
> 400 PB of collisions data



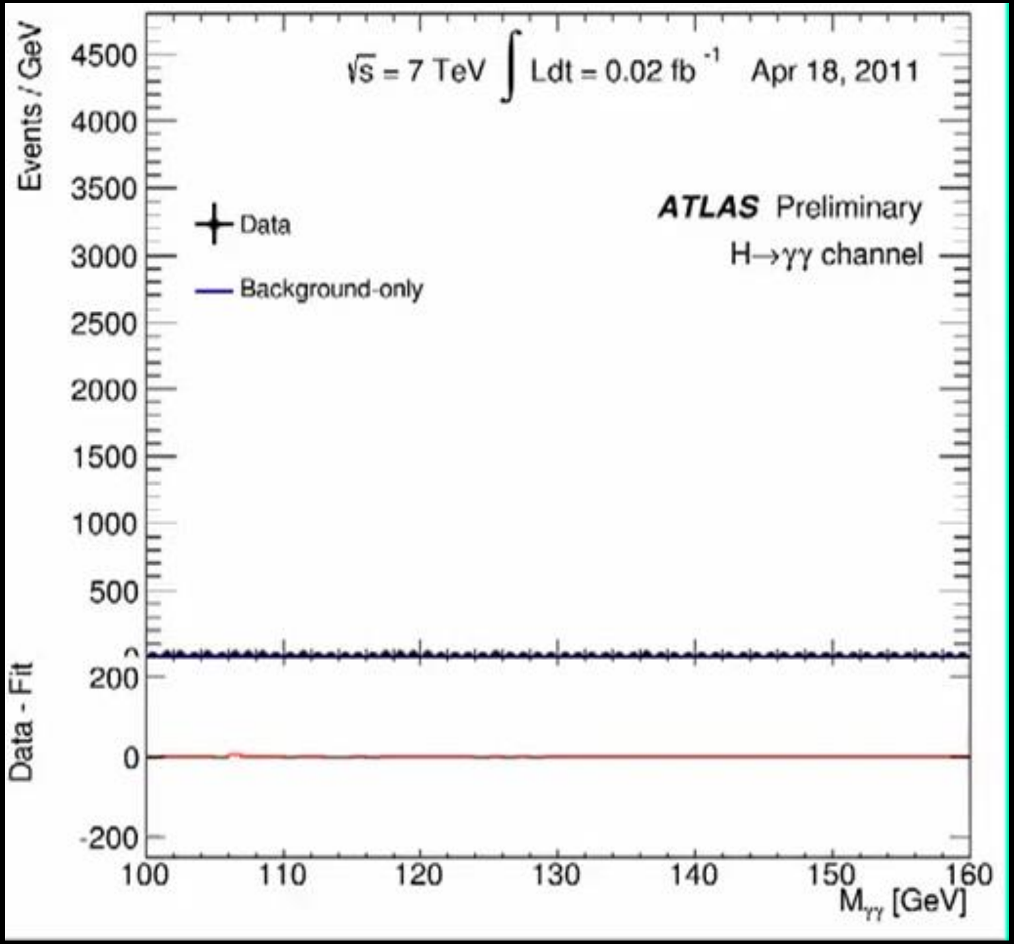
Physics object reconstruction

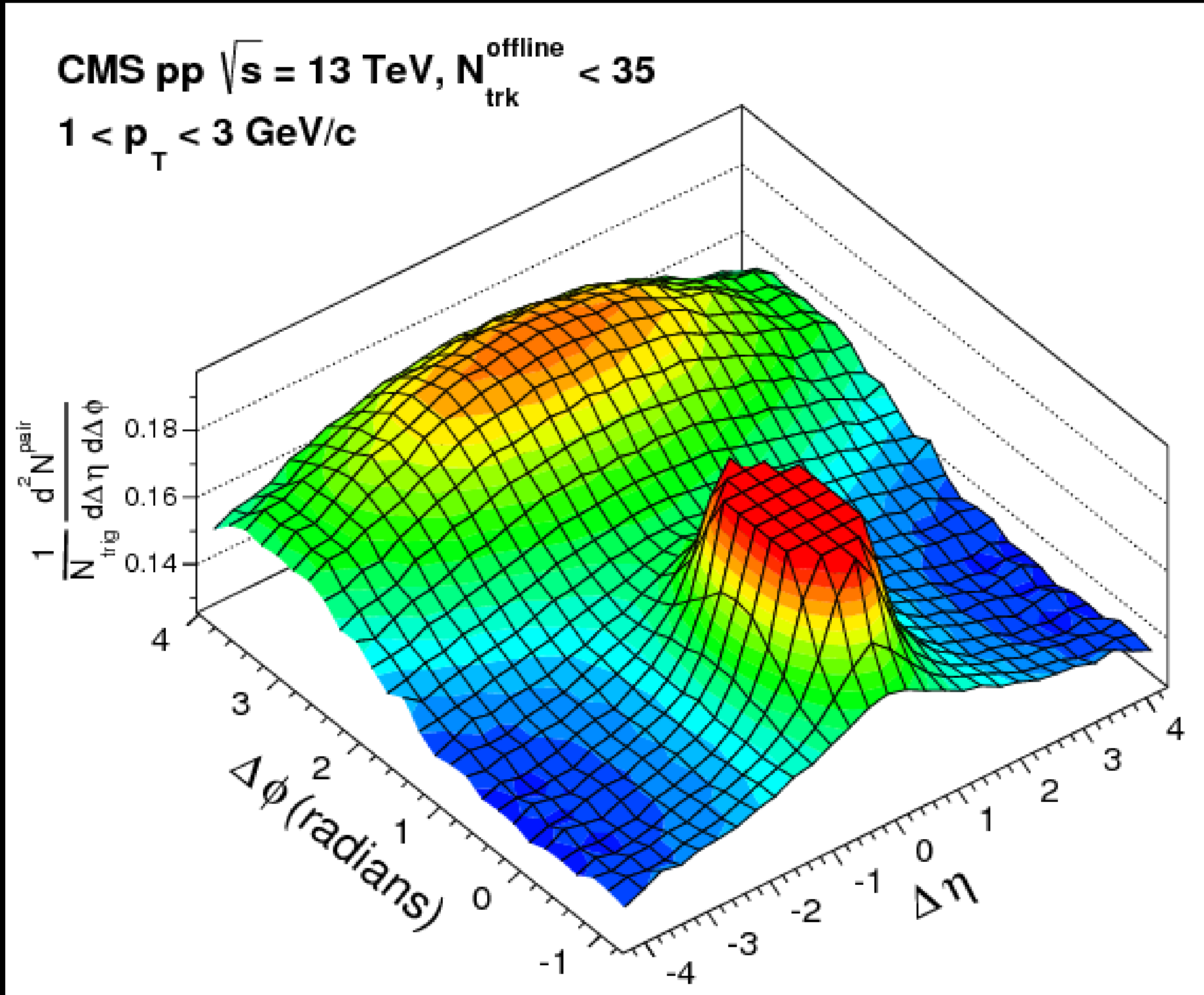
CMS public
2020 estimates





Data Analysis



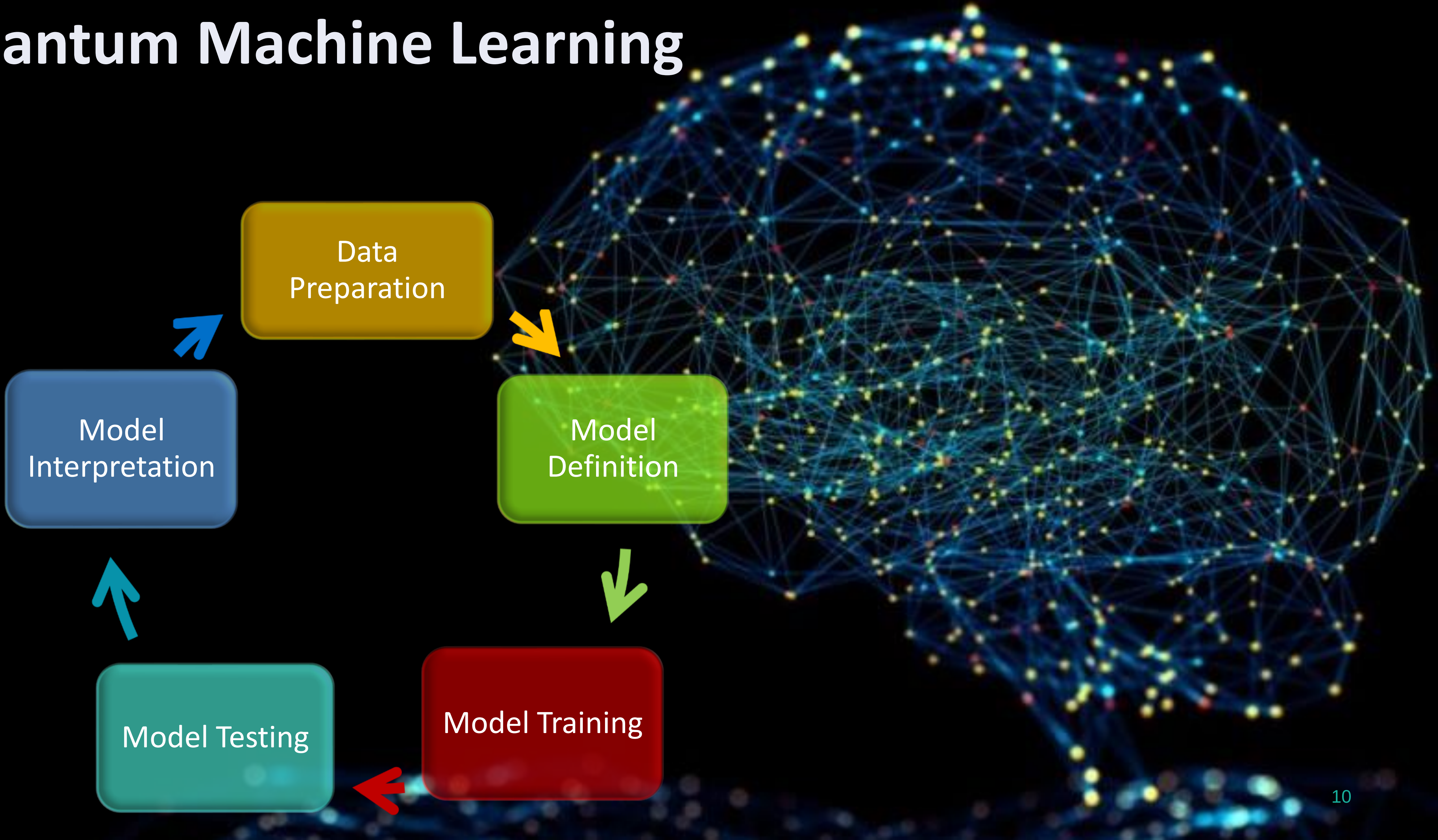


Khachatryan, Vardan, et al. *Physical review letters* 116.17 (2016): 172302.

