Quantum Computing at CERN

QUANTUM
TECHNOLOGY
INITIATIVE

Sofia Vallecorsa

AI and Quantum Research - CERN IT

CERN

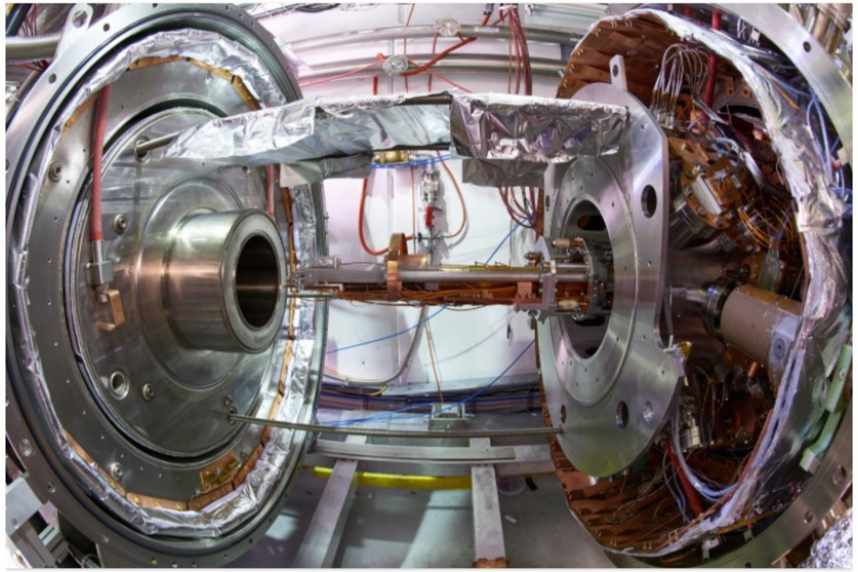
CERN Quantum Technology Initiative

Voir en français

CERN meets quantum technology

The CERN Quantum Technology Initiative will explore the potential of devices harnessing perplexing quantum phenomena such as entanglement to enrich and expand its challenging research programme

30 SEPTEMBER, 2020 | By Matthew Chalmers



The AEgIS 1T antimatter trap stack. CERN's AEgIS experiment is able to explore the multi-particle entangled nature of photons from positronium annihilation, and is one of several examples of existing CERN research with relevance to quantum technologies. (Image: CERN)

What **applications in HEP** can profit from quantum technologies?

High level objectives:

- **Scientific and Technical Development**
- **Community Building**
- **Co-development**
- **Integration** with national and international initiatives

2021 Roadmap: https://doi.org/10.5281/zenodo.5553774

Research Collaborations

Organizations and Projects

QUANTUM FLAGSHIP

QuantHEP

esa

Industry

Google

IBM Q-Net

intel

aws Amazon Braket

Microsoft

Xanadu

Atos

PASQAL

Cambridge Quantum Computing

QILIMANJARO QUANTUM · TECH

Academia, Research Labs and Agencies

DESY.

TUM

lrz

ETH zürich

EPFL

UNIVERSITÉ DE GENÈVE

UK NATIONAL QUANTUM TECHNOLOGIES PROGRAMME

cea

cnrs IN2P3

UAB

INFN Istituto Nazionale di Fisica Nucleare

Università degli Studi di Padova

Università degli Studi dell'Insubria

Università degli Studi di Milano Bicocca

iit Istituto Italiano di Tecnologia

QuTech

BSC

Universidad de Oviedo

Fermilab

Oak Ridge National Laboratory

instituto de telecomunicações

Politechnika Warszawska – Warsaw University of Technology

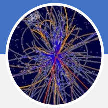
Helsingin yliopisto

Orta Doğu Teknik Üniversitesi – Middle East Technical University

University of Waterloo

ICEPP The University of Tokyo

Scientific Objectives



- Identify **areas of potential quantum advantage** in HEP
- Develop **common libraries of algorithms, methods, tools**; benchmark as technology evolves
- Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

Computing & Algorithms

- Identify and develop techniques for **quantum simulation** in collider physics, QCD, cosmology within and beyond the SM
- Co-develop quantum computing and sensing approaches by providing **theoretical foundations** to the identifications of the areas of interest

Simulation & Theory

- Develop and promote **expertise in quantum sensing** in low- and high-energy physics applications
- Develop quantum sensing approaches with emphasis on **low-energy particle physics measurements**
- Assess **novel technologies and materials** for HEP applications

Sensing, Metrology & Materials

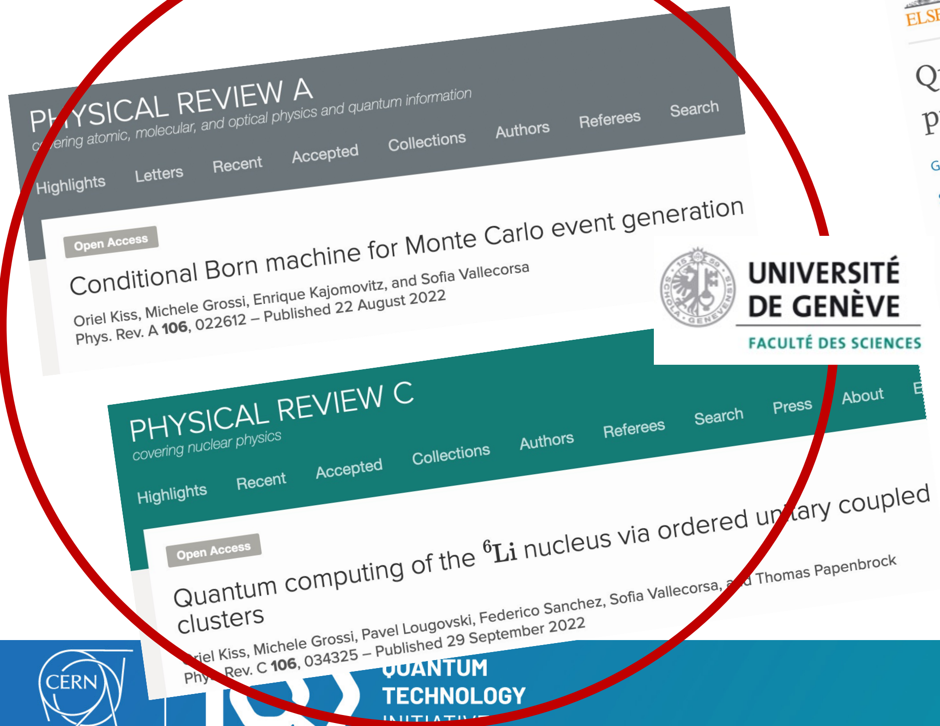
- **Co-develop CERN technologies relevant to quantum infrastructures** (time synch, frequency distribution, lasers)
- Contribute to the **deployment and validation of quantum infrastructures**
- Assess requirements and **impact of quantum communication on computing applications** (security, privacy)

Communications & Networks

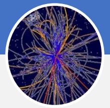
Scientific Production

- **More than 20 projects in all four quantum areas**
- **> 20 papers**

  >10 on peer-reviewed journals
- **More than 30 talks and presentations at conferences and workshops**



Quantum Computing Objectives at CERN

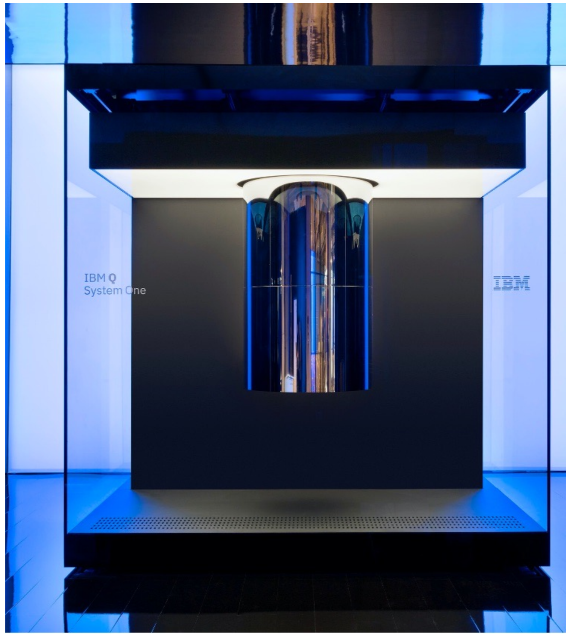


- Identify **areas of potential quantum advantage** in HEP (QML, classification, anomaly detection, tracking)
- Develop **common libraries of algorithms, methods, tools**; benchmark as technology evolves
- Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

Computing & Algorithms

- Baseline for application **prioritisation** and **systematisation**
- **Formal approach** to algorithms, methods, error characterisation and correction
  - **Quantum Machine Learning**
  - **Algorithms beyond QML**
- **Test different hardware**
- Contribute to the development of a **quantum infrastructure**

Quantum Computing Infrastructure and the Quantum Hub



A **quantum computing simulation cluster** with different simulators is available for initial investigations up to 20 qubits

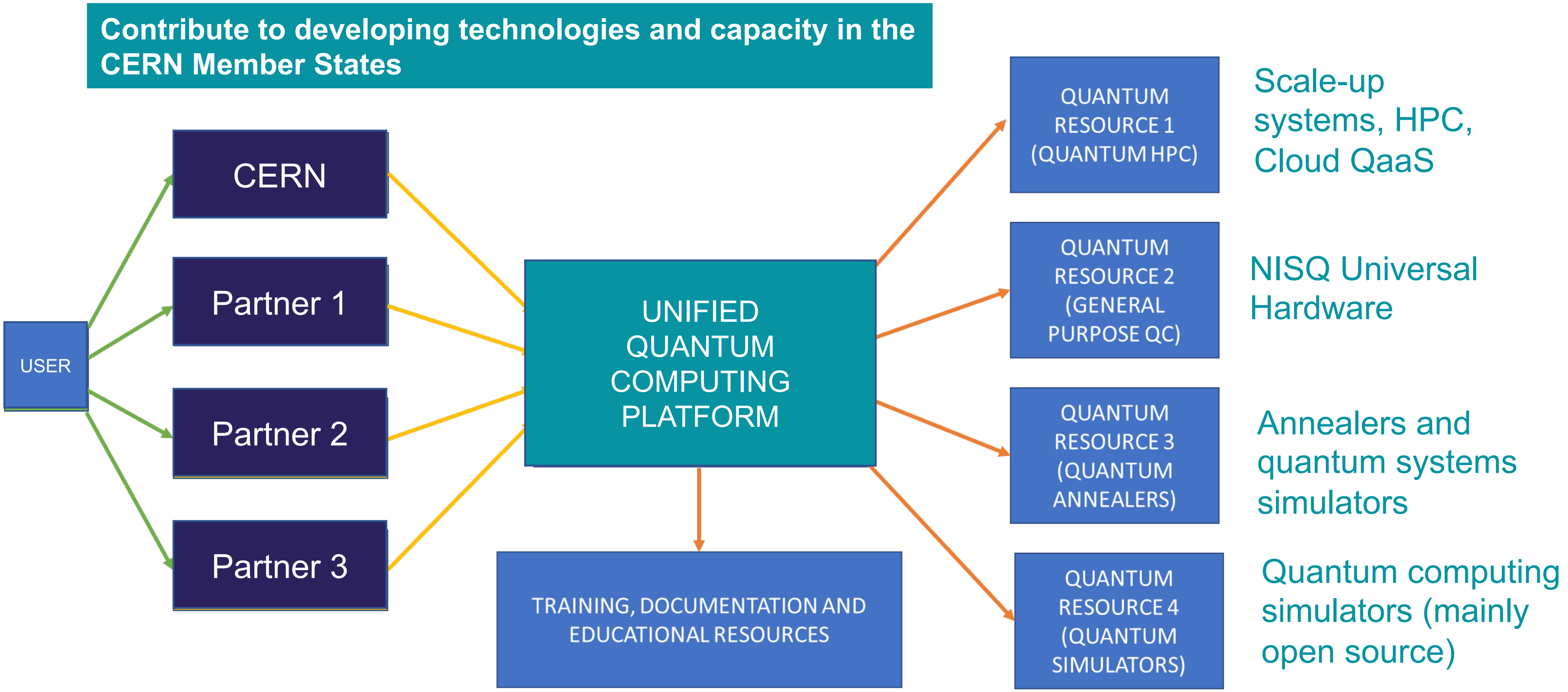
A **collaboration with Intel, TUM and the Munich Leibniz centre** is being set up to investigate applications of quantum simulation on HPC

CERN has acquired an **Atos QLM 34 simulation appliance** for projects requiring more than 30 qubits

CERN is a **Hub Member of the IBM Quantum Network** with quota access to all IBM quantum computers up to the recently released 127-qubit system

Collaborations with **cloud providers** for access to different quantum hardware are being discussed

