ICSC
Centro Nazionale di Ricerca in HPC,
Big Data and Quantum Computing

QUANTUM ML

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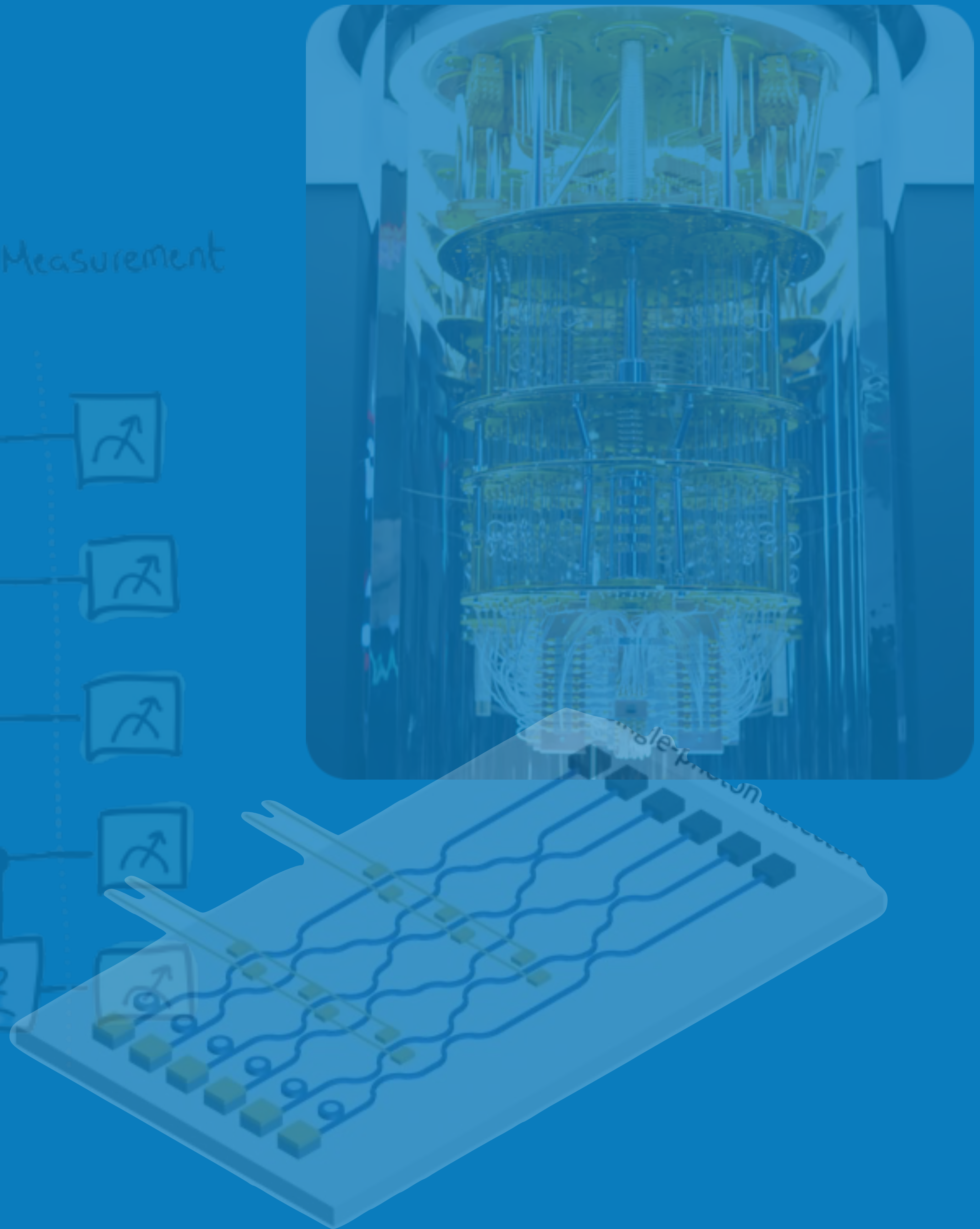

Workshop Computing@CSN5 - Bari - October 14-16th, 2024

INFN ROMA

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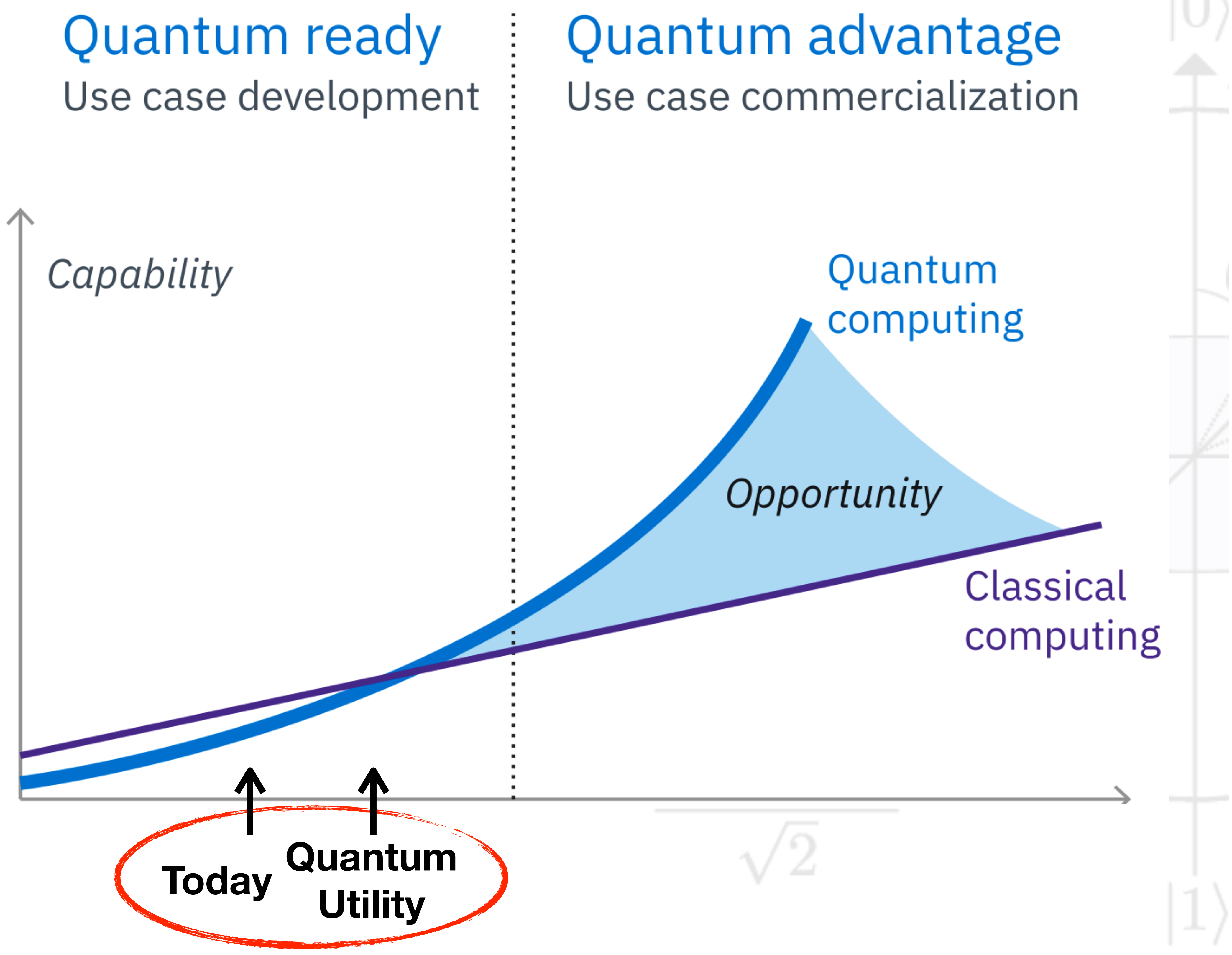
INTRODUCTION & OUTLOOK

- quantum computers offer an intriguing path for a paradigmatic change of computing in the natural sciences, with the potential for achieving a significant speed-up of numerical simulations and big data analysis
- INFN research activities can help realising and test this potential (and leverage it in the future) through a source of formidable challenging computational problems
- equipping classical ML algorithms with QC may offer the possibility of exploit QC acceleration with current NISQ devices, and find ways to prove quantum utility
- Outlook:
  - Quantum Computing & QML
  - Example applications
  - The road ahead & summary

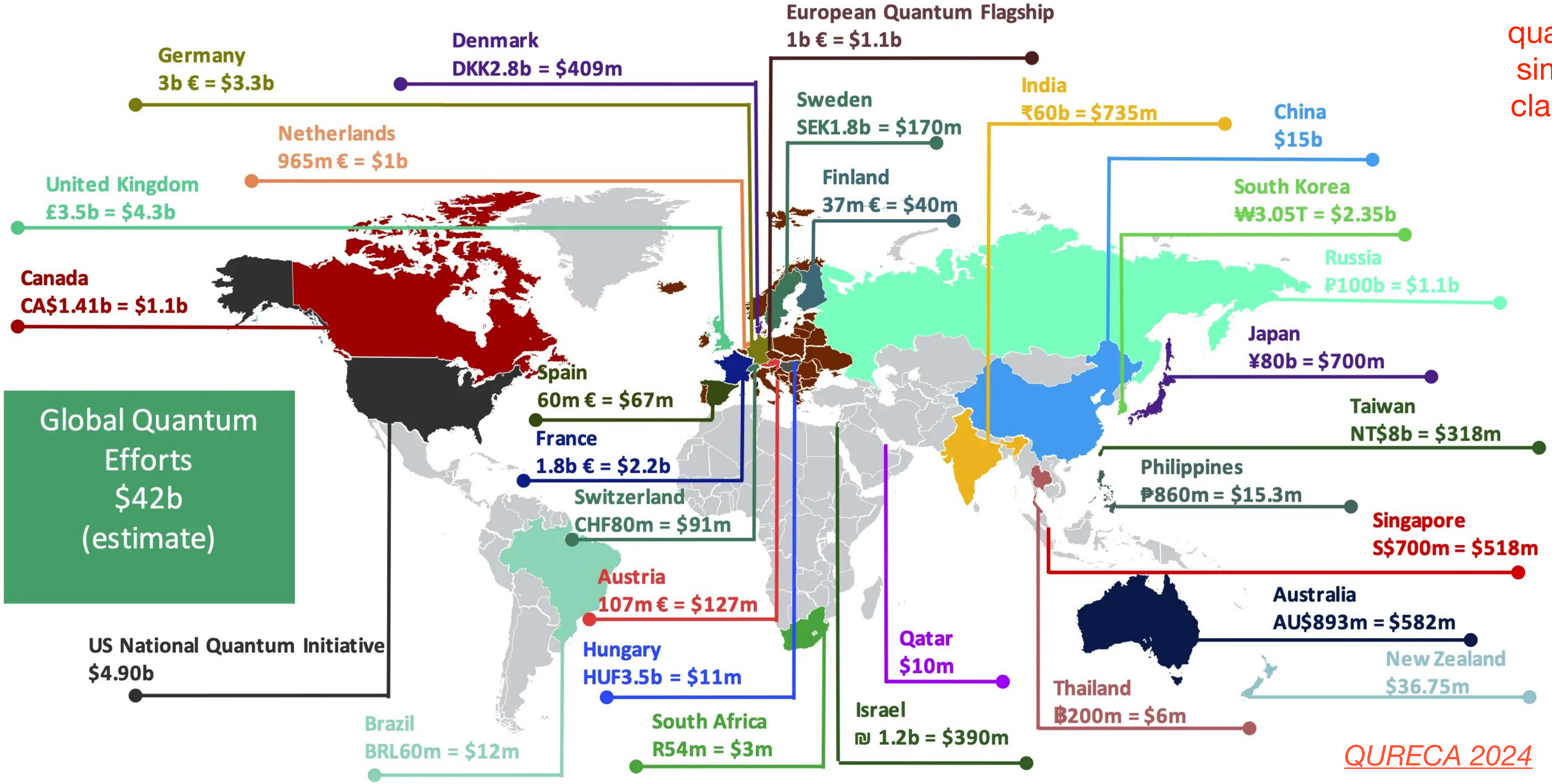


Recent reviews on QML:

- *Y.Wang, J.Liu, A comprehensive review of Quantum Machine Learning: from NISQ to Fault Tolerance, arXiv:2401.11351 [quant-ph]*
- *D.Peral Garcia et al, Systematic literature review: Quantum machine learning and its applications, Comp. Sci. Rev. 51 (2004) 100619*
- *Y. Gujju et al, Quantum machine learning on near-term quantum devices: Current state of supervised and unsupervised techniques for real-world applications, Phys. Rev. Applied 21, 067001*
- *A. Di Meglio et al, Quantum Computing for High-Energy Physics, Summary of the QC4HEP Working Group, arXiv:2307.03236 [quant-ph]*

QC (R)EVOLUTION AND EFFORT WORLDWIDE

quantum initiatives ongoing today in >40 countries
global Q-tecnology market projected to reach $106b by 2040



QURECA 2024

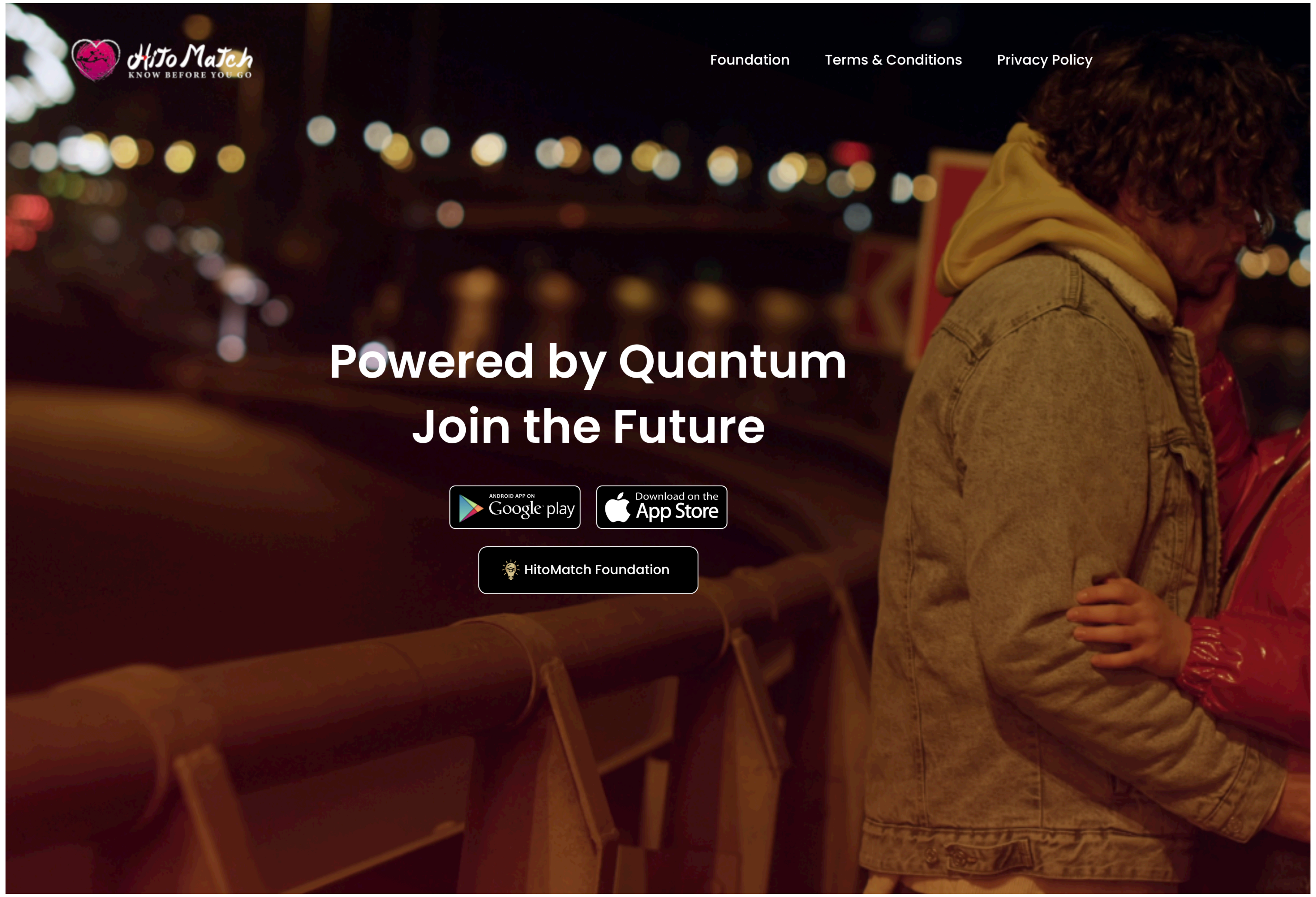
despite the fact that:

for practical applications, quantum computing today is at a similar stage of development as classical computers in the ‘50 …

AND QUANTUM HYPE …

BREAKING: Quantum computing enters online dating!

"Our quantum matching system helps you find a partner for a lifetime, not just a night."



https://hitomatch.com/

Testimonials

Here's what they have to say.

"

HitoMatch helped me find my soulmate. The quantum matches and profile videos made a huge difference.

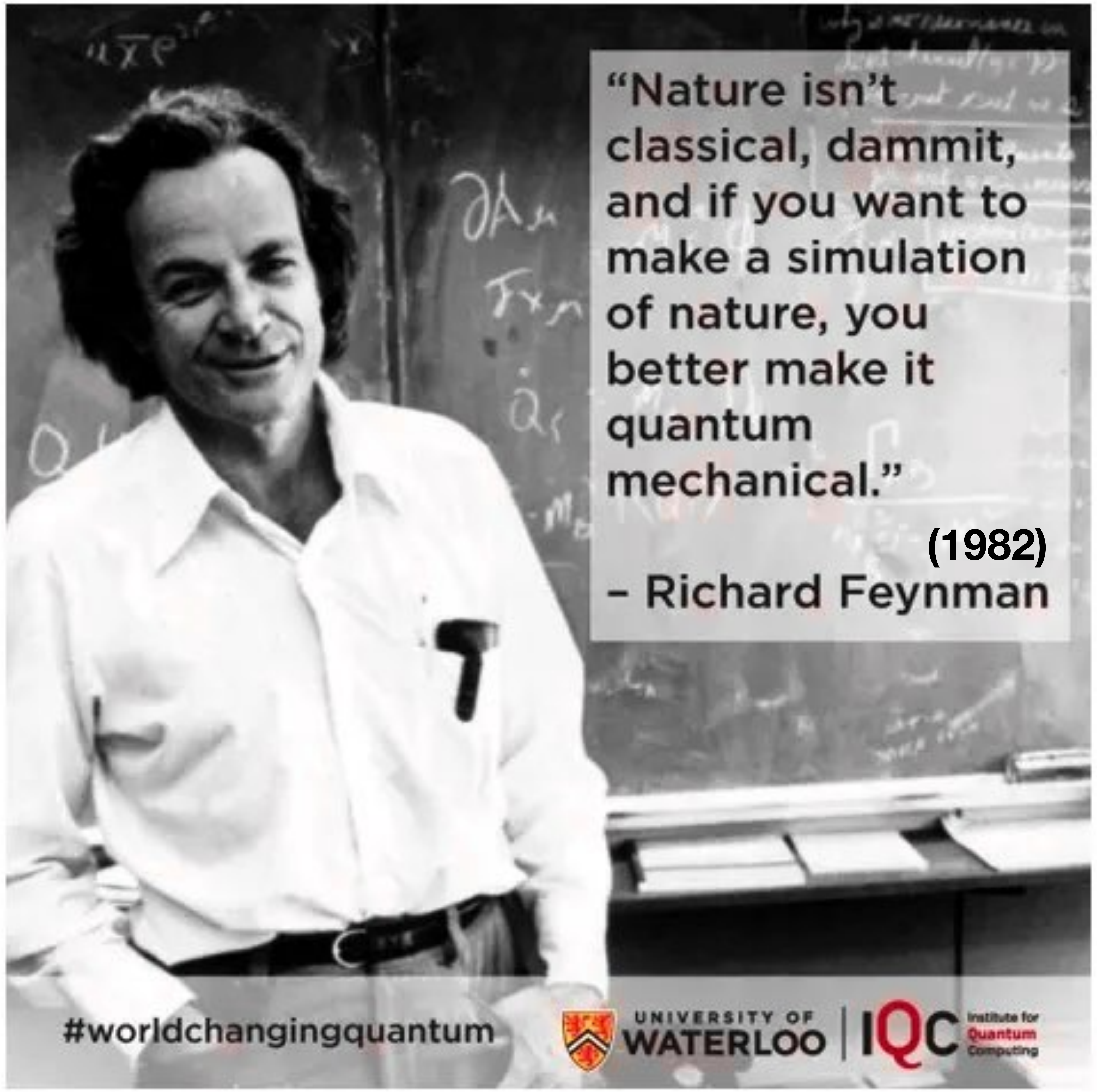
I couldn't be happier with the connection I've made!

John K.

if you believe Everett's multi worlds interpretation of QM, there's a version of you that will find your perfect match

in any case it is w/o doubts a spectacular random number generator …

HOW PARTICLE PHYSICS CAN HELP QUANTUM COMPUTING?



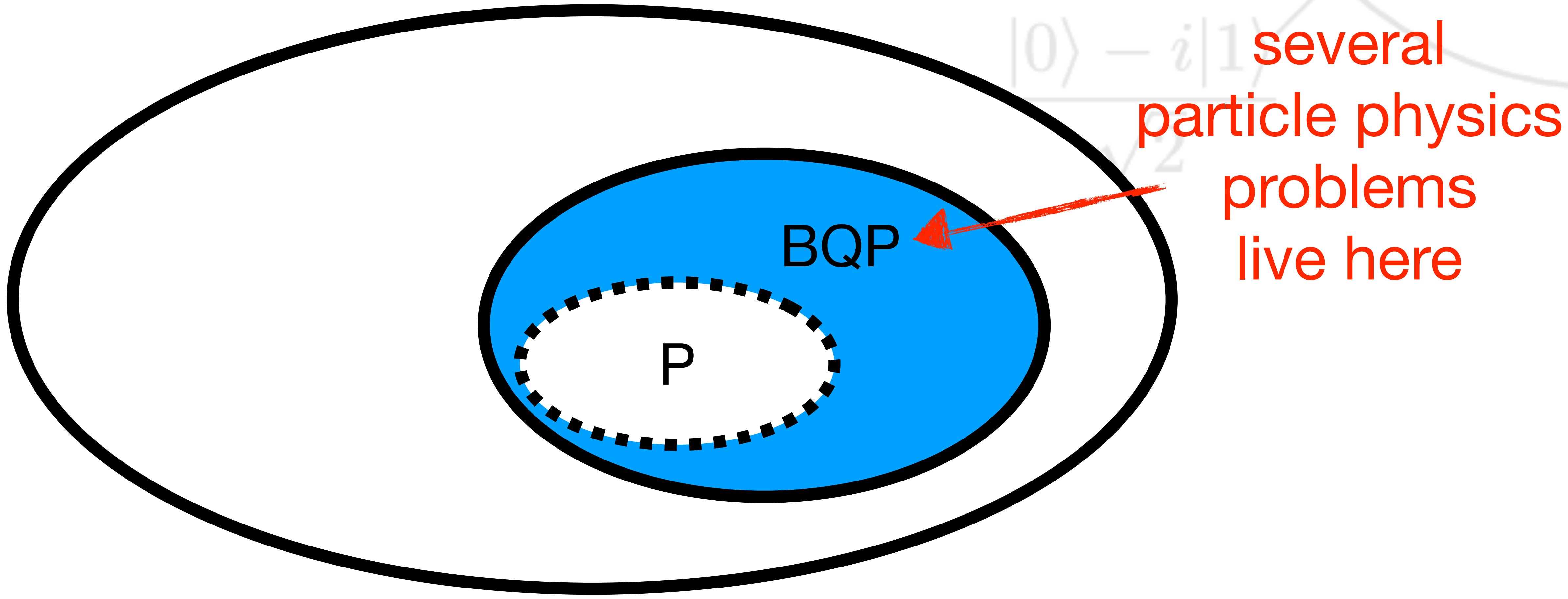
Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

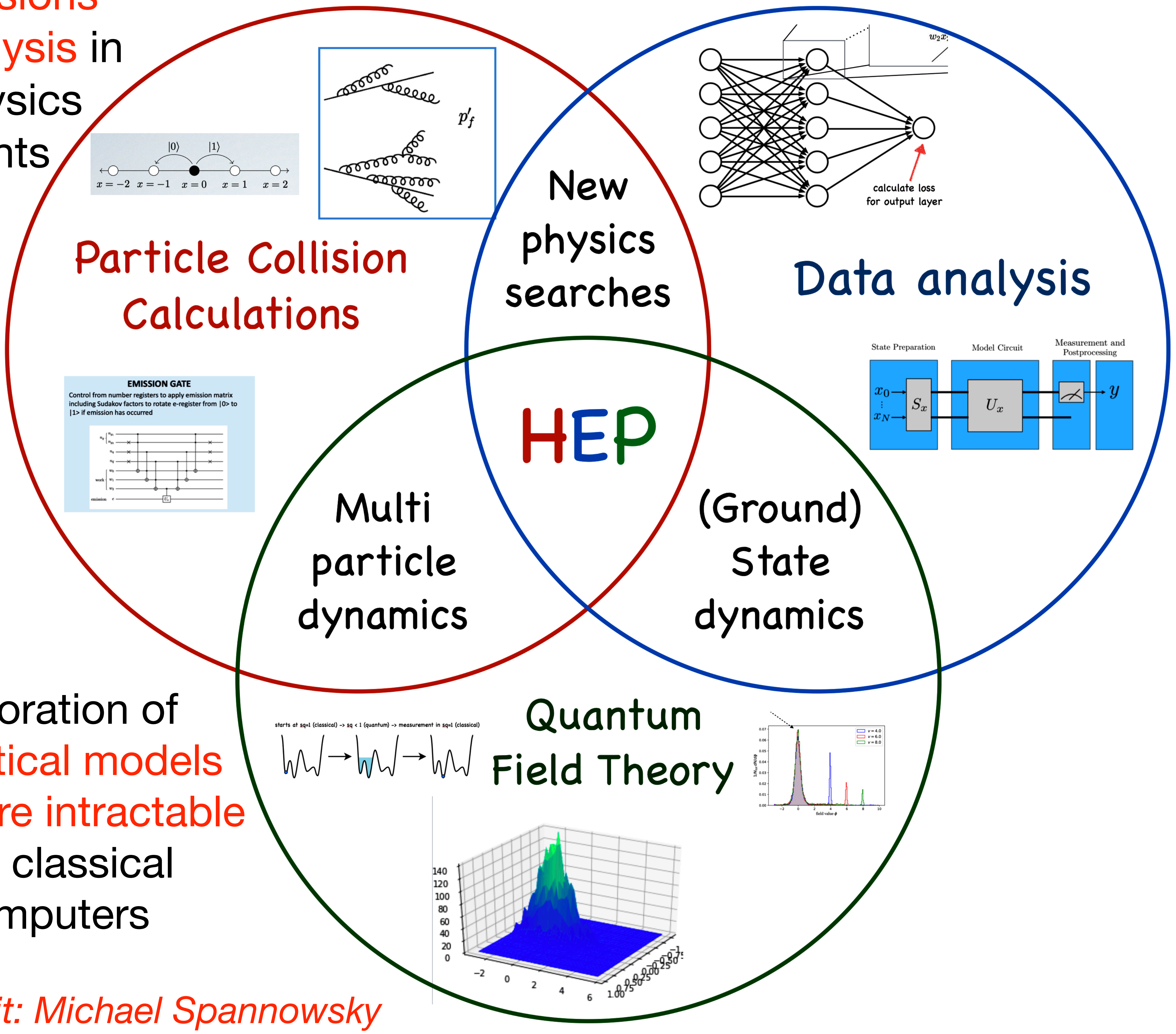
Particle Physics is inherently quantum mechanical, thus simulating theory and analysing experimental data with quantum computers seems a very good idea