Quantum Machine Learning :

Some basic concepts

Quantum Machine Learning

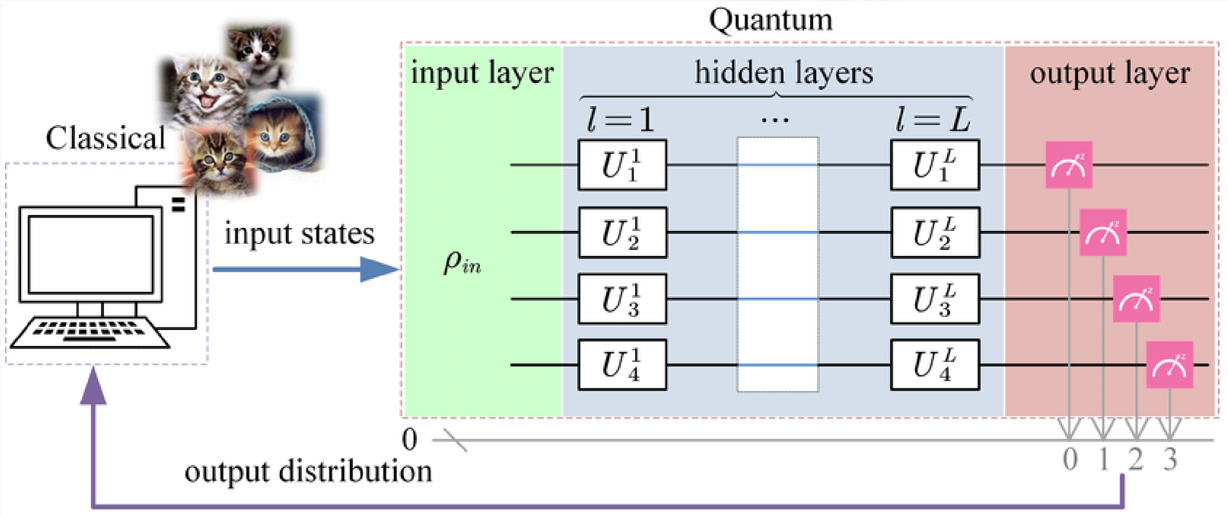


Quantum Machine Learning models

General algorithms applicable to different problems, implemented as quantum-classical hybrids, noise robust