Quantum Computing Platforms

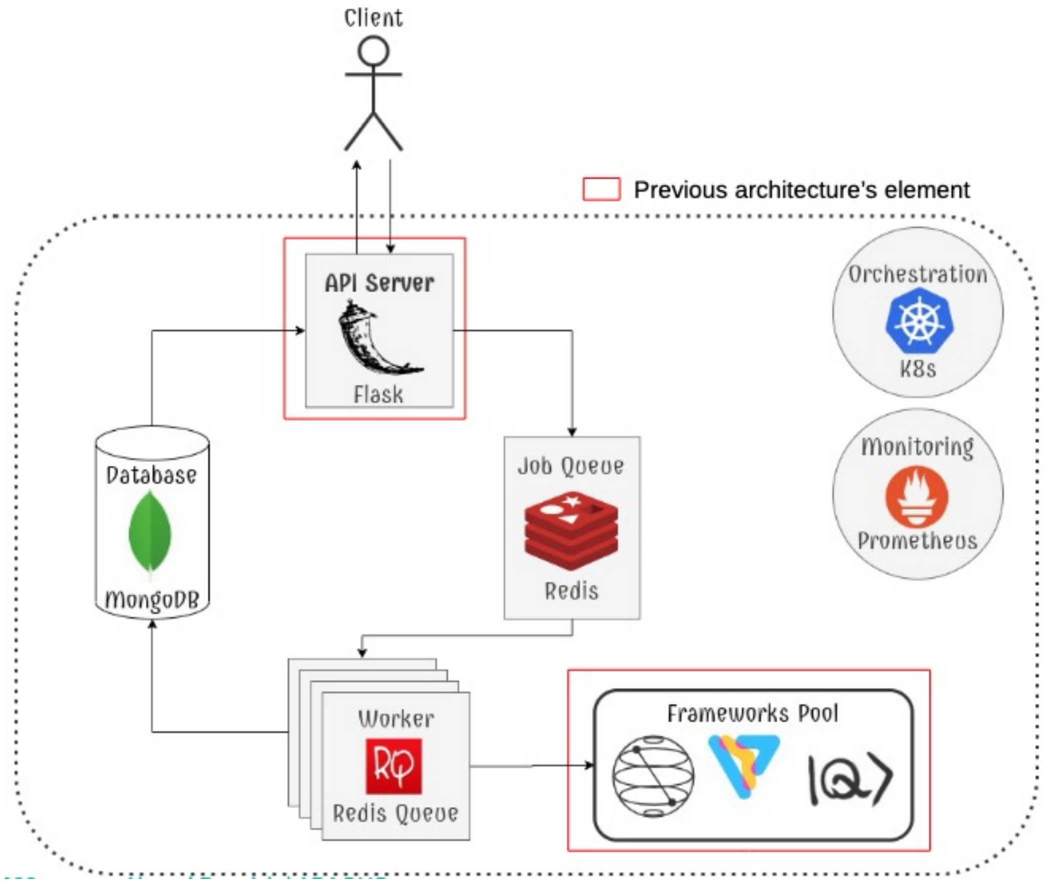


Ahmed Darwish "**ABAQUS**",
https://indico.cern.ch/event/1191490/contributions

ABAQUS

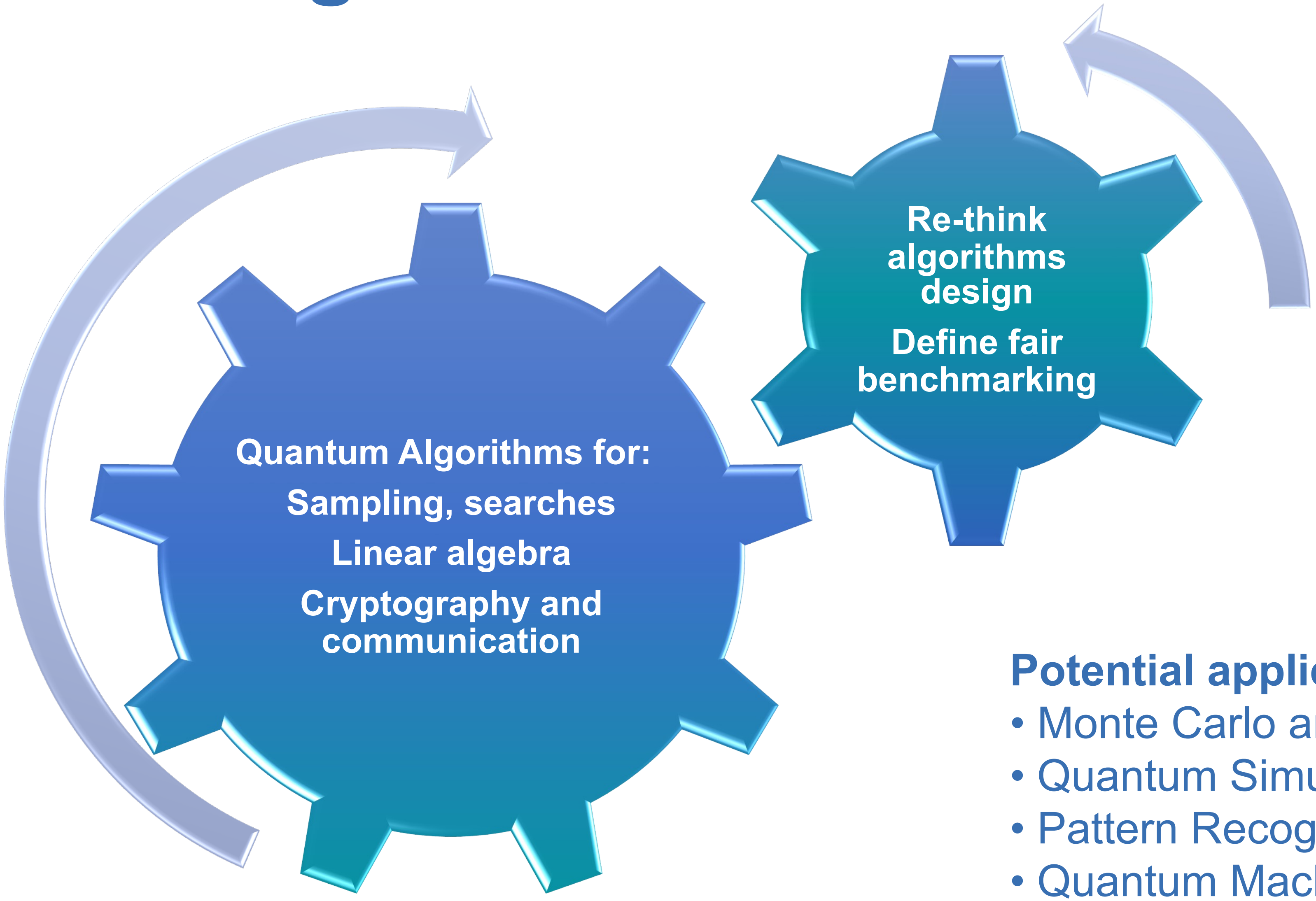
Automated Benchmarking of Algorithms for Quantum Systems

- **Open-source extensible**, **scalable** platform for running benchmarks on simulators (and quantum devices)
- **Community-based**
- Facilitate deployment on clusters (containers based)
- How the system works:
    1. User submits desired benchmarks to server.
    2. Server adds them to a queue of jobs to run.
    3. Workers serve the queue, execute the jobs and store results database.
    4. Server returns results to User.



Quantum Algorithms & Applications

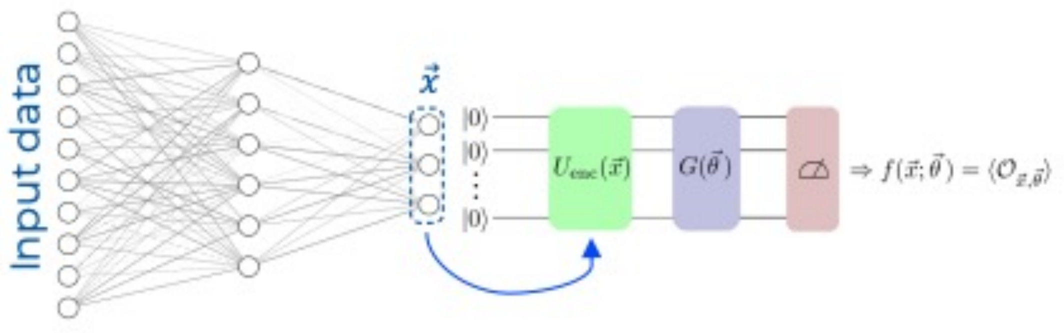
Quantum Algorithms for HEP



Potential applications:

- Monte Carlo and Event Generation
- Quantum Simulation
- Pattern Recognition
- Quantum Machine Learning

Quantum Machine Learning



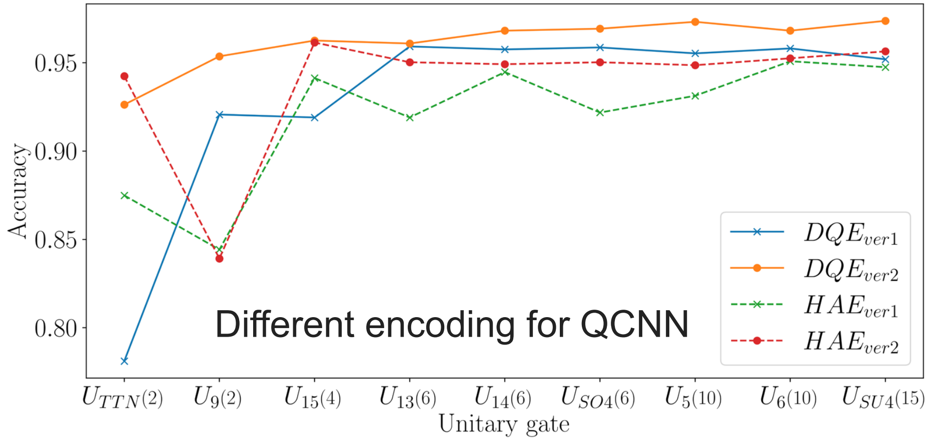
Use **Quantum Computing** to accelerate **ML/DL.**

Quantum circuits are **differentiable** and can be trained **minimizing a data dependent cost function:**

1. **Feature extraction** and **data encoding**
   - How to represent classical data in quantum states?
2. **Model definition** (kernel based or variational)
   - Design wrt data
3. **Optimisation** and **convergence in Hilbert space**
   - **Convergence vs expressivity**
   - Barren plateau and vanishing gradients
   - Classical optimisation via gradient-free or gradient-based optimisers
   - …

Belis, Vasilis, et al. "**Higgs analysis with quantum classifiers**." *EPJ Web of Conferences*. Vol. 251. EDP Sciences, 2021.

Feature selection + Model	AUC
AUC + QSVM	0.66 ± 0.01
PyTorch AE + QSVM	0.62 ± 0.03
AUC + SVM rbf	0.65 ± 0.01
PyTorch AE + SVM rbf	0.62 ± 0.02
KMeans + SVM rbf	0.61 ± 0.02



S.Y. Chang, poster at "**Quantum Tensor Network in Machine Learning**, NeurIPS 2021

Model definition

Variational algorithms

Flexible parametric ansatz: design can leverage data symmetries[1]

Trained using gradient-free or **gradient-based** optimization in a classical loop

Data Embedding $\mathcal{V}_\phi(x)$ can be **learned**

Better generalization[3]

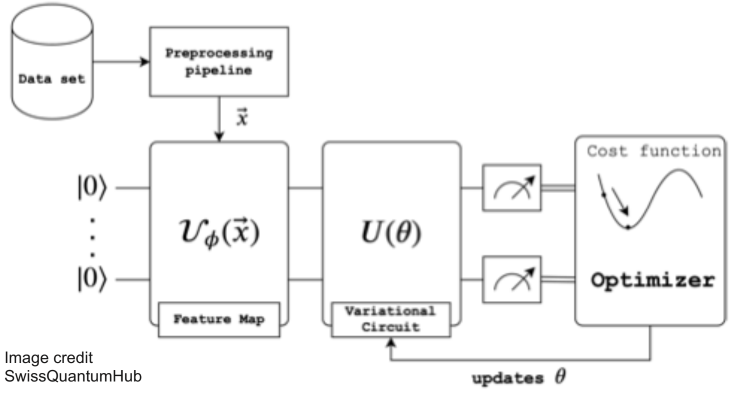


Image credit SwissQuantumHub

Kernel methods

Feature maps as **quantum kernels**

Identify kernel classes that relate to specific data **structures**[2]

Use classical **kernel-based training**

Better accuracy[3]

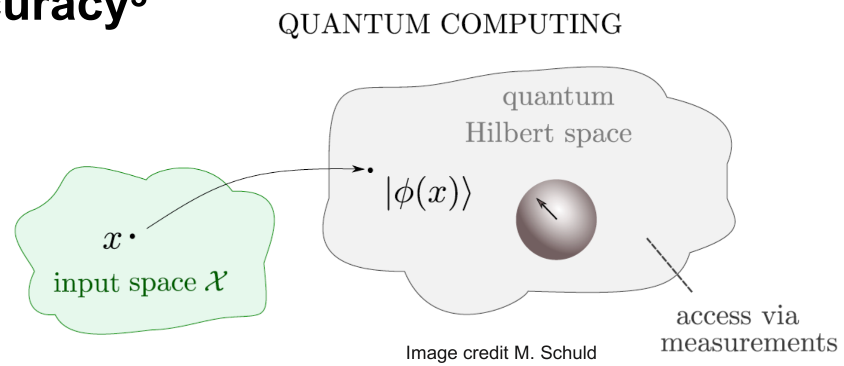


Image credit M. Schuld

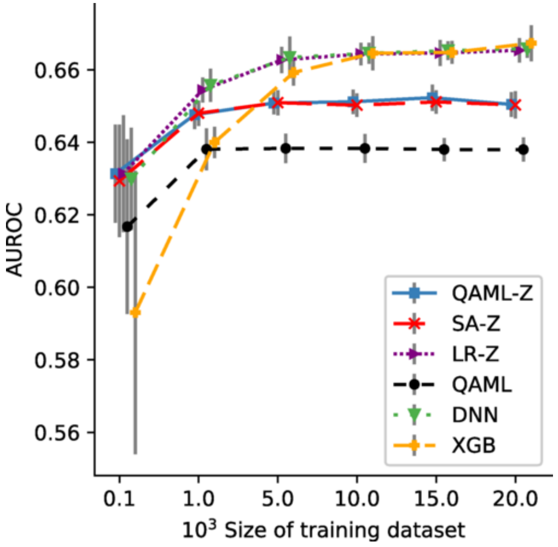
1 Bogatskiy, Alexander, et al. "**Lorentz group equivariant neural network for particle physics**." PMLR, 2020.