PARTICLE PHYSICS AND QC

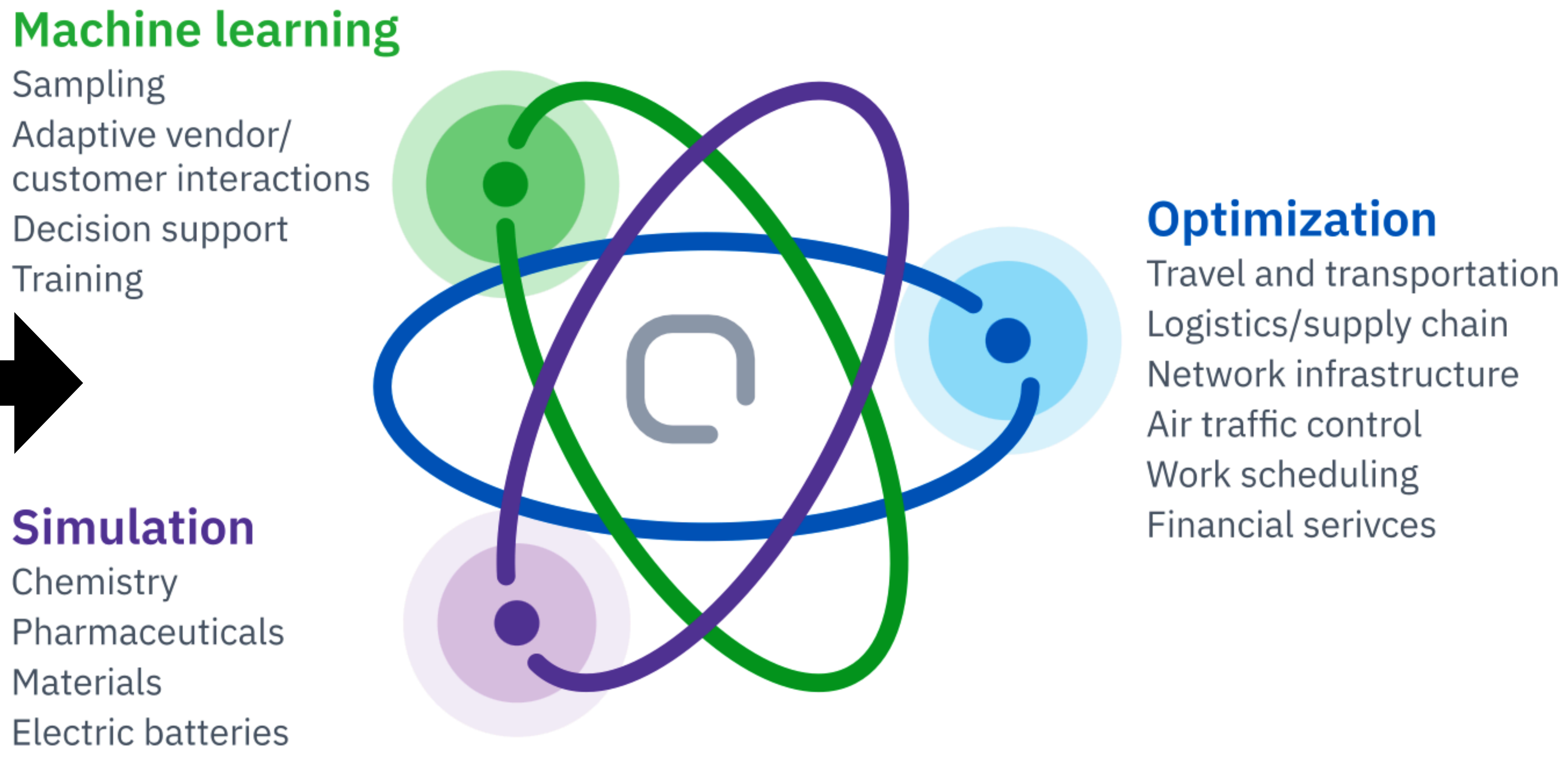
major application areas in HEP that may benefit from QC/QML

simulation of particle collisions and data analysis in particle physics experiments



exploration of theoretical models which are intractable with classical computers

credit: Michael Spannowsky



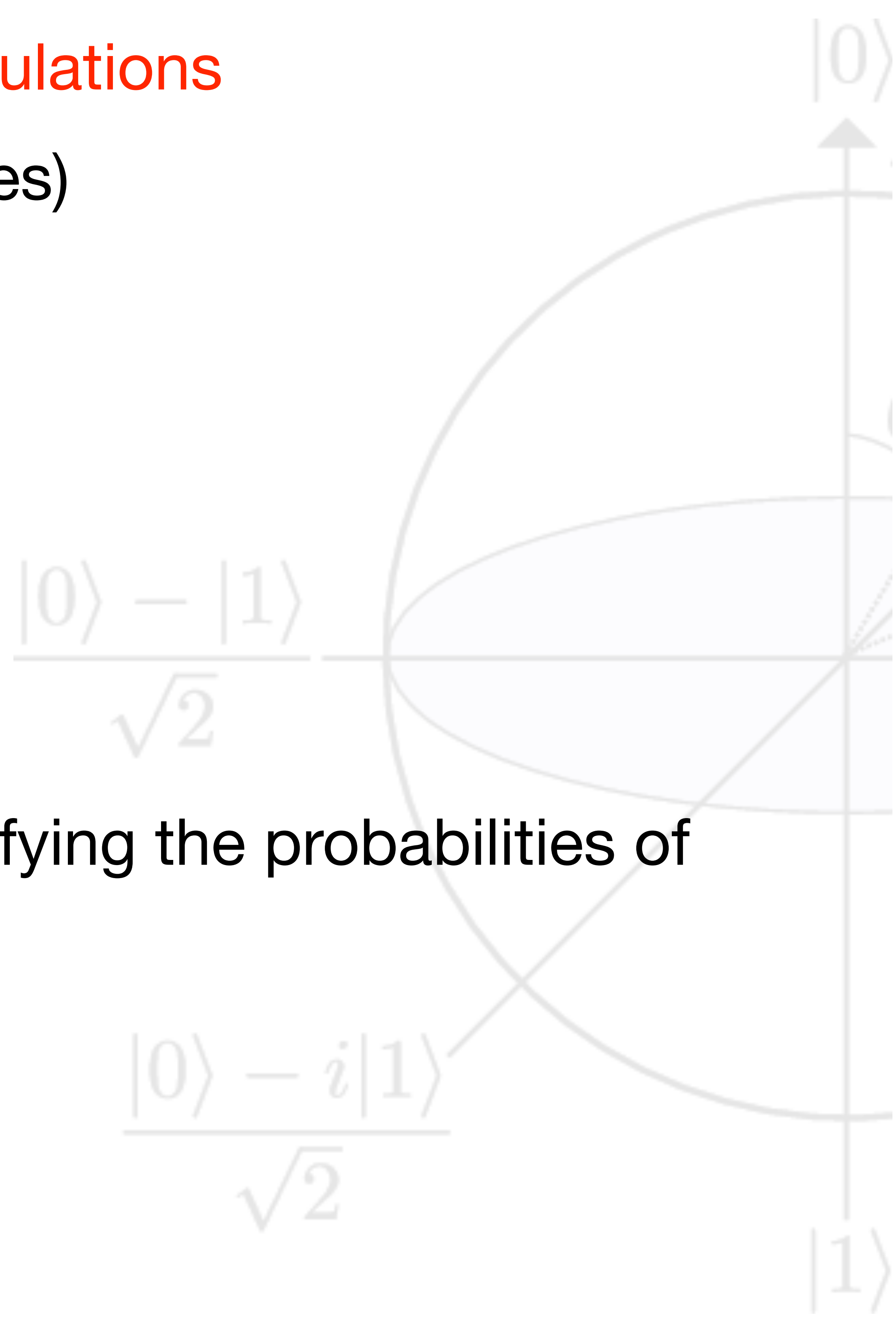
QC use-cases in 2023 for IBM

QUANTUM COMPUTING

- Computing paradigm that explicitly leverage quantum mechanical properties of matters to perform calculations
  - in contraposition to CC where QM enters only indirectly (eg. semiconductors in CPUs follow QM rules)
  - QC are not “faster” computers wrt CC, but systems that do computation in different ways
  - QC are not general purpose machines that speed up any problem wrt CC

- Takes advantage of:
  - **Superposition and Entanglement** → exponential representation power
  - **Constructive/destructive interference** → guide the computation toward the correct solution amplifying the probabilities of correct answers and reducing the probabilities of incorrect ones

- and other useful/problematic features:
  - Quantum operations (gates) as **unitary transformations** → reversible computing
  - Output is the result of a **quantum state measurement** according to Born rule → stochastic computation
  - **No-cloning** theorem → information security / complex/resource hungry error-correction
  - **Quantum state coherence and isolation** → computation stability and errors



ELEMENTS OF A QUANTUM CIRCUIT MODEL OF COMPUTATION

- in a general way any computation (classical or quantum) is based on three fundamental elements:

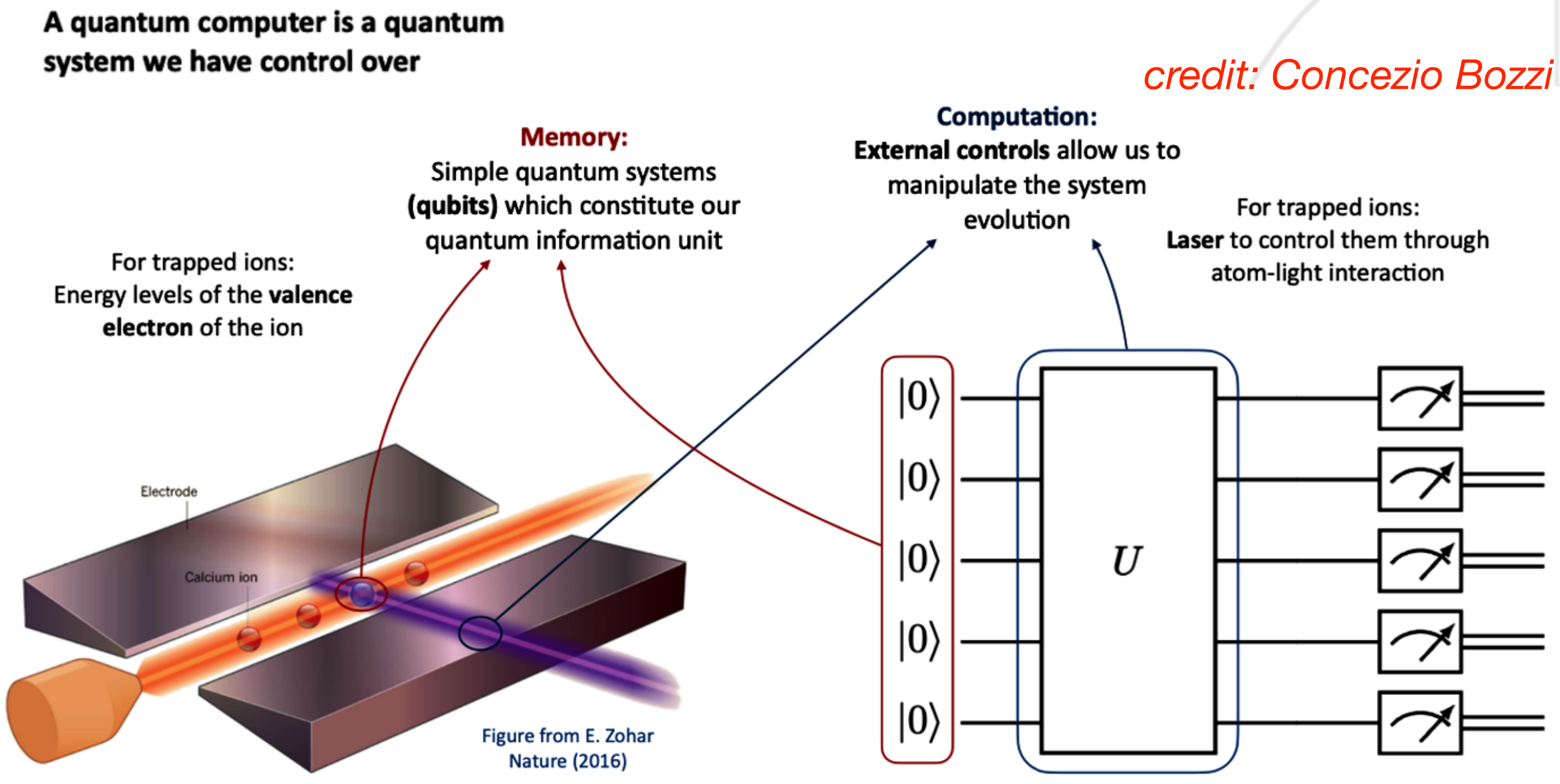
input data → operations on data → output results

- in a quantum circuit these elements are described by:

- **qubits** (quantum bits): basic unit of quantum information
  - store information as classical bits in a CC

- **quantum logic gates**: operators that transform quantum data
  - the building blocks of QC, like classical logic gates in CC

- **quantum measurement**: the operation that allows to access classically the resulting quantum state
  - reading out information from a quantum system generally change the state and destroy the computation that we are performing
  - can't predict the exact outcome of a quantum measurement, due to the probabilistic nature of QM all we can predict are only likelihood



credit: Concezio Bozzi

quantum circuit representation

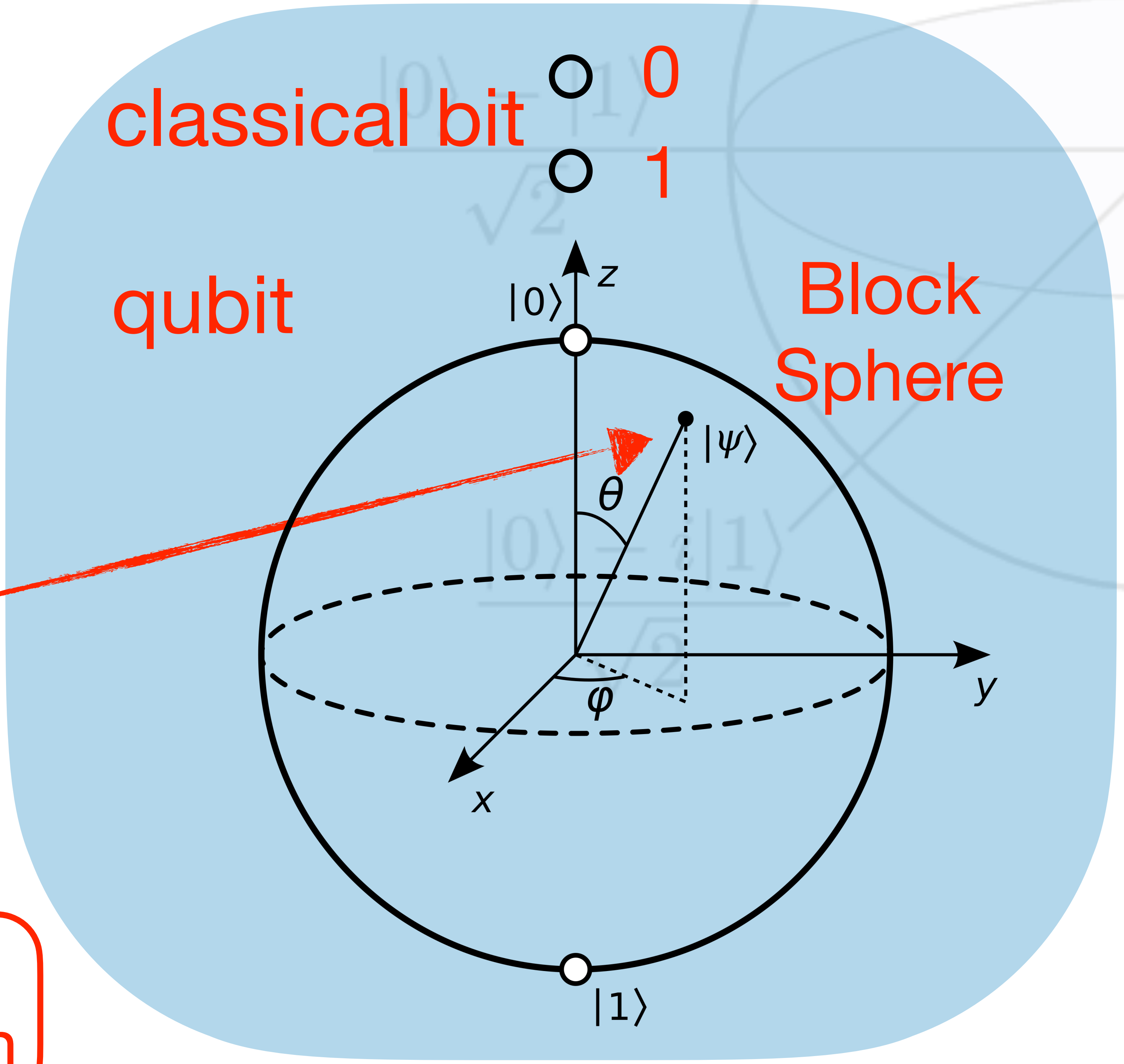
QUBIT: QUANTUM BIT

- basic unit of quantum computation representation
  - **classical bit**: binary ("0 or 1")
  - a generic quantum state (**qubit**) $|\psi\rangle$ can be written in a superposition of a Hilbert space basis: can "take" infinitely many different values in a continuum of states (but when we read it we always find 0 or 1)

computational basis typically used as canonical basis:

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \quad |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$$

$$|\psi\rangle = \begin{bmatrix}a_0\\a_1\end{bmatrix} = a_0\begin{bmatrix}1\\0\end{bmatrix} + a_1\begin{bmatrix}0\\1\end{bmatrix} = a_0|0\rangle + a_1|1\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$



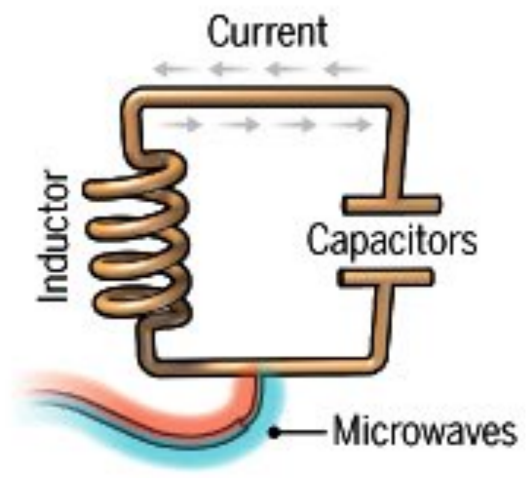
Extending this to a system of n qubits forms a 2^n-dimensional Hilbert Space
eg. 2^n complex numbers → a quantum system can contain much more information

TECHNOLOGIES FOR QUANTUM COMPUTERS

- not yet a standard way to implement qubits, unlike for classical bits encoded in transistors
  - physically, qubits can be any two-level systems: the spin of an electron, the polarization of a proton, two superconducting current directions …
  - current leading technology in the quantum computing commercial space: superconducting qubits

credit: Concezio Bozzi

Superconducting Loops

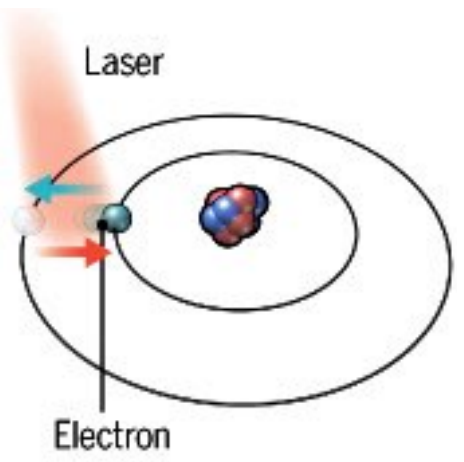


resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into superposition states

fast operations, built on existing SC industry

quick decoherence, must be kept cold

Trapped ions or neutral atoms arrays

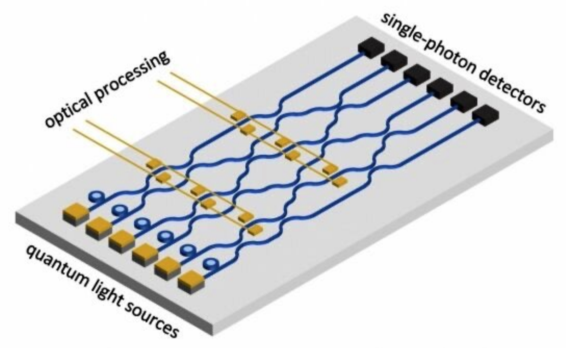


use the energy levels of electrons in neutral atoms or ions as qubits. Excite them with lasers to a higher energy level. Assign the qubit values based on their energy status

very stable, high gate fidelity, 2D and 3D

slower operation, complex laser technology required

Linear / non-linear optical QC

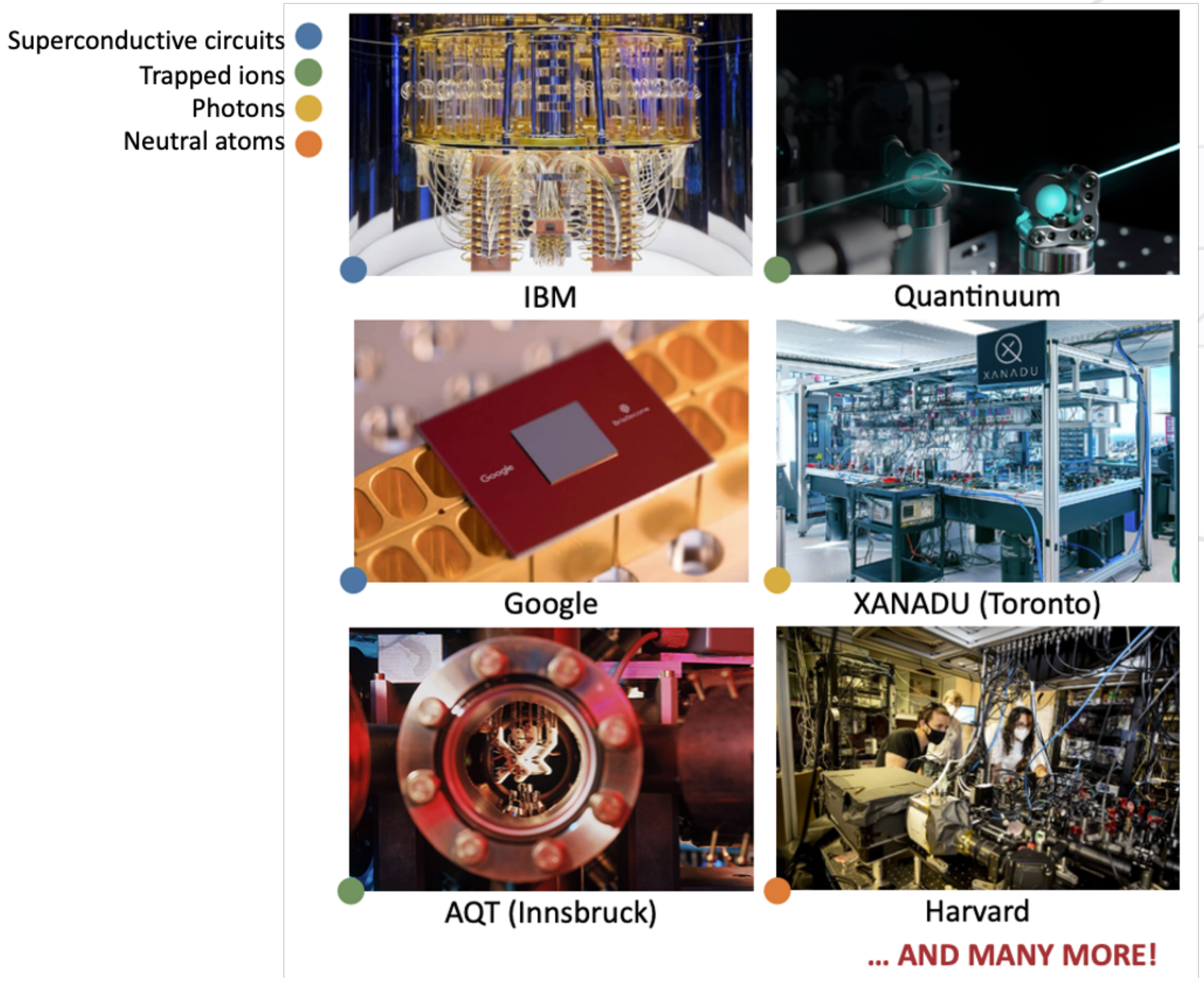


use particles of light to carry and process information. Qubits realised by processing states of different modes of light through both linear and nonlinear element (quantum microprocessor based on laser photonics)

operate at room temperature, photons less sensitive to env.

emerging technology, hard to build large number of gates, cannot stop photons …

O.Ezratty, Eur. Phys. J. A 59, 94 (2023)

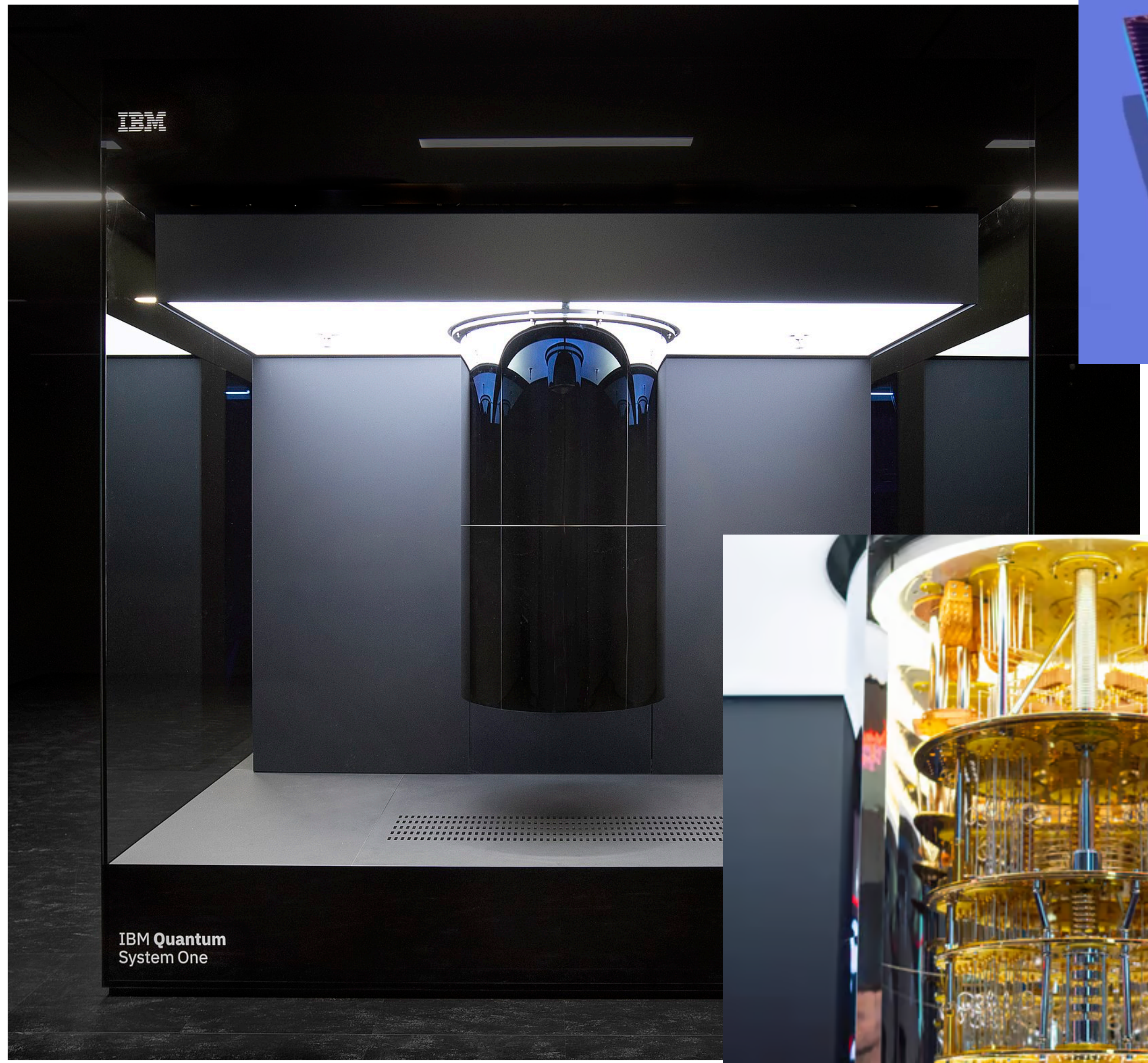


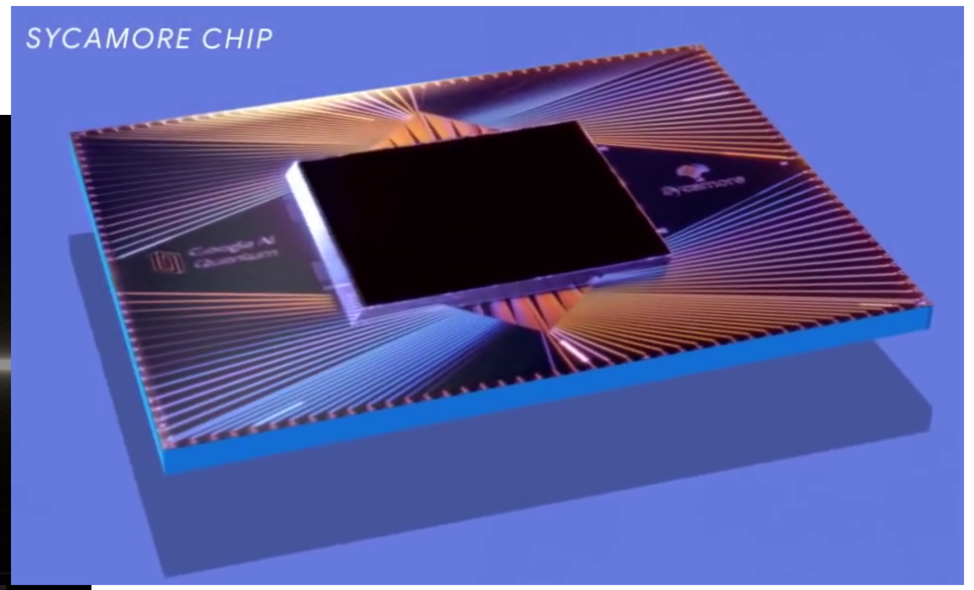
EXAMPLES OF QUANTUM COMPUTERS

IBM Q

Google

53/67 qubits





1121/133 (low error/ faster) qubits today
1000+ near-term

actual quantum processor is just O(2x2 cm^2)
needs cooling&protection from environment to preserve the quantum capabilities

source: IBM

PASQAL

100 qubits today
~1000 near-term

DWAVE

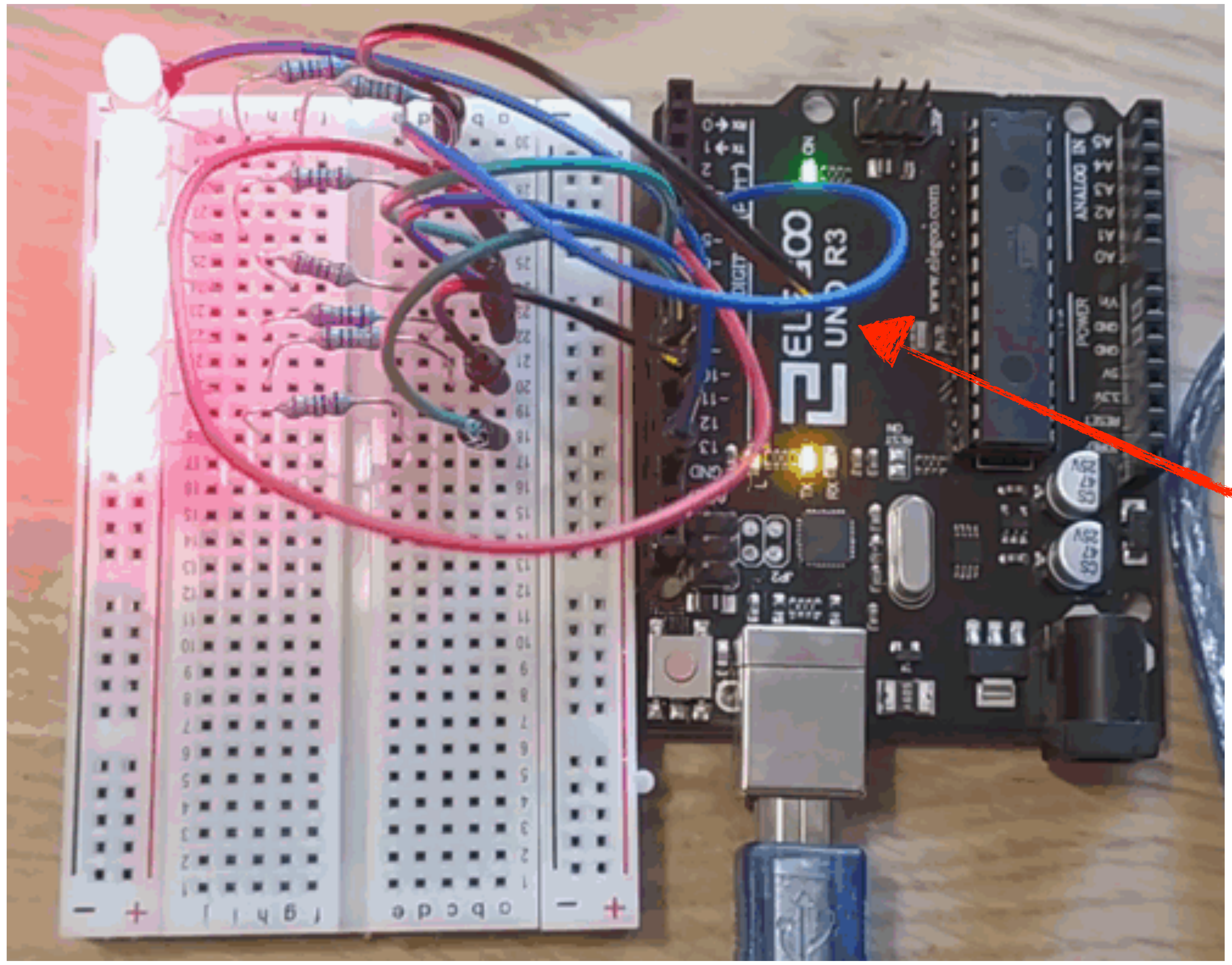
5000+ qubits today
(quantum annealers)