Variational algorithms

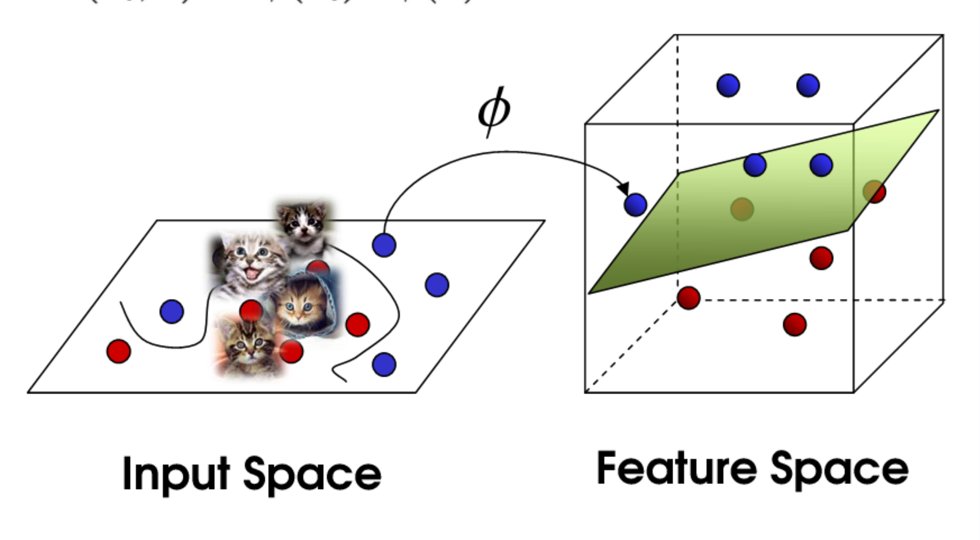
”equivalent” of a neural network



Kernel methods

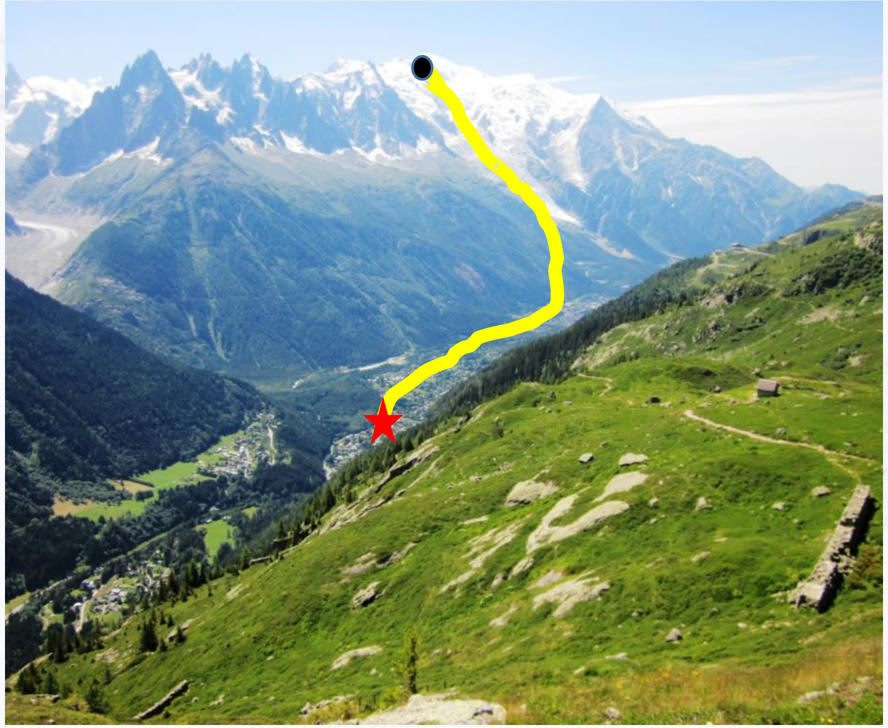
kernels defined by a quantum feature map:

$$k(x_i, x) := \phi(x_i)^\dagger \cdot \phi(x)$$

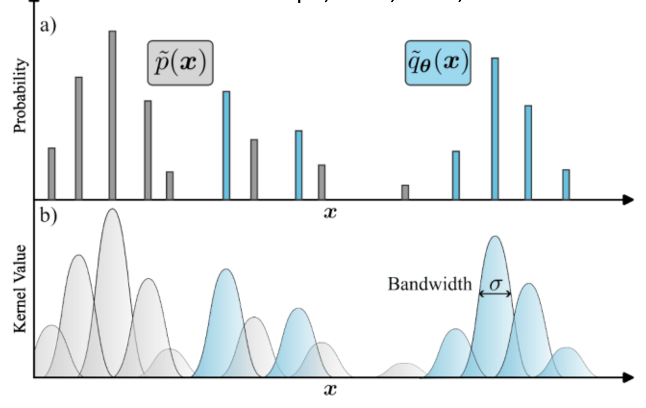


Learning in the quantum space

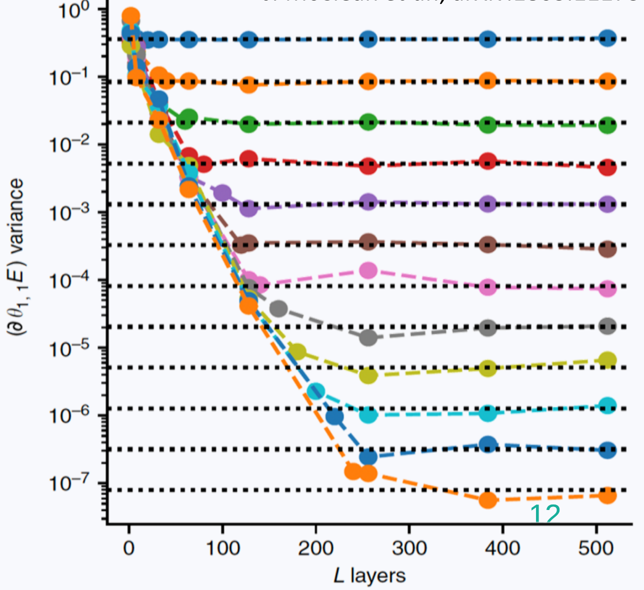
Vanishing gradients, kernels concentration, lack of generalization, trainability barriers….



Rudolph, M. S., *et al.*, *arXiv:2305.02881*.