2 Glick, Jennifer R., et al. "**Covariant quantum kernels for data with group structure**." *arXiv:2105.03406* (2021).

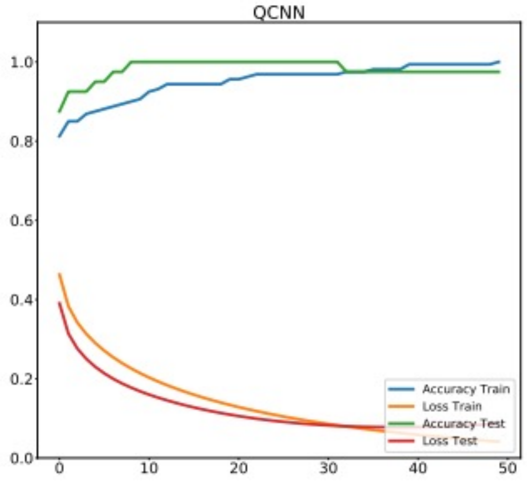
3 Jerbi, Sofiene, et al. "**Quantum machine learning beyond kernel methods**." *arXiv preprint arXiv:2110.13162* (2021).

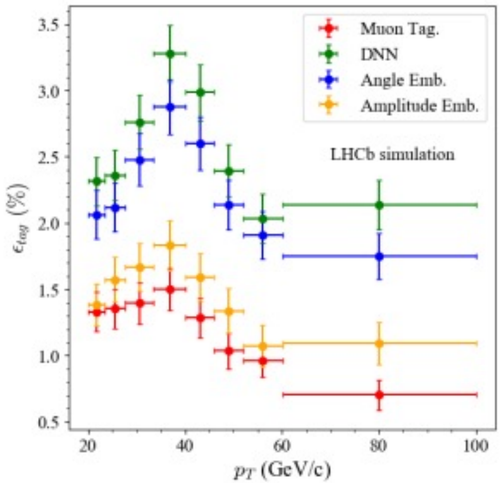
QML in High Energy Physics

Alexander Zlokapa, Alex Mott, Joshua Job, Jean-Roch Vlimant, Daniel Lidar, and Maria Spiropulu. **Quantum adiabatic machine learning by zooming into a region of the energy surface.** Physical Review A, 102:062405, 2020. DOI:10.1103/PhysRevA.102.062405.



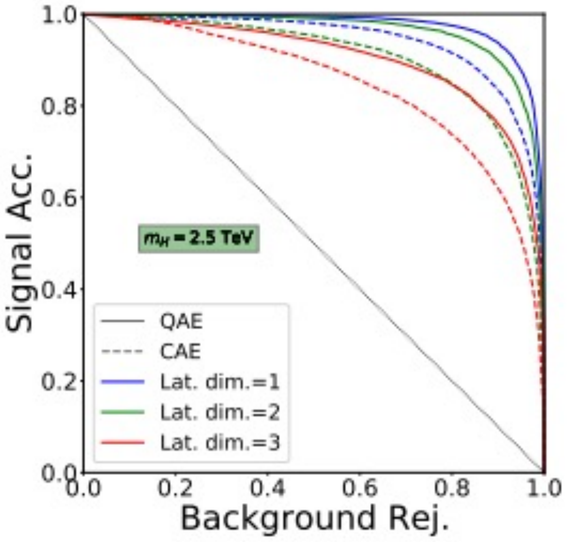
Samuel Yen-Chi Chen, Tzu-Chieh Wei, Chao Zhang, Haiwang Yu, and Shinjae Yoo. **Quantum convolutional neural networks for high energy physics data analysis.** arXiv preprint: 2012.12177, 2020.



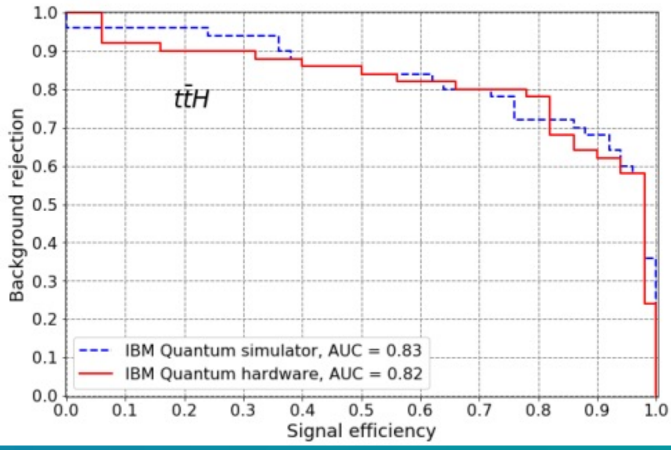


Alessio Gianelle, Patrick Koppenburg, Donatella Lucchesi, Davide Nicotra, Eduardo Rodrigues, Lorenzo Sestini, Jacco de Vries, and Davide Zuliani. **Quantum Machine Learning for b-jet identification.** arXiv:2202.13943, 2022.

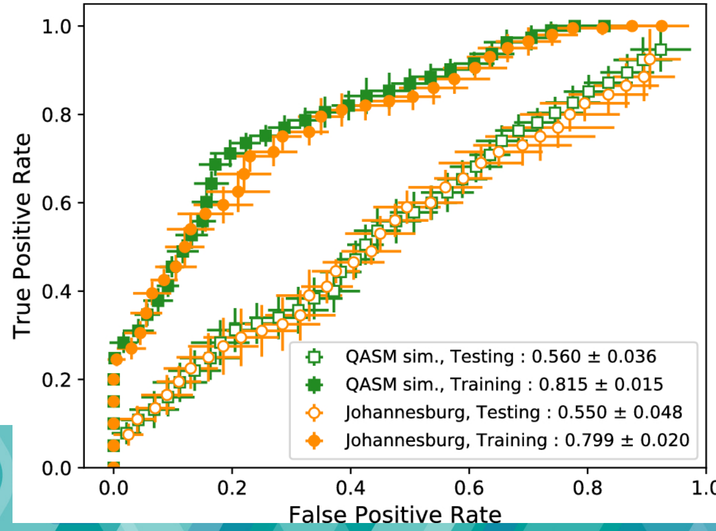
Vishal S Ngairangbam, Michael Spannowsky, and Michihisa Takeuchi. **Anomaly detection in high-energy physics using a quantum autoencoder**. arXiv preprint arXiv:2112.04958, 2021.



Sau Lan Wu, Jay Chan, Wen Guan, Shaojun Sun, Alex Wang, Chen Zhou, Miron Livny, Federico Carminati, Alberto Di Meglio, Andy C Y Li, and et al. **Application of quantum machine learning using the quantum variational classifier method to high energy physics analysis at the lhc on ibm quantum computer simulator and hardware with 10 qubits**. Journal of Physics G: Nuclear and Particle Physics, 48(12):125003, Oct 2021

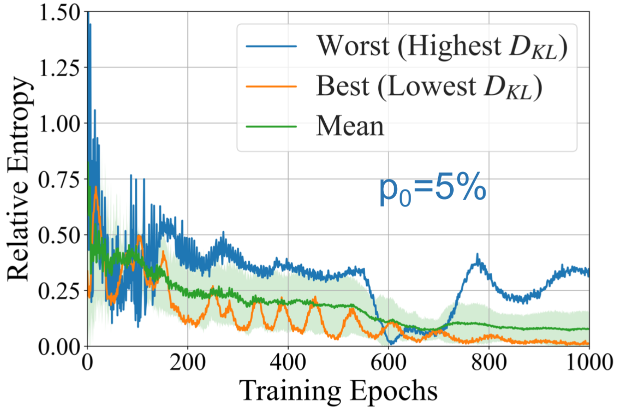


Koji Terashi, Michiru Kaneda, Tomoe Kishimoto, Masahiko Saito, Ryu Sawada, and Junichi Tanaka. **Event classification with quantum machine learning in 20 high-energy physics**. Computing and Software for Big Science, 5(1), January 2021.

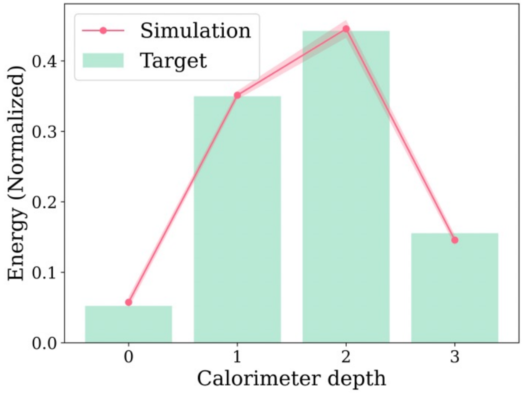


QML at CERN

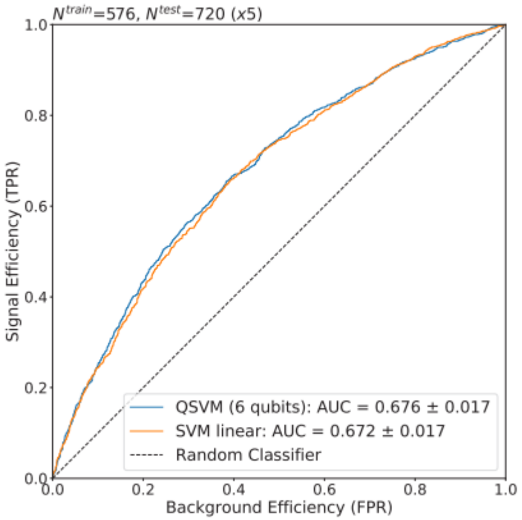
Borras, Kerstin, et al. "**Impact of quantum noise on the training of quantum Generative Adversarial Networks**." *arXiv preprint arXiv:2203.01007* (2022).



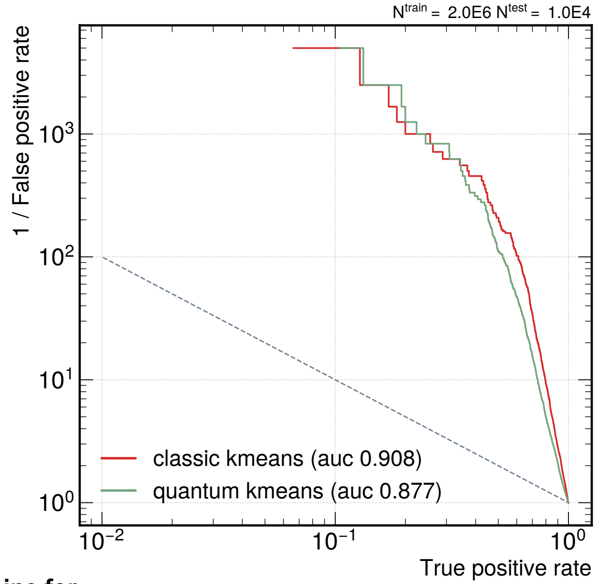
Chang S.Y. *et al.,* **Running the Dual-PQC GAN on Noisy Simulators and Real Quantum Hardware**, QTML2021, ACAT21



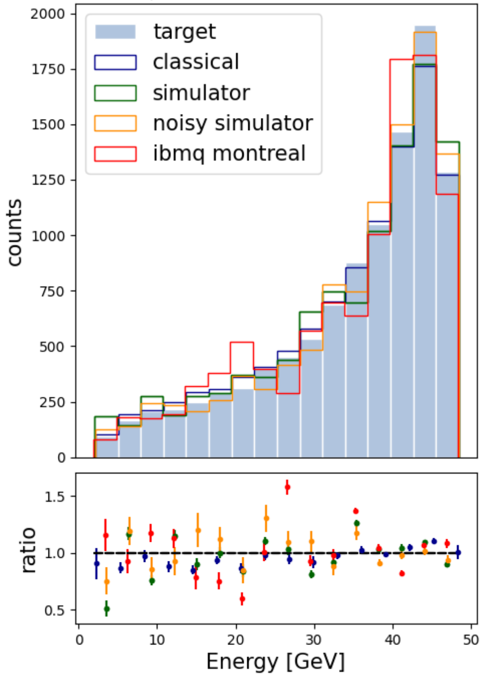
Vasilis Belis, Samuel González-Castillo, Christina Reissel, Sofia Vallecorsa, Elías F. Combarro, Günther Dissertori, and Florentin Reiter. **Higgs analysis with quantum classifi**ers. EPJ Web of Conferences, 251:03070, 2021