IONQ

36 qubits today
64+ near-future

EXAMPLES OF QUANTUM COMPUTERS …

- Quantum Computing on Arduino …



$10 - 7 qubits emulator
implements Hadamard, CNOT, X, Y, S, T and Z gates

Davide Gessa, github project

Elego Uno (a much cheaper version of Arduino Uno) processor

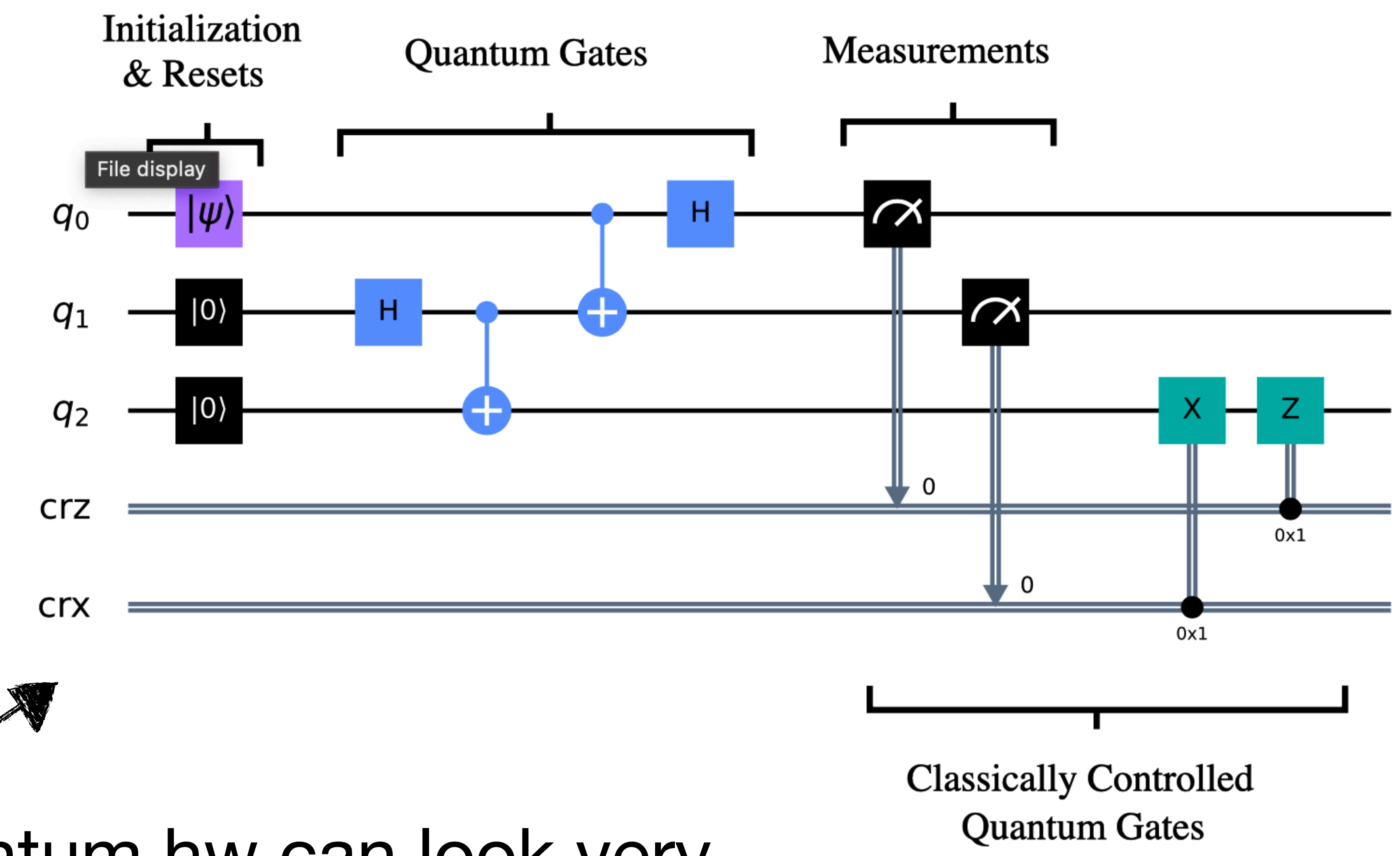
Disclaimer from the author: "This quantum emulator may not actually solve any real-world problems faster than a classical computer. But neither do most other quantum computers right now…

OPERATIONS OVER QUBITS: QUANTUM GATES&CIRCUITS

- quantum computation proceeds by applying physical operations on a quantum state of qubits inducing a change in the state, in a similar way as we operate on classical bits through logical operations
- a state-changing operator is called a quantum gate, and it is represented by a complex unitary matrix, eg length-preserving, linear transformation, which represent a rotation on the Bloch sphere:

$$|\psi'\rangle = U|\psi\rangle \quad \text{with } U \text{ unitary matrix:} \quad U : U^{\dagger}U = I$$

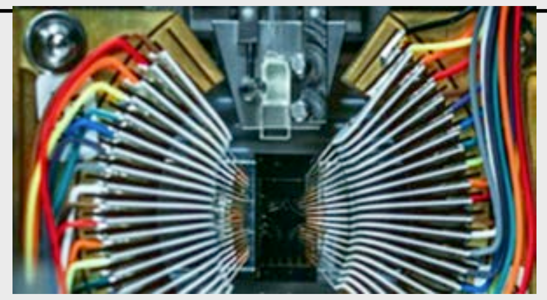
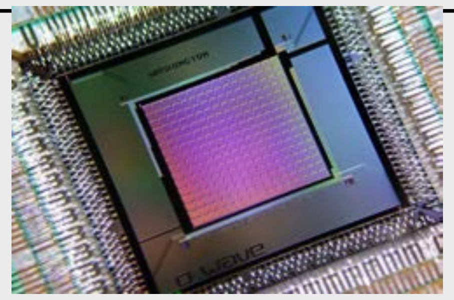
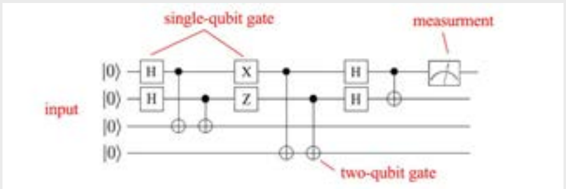
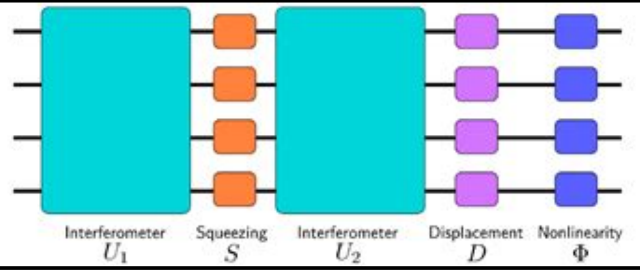
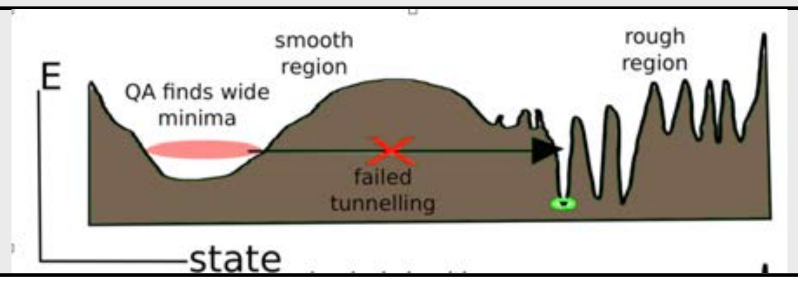
- **quantum circuit** = a collection of quantum gates that operates on qubits
- quantum software is programmed by building these circuits



NOTE: when ported to the real quantum hw can look very different from the initial design (circuit adaptation, transpiling)

Operator	Gate(s)	Matrix
Pauli-X (X) (NOT gate)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Identity/idle	I	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

QC PARADIGMS

Type	Discrete Gate (DG)	Continuous Variable (CV)	Quantum Annealer (QA)
Computing	Digital	Digital/Analog	Analog
Property	Universal (any quantum algorithm can be expressed)	Universal - GBS non-Universal	Not universal — certain quantum systems
Advantage	most algorithms and tech support	uncountable Hilbert (configuration) space	continuous time quantum process
How?	IBM - Qiskit ~500 Qubits	Xanadu Quantum Lab	DWave - LEAP ~7000 Qubits
What?			
			

- Universal gate-based quantum computers designed to tackle a wide range of problems, evolution decomposed in elementary gates
- Quantum Annealers designed specifically for optimization problems:
  - uses a network of qubits and couplers arranged to efficiently map optimization problems onto the quantum hardware
  - allows for the effective translation of optimization problems into Hamiltonian equations and the subsequent minimization of these equations by applying an annealing process

credit: Michael Spannowsky

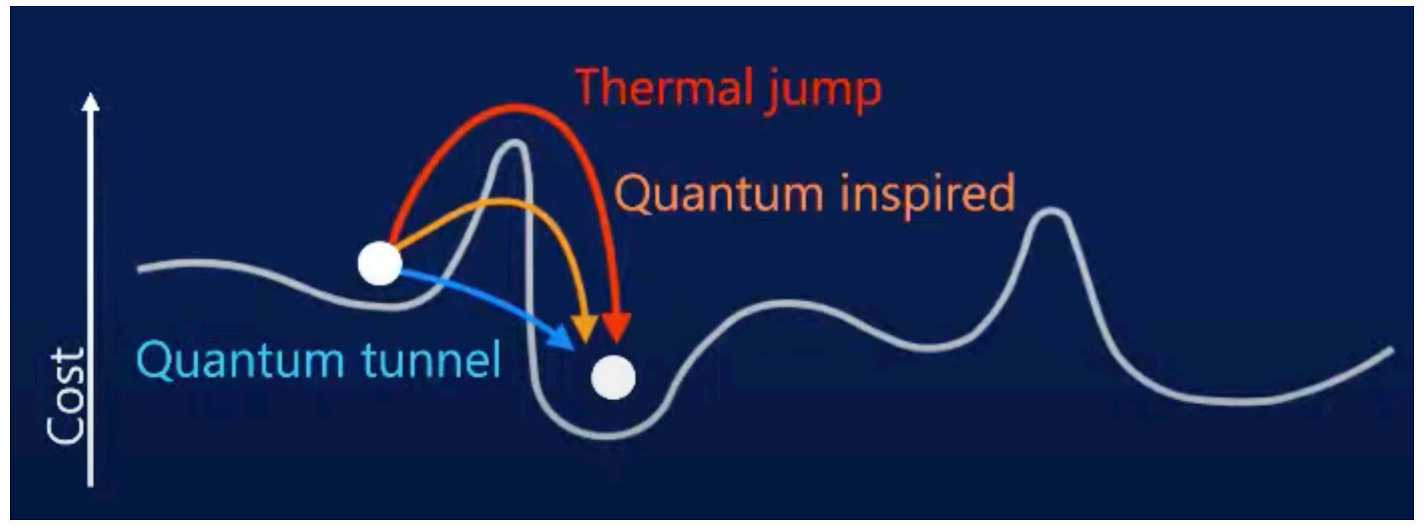
QUANTUM ALGORITHMS IN THE NISQ REGIME

- an entire zoo of sophisticated quantum algorithms that can offer speedups over classical algorithms has been proposed in literature assuming the availability of fault-tolerant quantum processors supporting a large number of qubits and quantum gates
  - Shor's (proved exponential speedup in factoring prime numbers), Grover's (polynomial (quadratic) speedup for searching in an unsorted db), Quantum MC, Quantum Fourier Transform …

60+ quantum algorithms with quantum speedup
https://quantumalgorithmzoo.org/

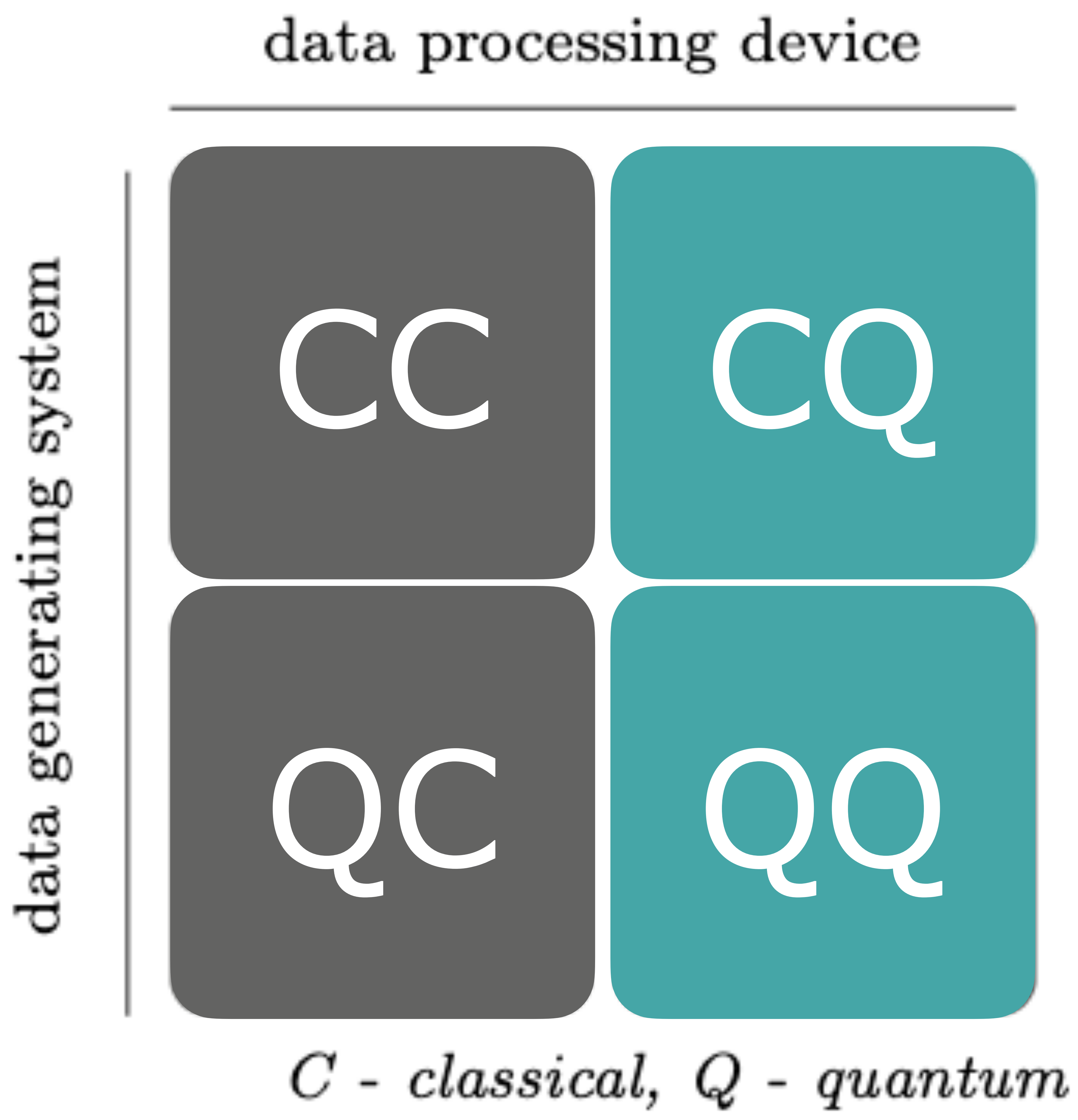
- **however current quantum computers** support only O($10^1 \div 10^3$) qubits, and **not all necessarily able to interact with each others**: these are the so called noisy intermediate-scale quantum devices **(NISQ)**:
  - no error correction: produce only approximate results of computations
  - algorithms limited to use only a few qubits and gates with deep impact on quantum algorithmic design and achievable performance

- interesting to narrow down the objective: finding computational problems that can be solved by NISQ device while possibly exhibiting some kind of advantage or utility wrt classical algorithms:
  - ex. find the ground-state energy of a many-body system (ex. a molecule) with quantum annealers
  - **ex. Quantum Machine Learning**



credit: M.Troyer - Quantum Colloquium 2021 - Simons Institute

APPROACHES TO COMBINE QC AND ML



different possibilities:

- CC: classical data being processed classically but with methods inspired by QC algorithms (like tensor networks)
- QC: quantum data processed with classical algorithms, eg use classical ML to help preparing and use QC (describe quantum state in a compact manner, state preparation, qubit error correction, …)
- CQ: classical data processed with quantum devices
- QQ: quantum data being processed by a quantum computer. Connected to CQ (just change the input data), becomes interesting with the development of quantum sensing

E.A. Gilles Brassard, S. Gambs: Machine learning in a quantum world. In: Advances in Artificial Intelligence, pp. 431–442. Springer (2006)

QML

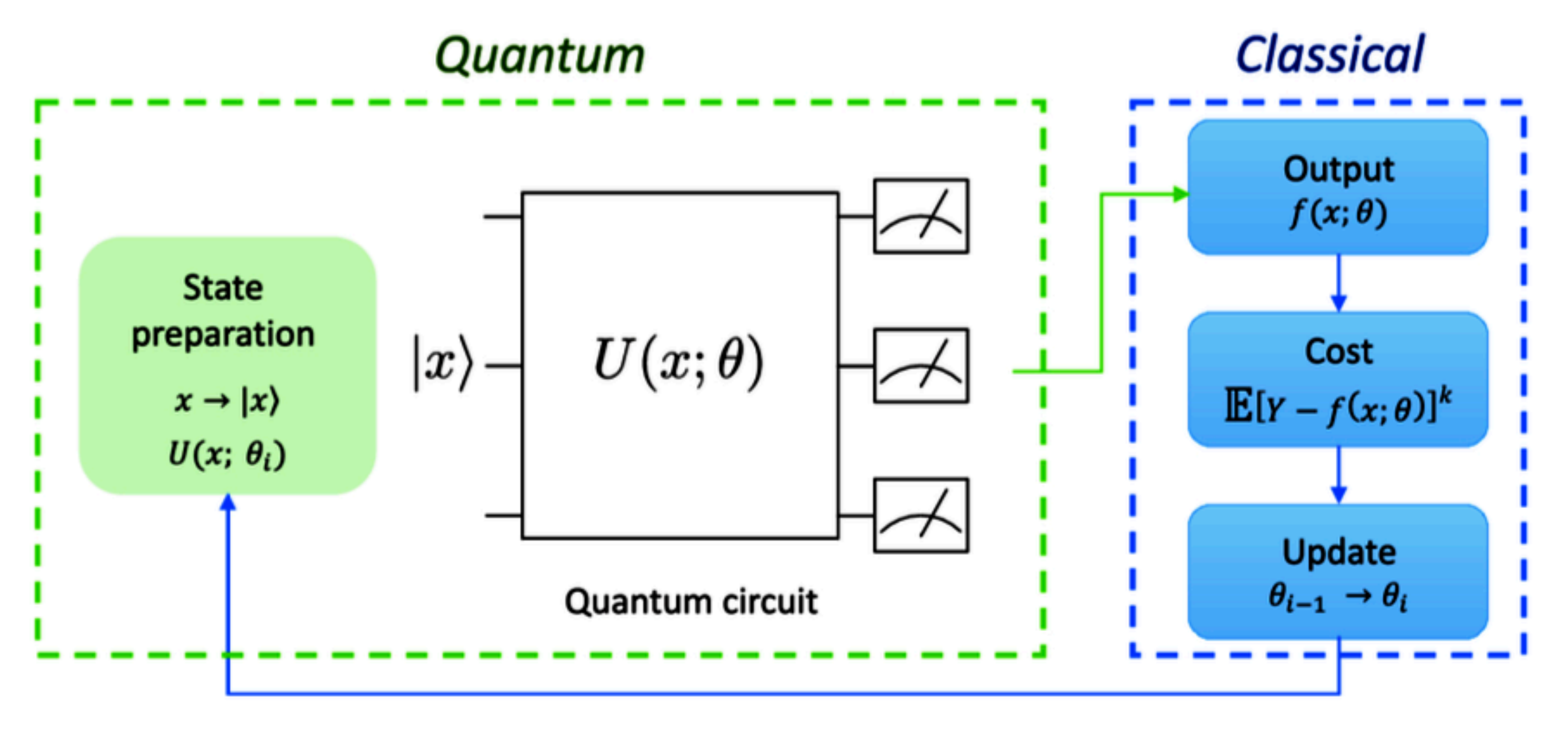
a set of algorithms inspired by classical ML that all share the same common idea:

encode the task into a parametrised cost function (ansatz)

- evaluated in a QC
- parameters optimised (trained) in a CC

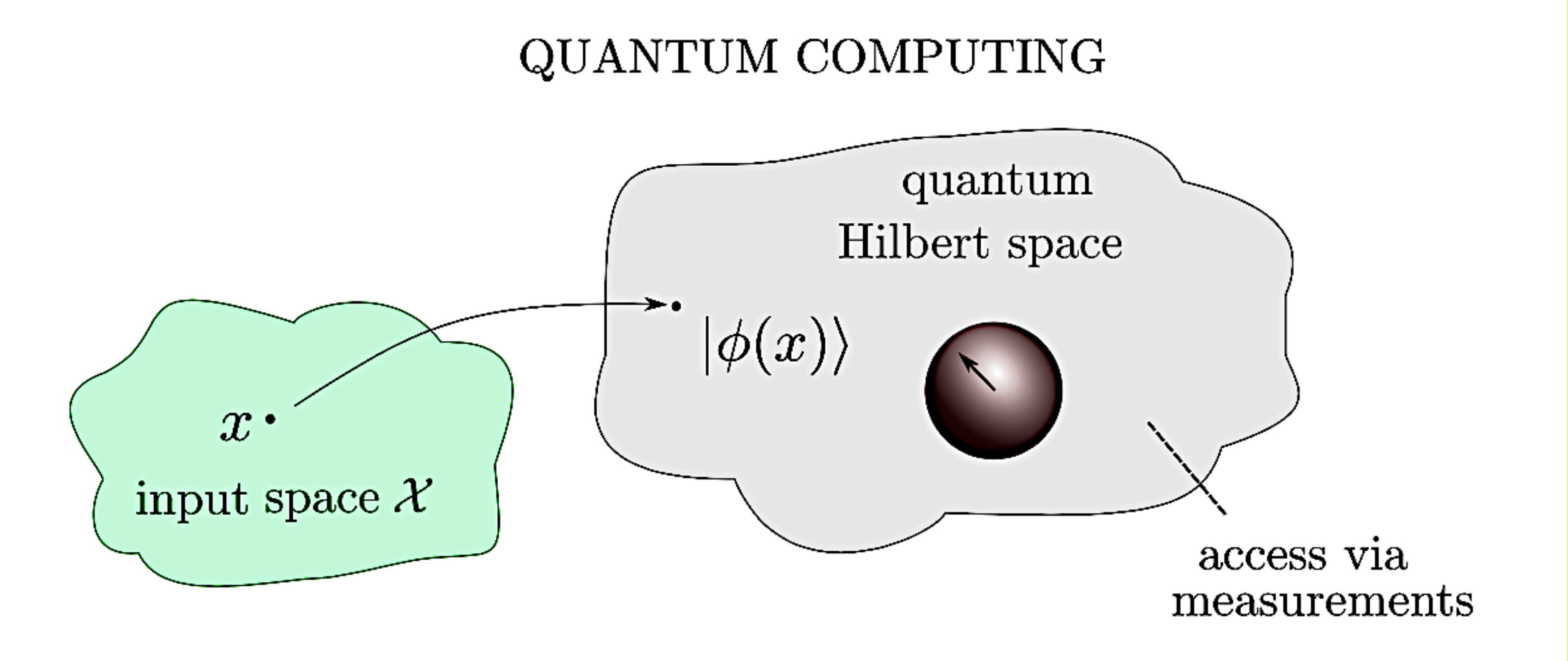
Variational Q-Algorithms

ex. Quantum-NN



Kernel Based

ex. Quantum-Support Vector Machines



$$|\phi(x)\rangle = U_\phi(x)|0\rangle$$
$$|\phi(x')\rangle = U_\phi(x')|0\rangle$$

$$|\langle\phi(x)|\phi(x')\rangle|^2 = K(x,x')$$

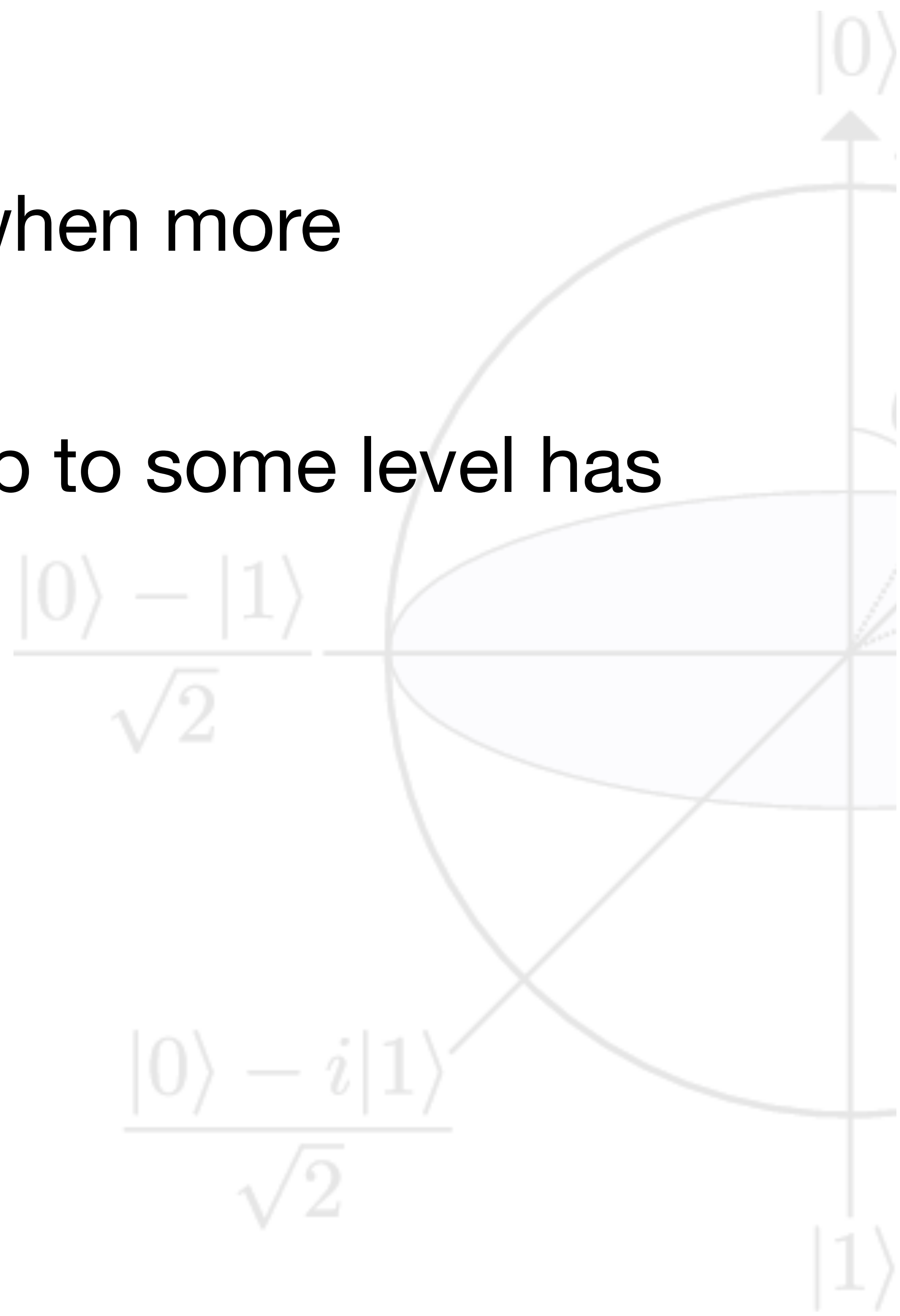
Energy Based

Finds the ground-state of a quantum system using a quantum-classical hybrid approach (ex. Quantum Boltzman Machines)

WHY QML?