J. McClean *et al.*, arXiv:1803.11173



Ideally we are looking for classically intractable models
In reality we compromise between "power" and convergence

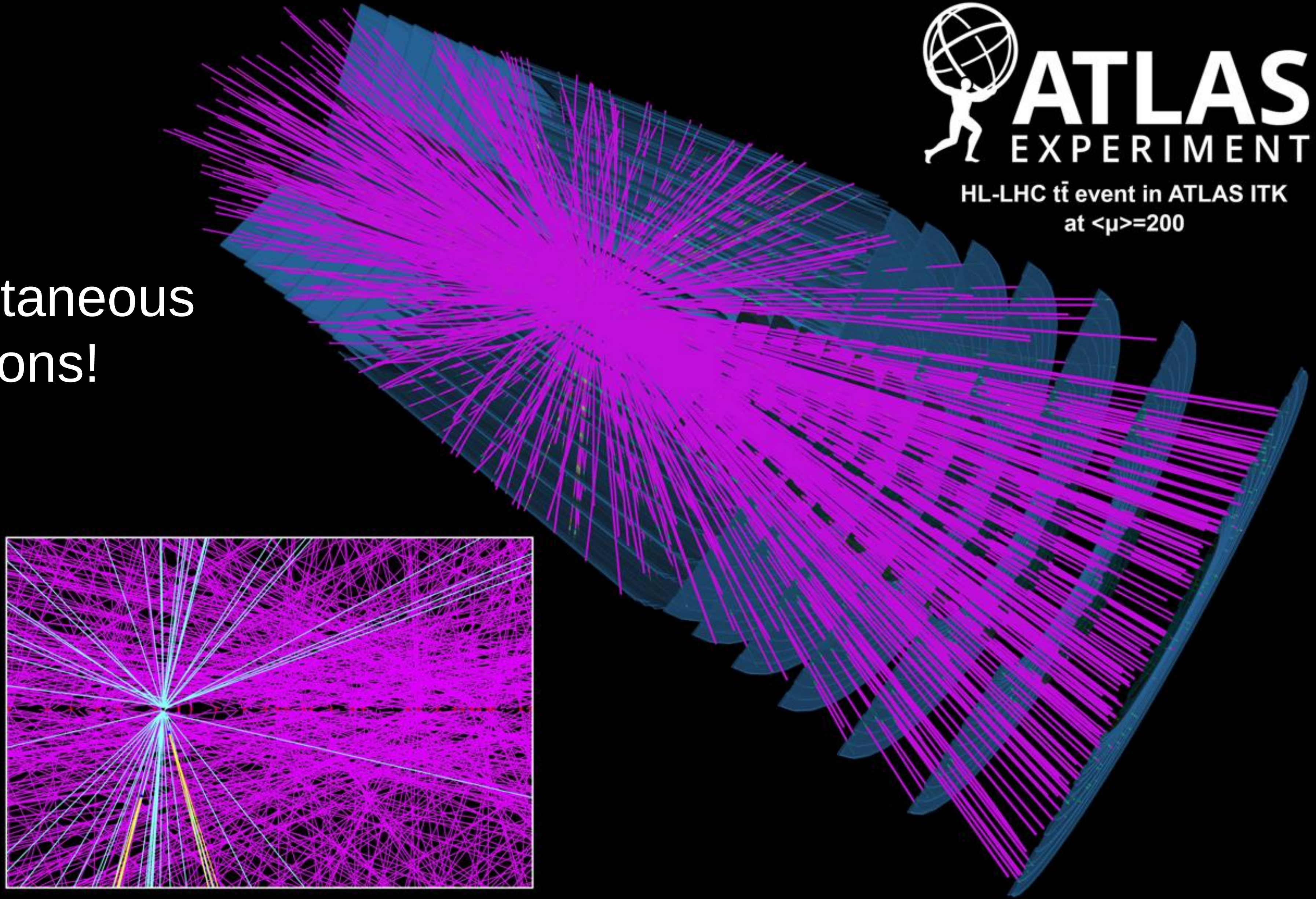
Quantum Machine Learning examples:

Anomaly Detection

Quantum anomaly detection in the latent space of proton collision events at the LHC
arXiv:2301.10780.

The curse of dimensionality

200 simultaneous collisions!