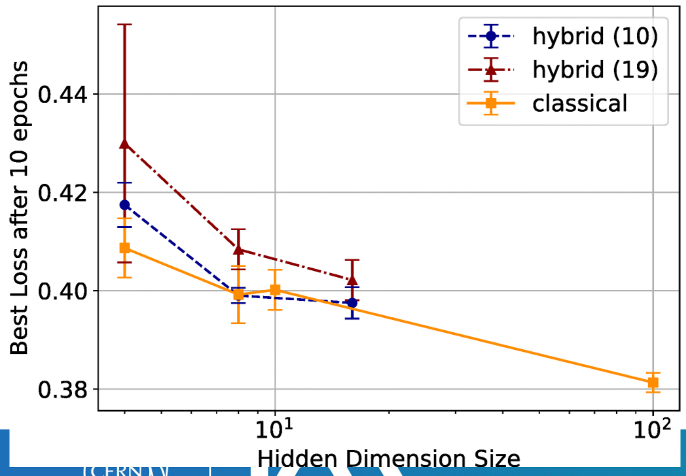
Kinga Wozniak, **Unsupervised clsutering for a Randall–Sundrum Graviton at 3.5TeV narrow resonance, 5th IML workshop, May 2022**



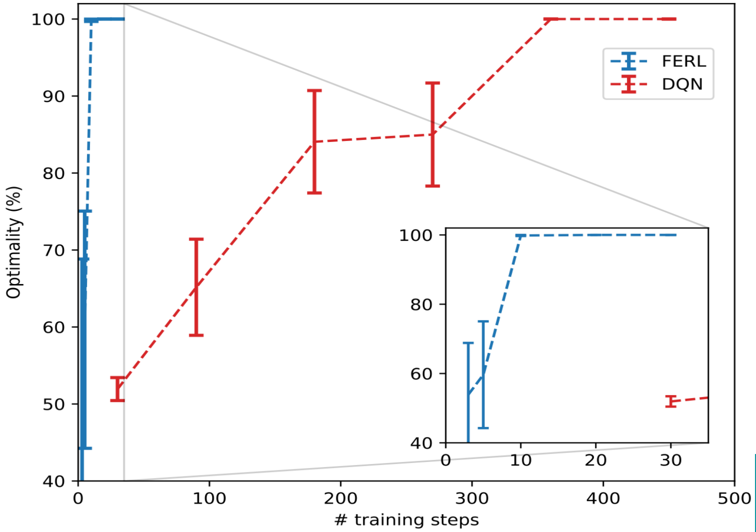
O. Kiss, **Quantum Born Machine for event generation**, ACAT2021



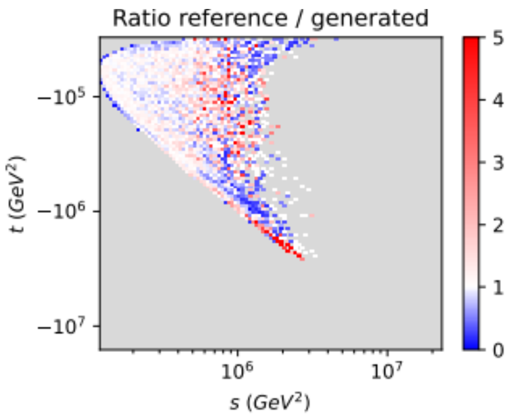
Tüysüz, Cenk, et al. "**Hybrid quantum classical graph neural networks for particle track reconstruction**." *Quantum Machine Intelligence* 3.2 (2021): 1-20.



M. Shenk, V. Kain, **Quantum Reinformcement Learning**, BQiT 2021, 2022 CERN openlab Tech Workshop



Bravo-Prieto, Carlos, et al. "**Style-based quantum generative adversarial networks for Monte Carlo events**." *arXiv preprint arXiv:2110.06933* (2021).



Our results so far..

- ⊕ Multiple QML prototypes for different applications
- ⊕ Increasing level of precision
- ⊕ Robustness against noise
- ⊕ Same initial hints at advantages

- ⊖ Scale is still a problem on current quantum hardware
- ⊖ Complex data pre-processing
- ⊖ Data discretization?

Representation Learning

- **Generative Models** learn the **representation** of an intractable probability distribution, p_{data} defined on $\mathbb{R}^n$
- Don't define explicit mathematical expression of $p_{model} \approx p_{data}$
- Trained as **generators** $\mathcal{g}: \mathbb{R}^m \rightarrow \mathbb{R}^n$ that map samples from a tractable distribution $\mathcal{Z}$ supported in $\mathbb{R}^m$ to points in $\mathbb{R}^n$
- **Different tasks**: data compression, anomaly detection, event generation, …
- **Multiple flavors**: Boltzman Machines, (Variational) Auto-Encoder, Generative Adversarial Networks, …

Brown, Tom, et al. "**Language models are few-shot learners**." Advances in neural information processing systems 33 (2020): 1877-1901.

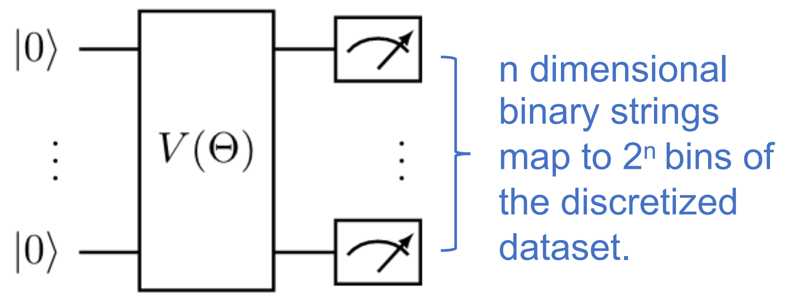
Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	3.0×10^{-4}
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

Quantum Generative Models

Delgado and Hamilton, arXiv:2203.03578 (2022)
Zoufal, et al., *npj Quantum Inf* **5**, 103 (2019)
Leadbeater et al., *Entropy* **2021**, *23*, 1281.
Amin, et al. *Physical Review X* 8.2 (2018): 021050.

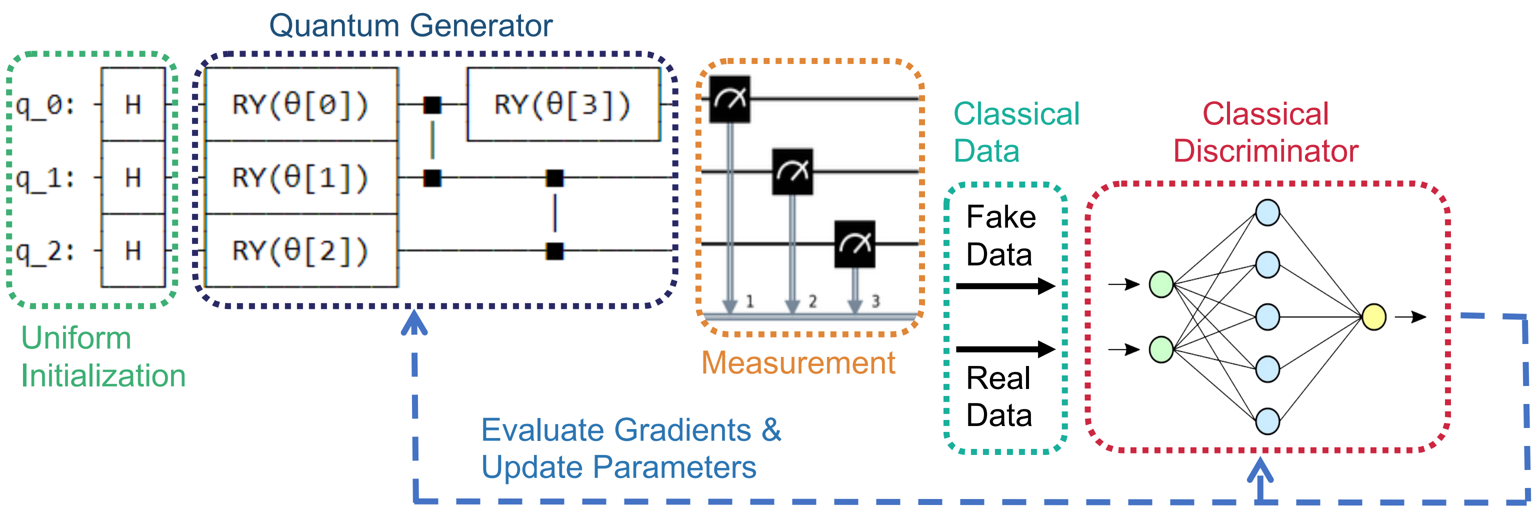
QCBM

Sample variational pure state $|\psi(\theta)\rangle$ by projective measurement through **Born rule**: $\mathbf{p}_{\boldsymbol{\theta}}(\mathbf{x}) = |\langle \mathbf{x}|\boldsymbol{\psi}(\boldsymbol{\theta})\rangle|^2$.



QGAN

Multiple implementations, mostly classical-quantum hybrid



QBM

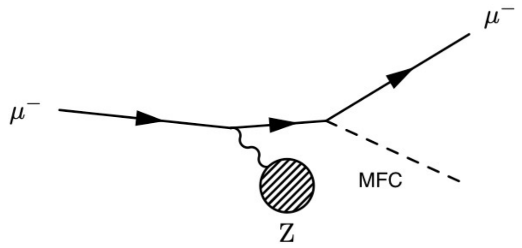
Network of stochastic binary units with a quadratic energy function that follows the Boltzman distribution (Ising Hamiltonian)

$$H = -\sum_a b_a \sigma_a^z - \sum_{a,b} w_{ab} \sigma_a^z \sigma_b^z$$

+ QVAE, general QNN…

QCBM for event generation

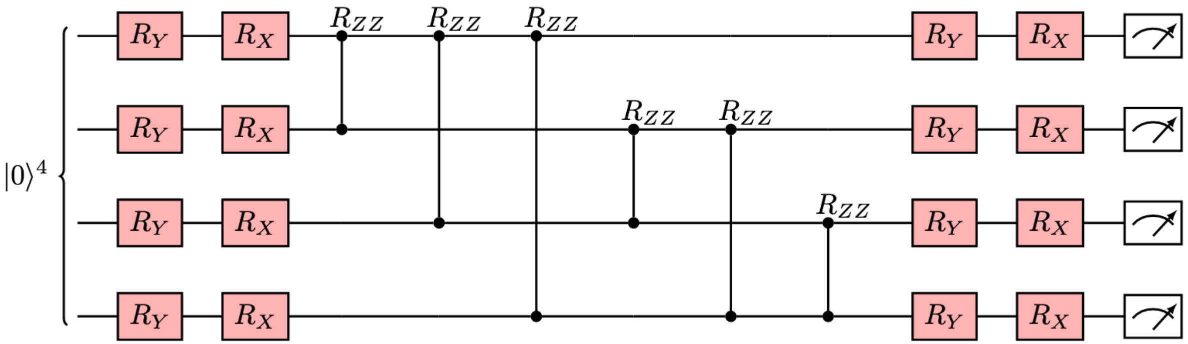
Muon Force Carriers, in muon fixed-target experiments (FASER) or muon interactions in calorimeters (ATLAS)[1].