- QML works well with NISQ:
  - flexible, can be implemented with a small number of qbits and then scaled up when more resources are available
  - more robust to noise (noise in differentiable optimisation works as regulariser, up to some level has been show that QML algorithms give the correct result)

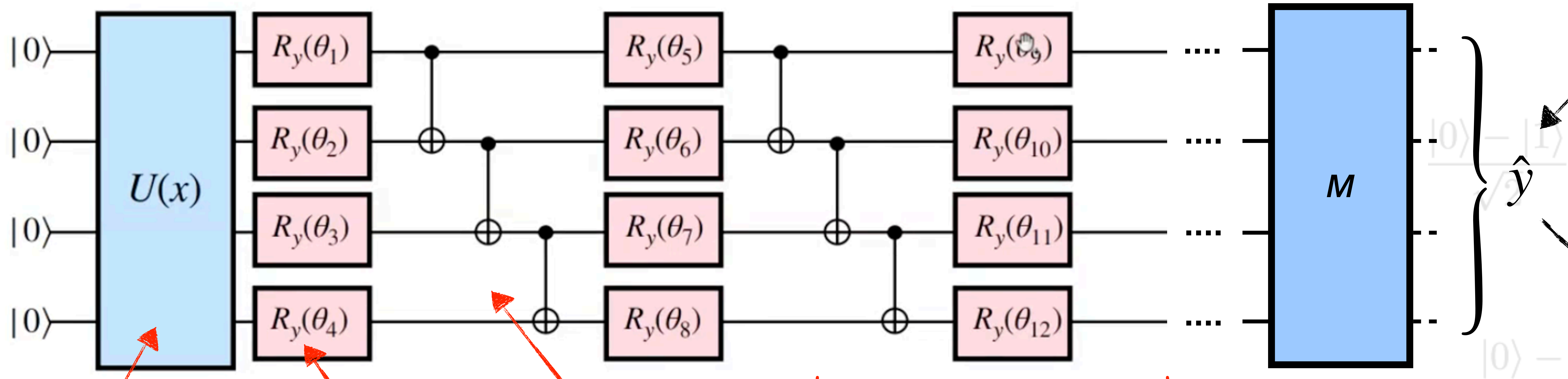
- and can in principle improve classical ML:
  - speed-up and complexity
  - sample efficiency
  - representational power
  - energy efficiency
  - …



QUANTUM NEURAL NETWORKS

- **typical example of a QNN:**

$$\hat{y} \doteq f(x, \theta) = \langle M \rangle =$$
$$= \langle x \,|\, V^{\dagger}(\theta) M V(\theta) \,|\, x \rangle$$



$$L(y, \hat{y} \,|\, \theta)$$

encoding classical input x

parametrised rotations (along y in this example)

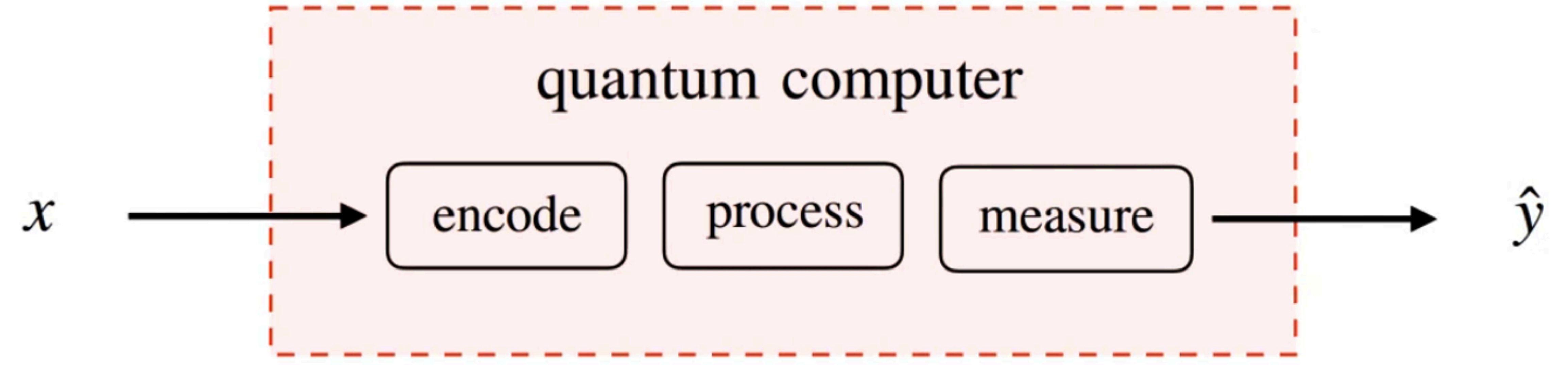
entanglement block via CNOT gates
creates non-classical correlations that hopefully will increase the expressibility of the circuit

repeated N-times (N-layers) to increase expressibility

$$\theta^* = \arg\min \sum_{i \in D} L(y_i, f(x_i, \theta))$$

ENCODING CLASSICAL DATA

- encoding of classical data is a crucial step in implementing CQ-QML algorithms

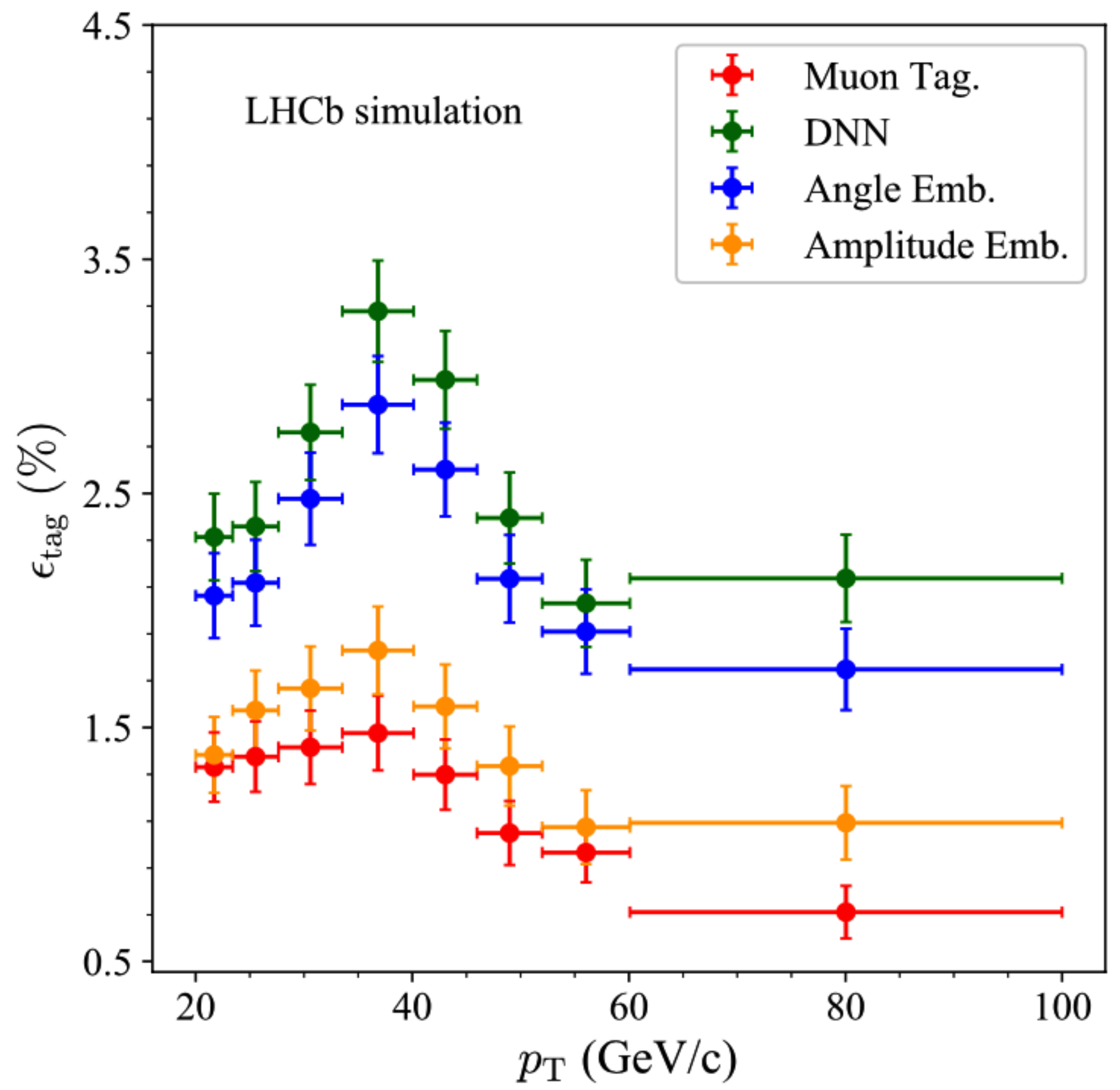


- several way to do it, ranging from conceptually simple but resources hungry (# qubits), to more efficient but also more complex (tradeoff between compression and circuit depth)

- example: amplitude encoding

$$x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \rightarrow |x\rangle = \frac{1}{\|x\|}(x_0|0\rangle + x_1|1\rangle) = \frac{1}{\|x\|}\sum_{i=0}^{N} x_i|i\rangle$$

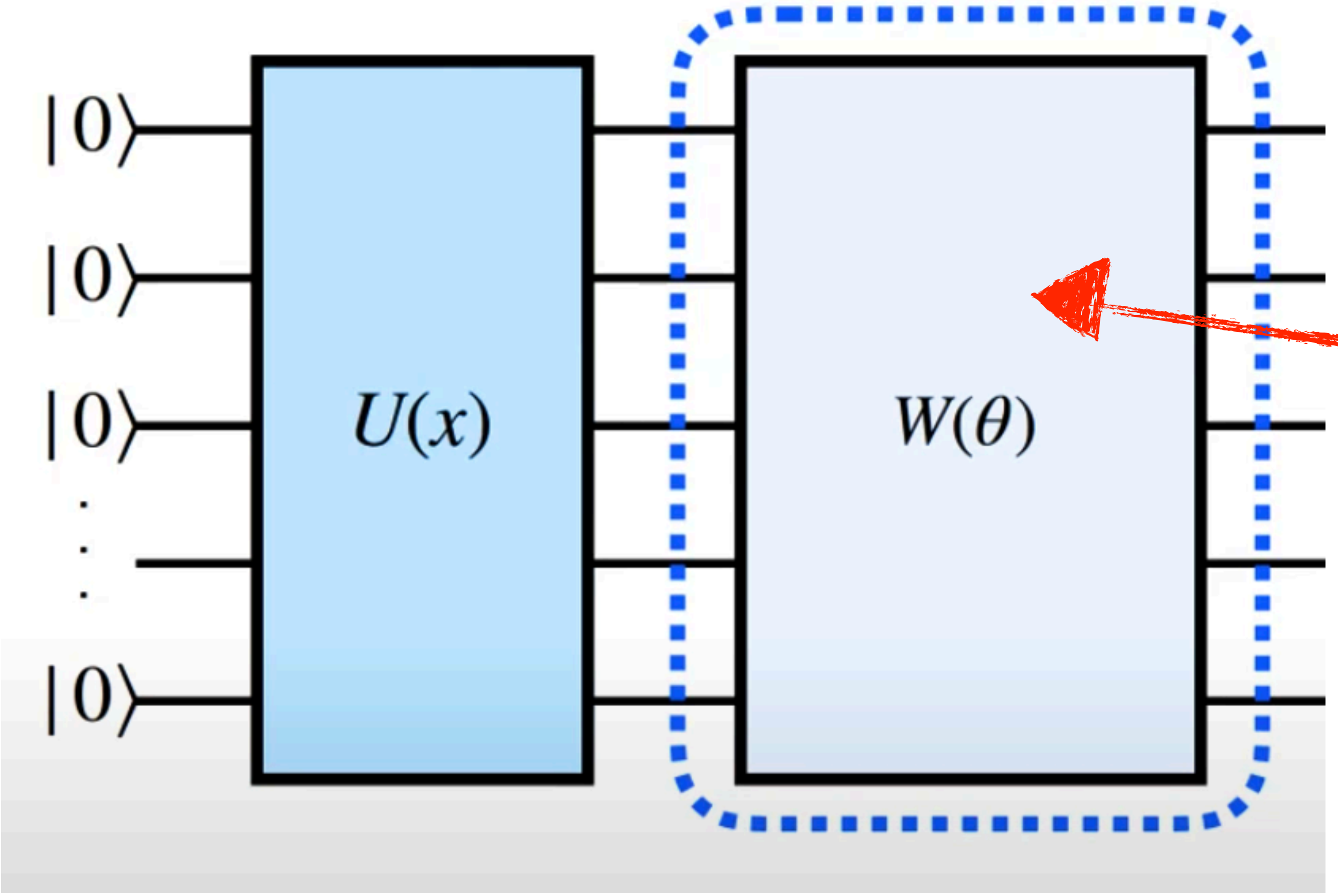
  - fewer qubits needed: exponential compression $n_q \propto O(\log N)$
  - more complex preparation and readout: # of gates $n_g \propto O(\text{poly}(N))$



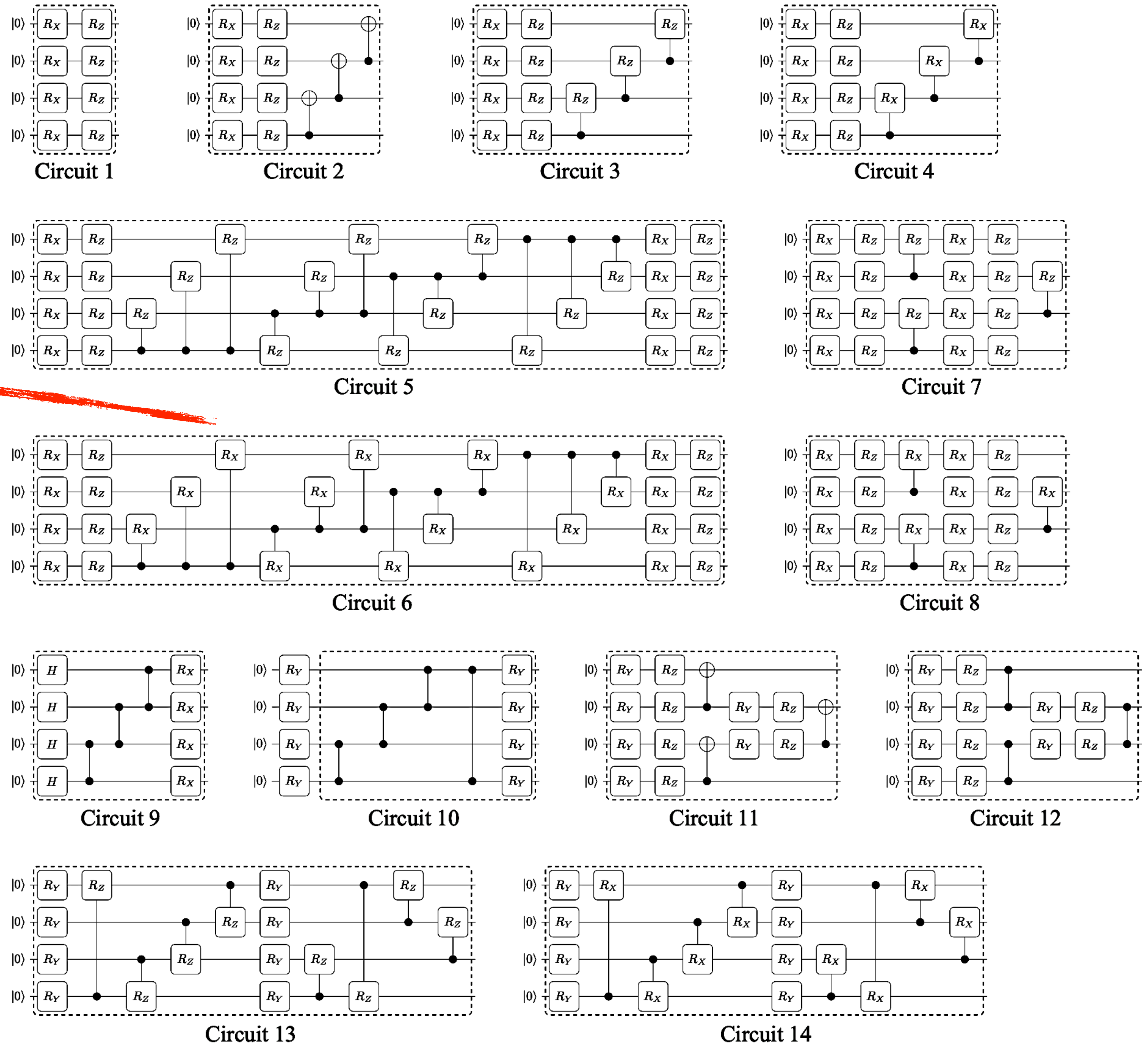
A.Gianelle et al, JHEP 2022, 14

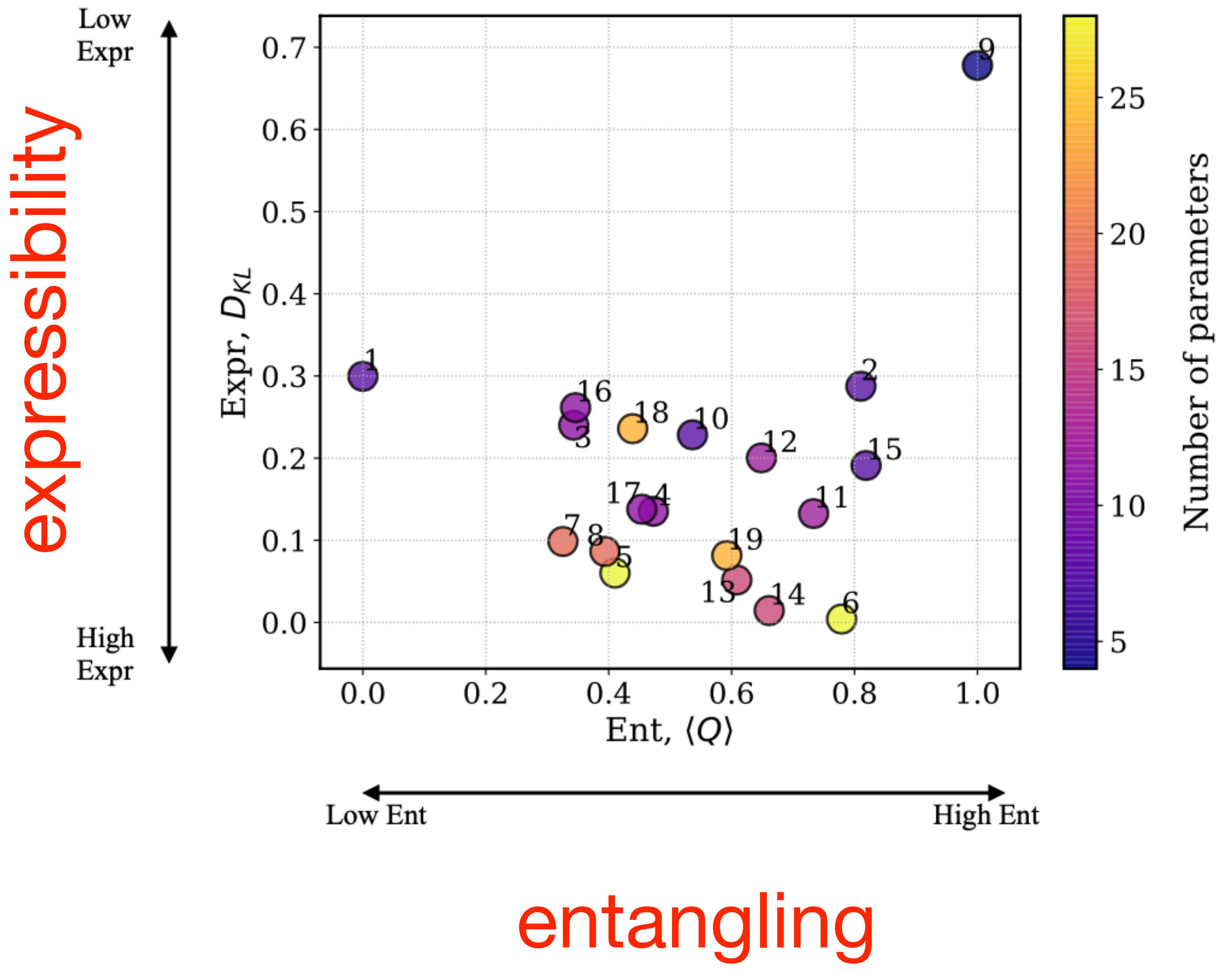
EXPRESSIVE POWER OF PARAMETRISED QUANTUM CIRCUITS

- several studies in literature on how to choose the circuit ansatz in order to maximise expressibility and entangling capabilities (eg ability to efficiently represent the solution space for the tasks at hand and to capture non-trivial correlation in the quantum data)



encoding PQC





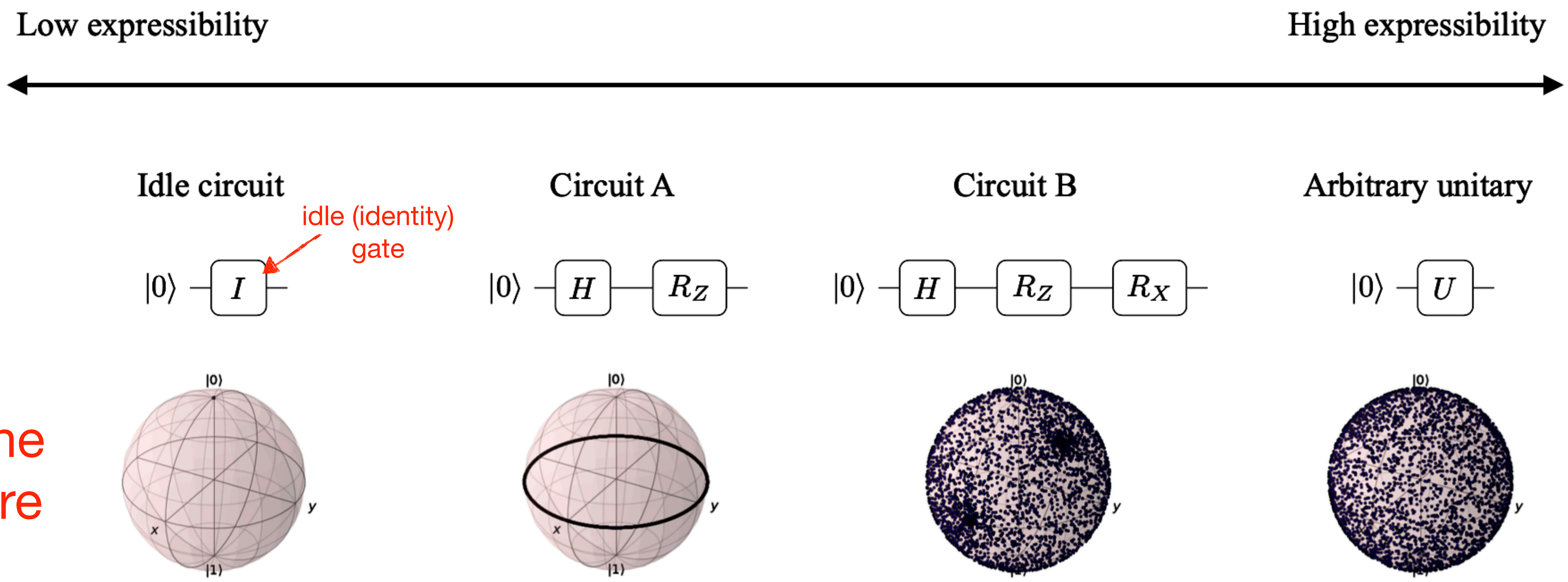
S. Sim et al: arXiv:1905.10876

EXAMPLE: EXPRESSIBILITY FOR A SINGLE QUBIT

- expressibility: circuit's ability to generate (pure) states that are well representative of the Hilbert space
- in the case of a single qubit, the expressibility corresponds to the circuit's ability to explore the Bloch sphere

circuit

points on the block sphere



S. Sim et al: arXiv:1905.10876

EXPRESSIBILITY VS TRAINABILITY: THE BARREN PLATEAUS PROBLEM

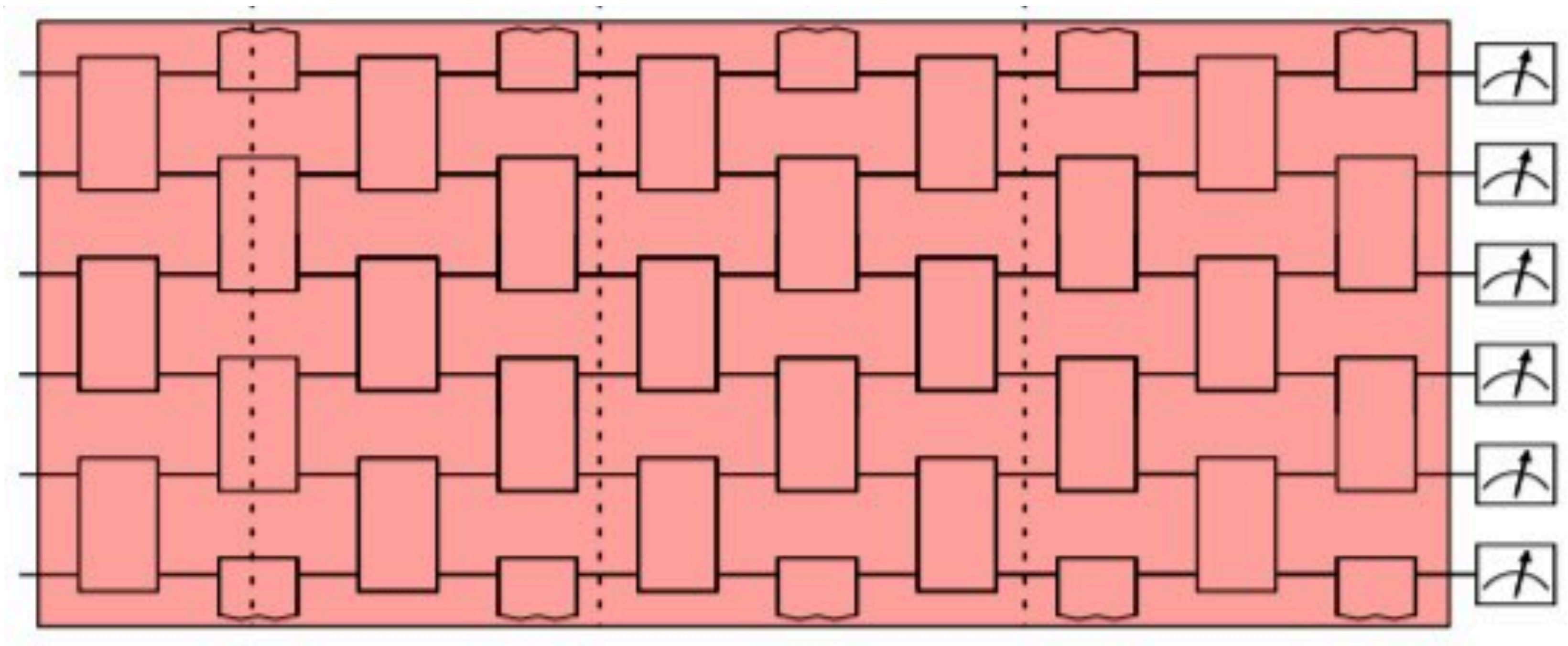
- variational circuits are affected by the presence of large regions in the loss landscape where the variance of the gradient is almost 0 (flat loss landscape)
- a circuit initialised in one of these areas will be untrainable using any gradient-based algorithm
- it can be shown that the gradient's variance exponentially decrease with the # of qubits

$$\langle \partial_\theta L \rangle \simeq 0$$

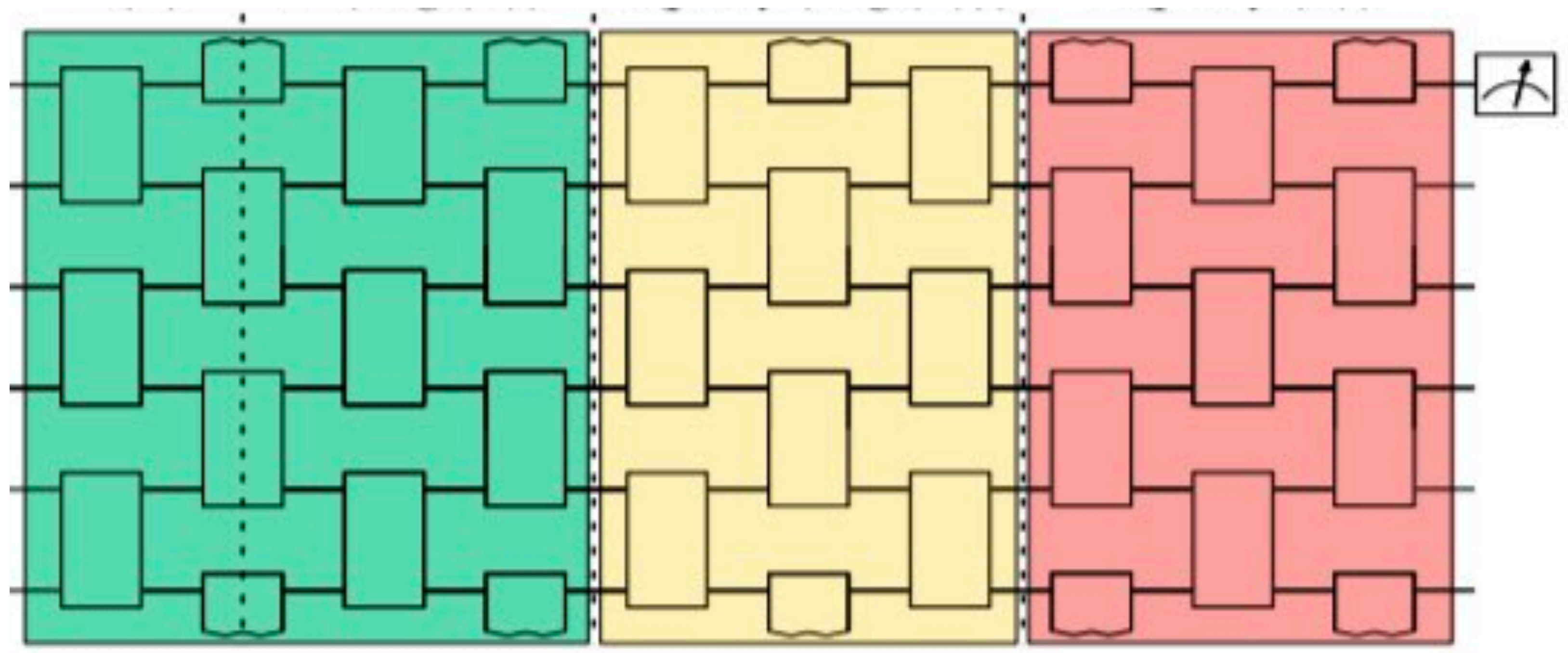
$$\text{Var}[\partial_\theta L] \sim 2^{-n}$$

J.R. Mc Clean et al., Nat. Comm.

- a possible mitigation strategy: use local cost functions that only have information from part of the circuit coupled with not too-deep circuits and not too much entanglement:



global loss



local loss

$$\text{Var}[\partial_\theta L] \gtrsim \text{poly(n)}^{-1}$$

Cerezo et al: arXiv:2001.00550

QML AND QUANTUM ADVANTAGE

Quantum Convolutional Neural Networks are (Effectively) Classically Simulable

Pablo Bermejo, Paolo Braccia, Manuel S. Rudolph, Zoë Holmes, Lukasz Cincio, M. Cerezo

P. Bermejo et al, arXiv:2408.12739

our work can not, and does not intend to, prove that there is no scenario whatsoever where it may be necessary to train a QCNN on a quantum computer. However, the burden of proof now rests firmly in the hands of any proponent of QCNNs to identify such cases and until then it is good practice to maintain a healthy skepticism that such cases can be found. Hence we boldly claim: *There is currently no evidence that QCNNs will work on classically non-trivial tasks, and their place in the upper echelon of promising QML architectures should be seriously revised.*

M.Cerzo et al, QTML 2024

Does provable absence of barren plateaus imply classical simulability? Or, why we need to rethink variational quantum computing

M. Cerezo, Martin Larocca, Diego García-Martín, N. L. Diaz, Paolo Braccia, Enrico Fontana, Manuel S. Rudolph, Pablo Bermejo, Aroosa Ijaz, Supanut Thanasilp, Eric R. Anschuetz, and Zoë Holmes

This provokes the question: *Could the very same structure that allows one to provably avoid barren plateaus be leveraged to efficiently simulate the loss function classically?* Here we argue that the answer to this question is 'yes'. *Specifically, we claim that loss landscapes which provably do not exhibit barren plateaus can be simulated using a classical algorithm that runs in polynomial time.* Importantly, this simulation might still necessitate

is the quantum advantage the right goal for QML? M. Schuld, N.Kiloran PRX Quantum 2 030101

Until error correction will be available (2030?) better to focus on an intermediate milestone: **quantum utility ...**

QUANTUM UTILITY

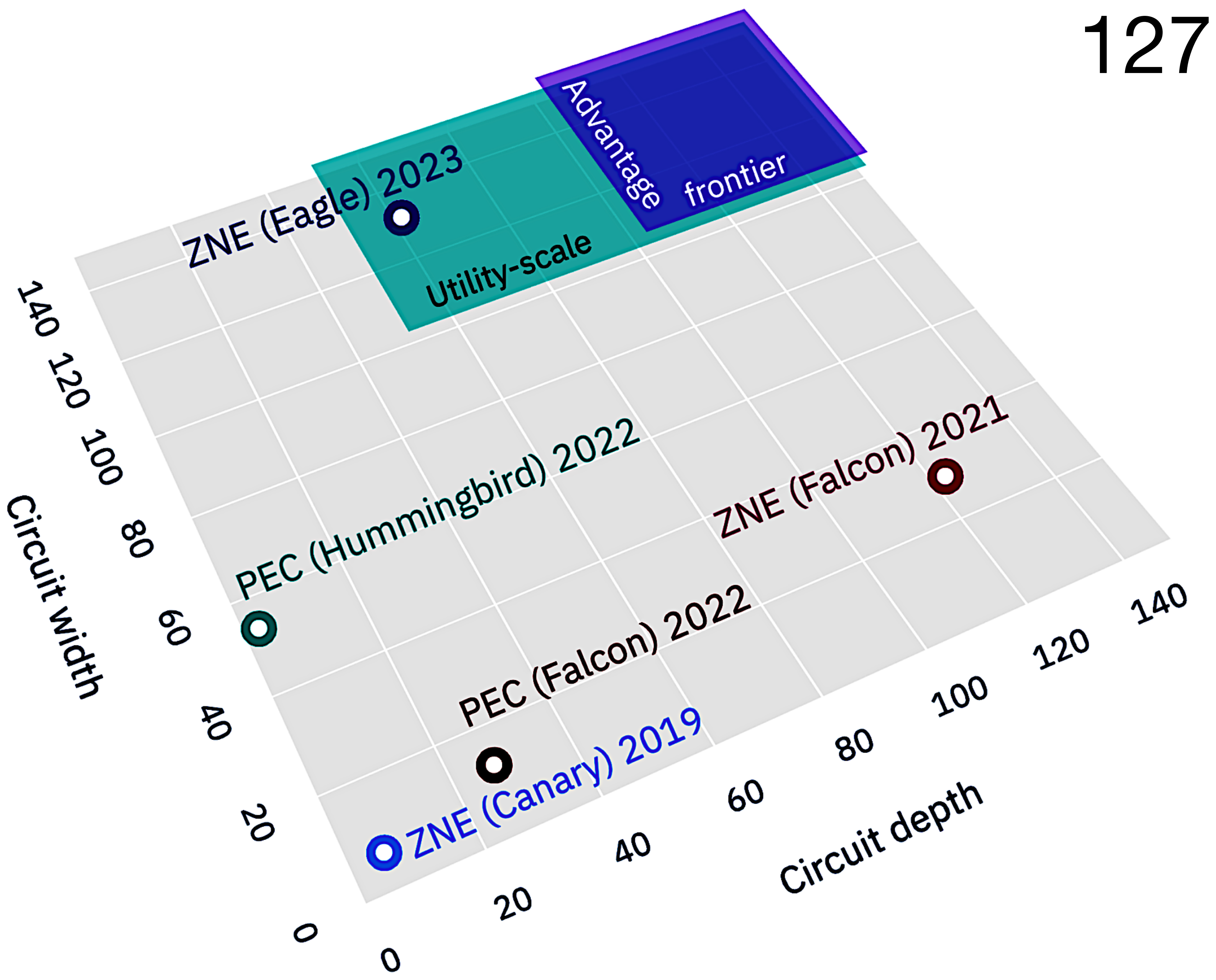
High-fidelity quantum computation outside the reach of exact classical simulation methods

It is the first major milestone on the path to Quantum Advantage.