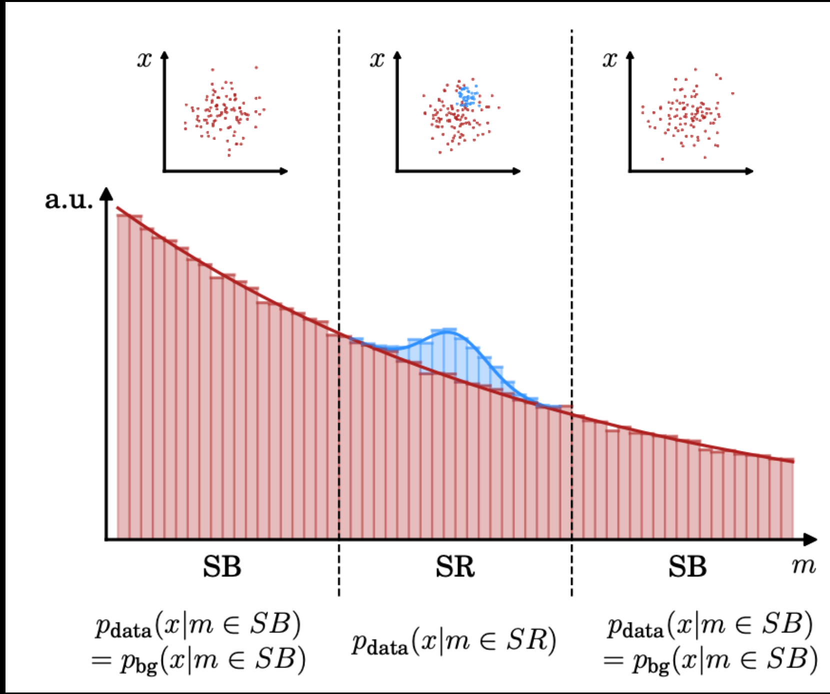


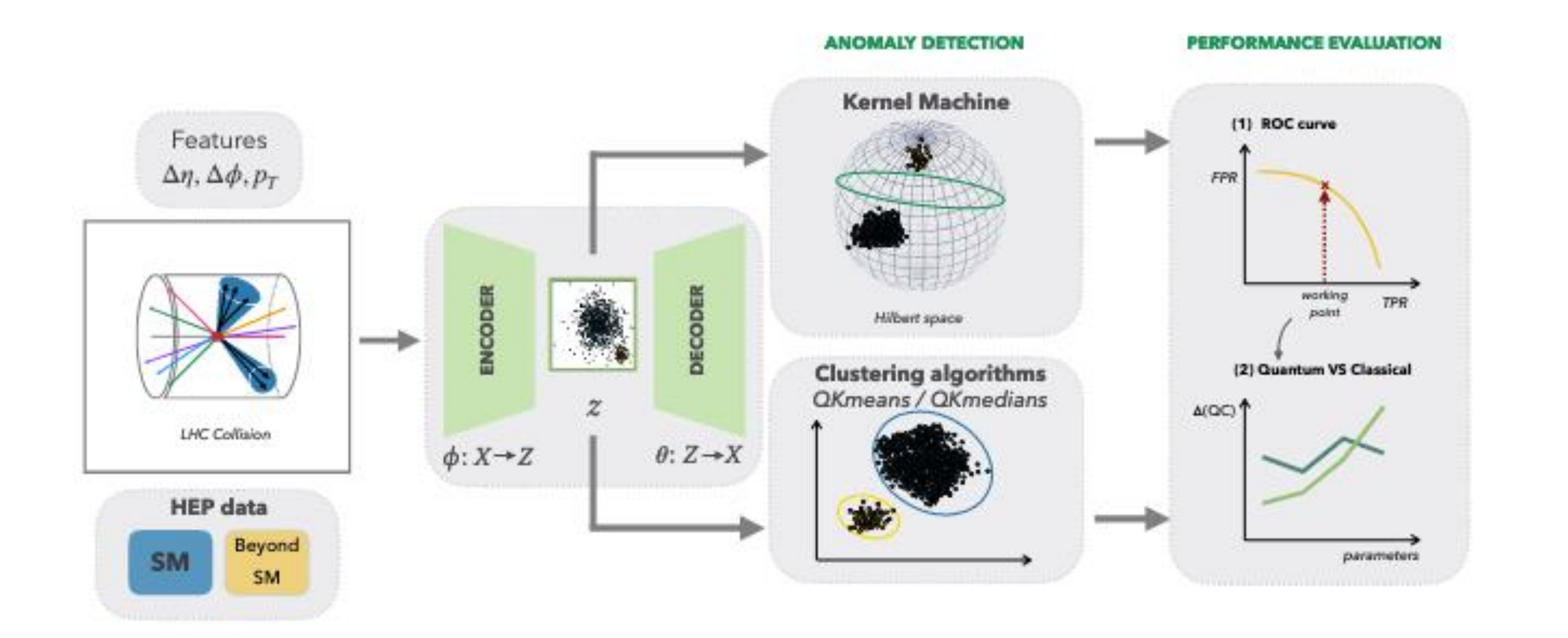
ATLAS EXPERIMENT

HL-LHC $t\bar{t}$ event in ATLAS ITK at <μ>=200

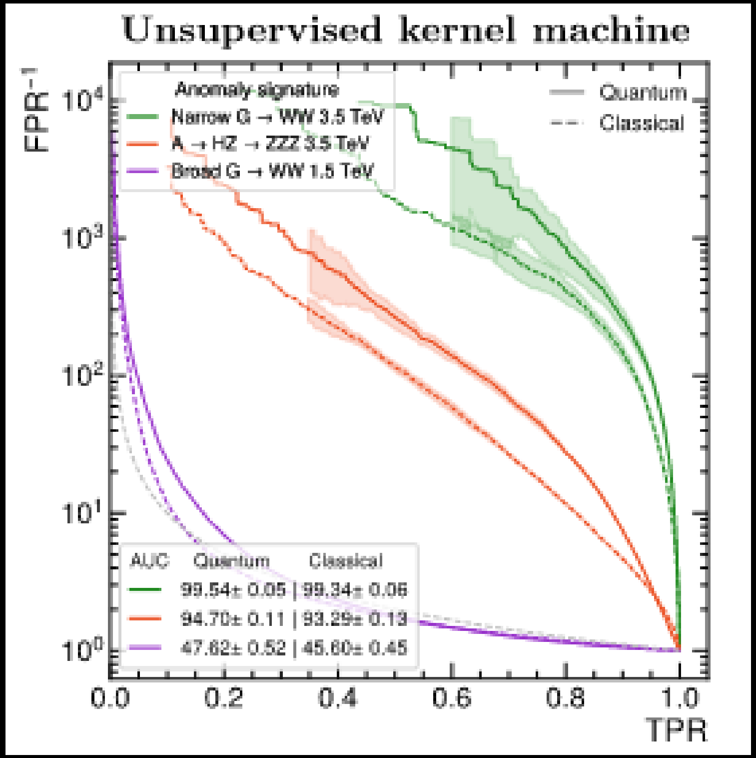
Quantum Machine Learning for Anomaly Detection

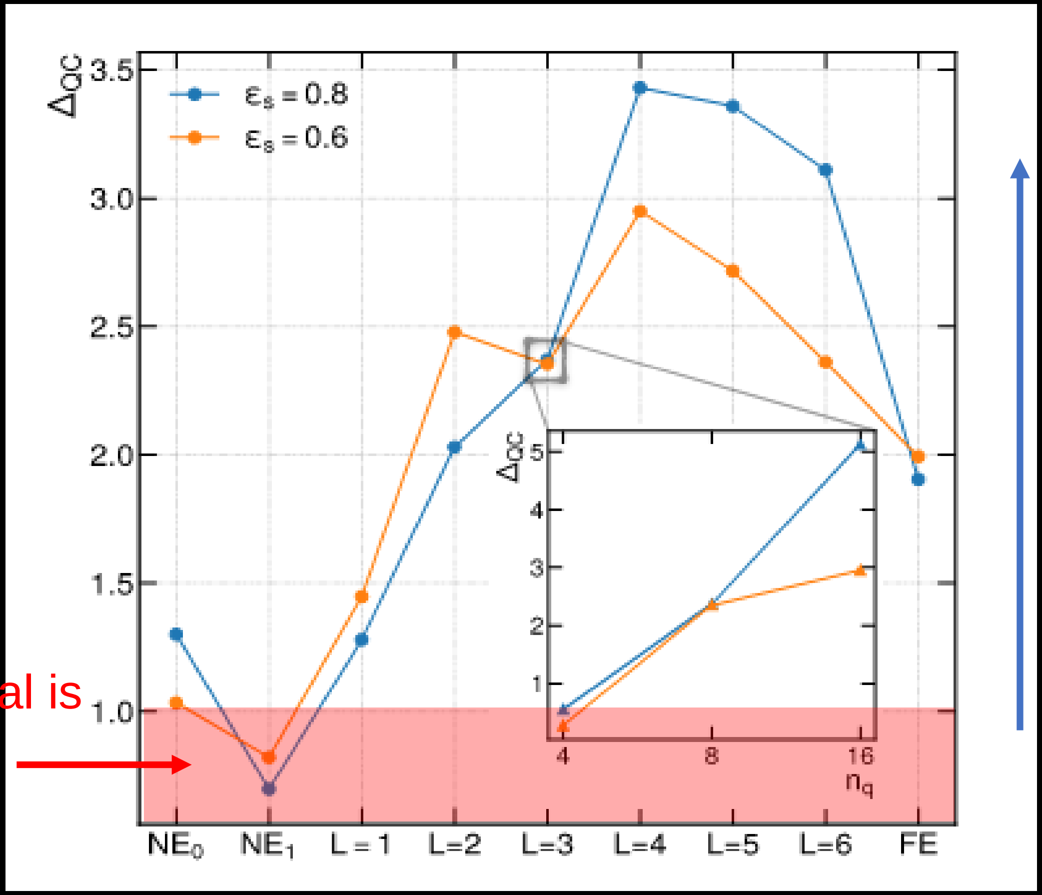
Anomaly detection can point to new physics at the LHC