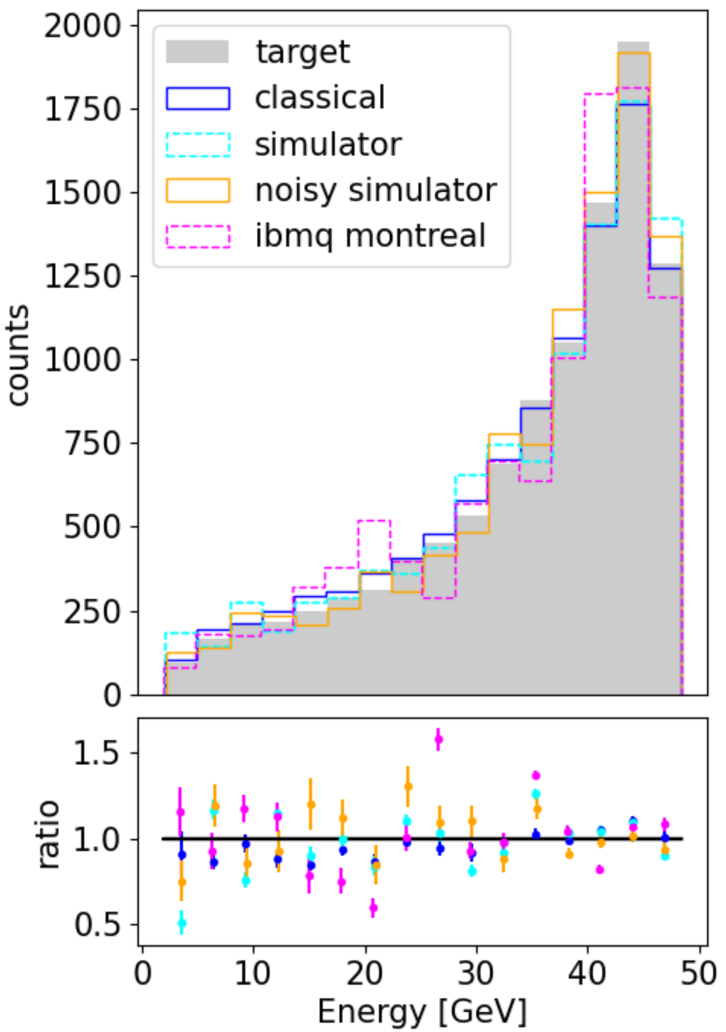


Generate multivariate distribution (E, p_t, η)

Maximum Mean Discrepancy for training

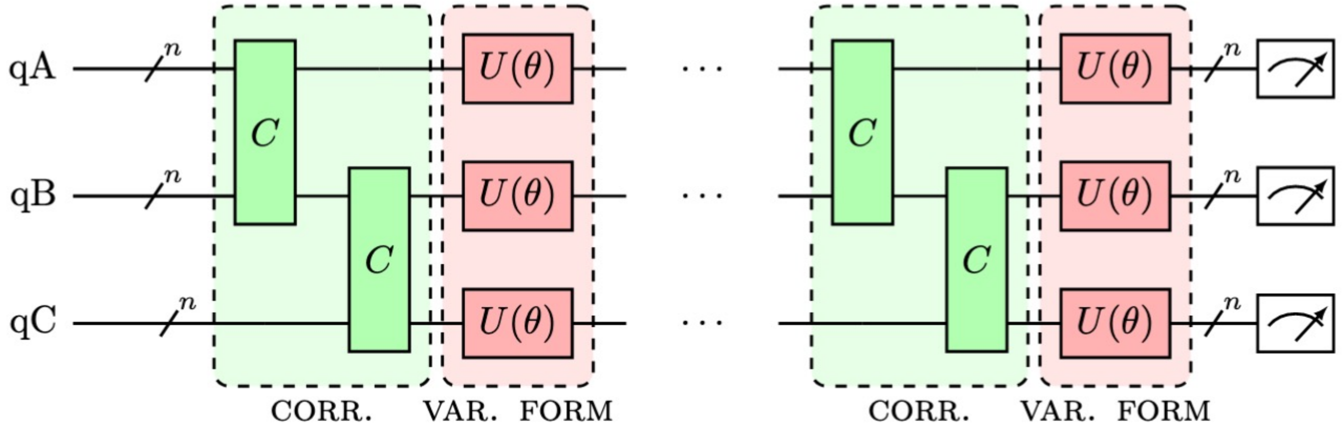
$$\mathrm{MMD(P,Q)} = \mathbb{E}_{\substack{X\sim P\\ Y\sim P}}[K(X,Y)] + \mathbb{E}_{\substack{X\sim Q\\ Y\sim Q}}[K(X,Y)] - 2\mathbb{E}_{\substack{X\sim P\\ Y\sim Q}}[K(X,Y)]$$





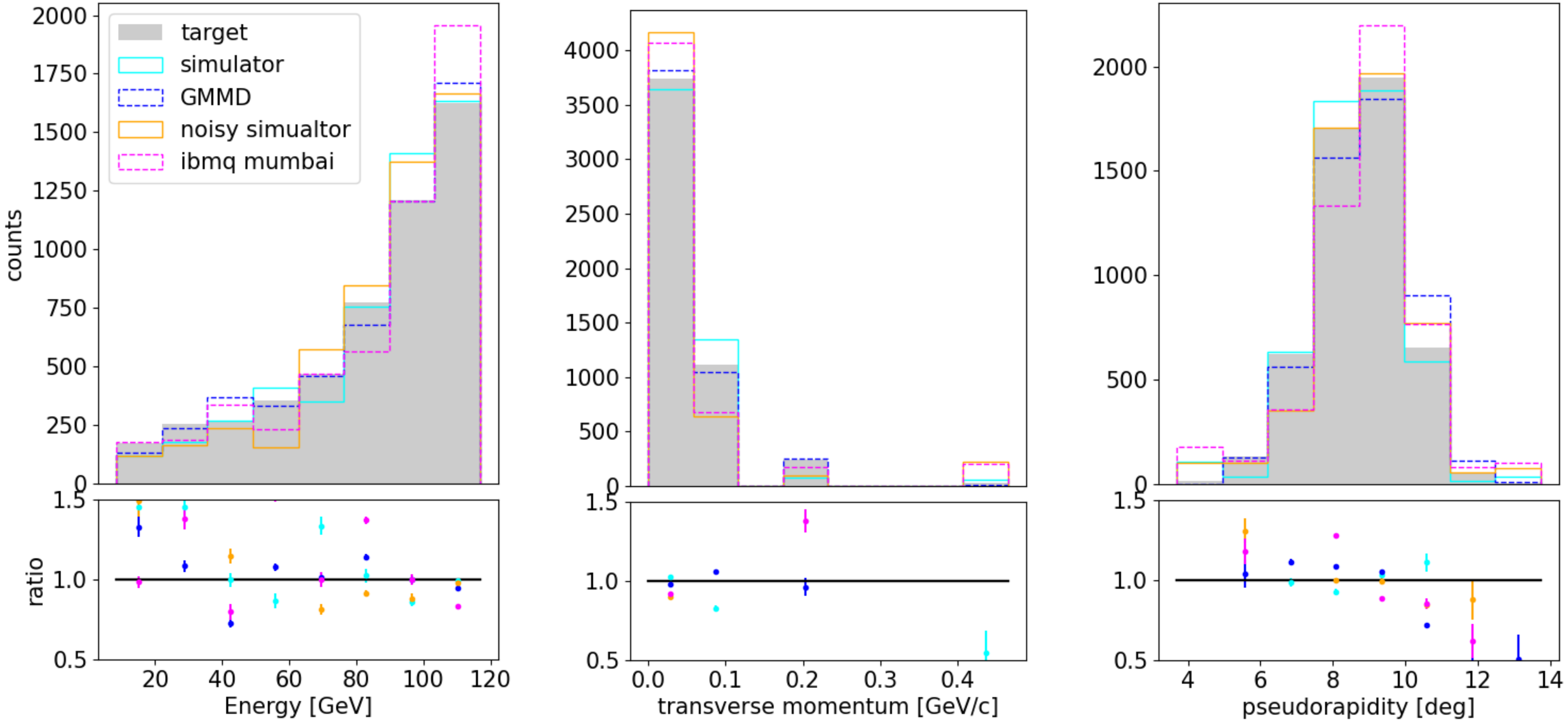
1 Galon, I, Kajamovitz, E et al. "Searching for muonic forces with the ATLAS detector". In: Phys. Rev. D 101, 011701 (2020)

Multivariate probability distribution



Simulation	Noisy simulation	IBMQ Mumbai	Classical
0.12	0.06	0.06	0.01

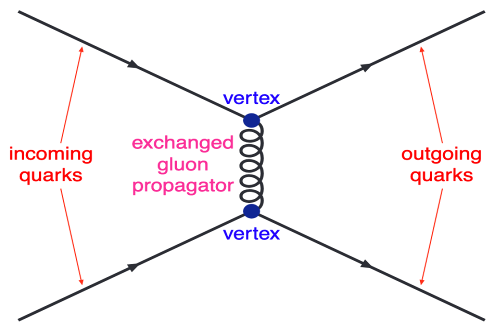
Mean difference between the correlations in the MC and generated samples



+ Implement conditional $\boldsymbol{p(y|x)}$ wrt incoming particle energy E_{in}.

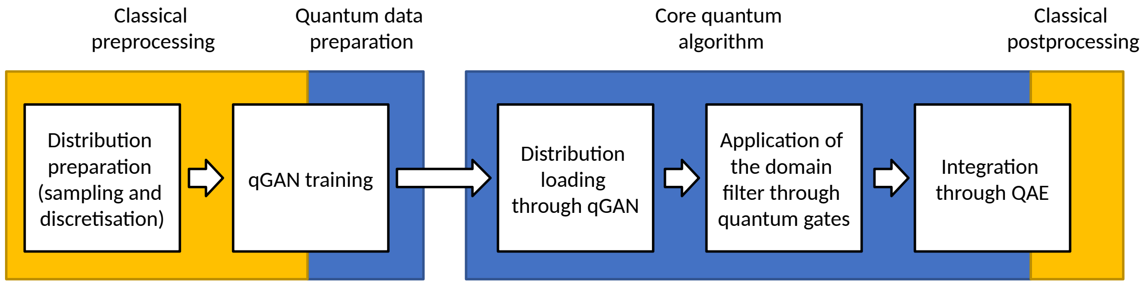
Agliardi, Gabriele, et al. "**Quantum integration of elementary particle processes.**" *arXiv preprint arXiv:2201.01547* (2022)

qGAN as a data loader



Cross section integration using **Quantum Amplitude Estimation**

Focus on electroweak process



phase-space factor

$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

matrix element

phase-space cuts

Data encoding in quantum states affects quality of integration

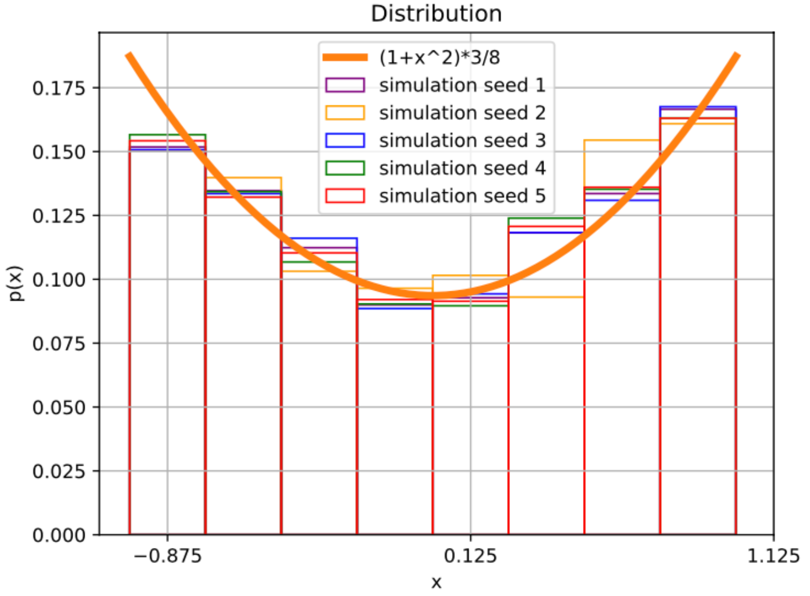
Test **QGAN** for data embedding and compare to direct loading

Test on $1 + x^2$ distribution:

- 10k events, 3 qubits, circular entanglement

$$G(\phi)\,|\psi_{in}\rangle = |g(\phi)\rangle = \sum_{i=0}^{N-1} \sqrt{p_g^i(\phi)}\,|i\rangle$$