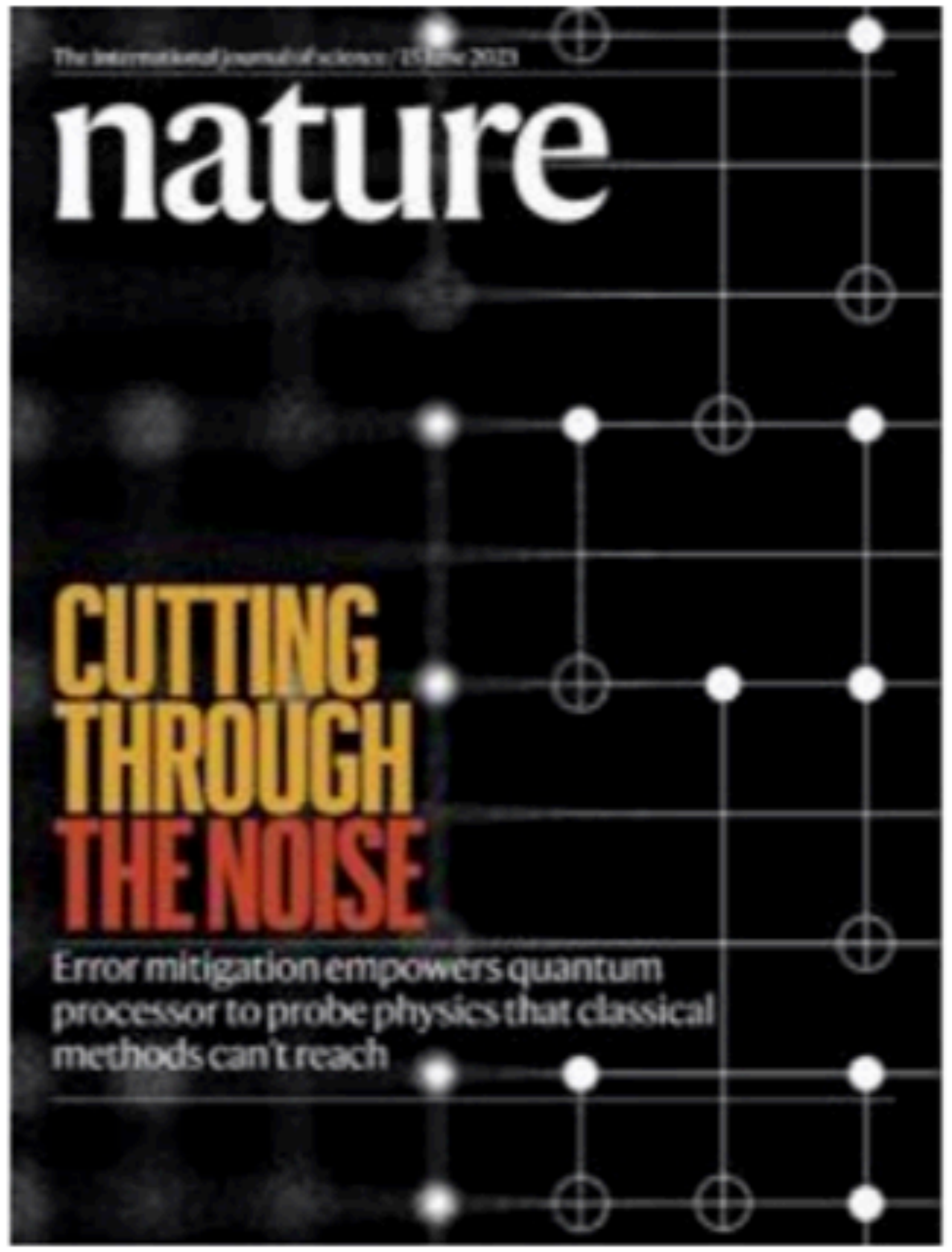
Useful quantum computation requires utility-scale hardware and co-designed scalable software capabilities.

This means systems larger than 100 qubits, where simulations are not a viable alternative.

IBM quantum 2024

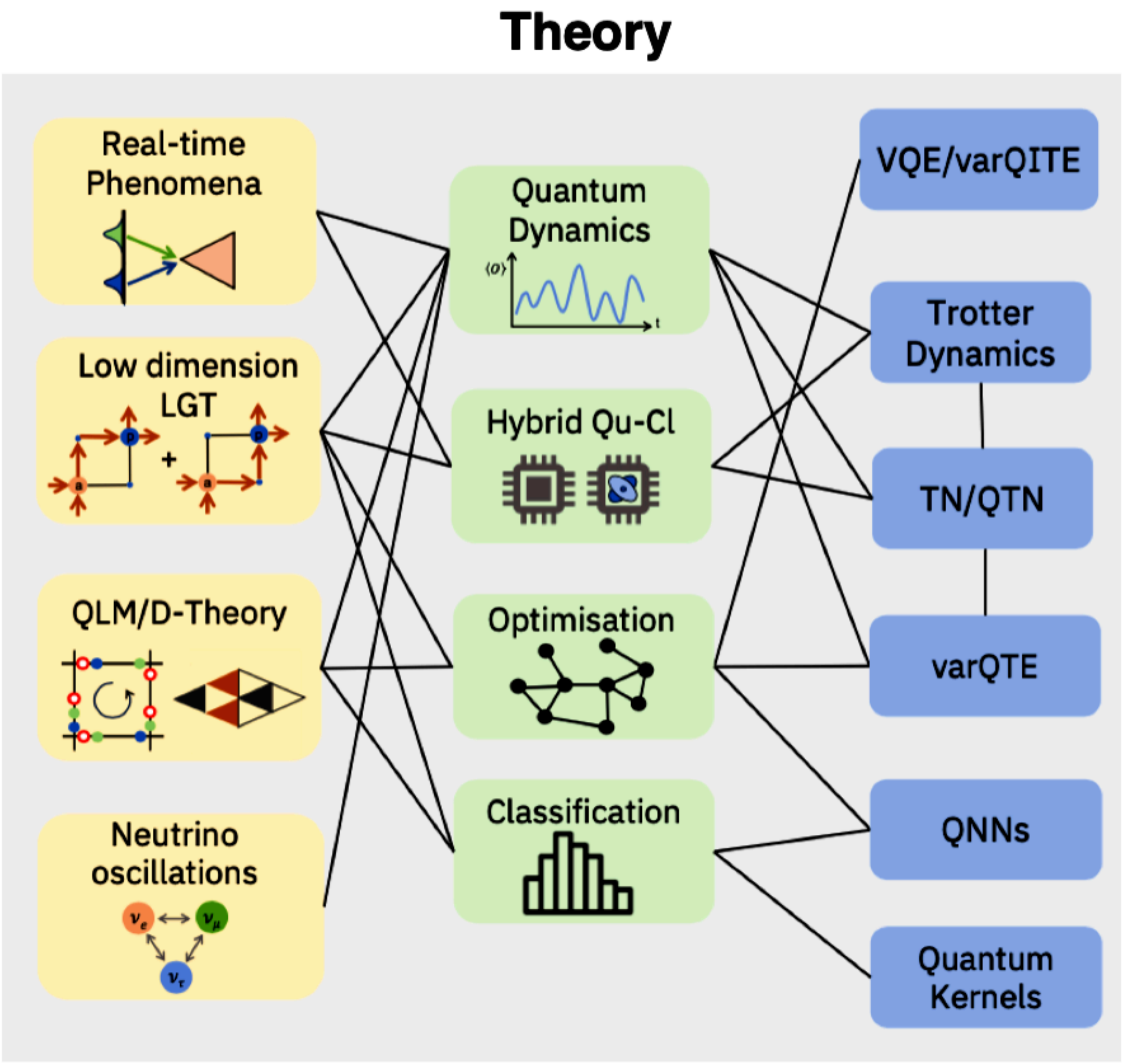


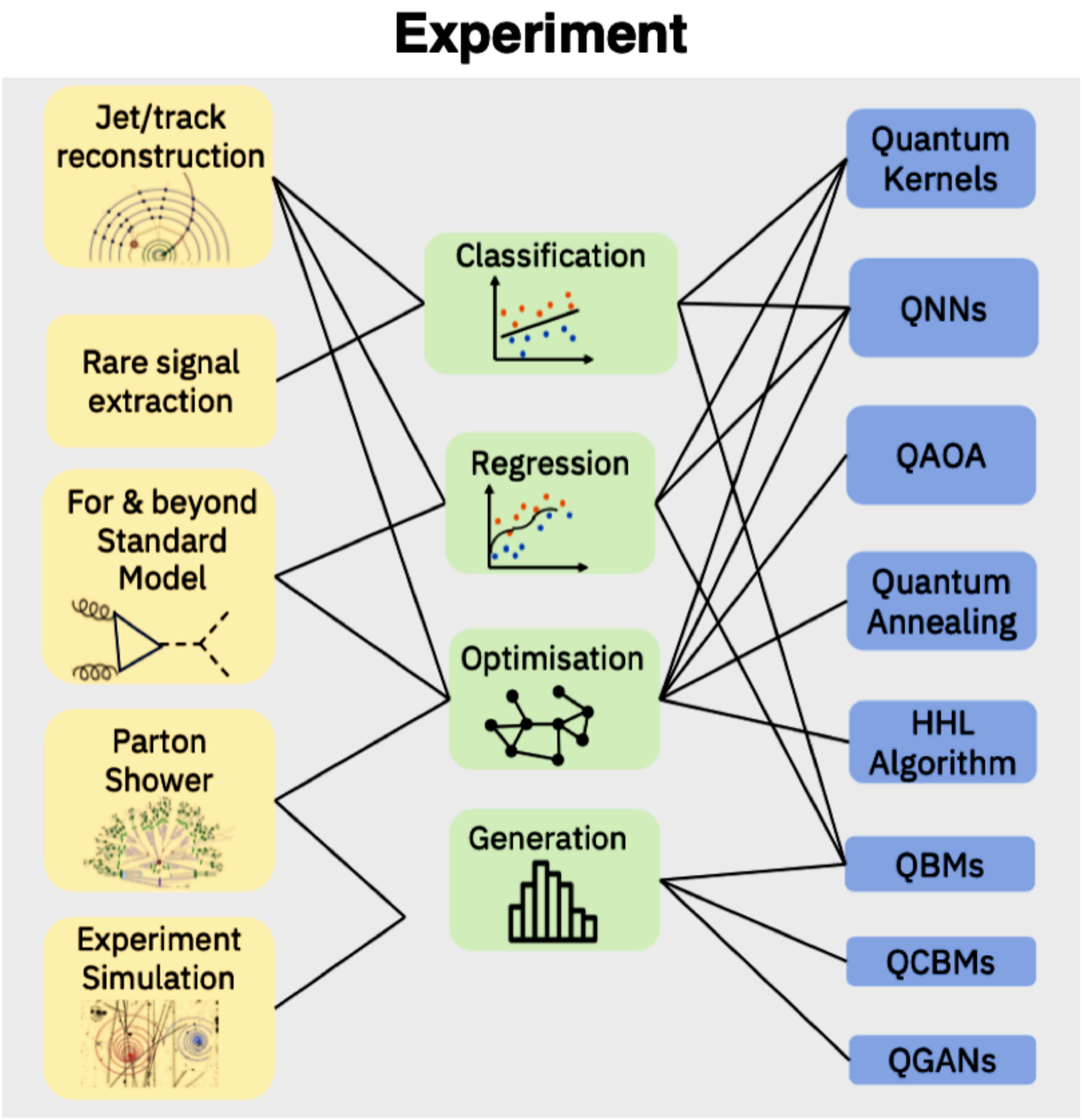
Evidence for the utility of QC before fault tolerance
127 qubits / 2880 CX gates



Nature, 618, 500 (2023)

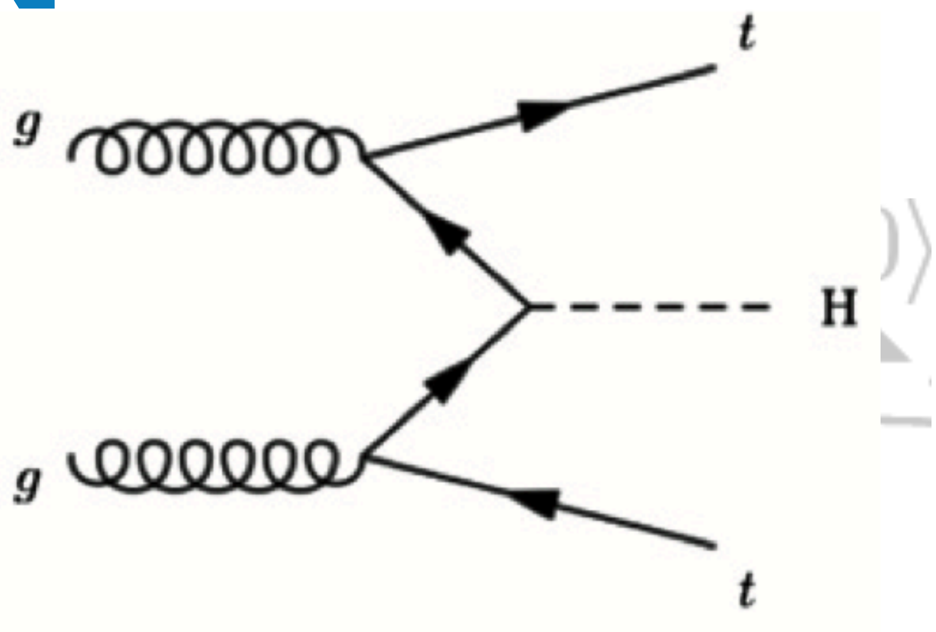
EXEMPLES OF QML APPLICATIONS IN HEP





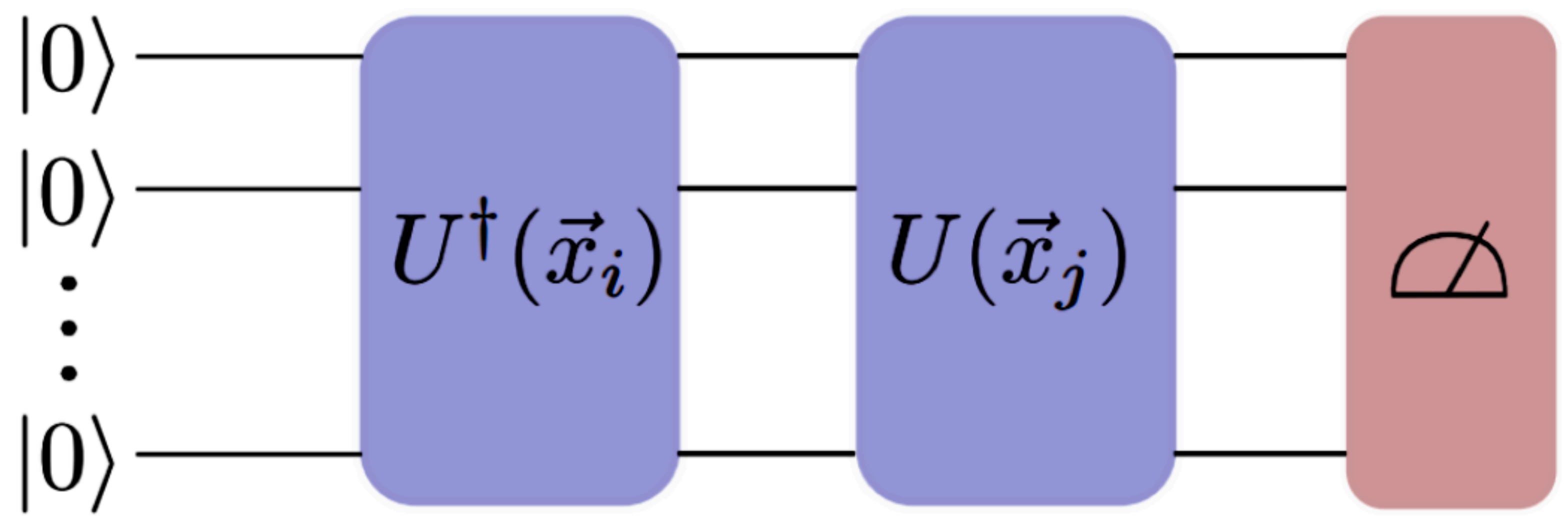
A. Di Meglio et al: arXiv:2307.03236 [quant-ph]

QML IN HEP: HIGGS CLASSIFICATION



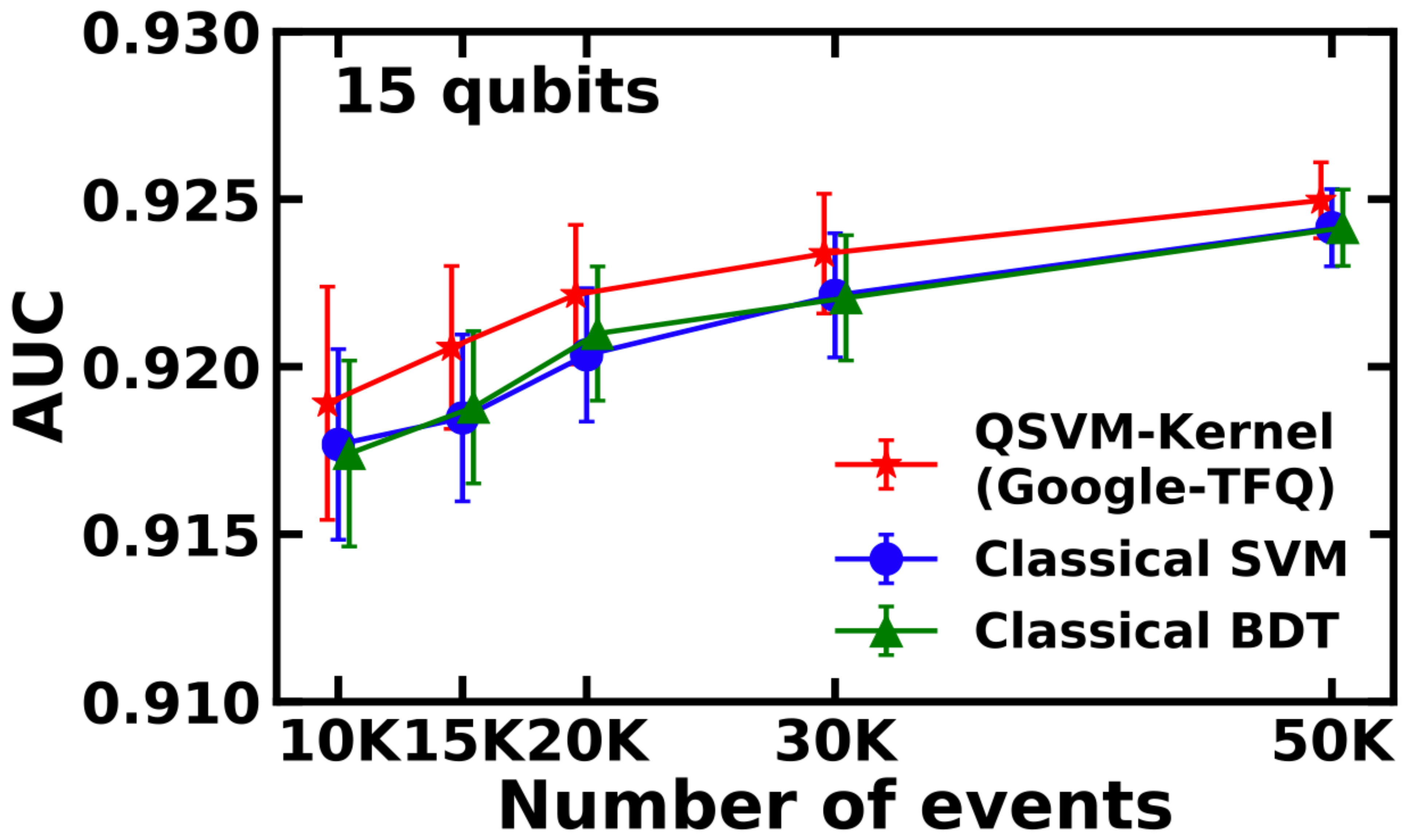
- Classical Support Vector Machine with Quantum Kernels acceleration employed in probing of the Higgs boson coupling to the top quark with the $t\bar{t}H(\to \gamma\gamma)$ channel

QSVM



$$y' = sgn(\sum_{i=1}^{t} \alpha_i y_i k(\vec{x}_i, \vec{x}') + b)$$ SVM output

$$\Rightarrow \quad k(\vec{x_i}, \vec{x_j}) = |\langle \Phi(\vec{x_i}) | \Phi(\vec{x_j}) \rangle|^2 = |\langle 0^{\otimes N} | \mathcal{U}^{\dagger}_{\Phi(\vec{x_i})} \mathcal{U}_{\Phi(\vec{x_j})} | 0^{\otimes N} \rangle|^2$$



Dataset:

- signal and dominant backgrounds considered, simulated with Delphes
- input features: 23 object-based kinematic variables from the ATLAS analysis

Sau Lan Wu et al, arxiv:2104.05059

A QUANTUM ANNEALER EXAMPLE: HIGGS CLASSIFICATION

- an alternative approach: using a programmable quantum annealer …
- task: classification of $H \rightarrow \gamma\gamma$ versus di-photon background

Quantum Annealing:

- define an ensamble of week classifiers $C_i(x) = \pm 1/N_c$
- maps the solution of the problem to the ground state of an Ising Hamiltonian

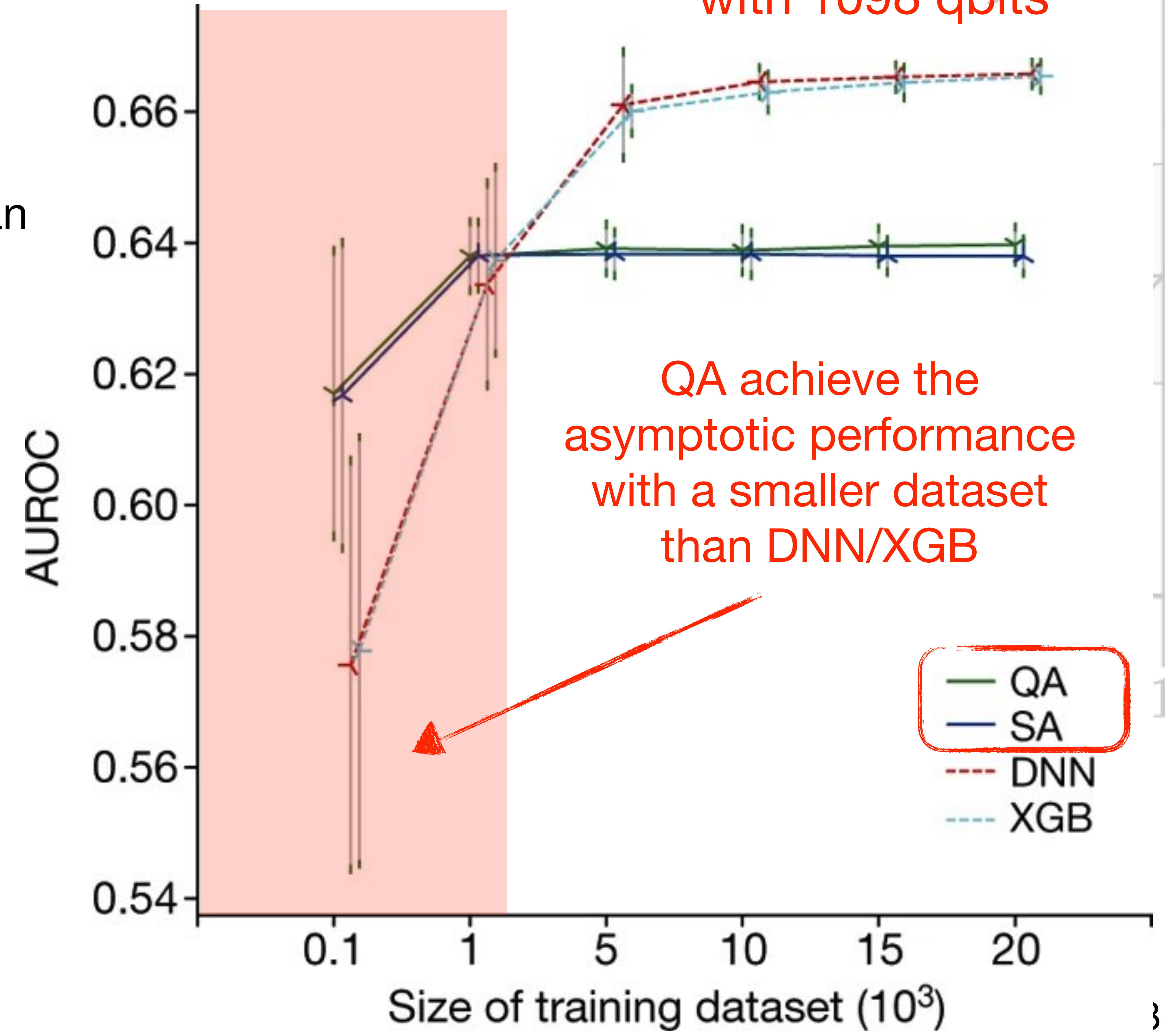
$$H = \sum_{i,j} J_{ij} s_i s_j + \sum_i h_i s_i \qquad C_i = \sum_t C_i(x_t) y_t$$

$$C_{ij} = \frac{1}{4} \sum_t C_i(x_t) C_j(x_t) \qquad h_i = \lambda - C_i + \frac{1}{2} \sum_j C_{ij}$$