Anomaly Detection





Classical is better

Higher is better

Increasing entanglement & expressivity

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

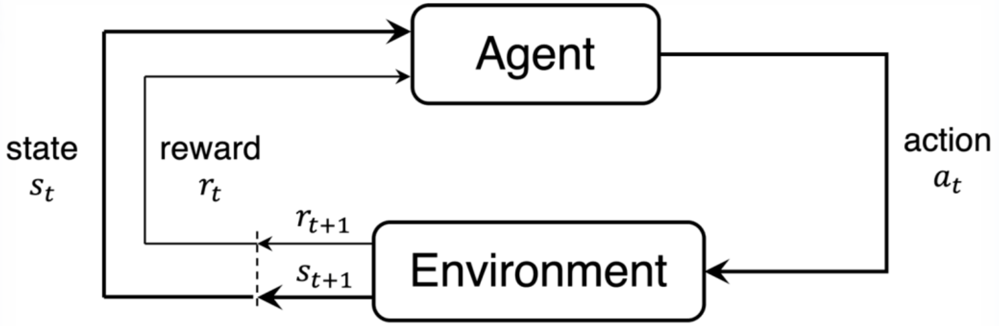
Quantum Machine Learning examples:

Reinforcement Learning

Schenk, M *et al.* Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines. *arXiv preprint arXiv:2209.11044.*, CHEP2023

Reinforcement learning

... in a nutshell



RL book: Sutton & Barto

Trial-and-error learning

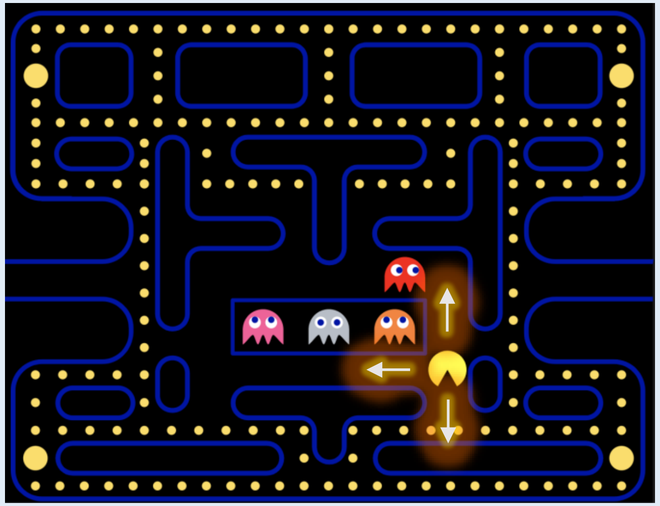
- Agent **takes actions** in environment and **collects rewards**

Q-learning

- Estimate **return using Q-function** $\mathrm{Q}(\boldsymbol{s}, \mathbf{a})$
- **Learn iteratively** using **collected interactions**
- Once trained, **select action greedily**

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

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**

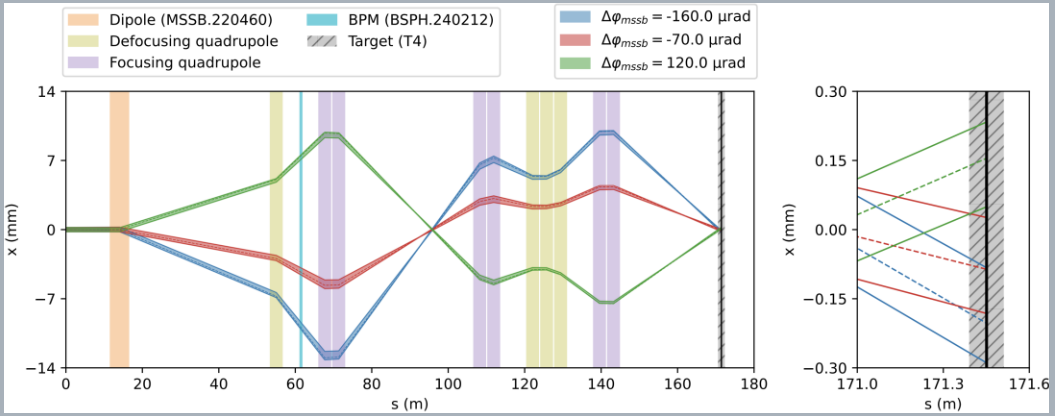
- **Classical Deep Q-learning (DQN)**
  Feed-forward neural net
- **Free-energy based RL (FERL)**
  Quantum Boltzmann machine (QBM)