Loading	Difference per bin [%] Min.	Max.	Average	σ_x
Direct	$+0.207$	-1.88	1.35	1.80×10^{-3}
qGAN default	$+2.36$	-21.1	8.51	0.0118
qGAN optimised	-0.995	-12.4	4.65	7.00×10^{-3}



qGAN for event generation

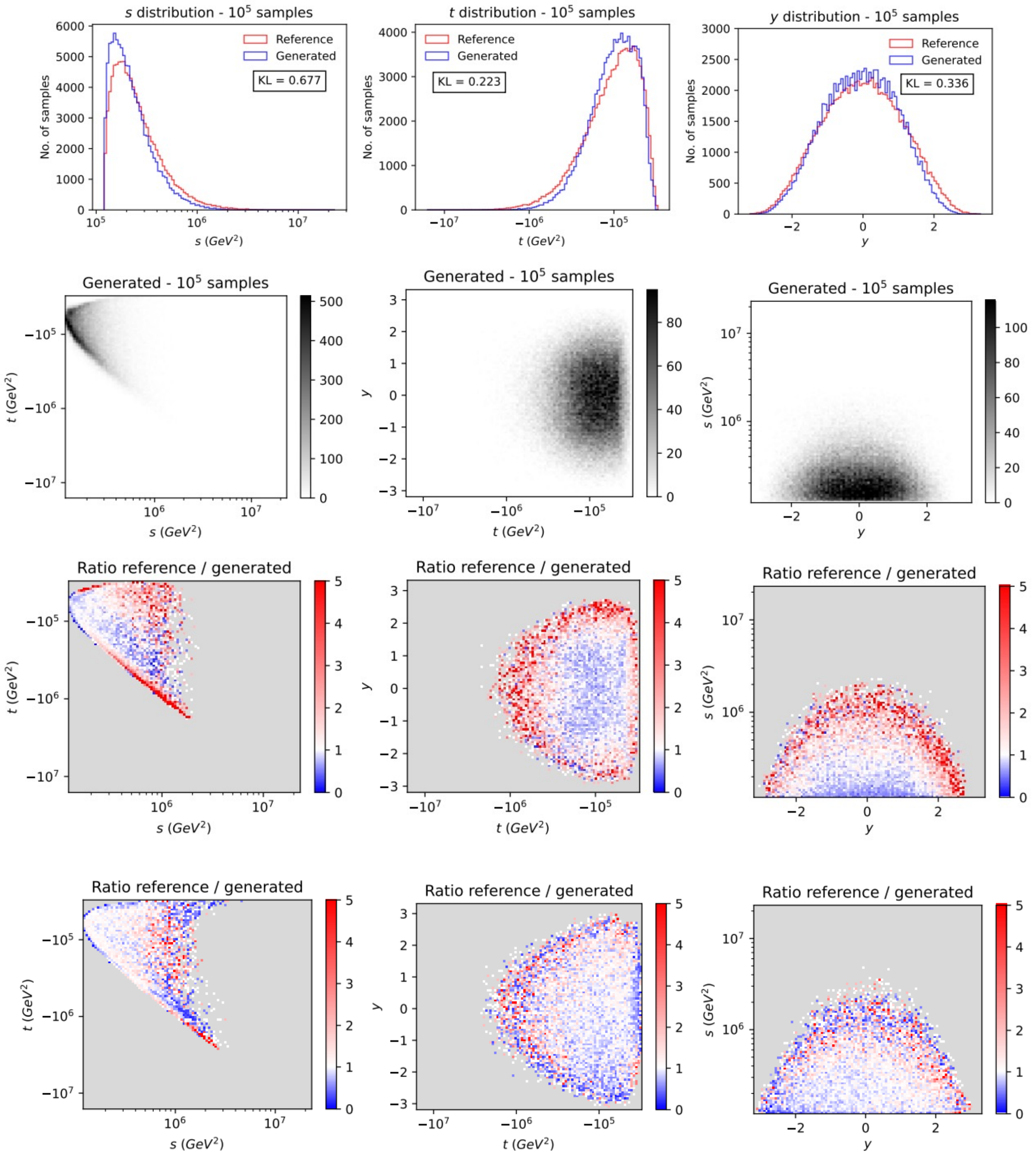
Generate Mandelstam (s,t) + y variables for t-tbar production

Introduce a style-based approach

	$pp \rightarrow t\bar{t}$ **LHC events**
Qubits	3
D_{latent}	5
Layers	2
Epochs	3×10^4
Training set	10^4
Batch size	128
Parameters	62
U_{ent}	2 sequential CR_y gates

IBM Q Santiago

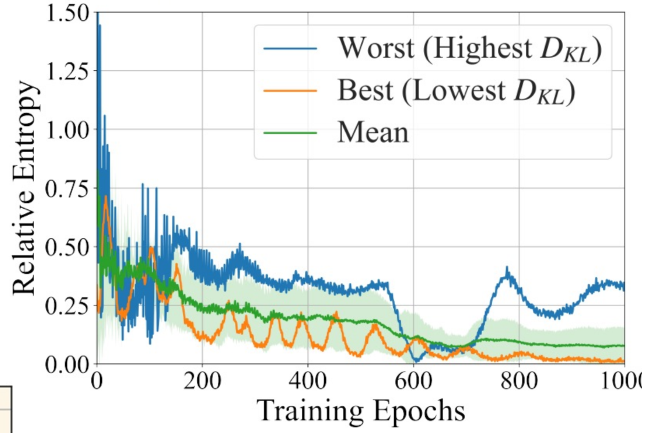
Quantum simulator

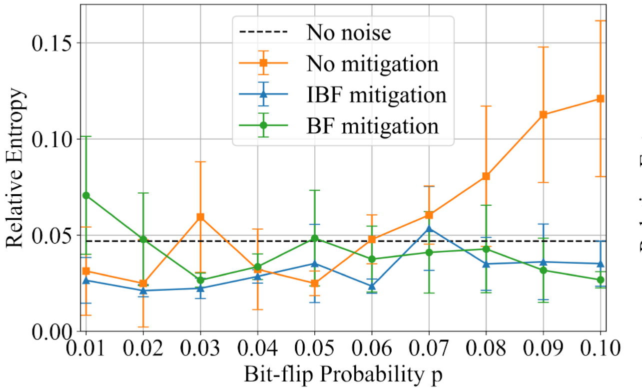


Bravo-Prieto et al. "**Style-based quantum generative adversarial networks for Monte Carlo events**." Quantum 6, 777 (2022) , *arXiv preprint arXiv:2110.06933* (2021).

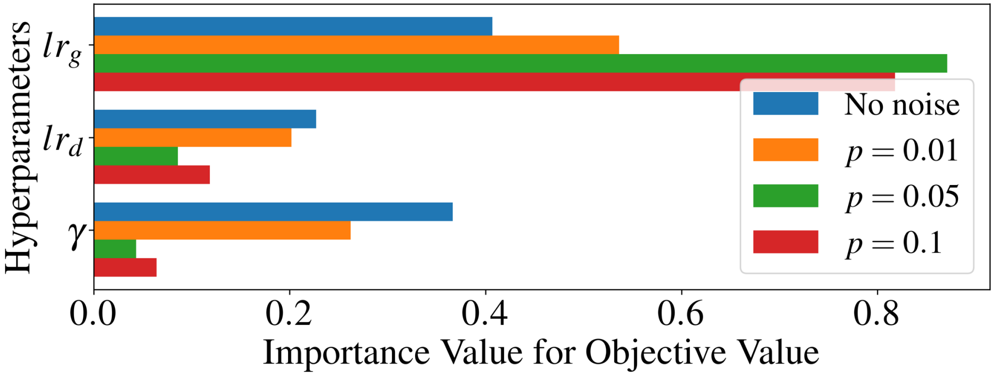
Robustness against noise

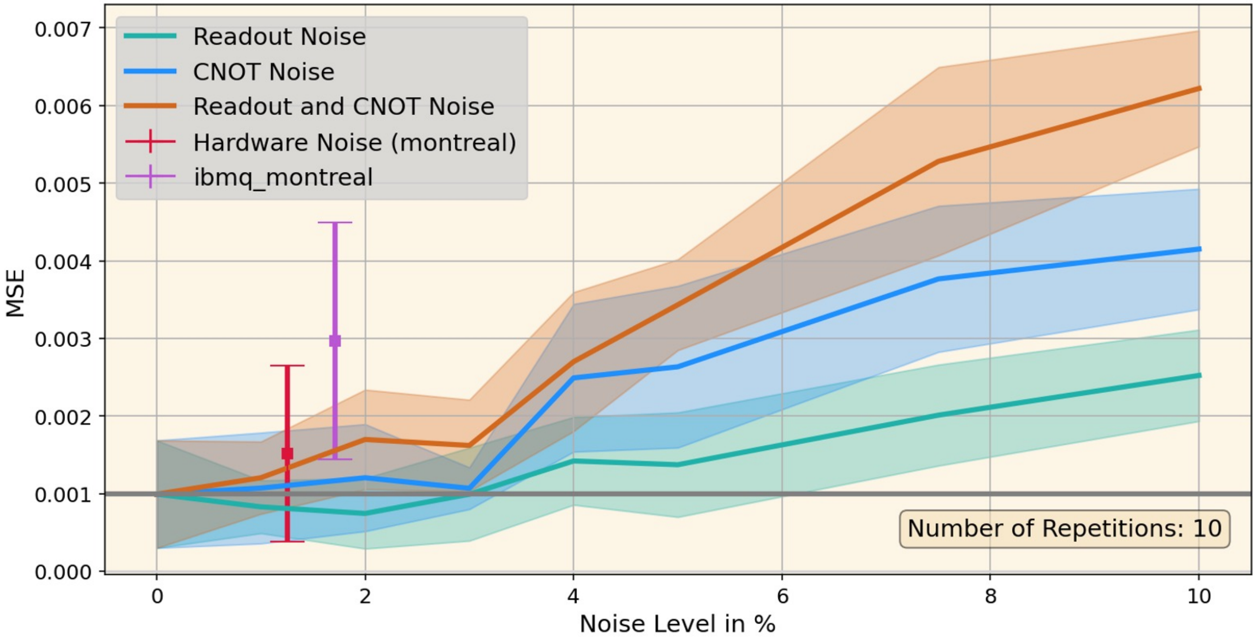
QML training process is robust against noise (error mitigation is needed in extreme cases)





Borras, Kerstin, et al. "**Impact of quantum noise on the training of quantum Generative Adversarial Networks**." ACAT2021, *arXiv preprint arXiv:2203.01007* (2022).





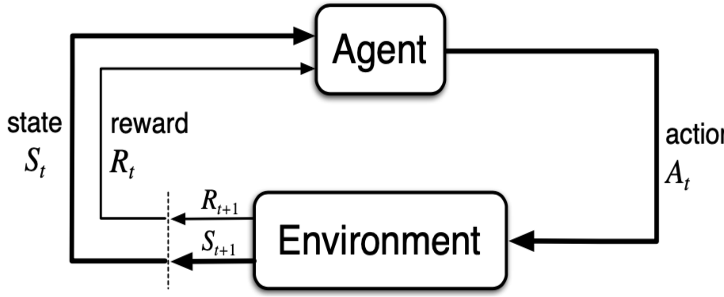
Borras, Kerstin, et al. "**Impact of quantum noise on the training of quantum Generative Adversarial Networks**."

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

Quantum Reinforcement Learning

Agent interacts with environment

- Follow **policy** $\boldsymbol{\pi}$: $S \to A$
- Find policy π^* **maximizing reward:** $G_t = \sum_k \gamma^k R_{t+k}$

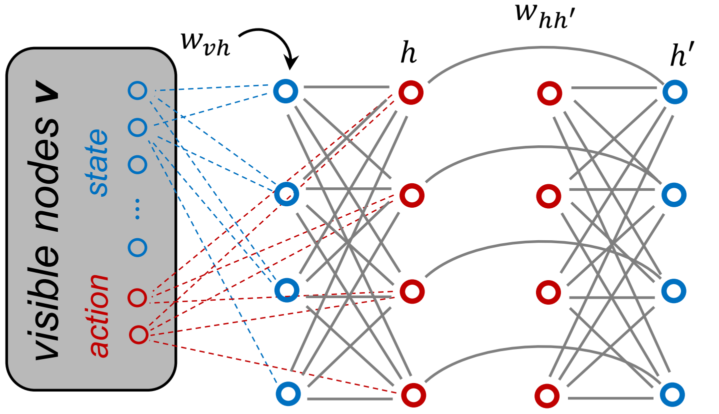


RL book: Sutton & Barto

Expected reward is estimated by ***value function*** $\boldsymbol{Q(s,a)}$

- **DQN:** Deep Q-learning *(feed-forward neural network)*
- **FERL:** Free energy based RL *(clamped Quantum Boltzmann Machine)*

Clamped QBM



Clamped QBM (visible nodes are treated as biases)

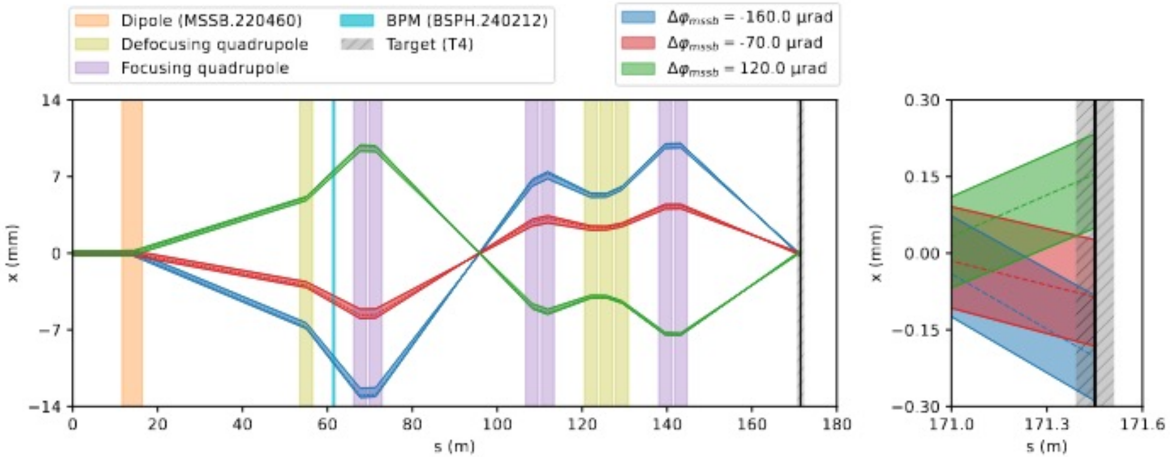
- $\boldsymbol{\hat{Q}(s,a)} \approx$ **negative free energy** of classical spin configurations c
- **Sampling** c using **(simulated) quantum annealing**
- **Discrete, binary-encoded** state and action spaces

$$\hat{Q}(s,a) \approx -F(\boldsymbol{v}) = -\langle H_{\boldsymbol{v}}^{\text{eff}} \rangle - \frac{1}{\beta} \sum_c \mathbb{P}(c|\boldsymbol{v}) \log \mathbb{P}(c|\boldsymbol{v})$$