- minimize H and return the ground state, building a strong classifier as:

$$R(x) = \sum_i s_i^* c_i(x) \in [-1,1]$$

D-wave hardware with 1098 qbits

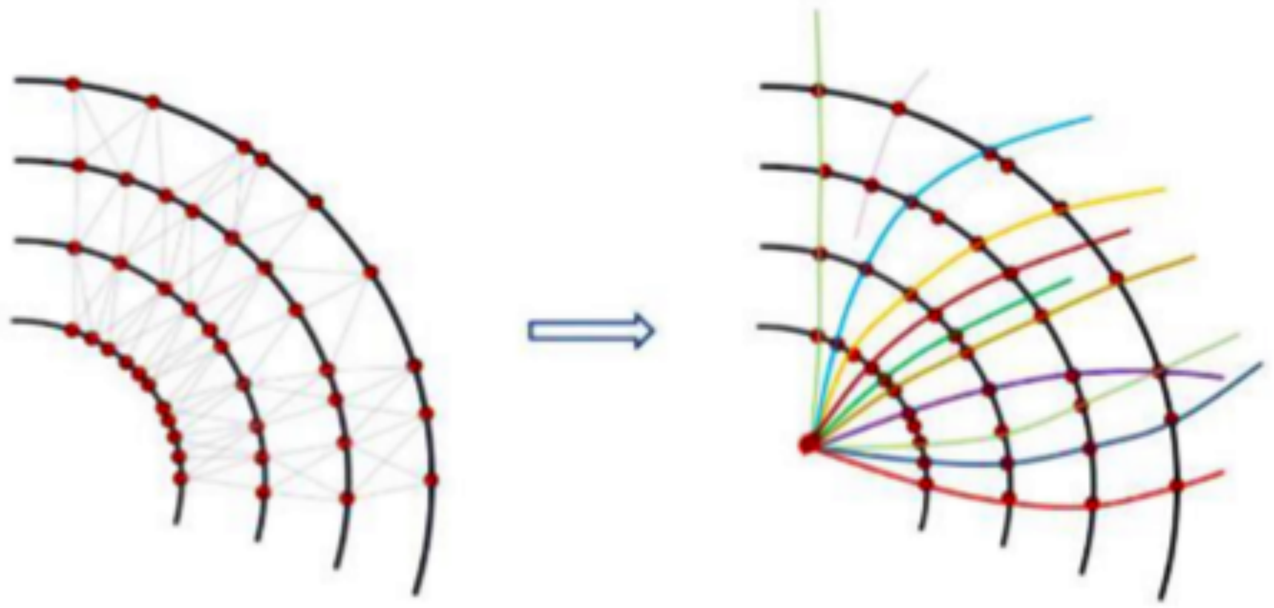


A. Mott et al, Nature volume 550, pages 375–379 (2017)

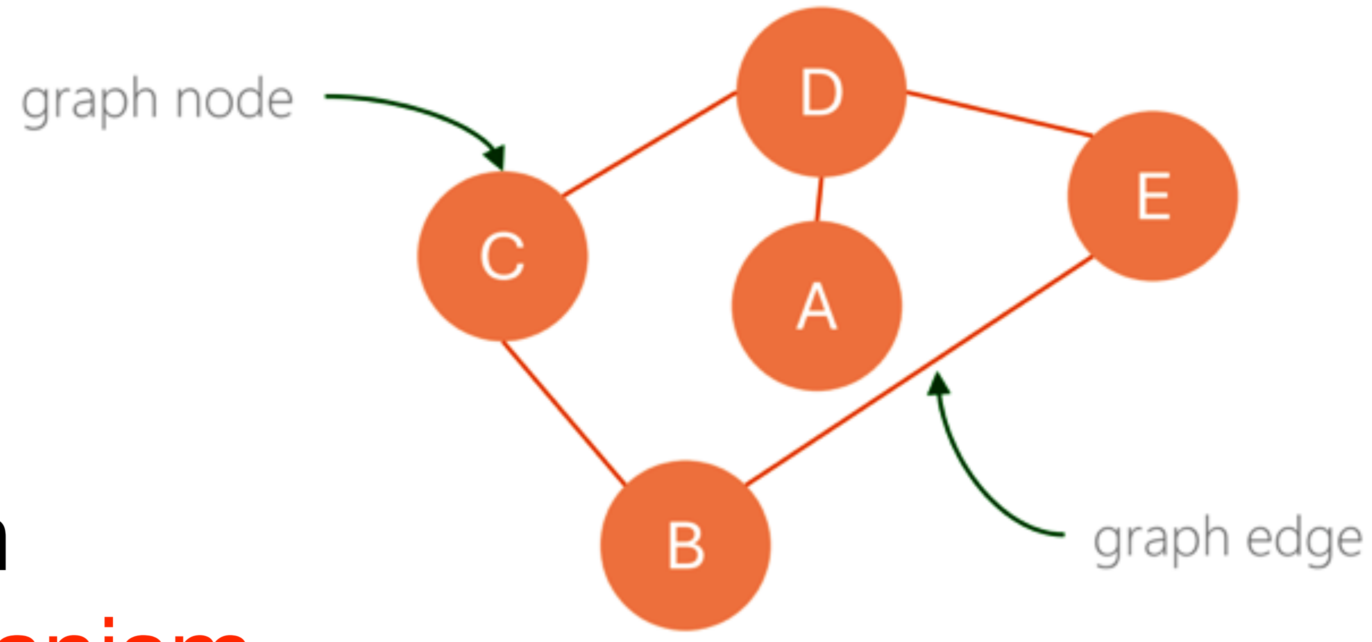
QML: HYBRID QUANTUM GNN FOR TRACK RECONSTRUCTION

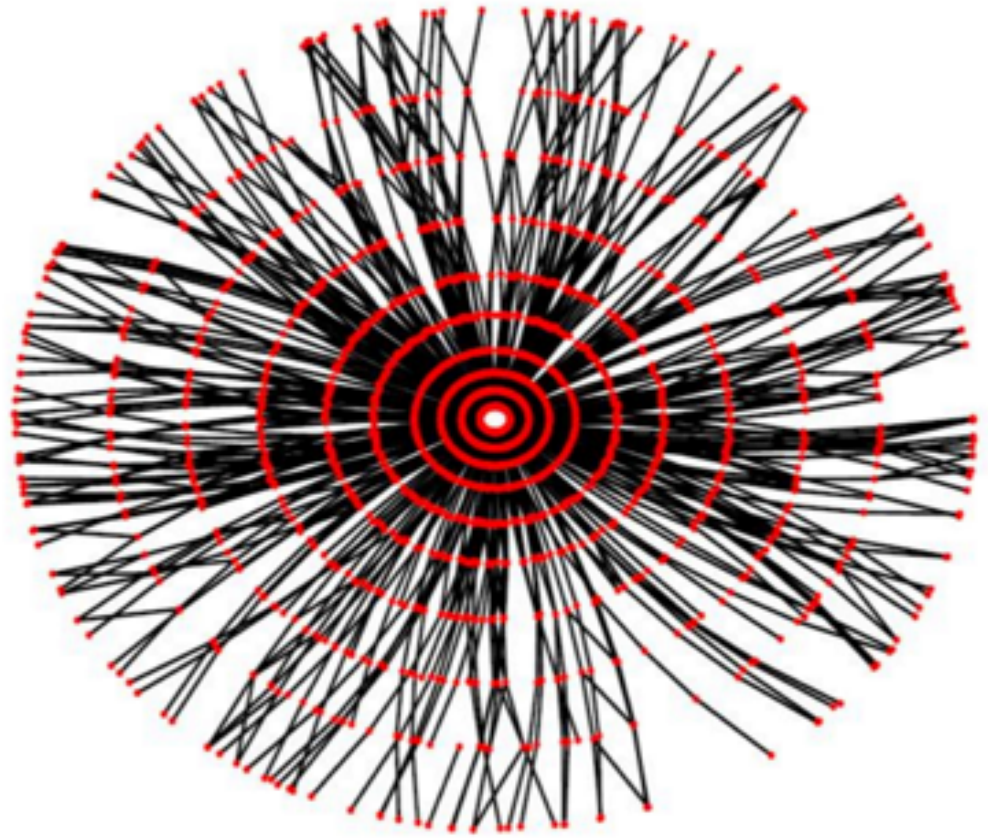
- one of the hard challenges at the future HL-LHC upgrade, when the increase in the instantaneous rate of particle collisions will yield many more detector hits, and thus measurements will pose a combinatorial challenge to track reconstruction algorithms

- idea: explore the possibility to speedup the task by implementing an hybrid classical-quantum Graph Neural Network trained to determine charged particle trajectories from hits in a LHC inner tracker detector



- charged particle tracks are represented as a graph over the detector hits
  - nodes: hits in a detector layer
  - edges: track segments
  - nodes and edges information is updated trough message passing leveraging an attention mechanism to identify most relevant nodes



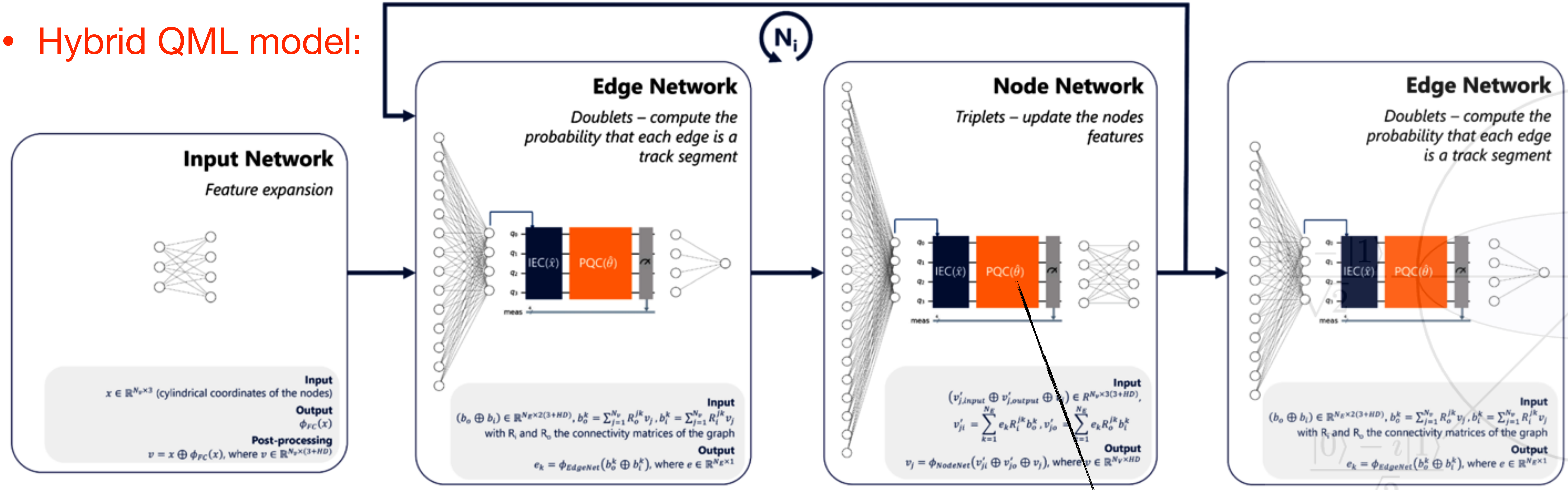


INFN-Ferrara: V.Amitrano, M.Argenton, C.Bozzi, E.Calore, L.Cappelli, F.Schifano

QML: HYBRID QUANTUM GNN FOR TRACK RECONSTRUCTION

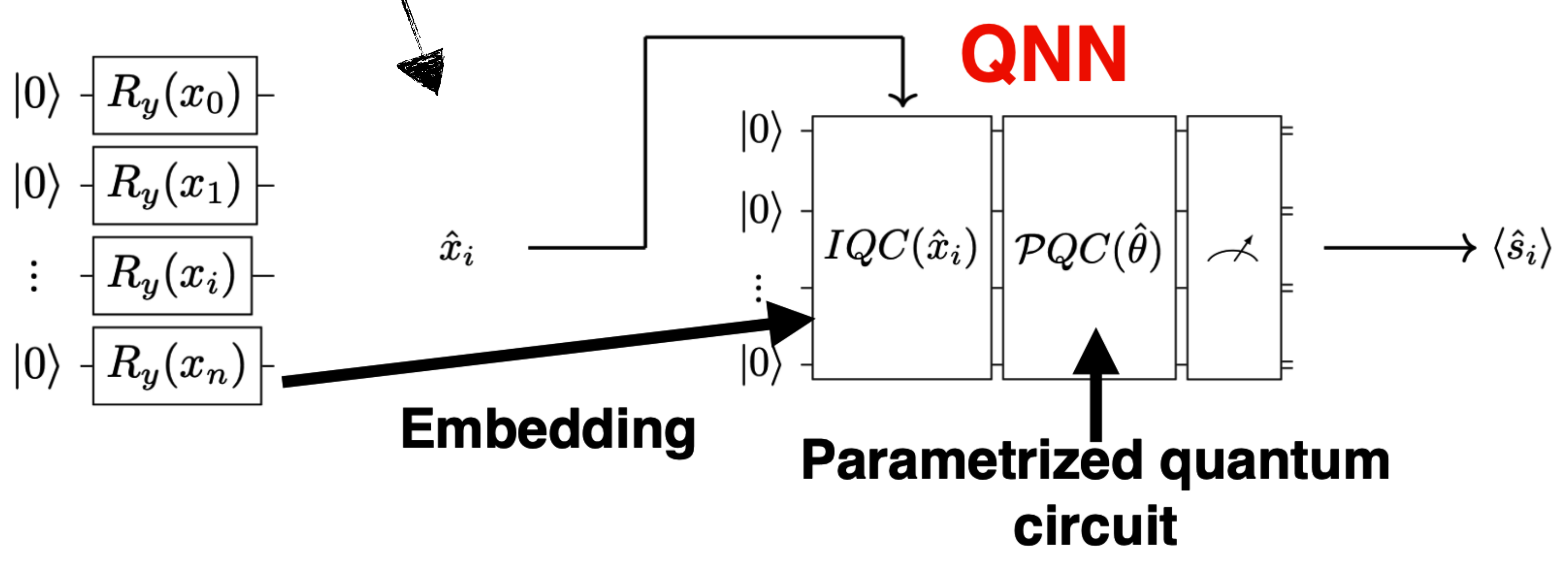
first implemented by [Cenk Tüysüz et al, arXiv:2012.01379]

- Hybrid QML model:



Edge network: QNN with edges as inputs, outputs probabilities for edges to be true (edge features)

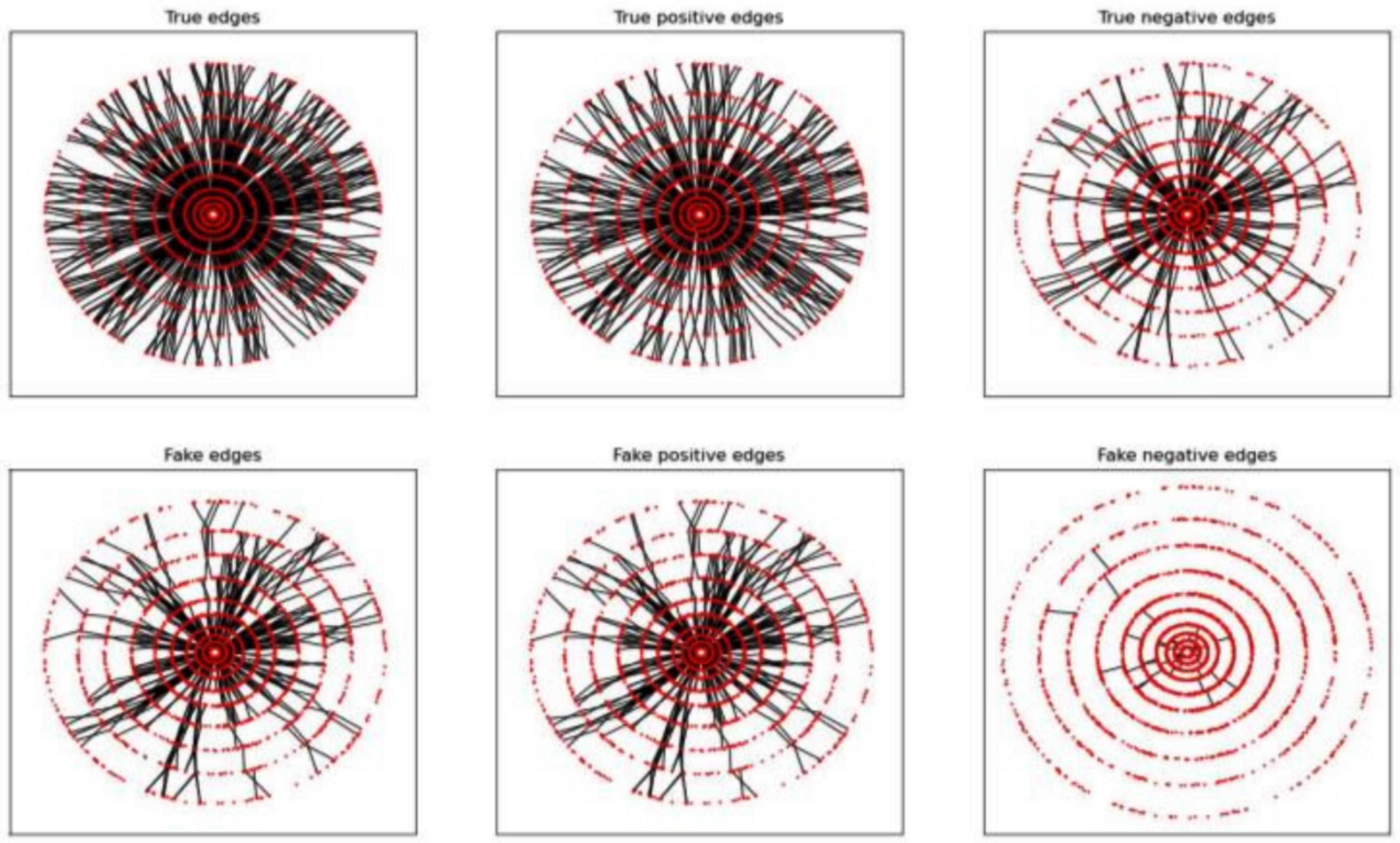
Node network: Edges are weighted with edge features. Triplets of connected nodes are built, and fed to a QNN. QNN provides updated nodes as outputs.

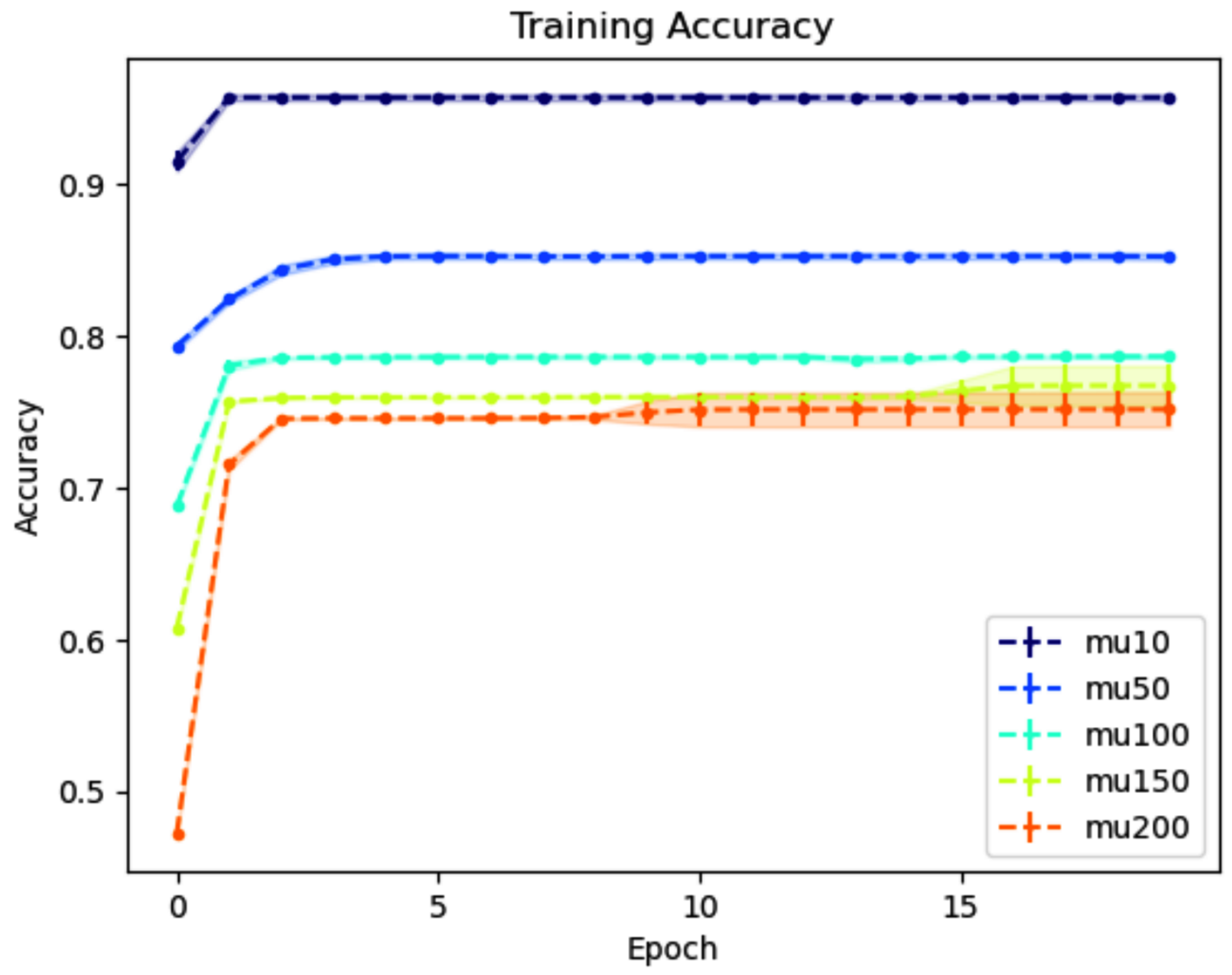


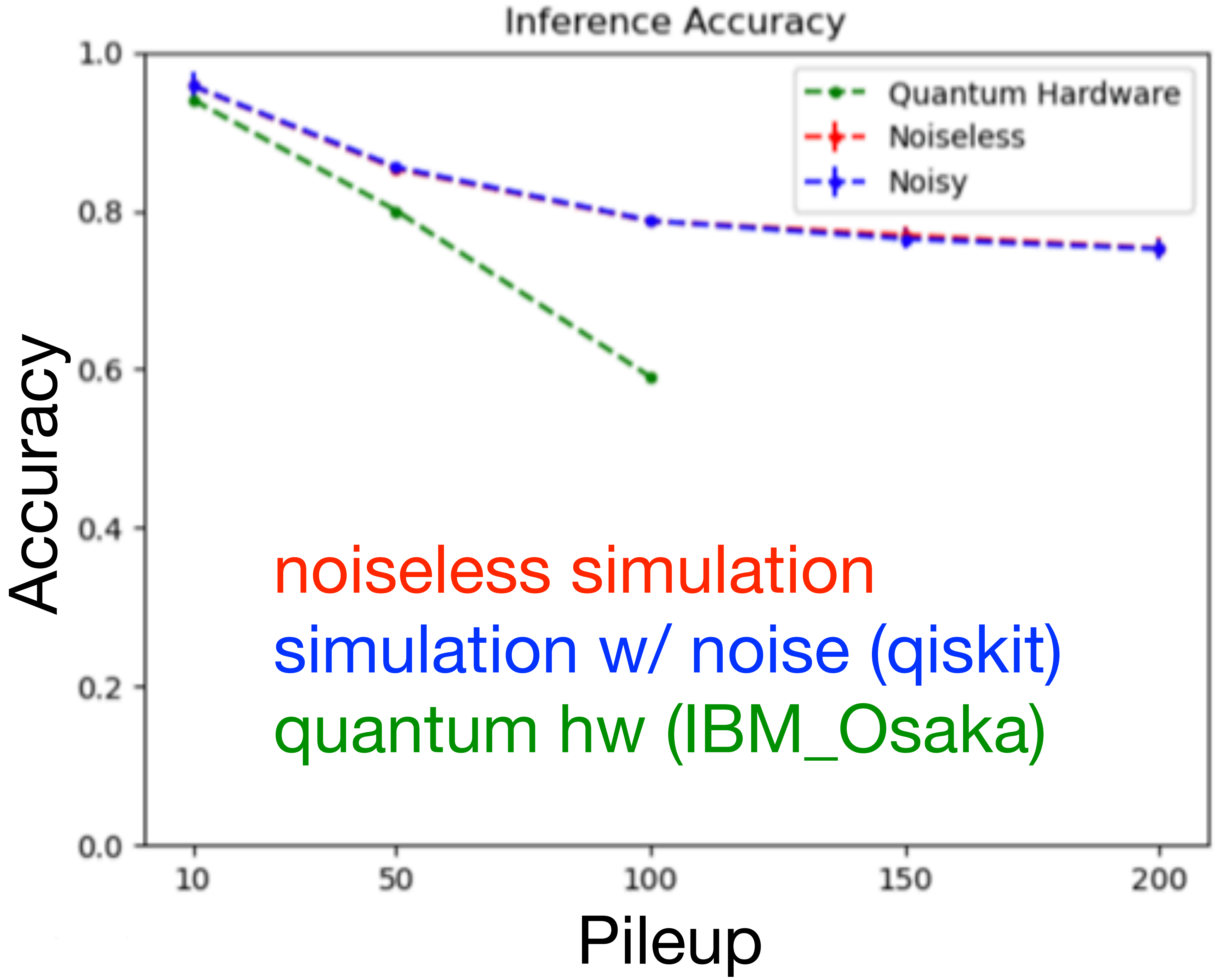
INFN-Ferrara: V.Amitrano, M.Argenton, C.Bozzi, E.Calore, L.Cappelli, F.Schifano

QML: HYBRID QUANTUM GNN FOR TRACK RECONSTRUCTION

Accuracy is, as expected, higher with lower pileup







INFN-Ferrara: V.Amitrano, M.Argenton, C.Bozzi, E.Calore, L.Cappelli, F.Schifano

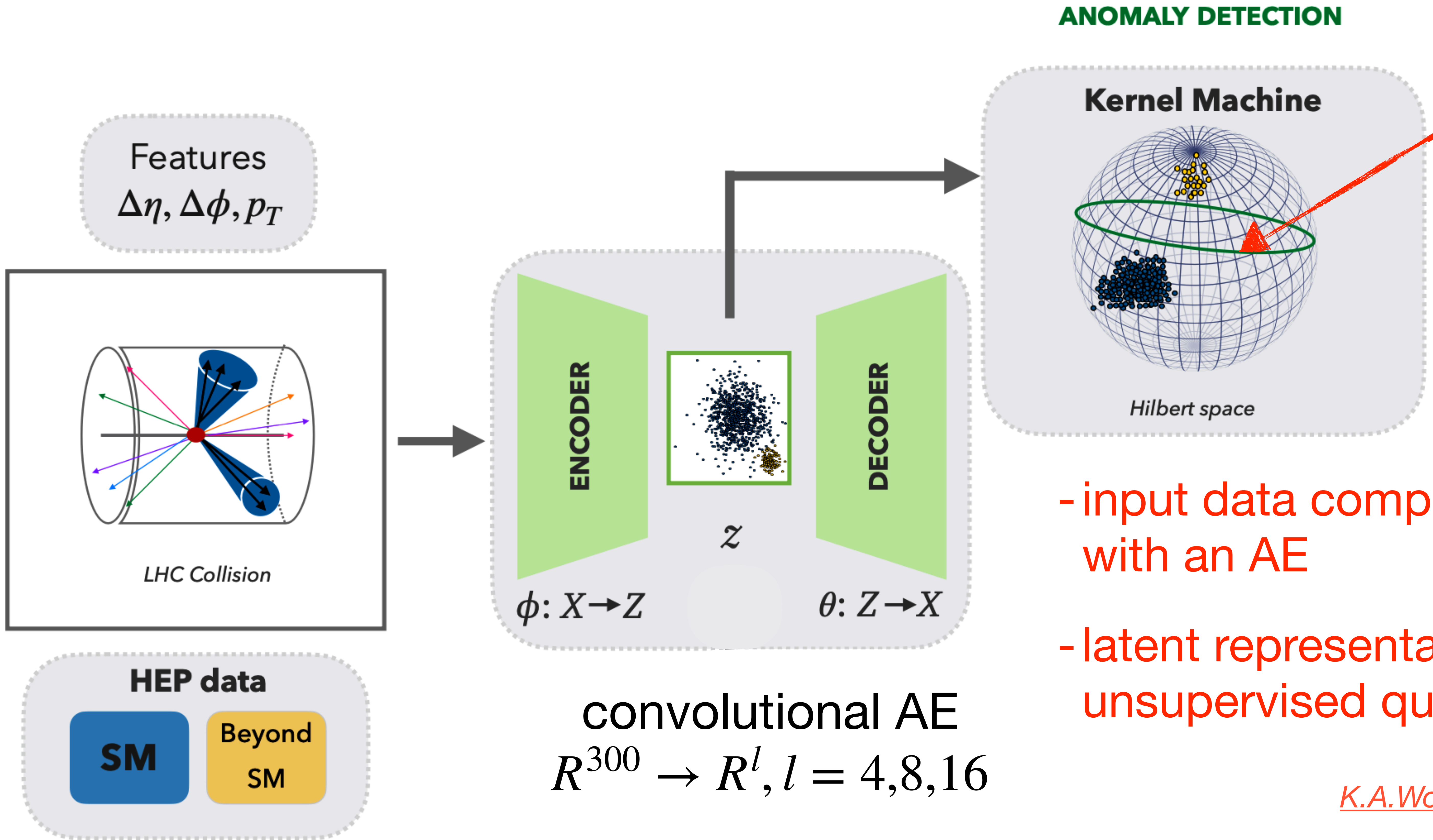
QUANTUM ANOMALY DETECTION FOR QCD JETS

- Anomaly Detection describes a class of algorithms that aims at the identification of rare items, events or observations, which deviate significantly from the majority of the data and do not conform to a well-defined notion of normal behavior

- Gained increasing interest recently in experiments at the LHC, as a viable ML approach to implement signal model-independent searches for NP effects

Use case:

- QCD multijets at the LHC
- delphes simulation
- build jets from 100 highest pt particles
- apply realistic event selection



convolutional AE

$R^{300} \to R^l, l = 4,8,16$

find the hyperplane that maximise the distance of the data from the origin of the feature vector space

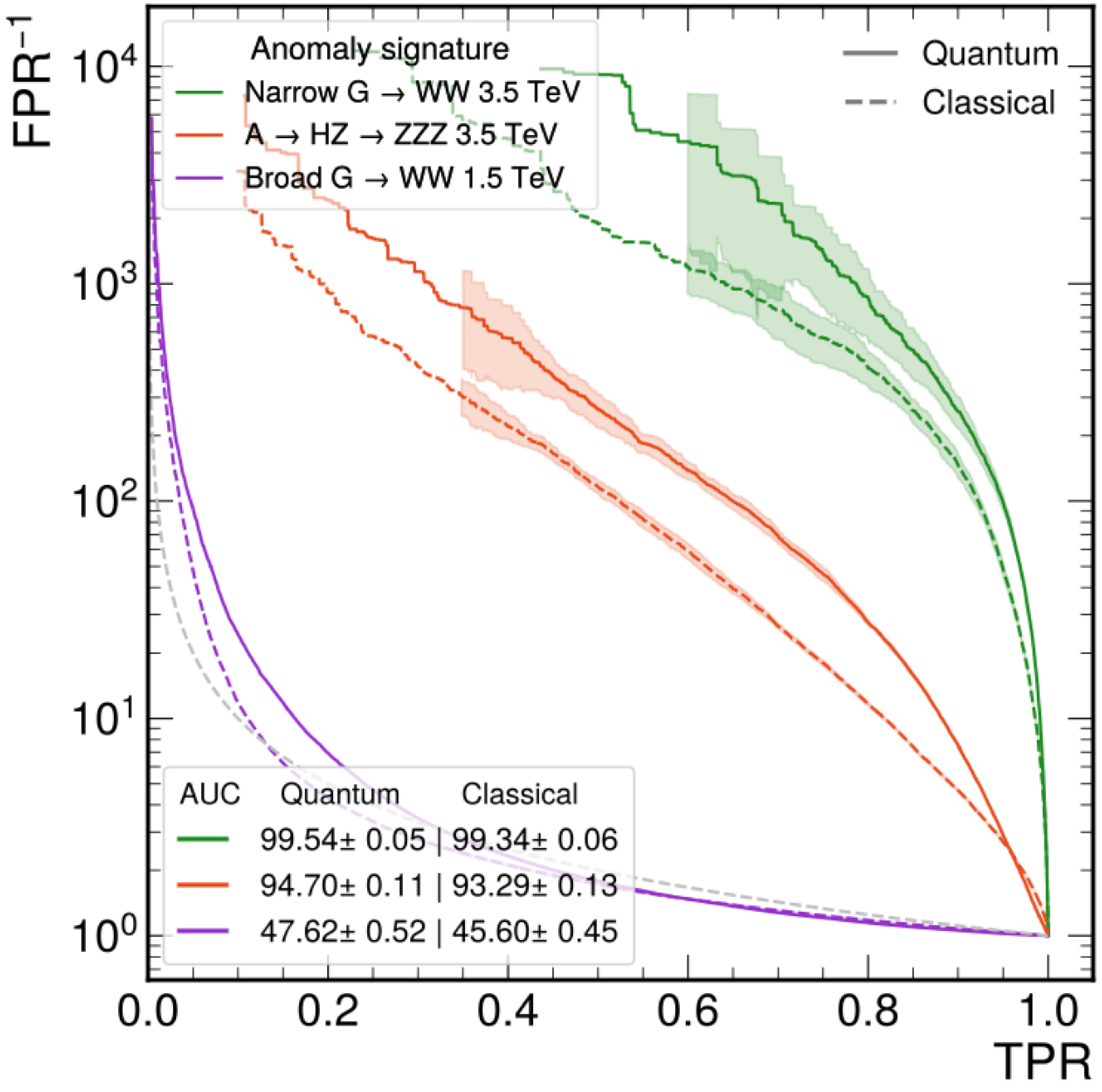
- input data compressed classically with an AE
- latent representation analysed by an unsupervised quantum kernel