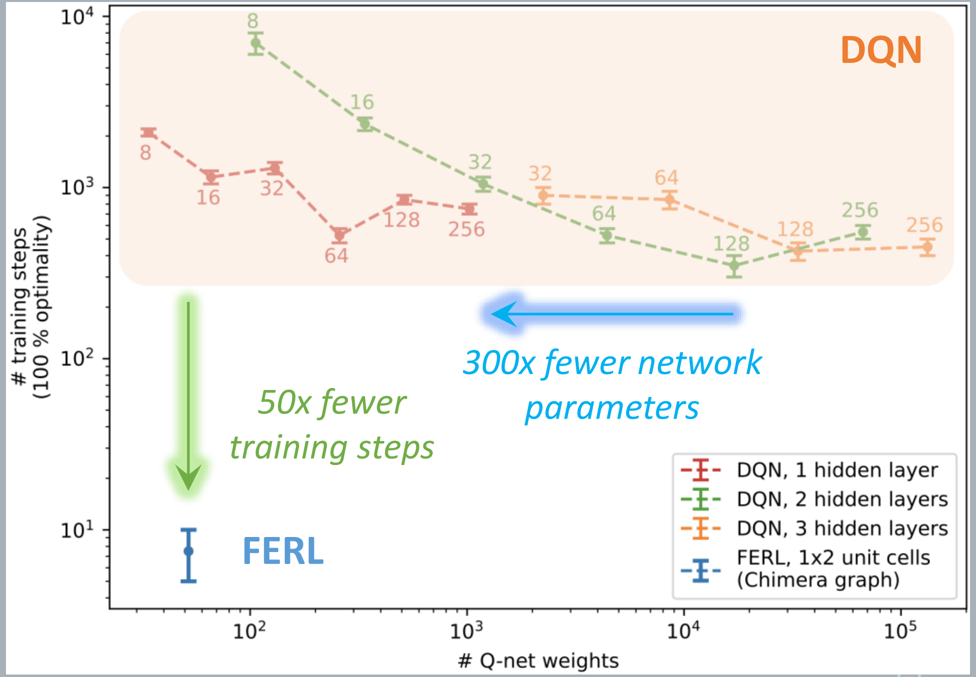
Key concept: sample-efficiency

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

1st study: 1D beam steering

CERN *North Area transfer line (discrete action space)*





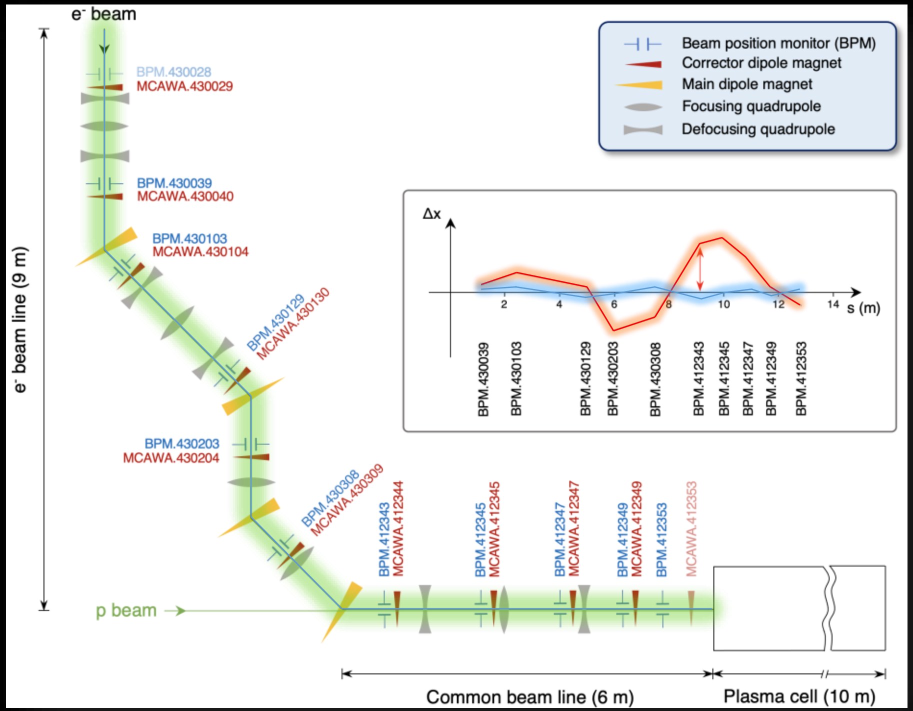
Schenk, M *et al.* Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines. *arXiv preprint arXiv:2209.11044.*, CHEP2023

2nd study: 10D continuous beam steering

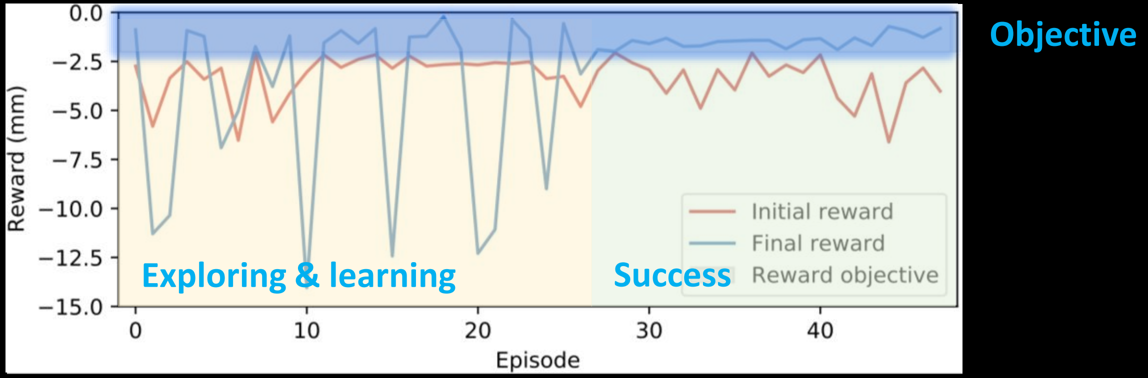
Environment: e⁻ beam line of AWAKE

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

AWAKE: Advanced Proton Driven Plasma Wakefield Acceleration Experiment

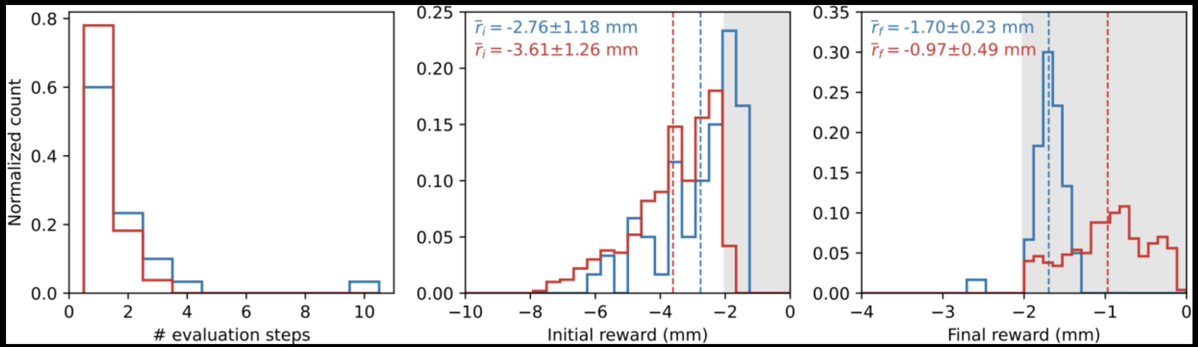


Training: on D-Wave Advantage quantum annealer (QA)



Evaluation: on actual beam line

Real vs. simulated QA



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

Quantum Machine Learning examples:

Phase Transitions identification

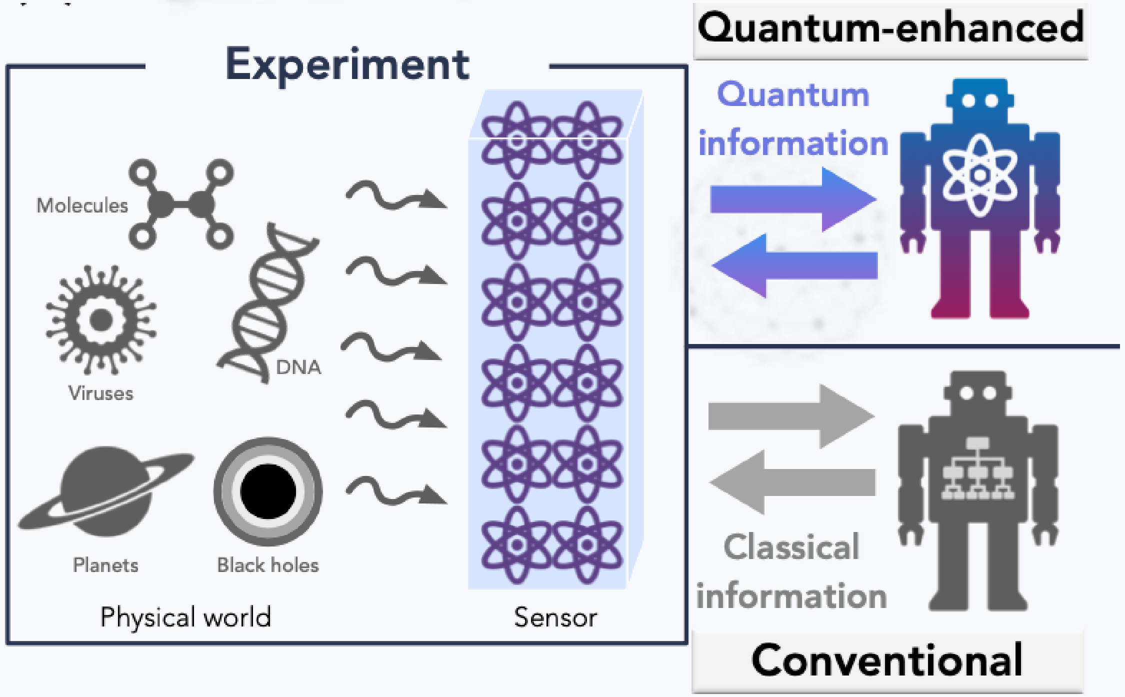
Saverio Monaco et al., **Quantum phase detection generalisation from marginal quantum neural network models**, arXiv:2208.08748v1.