Michael Schenk et al., **Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines**, e-Print: 2209.11044 [quant-ph]

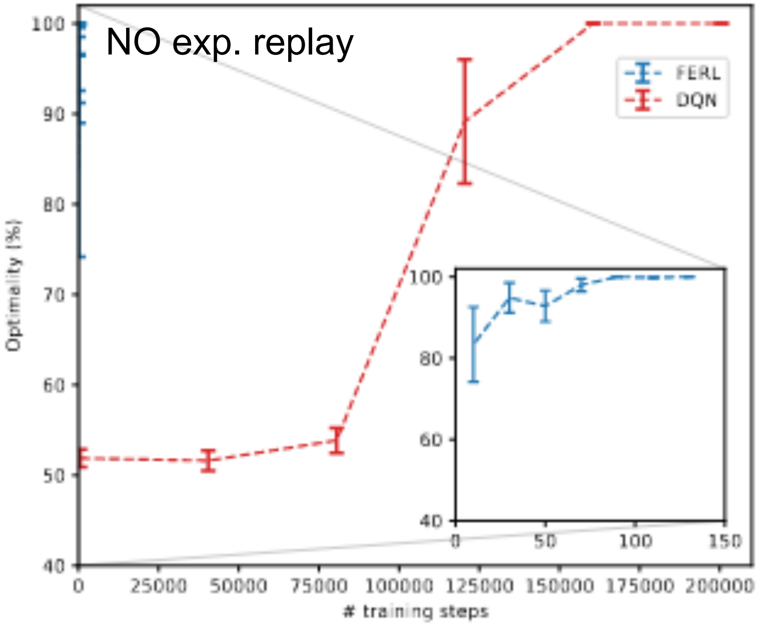
Beam optimisation in linear accelerators

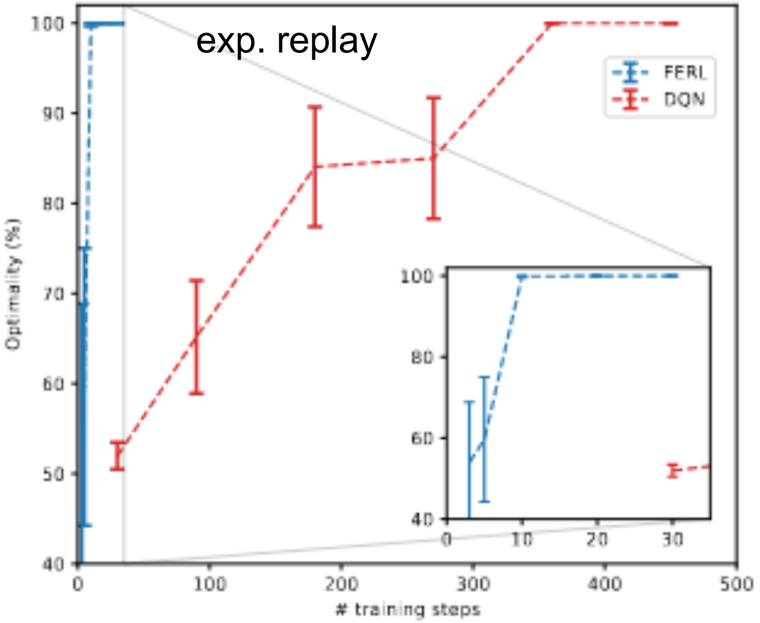
- **Action: (discrete) deflection** angle
- **State: (continuous) BPM** position
- **Reward: integrated beam intensity on target**
- **Optimality**: what fraction of possible states does agent take the right decision



One-dimensional beam target steering task at the CERN TT24-T4 beam line

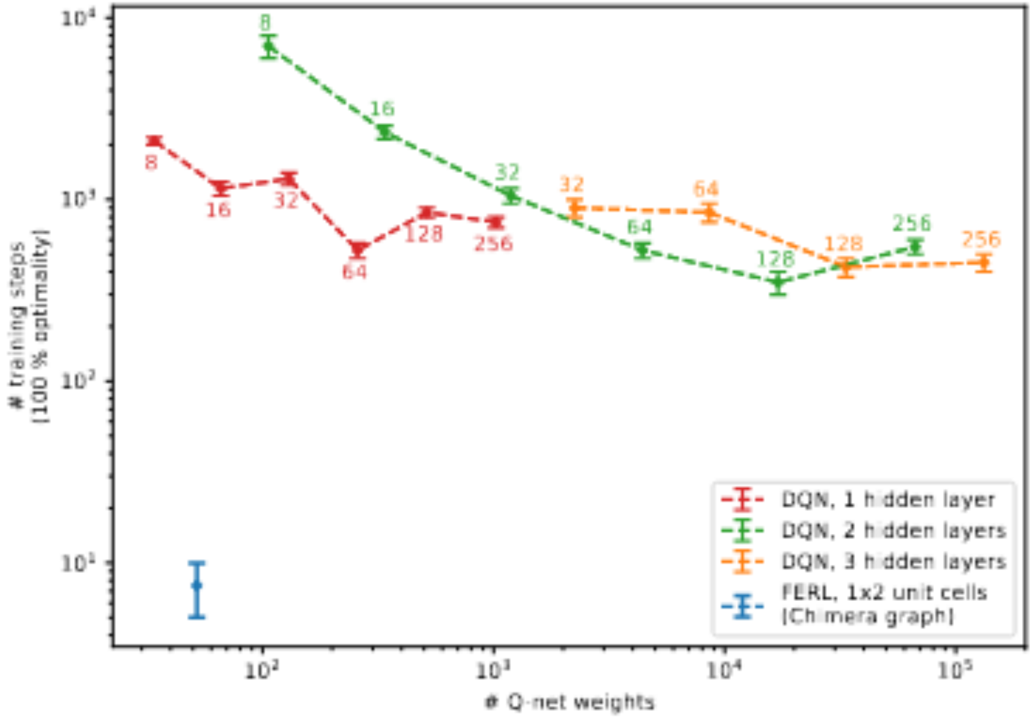
- **Training efficiency:** FERL **massively** outperforms classical Q-learning *(8±2 vs. 320±40 steps with experience replay)*





Expressive models

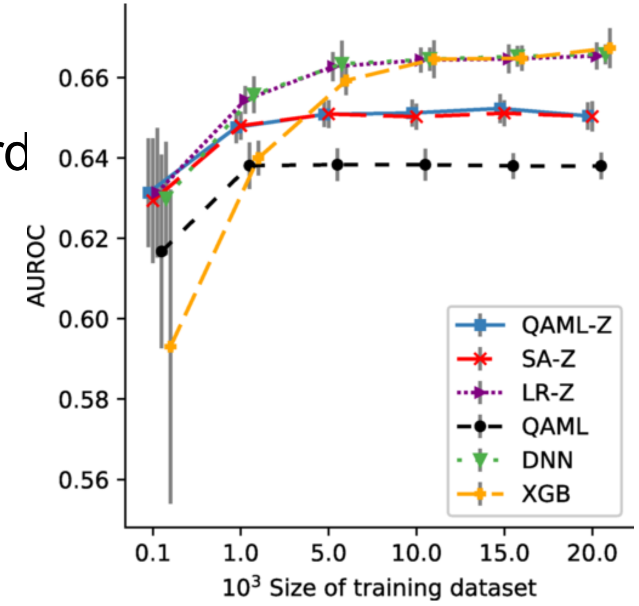
High effective dimension yields fewer parameters than classical case



Michael Schenk, Elías F. Combarro, Michele Grossi, Verena Kain, Kevin Shing Bruce Li, Mircea-Marian Popa, Sofia Vallecorsa, **Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines.** arXiv:2209.11044

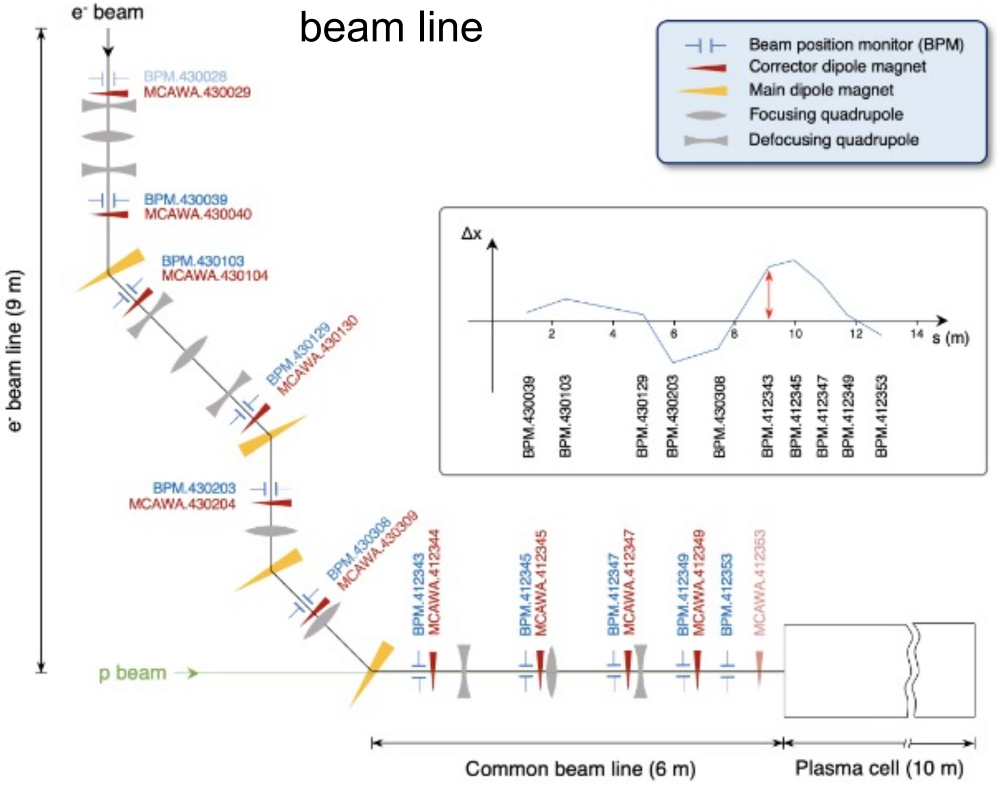
Alexander Zlokapa, Alex Mott, Joshua Job, Jean-Roch Vlimant, Daniel Lidar, and Maria Spiropulu. **Quantum adiabatic machine learning by zooming into a region of the energy surface.** Physical Review A, 102:062405, 2020. DOI:10.1103/PhysRevA.102.062405.

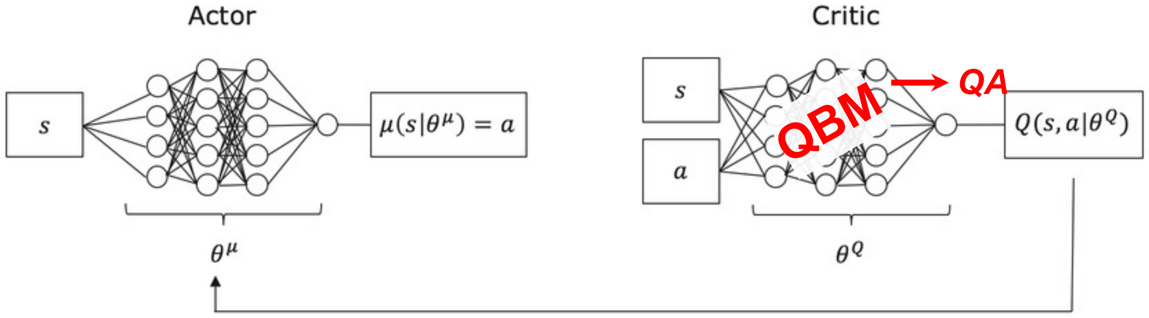
Early work pointed toward possible advantage in terms of **sample complexity and/or fast convergence**



CERN AWAKE facility

2GeV electron beam line





Policy Gradient: $\nabla_{\theta^\mu}\mu = \mathbb{E}_\mu[\nabla_{\theta^\mu} Q(s, \mu(s|\theta^\mu)|\theta^Q)] = \mathbb{E}_\mu[\nabla_a Q(s, a|\theta^Q) \cdot \nabla_{\theta^\mu}\mu(s|\theta^\mu)]$

Actor-Critic Q-learning training D-Wave Advantage

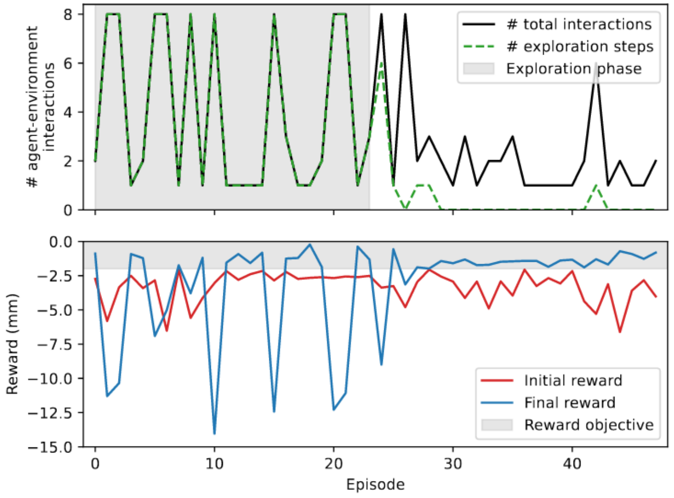
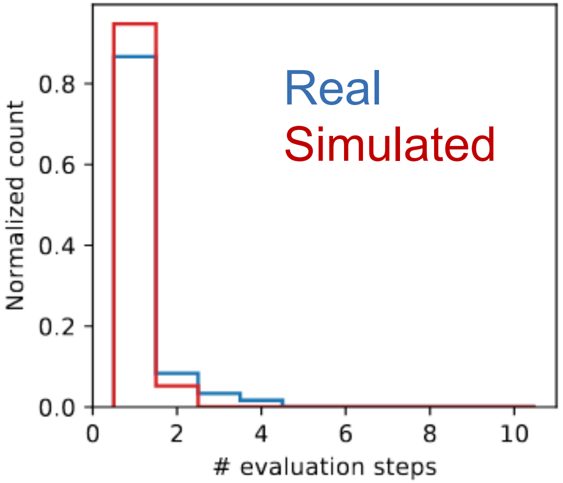


Figure 11: Single RL agent training evolution on D-Wave Advantage Systems using the simulated AWAKE environment with a reward objective of -2 mm.