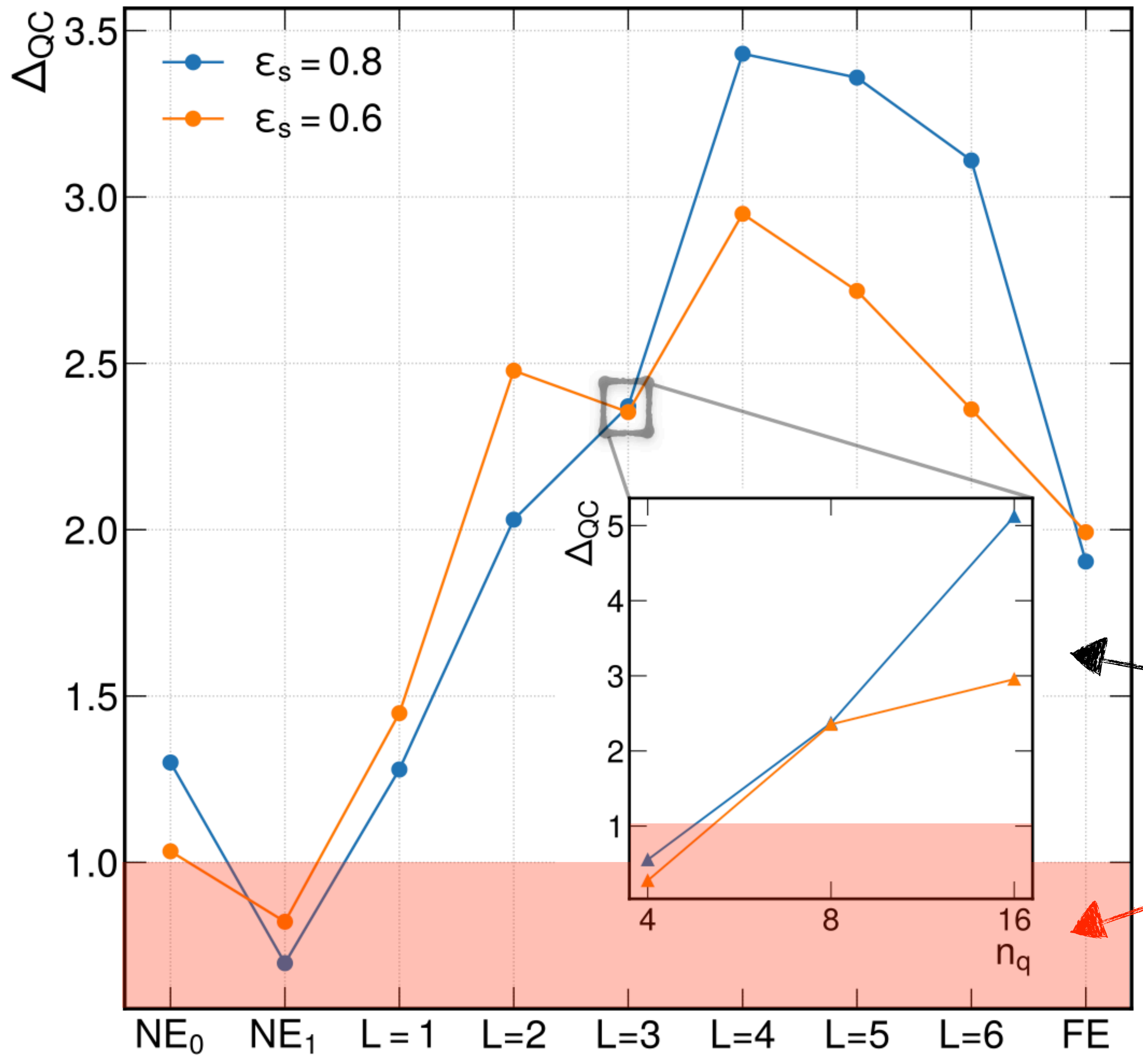
K.A.Wozniak et al, arXiv:2301.10780

QUANTUM ANOMALY DETECTION FOR QCD JETS

$$\Delta_{QC}(\epsilon_s) = \frac{\epsilon_b^{-1}(\epsilon_s; Q)}{\epsilon_b^{-1}(\epsilon_s; C)}$$

background rejection (FPR^{-1}) at a working point ϵ_s (TPR) given a specific quantum (Q) or classical (C) anomaly detection model





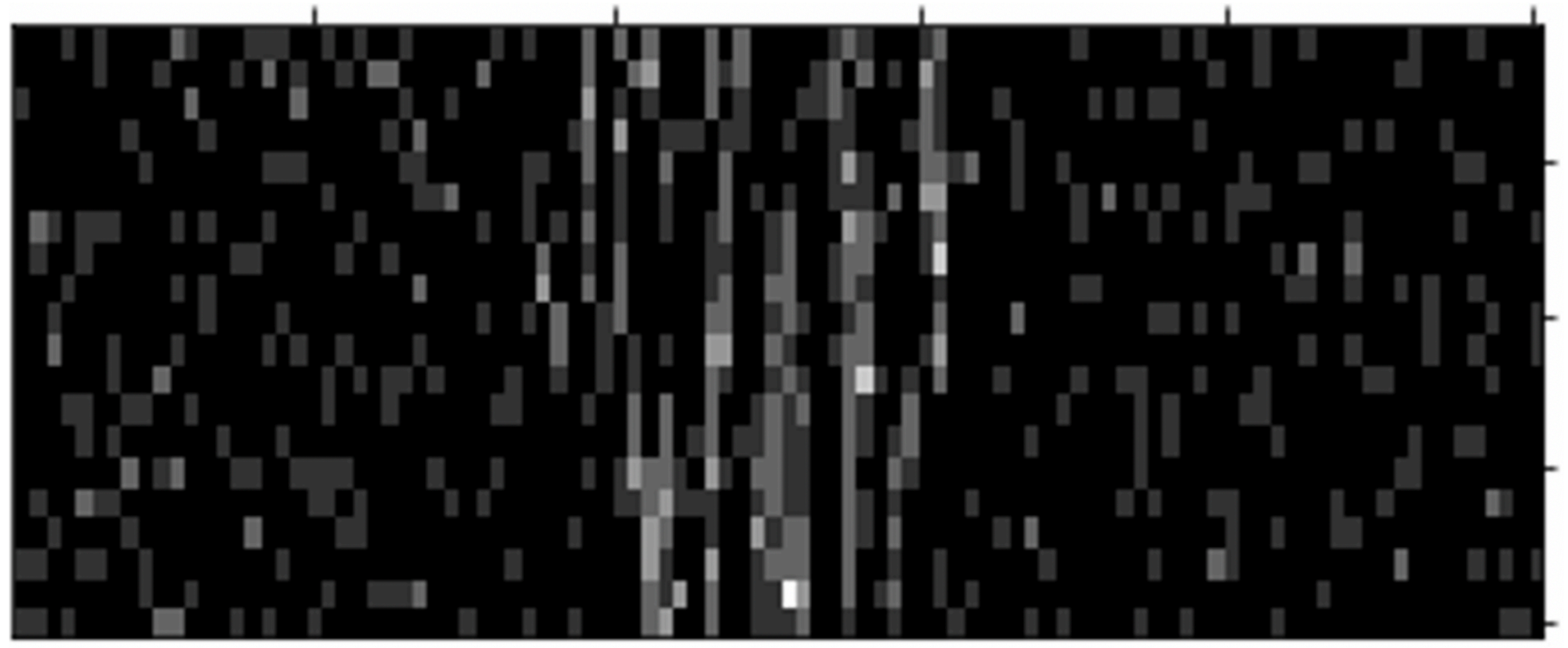
K.A.Wozniak et al, arXiv:2301.10780

QUANTUM ANOMALY DETECTION FOR LONG LIVED PARTICLES

- Design and train a Quantum-AE able to identify highly displaced decays using the ATLAS muon spectrometer information

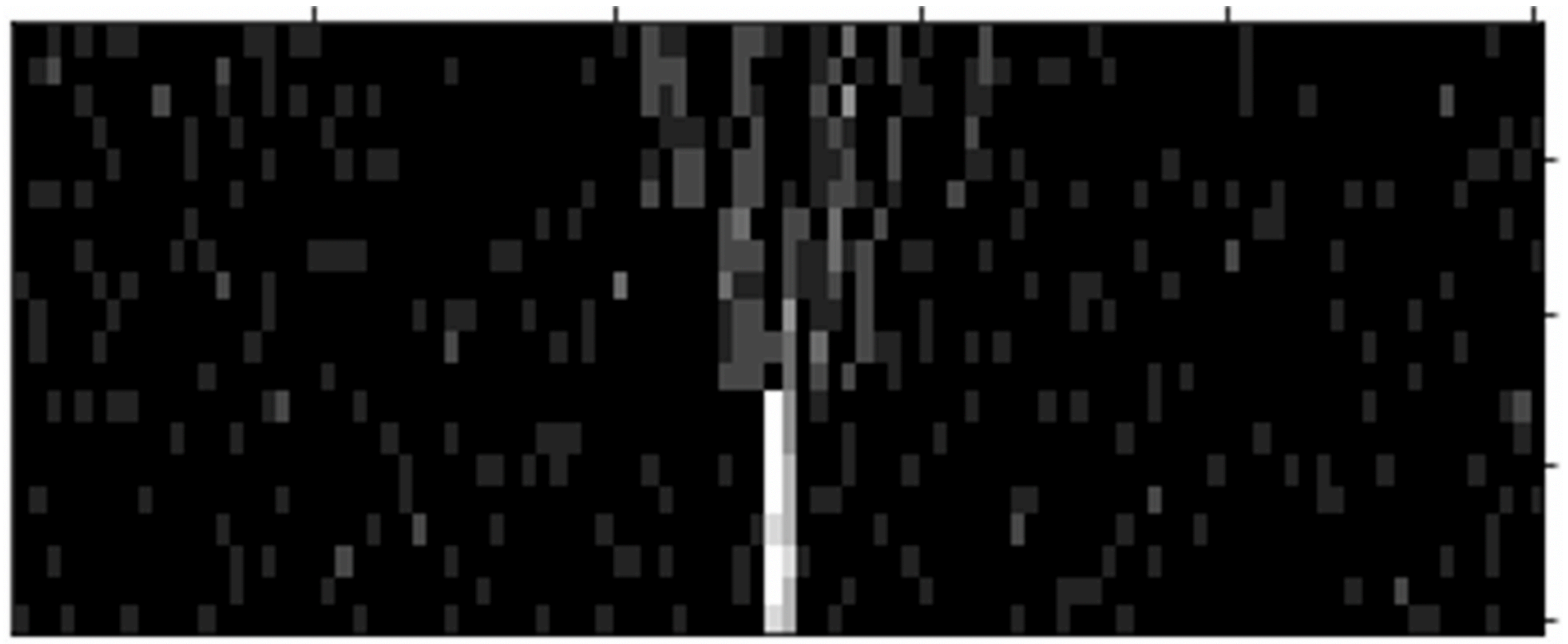
NORMAL event

“image” representation of a prompt decay in multi-muons

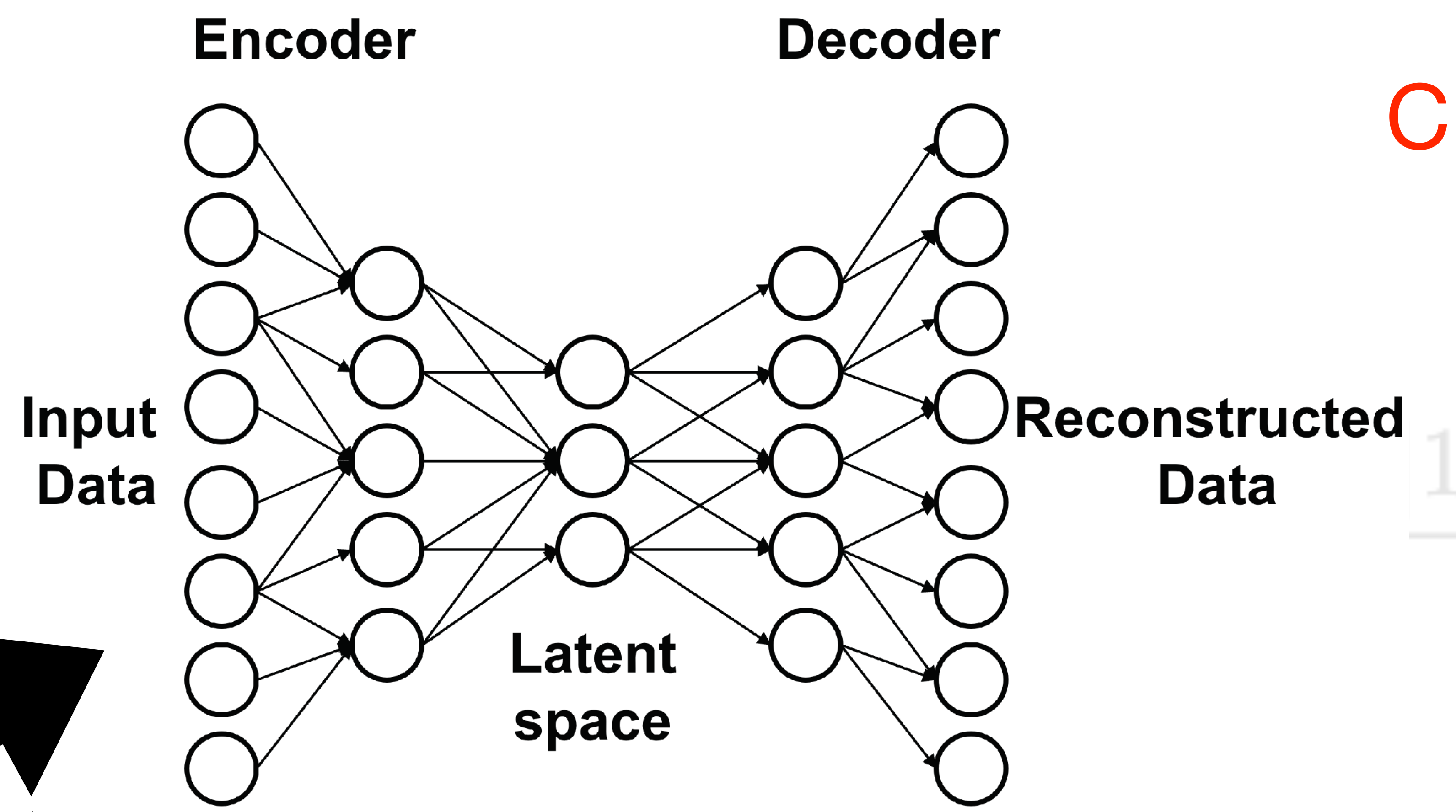


ANOMALOUS event

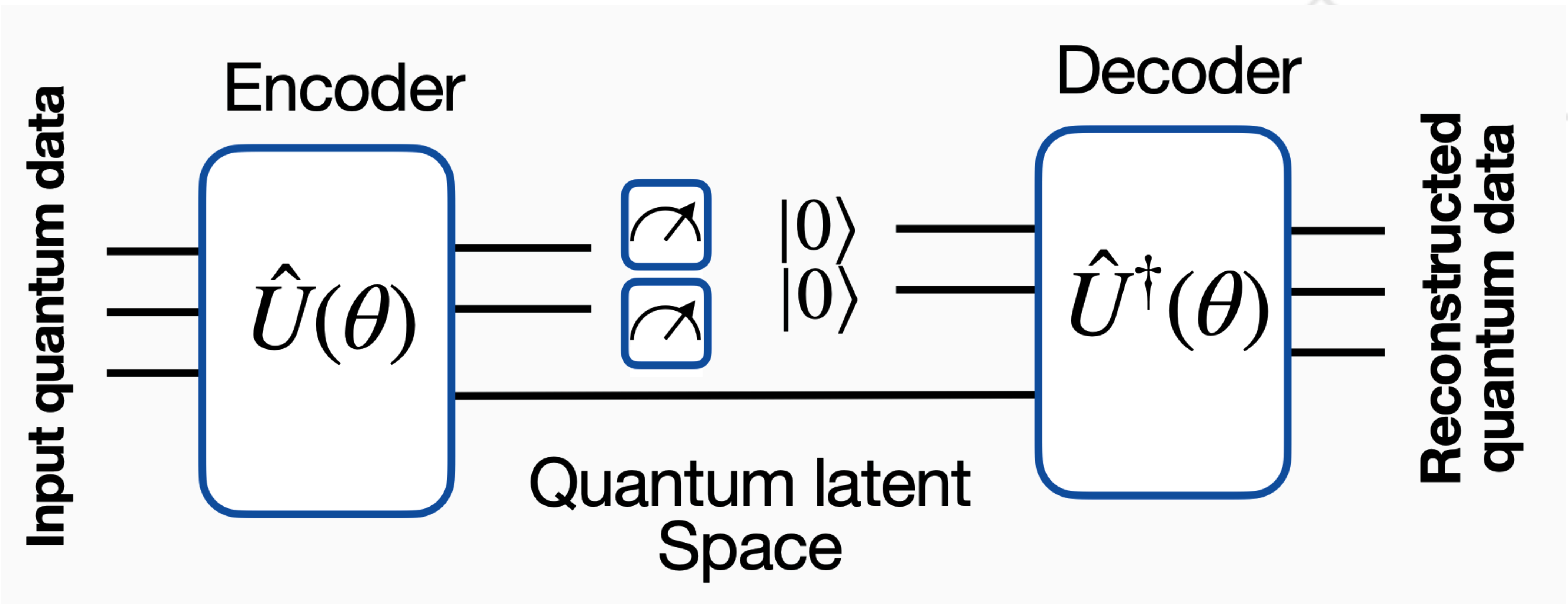
“image” representation of a highly displaced decay in multi-muons



Classical AE



Quantum-AE



S.Bordoni et al, Particles 2023, 1, 1–15

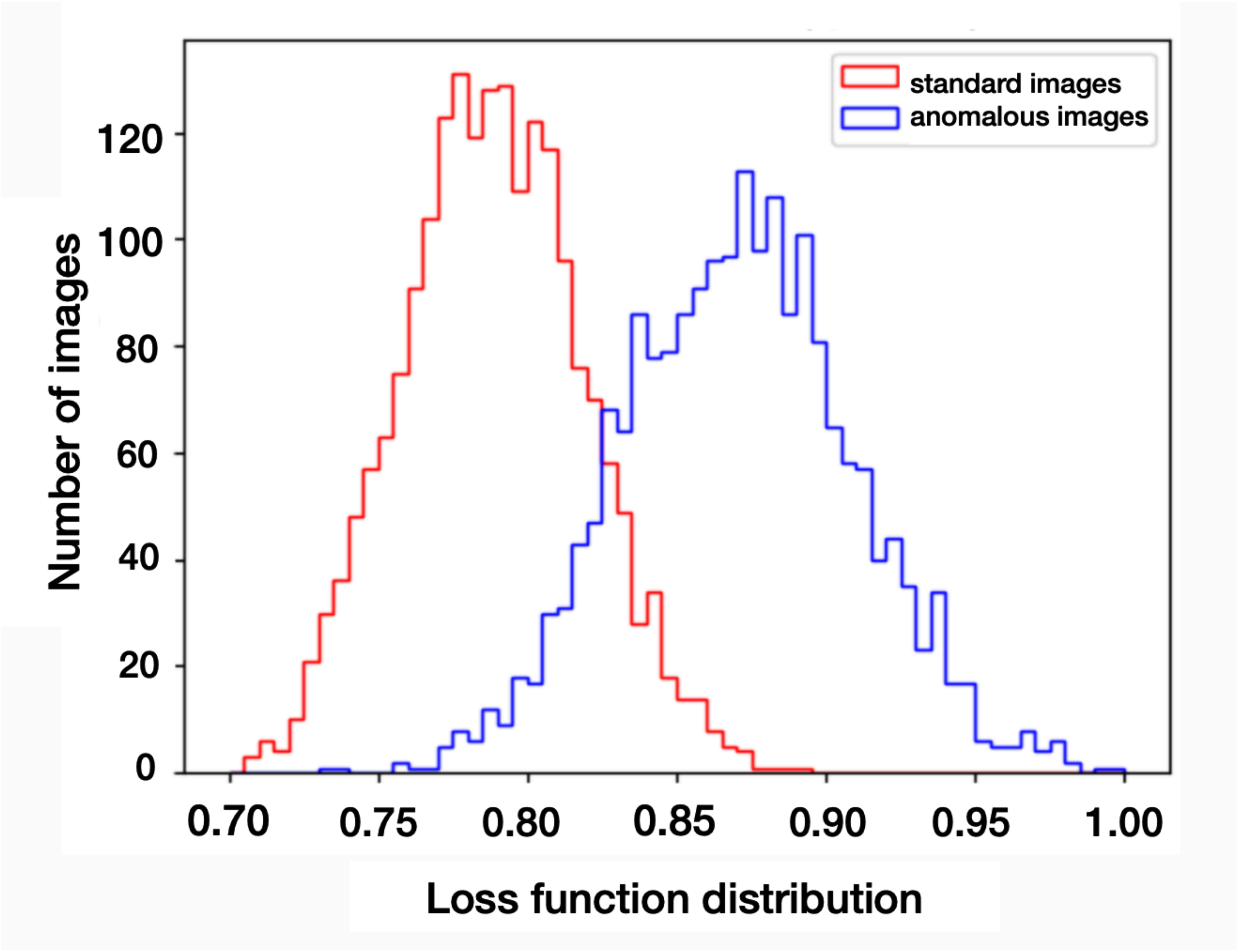
QML IN HEP: ANOMALY DETECTION FOR LONG LIVED PARTICLES

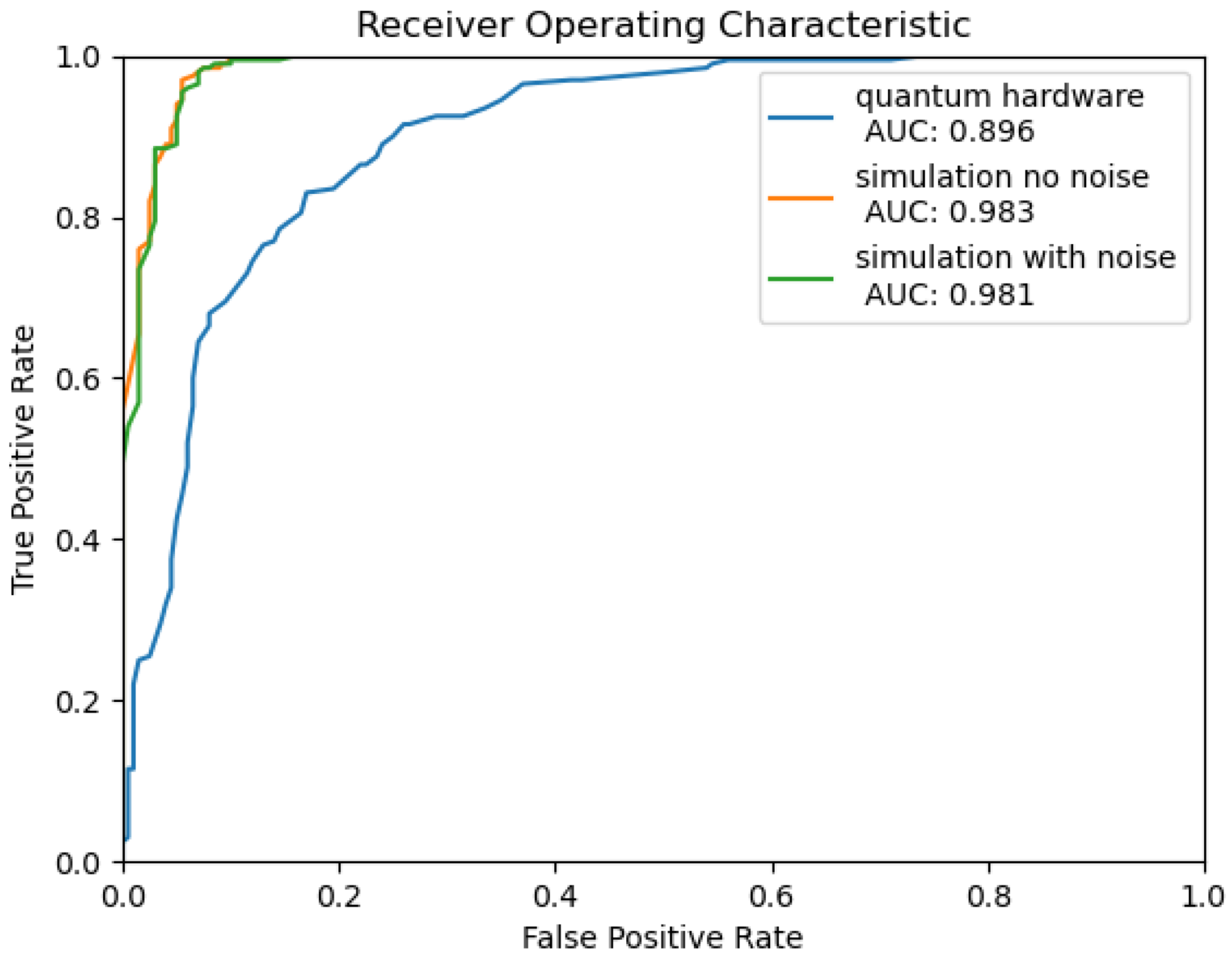
$U(\theta)$

```
q0:     ─RX─RY─RZ─o───────────X─RX─RY─RZ─o───────────X─RX─RY─RZ─o───────────X─RX─RY─  ...
q1:     ─RX─RY─RZ─X─o─────────|─RX─RY─RZ─X─o─────────|─RX─RY─RZ─X─o─────────|─RX─RY─  ...
q2:     ─RX─RY─RZ───X─o───────|─RX─RY─RZ───X─o───────|─RX─RY─RZ───X─o───────|─RX─RY─  ...
q3:     ─RX─RY─RZ─────X─o─────|─RX─RY─RZ─────X─o─────|─RX─RY─RZ─────X─o─────|─RX─RY─  ...
q4:     ─RX─RY─RZ───────X─o───|─RX─RY─RZ───────X─o───|─RX─RY─RZ───────X─o───|─RX─RY─  ...
q5:     ─RX─RY─RZ─────────X─o─RX─RY─RZ─────────X─o─RX─RY─RZ─────────X─o─RX─RY─  ...

q0: ... RZ─o───────────X─RX─RY─RZ─o───────────X─RX─RY─RZ─o───────────X─RX─RY─RZ─
q1: ... RZ─X─o─────────|─RX─RY─RZ─X─o─────────|─RX─RY─RZ─X─o─────────|─RX─RY─RZ─
q2: ... RZ───X─o───────|─RX─RY─RZ───X─o───────|─RX─RY─RZ───X─o───────|─RX─RY─RZ─
q3: ... RZ─────X─o─────|─RX─RY─RZ─────X─o─────|─RX─RY─RZ─────X─o─────|───────────
q4: ... RZ───────X─o───|─RX─RY─RZ───────X─o───|─RX─RY─RZ───────X─o───|───────────
q5: ... RZ─────────X─o─RX─RY─RZ─────────X─o─RX─RY─RZ─────────X─o─────────────────
```

parametric quantum circuit ansatz





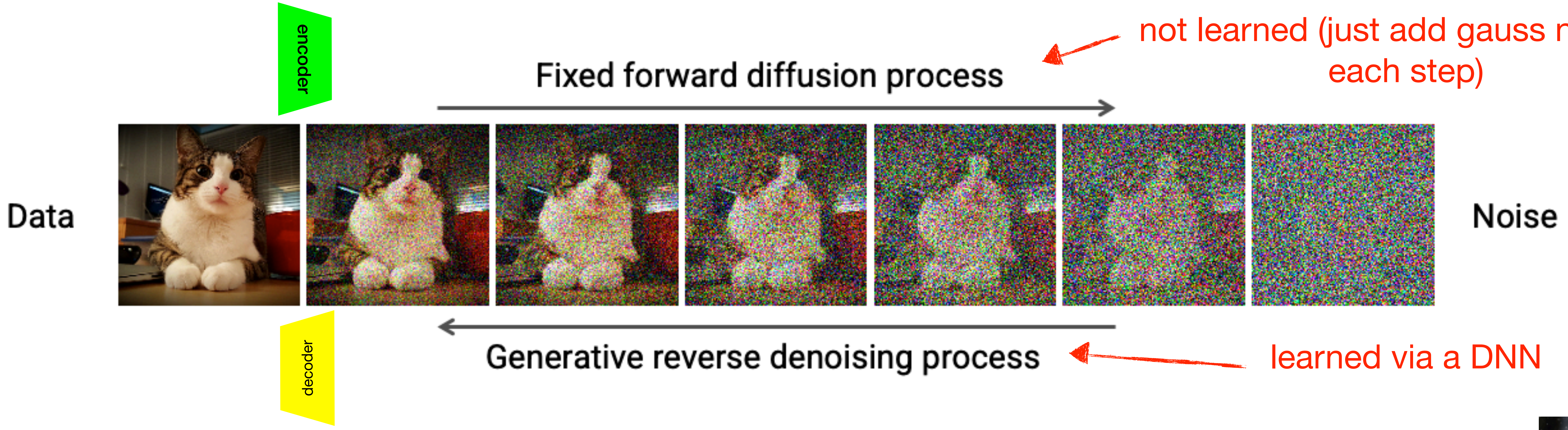
description of the quantum noise and quantum error correction

a crucial issues still to be solved …

S.Bordoni et al, Particles 2023, 1, 1–15

GENERATIVE QML: QUANTUM DIFFUSION MODELS

- Probabilistic Diffusion Models are generative models, inspired by non-equilibrium thermodynamics, that use artificial neural networks to gradually remove noise added to the data, with the goal of subsequently generating high-quality data samples



not learned (just add gauss noise at each step)

learned via a DNN

$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) \quad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

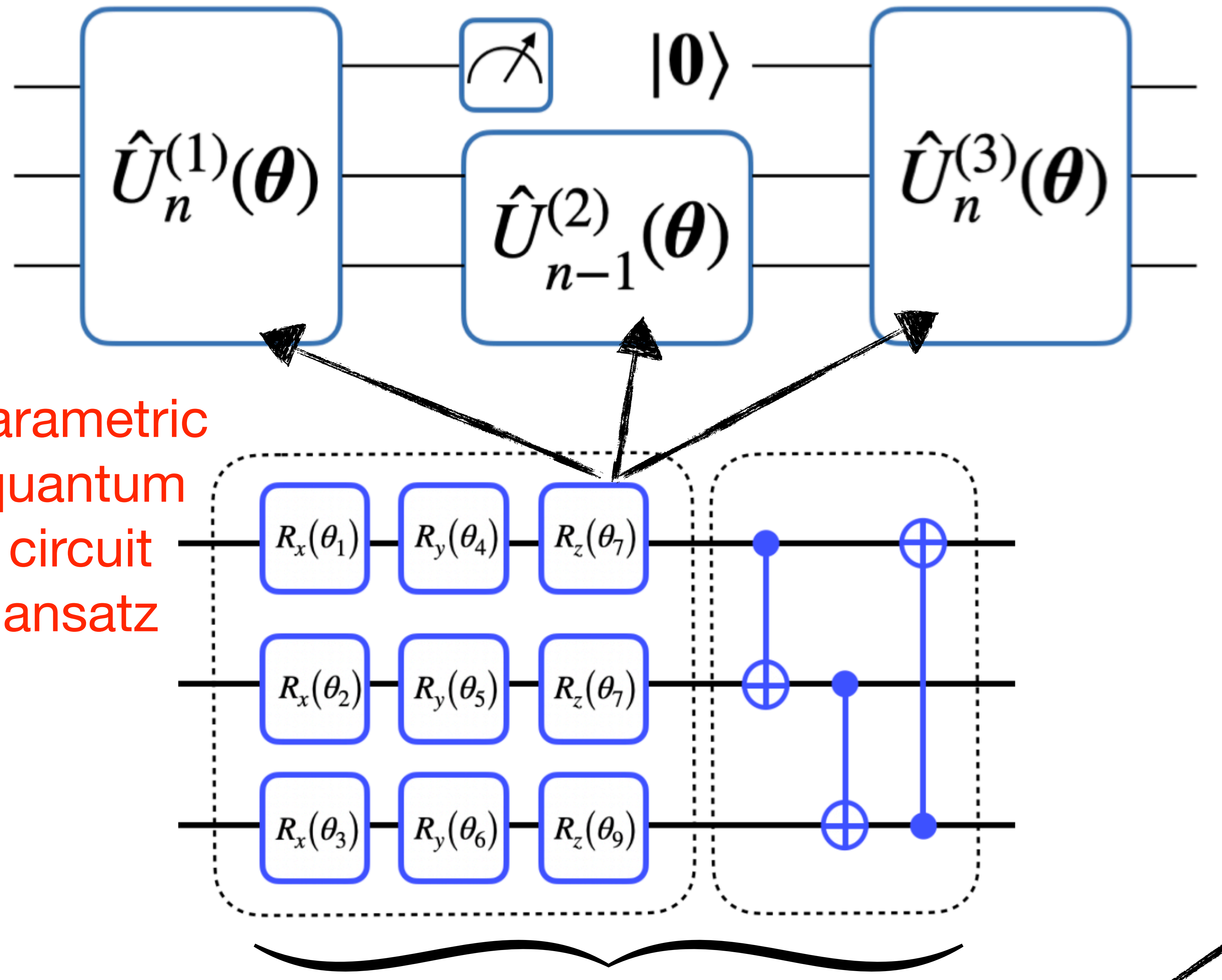
PDM are incremental updates where the assembly of the whole gives us an encoder-decoder structure, and in which the transition from one state to another is realized by a denoiser