Classifying quantum data

Generate **quantum states** directly on the device

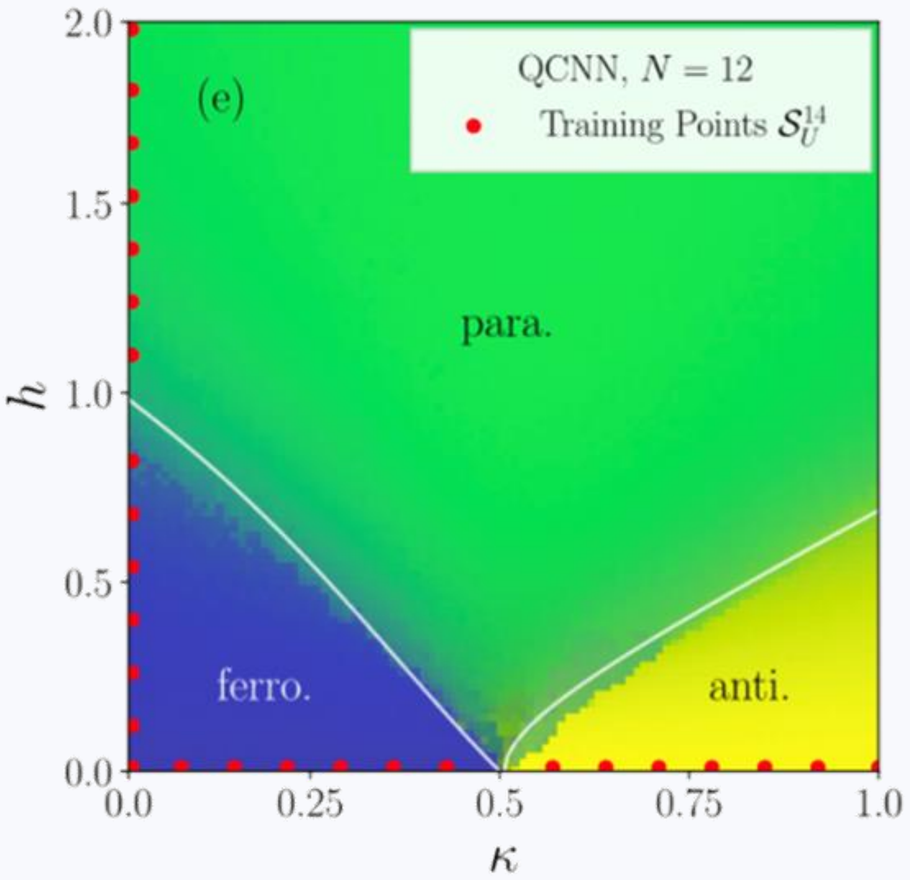
Train QCNN to **classify quantum states**

Use marginal datasets → **OOD generalization !**



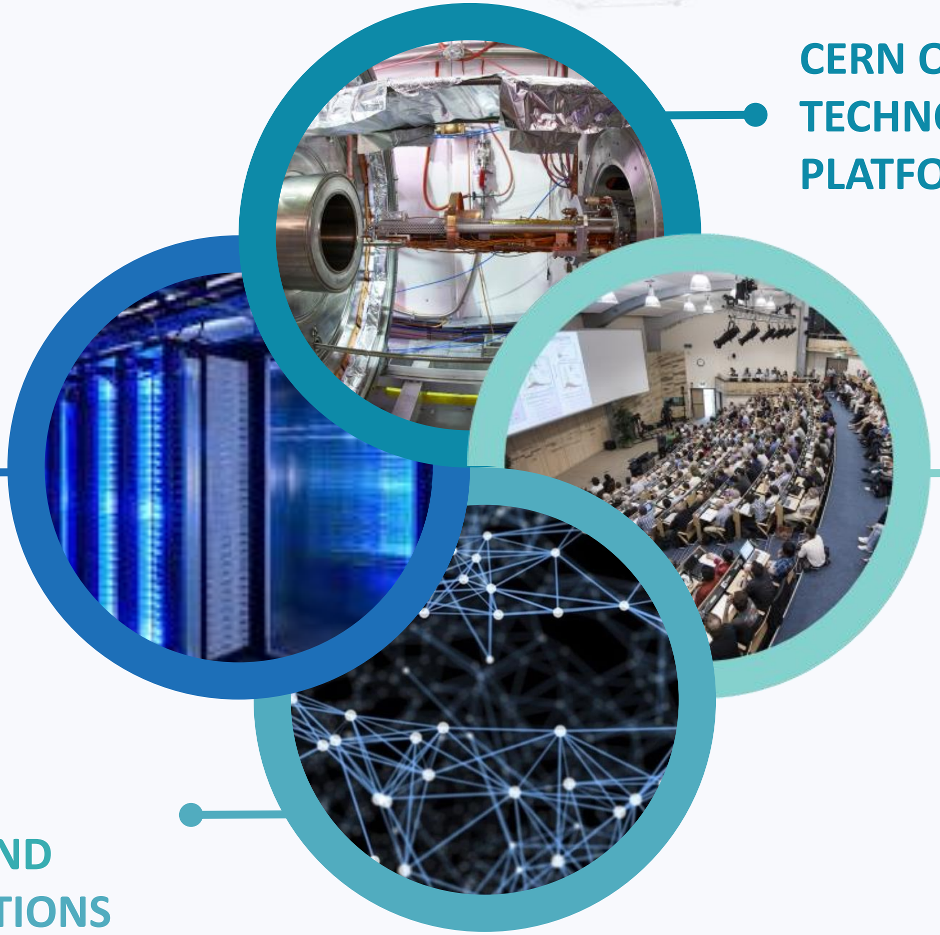
Out of Distribution Generalization

M..Caro et al., Out-of-distribution generalization for learning quantum dynamics, arxiv:2204.10268



The CERN Quantum Technology Initiative

Phase 2 :2024-2028



CERN QUANTUM TECHNOLOGY PLATFORMS

HYBRID QUANTUM COMPUTING AND ALGORITHMS

COLLABORATION FOR IMPACT

QUANTUM NETWORKS AND COMMUNICATIONS

Outlook and open questions

- Quantum computing offers great opportunties while HEP provides challenging problems
  - **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?
- CERN is committed to creating impact on QT research in the coming years

CERN

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