- today at the core of many AI applications: image generation (ex. text-conditional image generators like DALL-E, Stable Diffusion, …), image denoising, inpainting, super-resolution,

GENERATIVE QML: QUANTUM DIFFUSION MODEL

- Quantum Diffusion Models: data points encoded into quantum states. Markov chain implemented by a quantum circuit acting as a denoiser
- can be used in a full quantum or in an hybrid mode, where the quantum circuit is trained in the latent space of a classical AE
- conditioning achieved by adding ancillary qubits to encode labels

Quantum Denoiser



parametric quantum circuit ansatz

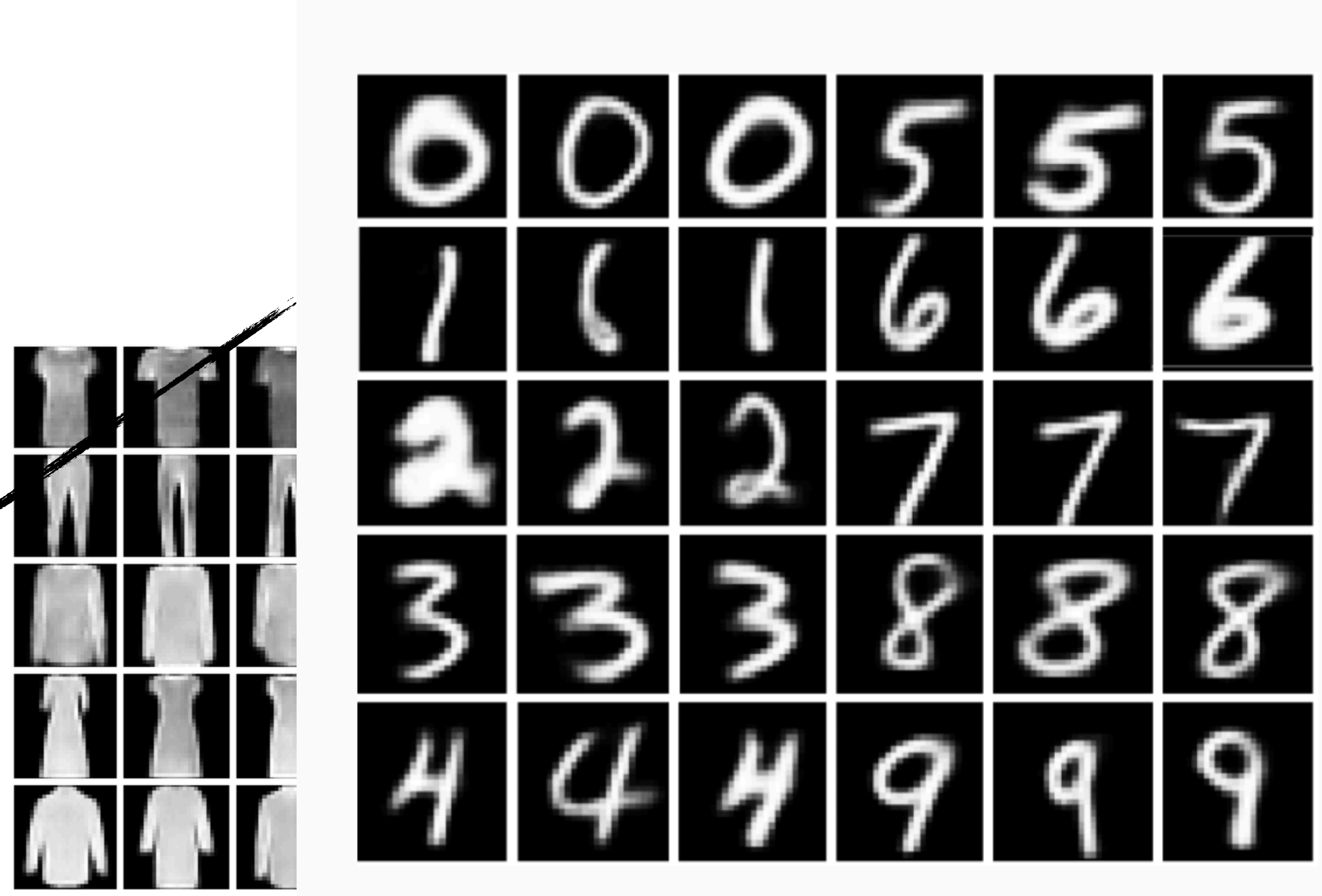
xL-layers

$$P(\theta, t)\,|\mathbf{x}_t\rangle = |\mathbf{x}_{t-1}\rangle \Rightarrow$$

$$P(\theta,1)\cdots P(\theta,T)\;|\mathbf{x}_T\rangle = |\mathbf{x}_0\rangle$$

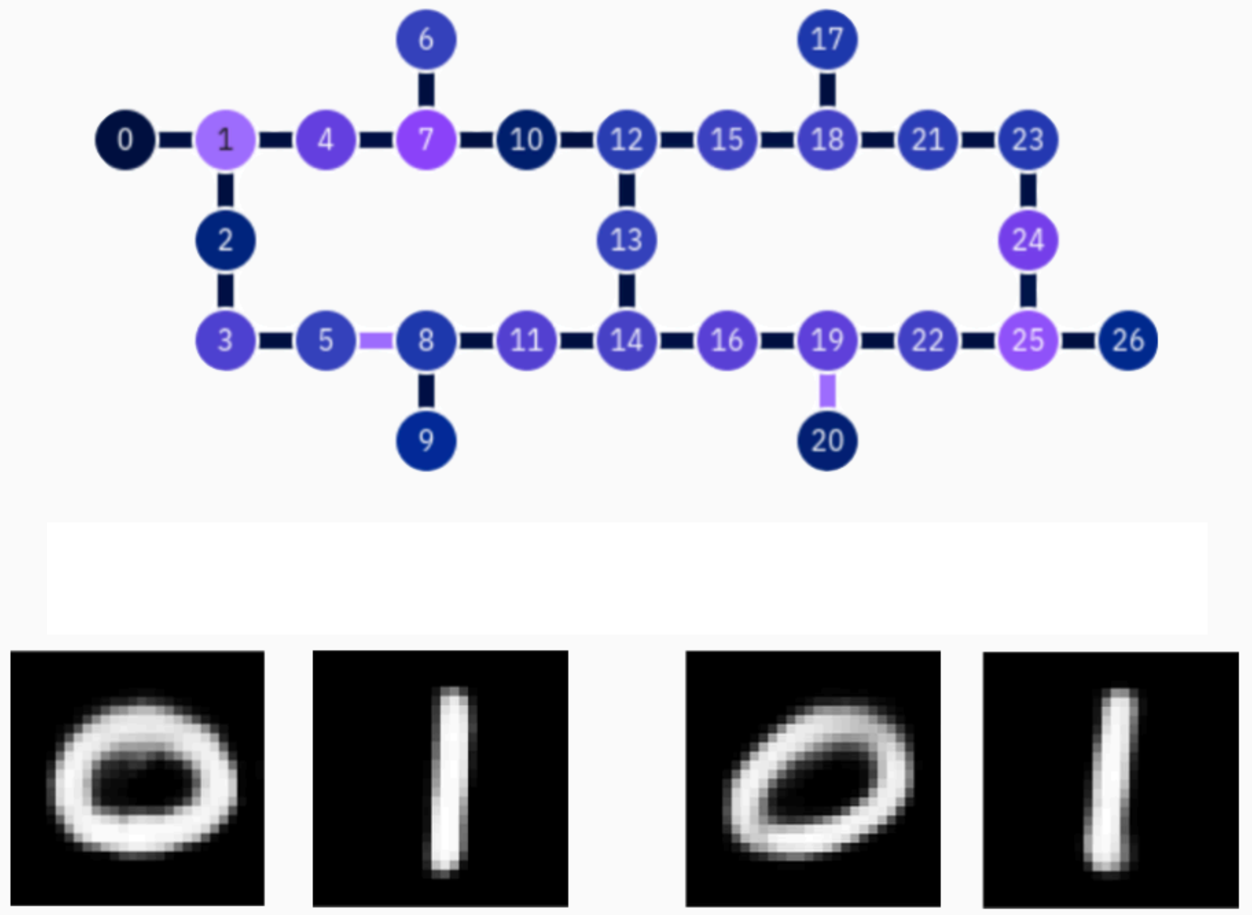
$$Loss = 1 - \mathbb{E}[F]$$ quantum in-fidelity

In quantum Simulation



Tested on quantum hw

IBM_hanoi quantum chip

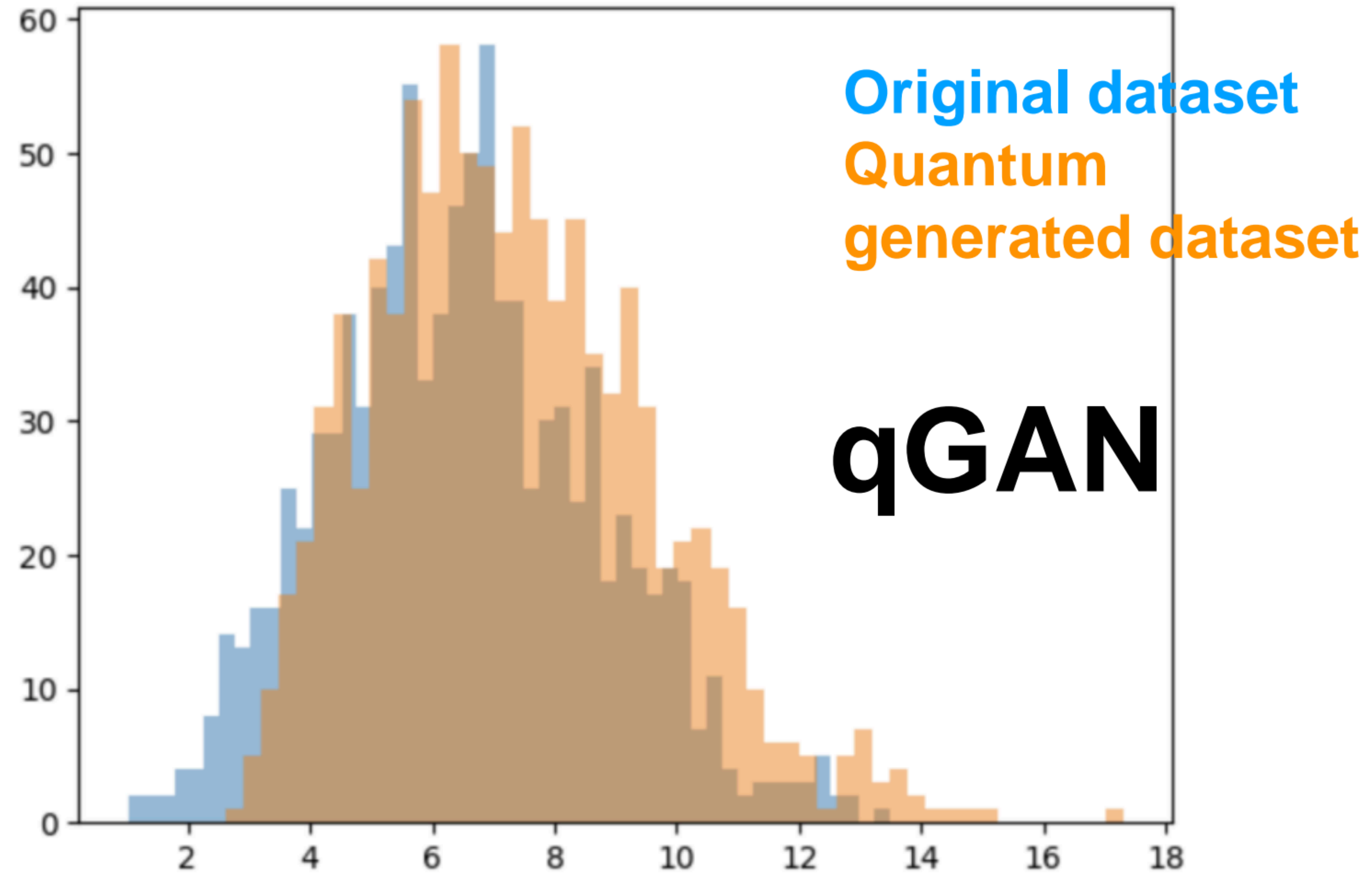


Digit	0	1	2	3	4	5	6	7	8	9
AUC	0.951	0.977	0.983	**0.989**	**0.857**	0.899	0.975	0.928	0.908	0.933

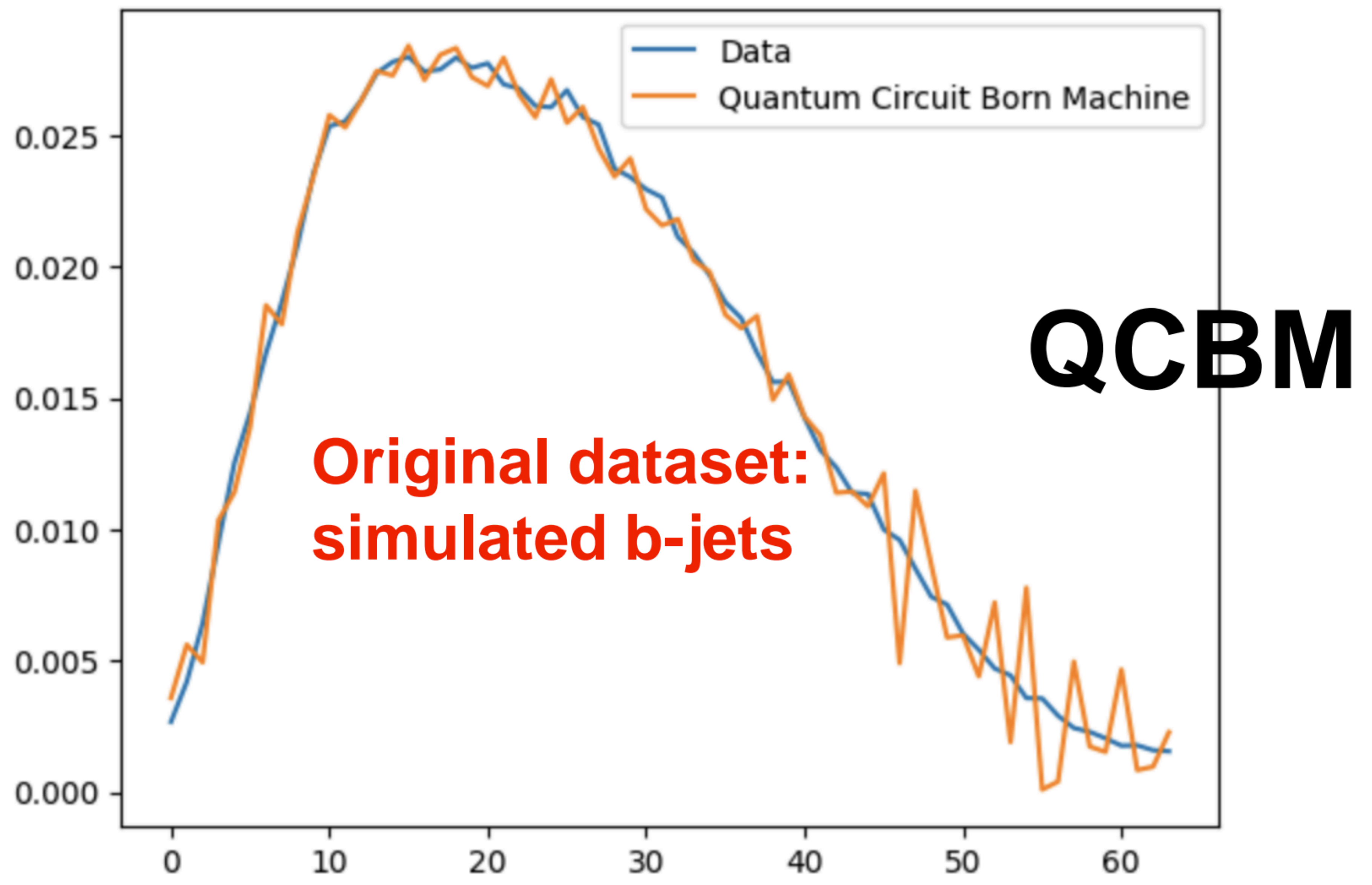
A. Cacioppo et al. arXiv:2311.15444 [quant-ph]

GENERATIVE QML: FIRST APPLICATIONS IN HEP

- Simulation of the LHCb calorimeter module: Quantum-GAN
- Simulation of a b-jet dataset with a Quantum Circuit Born Machine



Total energy measured by the module [arbitrary units]



Measured b-hadron decay distance from PV [mm]

work in progress: dealing with instabilities in the qGAN training and needs for large number of qubits …

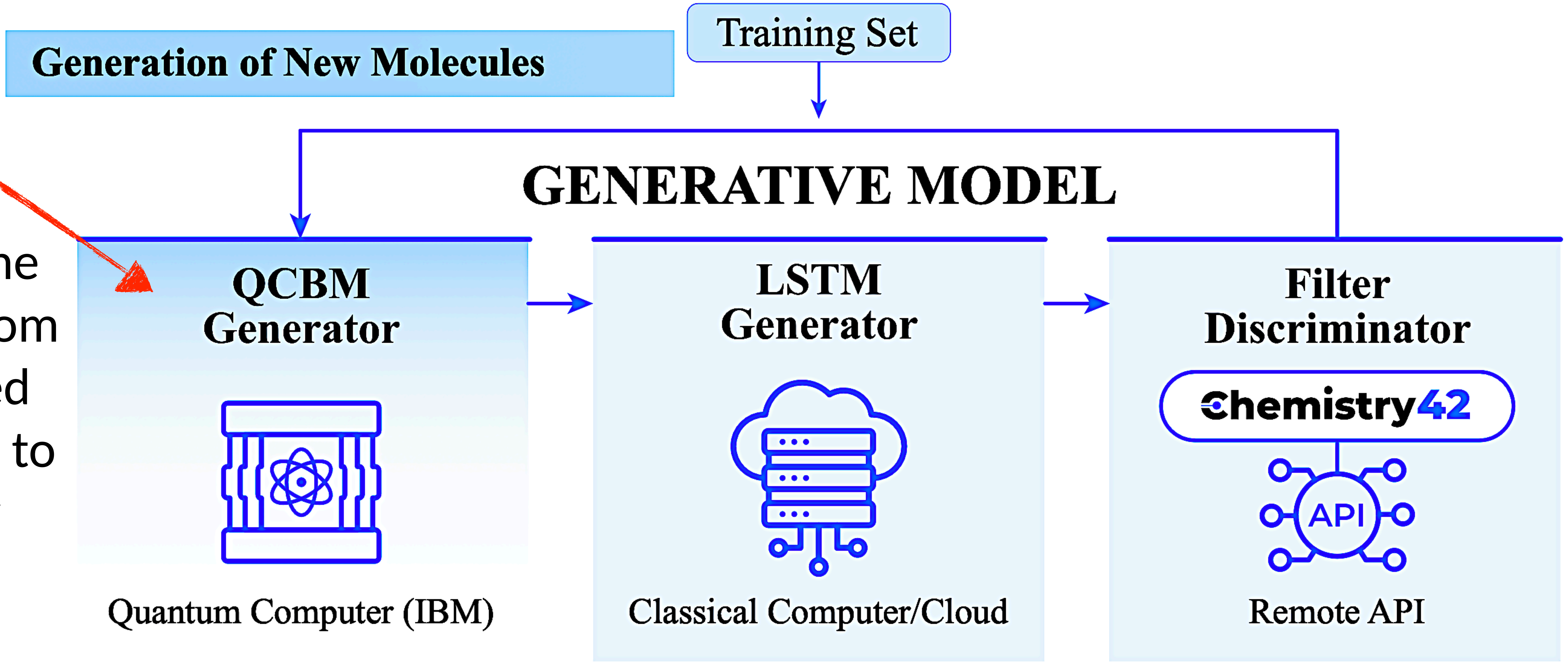
INFN-Padova: A. Gianelle, J.Hagen, D.Lucchesi, L.Sestini, D.Zuliani

GENERATIVE QML: FIRST APPLICATIONS IN DRUGDISCOVERY

- generative model running on quantum hardware that surpasses the best classical models in generating potential drug candidates for cancer. A hybrid classical AI-QuantumML model was used to simulate millions of drug candidates (KRAS inhibitors).

Quantum Circuit Born Machine
(learn and generate high-dimensional and complex probability distribution)

- The two molecules generated by the model were found to be distinct from existing KRAS inhibitors and showed superior binding affinity compared to the molecules generated by purely classical models.



- an indication of how quantum computing and AI can already integrate to provide innovative state-of-the-art solutions

M.G. Vakili et al, arXiv:2402.08210 [quant-ph]

THE ROAD AHEAD (CONCLUSION)

- Quantum computing may offer great opportunities for researcher in INFN:
  - exciting field supported in the public and private sectors
  - a lot of space for original ideas and new algorithms yet to be discovered

- Many questions need to be answered:
  - what are the really promising applications (in our field, and outside)?
  - how we benchmark performances?
  - how to cope with classical data encoding/reduction?
  - QML trainability?
  - …

- quantum advantage in real-word applications will require a new generation of quantum computers and algorithms in terms of size, fault tolerance, connectivity and quantum gates implementation, but already today we are entering the quantum utility regime …

SOME RECENT PROMISING RESULTS …

[Submitted on 19 Sep 2024]

Hardware-efficient quantum error correction using concatenated bosonic qubits

Harald Putterman, Kyungjoo Noh, Connor T. Hann, Gregory S. MacCabe, Shahriar Aghaeimeibodi, Rishi N. Patel, Menyoung Lee, William M. Jones, Hesam Moradinejad, Roberto Rodriguez, Neha Mahuli, Jefferson Rose, J
Arriola, James Barnett, Przemyslaw Bienia
Cosmic, Ana Valdes Curiel, Erik Davis, La
Michael T. Fang, Yawen Fang, Matthew J.
Justin Hand, Yuan He, Mike Hernandez, D
Karabalin, Peter J. Karalekas, Andrew J. K
Guillaume Marcaud, Gavin McCabe, Cody
Pagdilao, Nicola Pancotti, Ashley Panduro
Resnick, Alex Retzker, Omar A. Reyna, M

AWS Center for QC @ Caltech: arXiv:2409.13025

Landmark IBM error correction paper published on the cover of Nature

IBM has created a quantum error-correcting code about 10 times more efficient than prior methods — a milestone in quantum computing research.

https://www.nature.com/articles/s41586-024-07107-7

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NEWS | 09 October 2024

Google uncovers how quantum computers can beat today's best supercomputers

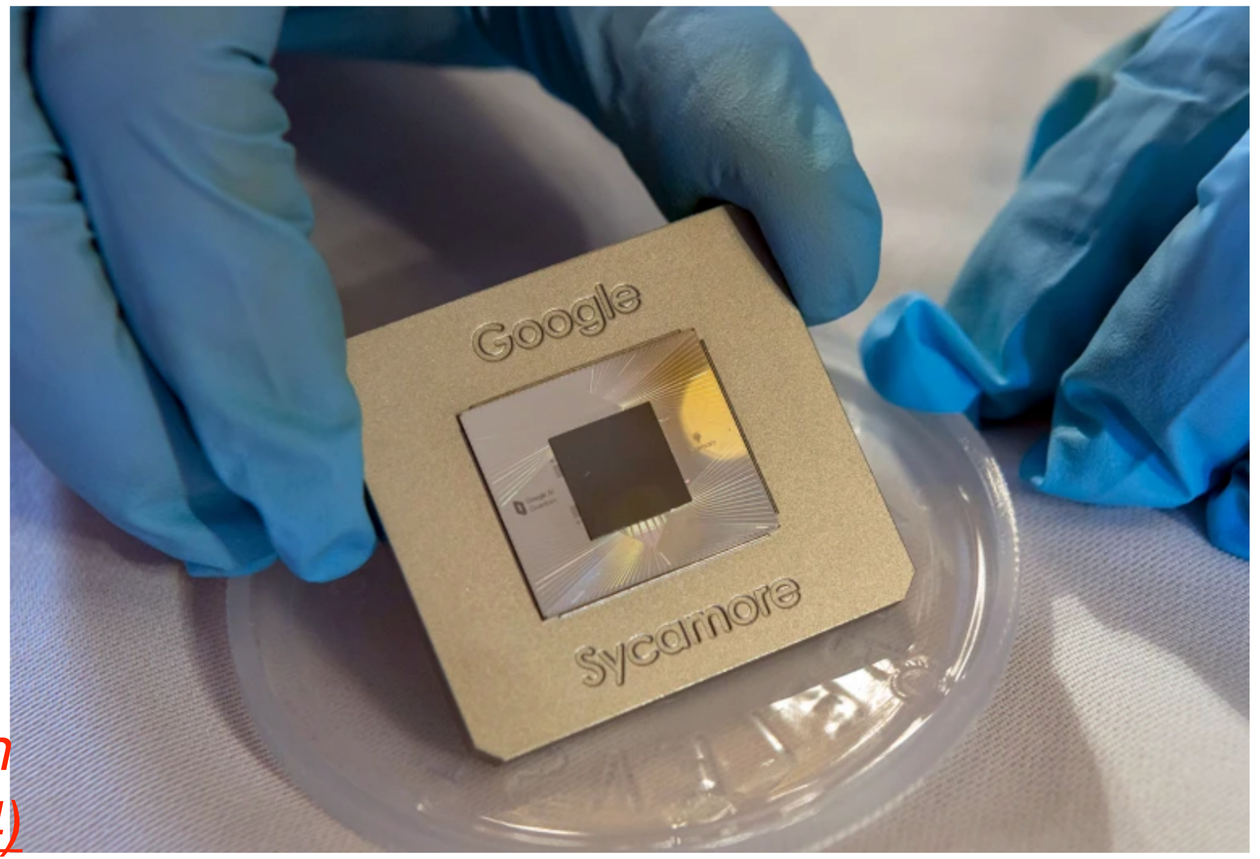
Quantum machines have a noise threshold past which classical machines cannot best them, researchers have learnt.

By Dan Garisto

An in-principle super-polynomial quantum advantage for approximating combinatorial optimization problems via computational learning theory

NIKLAS PIRNAY, VINCENT ULITZSCH, FREDERIK WILDE, JENS EISERT, AND JEAN-PIERRE SEIFERT Authors Info & Affiliations

SCIENCE ADVANCES • 15 Mar 2024 • Vol 10, Issue 11 • DOI: 10.1126/sciadv.adj5170



N.Pirnay et al, Sci.Adv. 2024 (arXiv:2212.08678)

A. Morvan et al, Phase transitions in random circuit sampling. Nature 634, 328–333 (2024)

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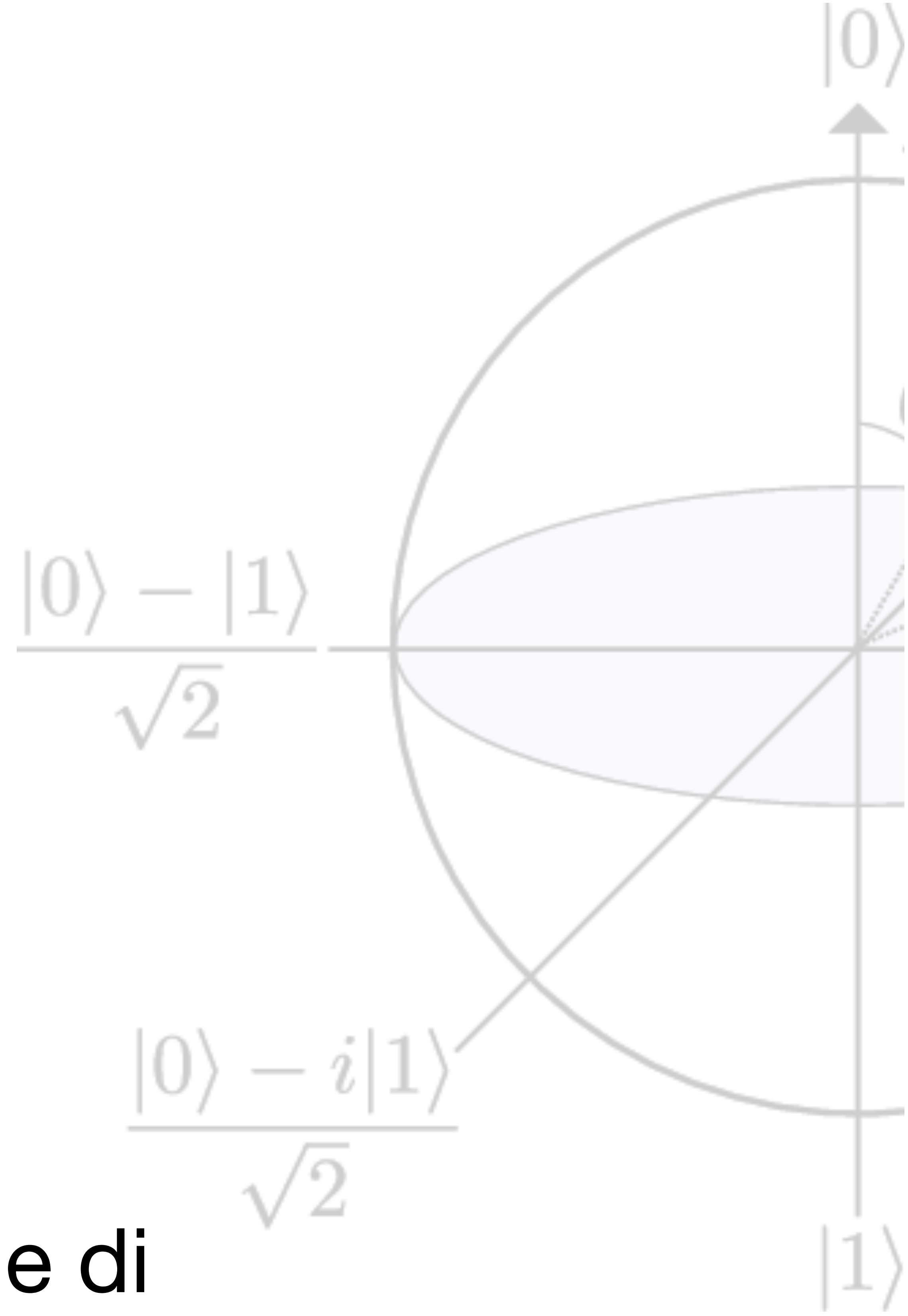

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