Successful evaluation the real beam-line



Michael Schenk et al., **Hybrid actor-critic algorithm for quantum reinforcement learning at CERN beam lines**, e-Print: 2209.11044 [quant-ph]

Research directions

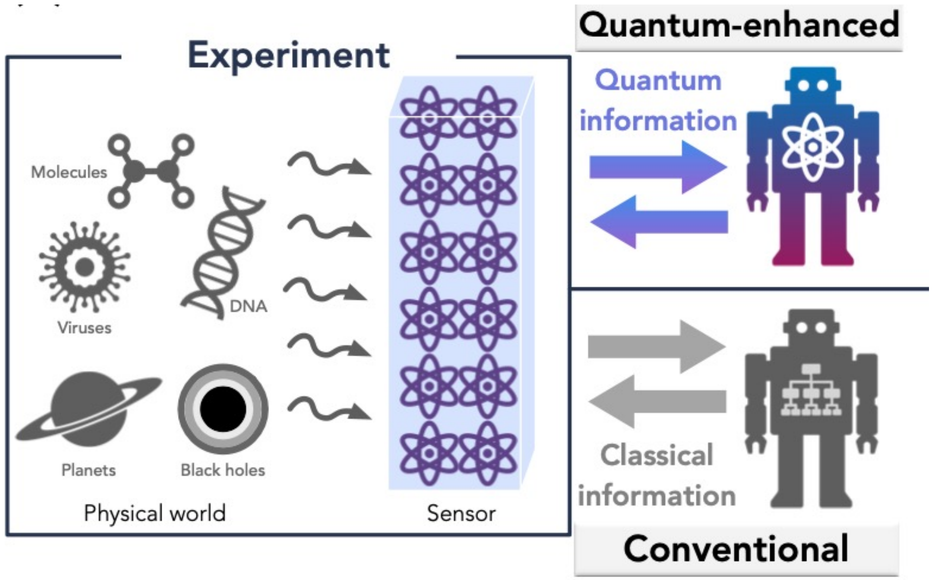
Quantum vs classical data

Correlate expected model performance to dataset properties

Convergence vs expressivity robustness studies

Algorithms beyond QML

Quantum machine learning for quantum data



Huang, *et al.*, *Science* **376**, 6598 (2022)

Work directly with quantum states.

Task: Drawing phase diagrams

1. **Supervised classification** using a convolutional QNN using the groundstates as input data.
2. Advantageous since quantum states are **exponentially hard to save classically**.
3. **Bottleneck**: we need access to classical training labels! Interpolation does not work

Cong, *et al.*, *Nat. Phys.* **15**, 1273–1278 (2019)

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

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Our solution:

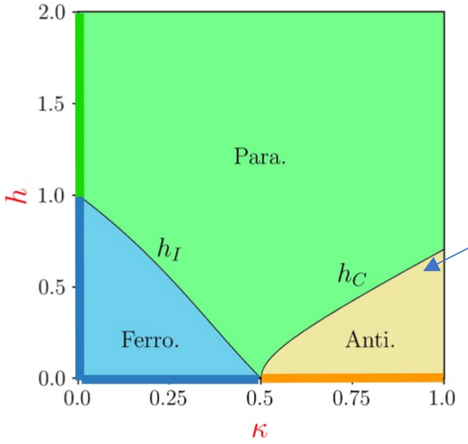
Train in easy subregions, where the model is integrable, and generalize.

Model: Axial Next Nearest Neighbor Ising (ANNNI) Hamiltonian:

Senk, *Physics Reports*, **170**, 4 (1988)

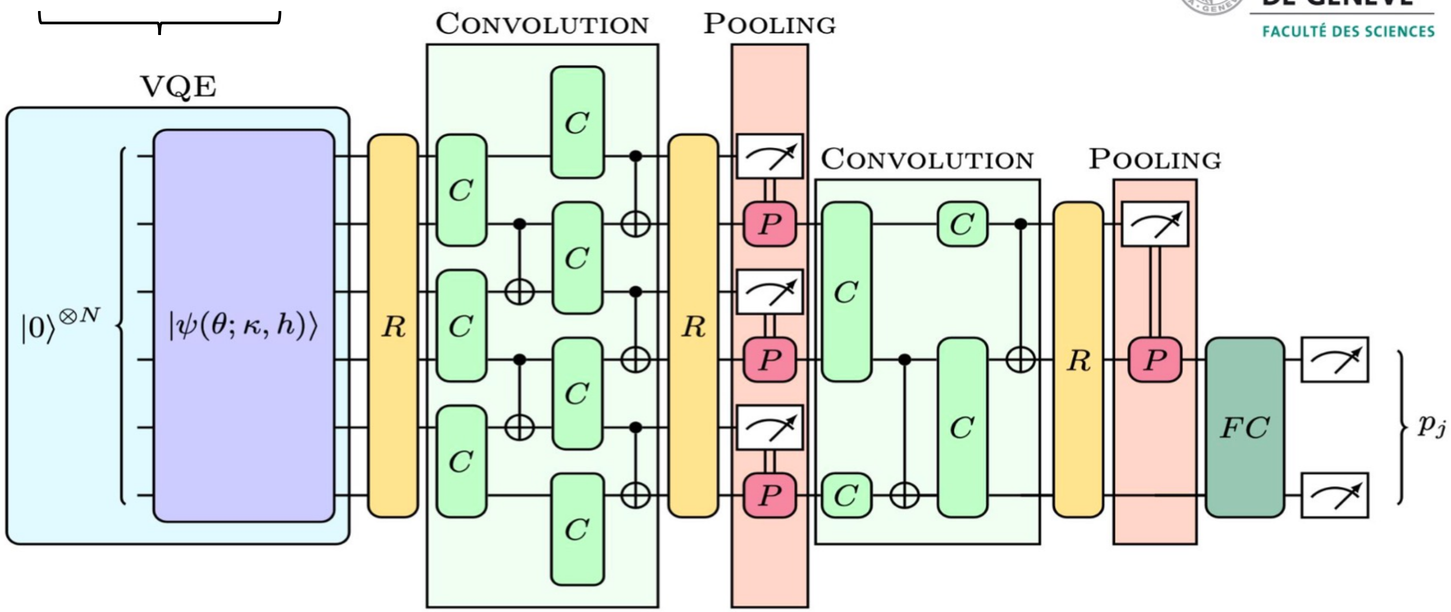
$$H = J \sum_{i=1}^{N} \sigma_x^i \sigma_x^{i+1} - \kappa \sigma_x^i \sigma_x^{i+2} + h \sigma_z^i,$$

Which is integrable for $\kappa = 0$ or $h = 0$.



Monte Carlo, DMRG

Variational quantum data



Binary Cross-entropy

Loss: $$\mathcal{L} = -\frac{1}{|\mathcal{S}_X^n|} \sum_{(\kappa,h)\in\mathcal{S}_X^n} \sum_{j=1}^{K} y_j(\kappa, h) \log\left(p_j(\kappa, h)\right)$$

Labels:

- [0,1] ferromagnetic
- [1,0] antiphase
- [1,1] paramagnetic
- [0,0] trash label

Some results

Learn a similarity function between the data.
Kottman, *et al., Phys. Rev. Research* **3**, 043184 (2021))

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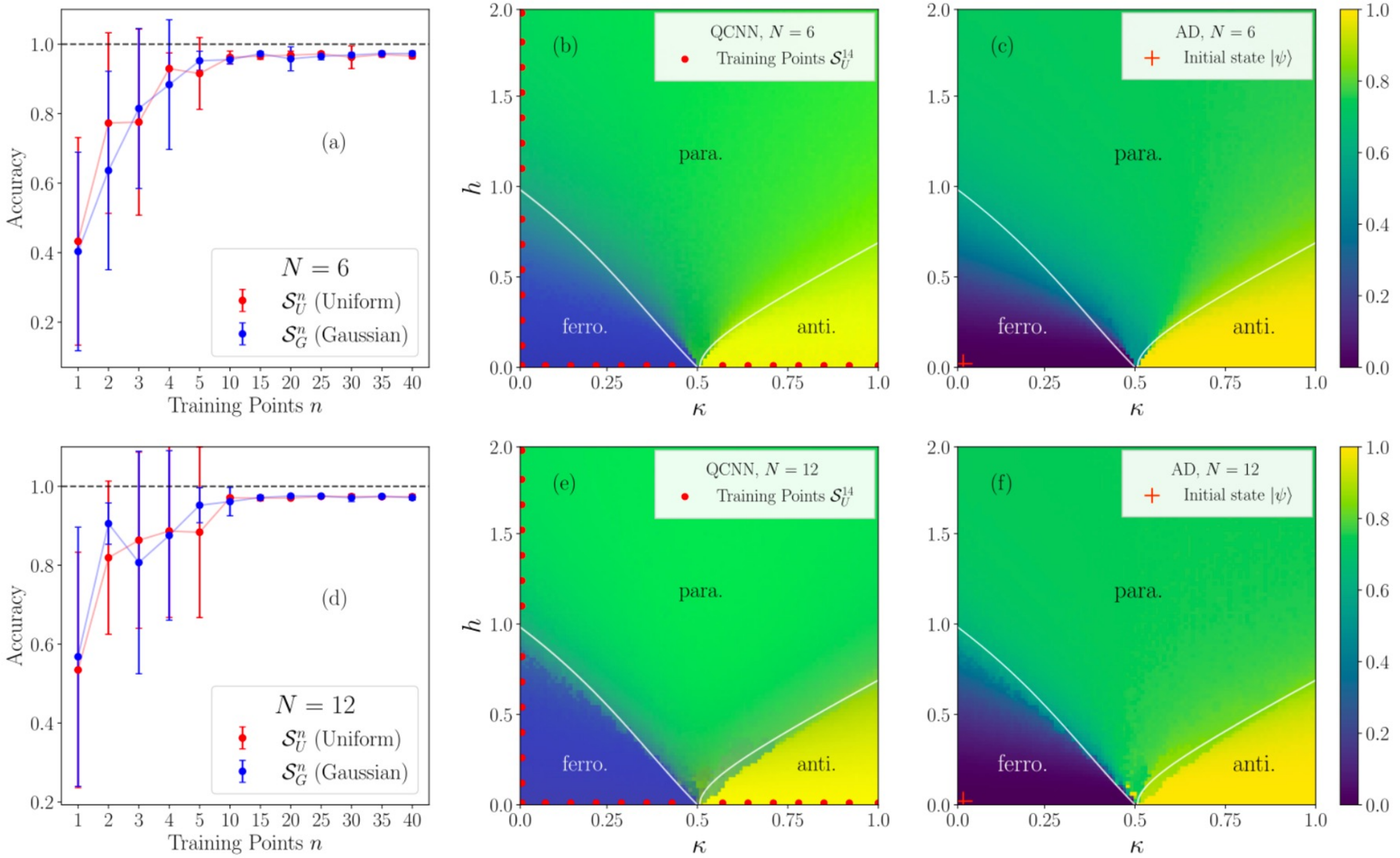
Size of training set | QCNN (95%) | Autoencoder

N = 6

N = 12



1. **Generalisation** from few training data Caro et al., *Nat Commun* **13**, 4919 (2022).
2. Performance increases with **system size**.
3. **No need for expensive training labels.**
4. QCNN gives **quantitative** predictions.

5. Both techniques are unable to find the floating phase.

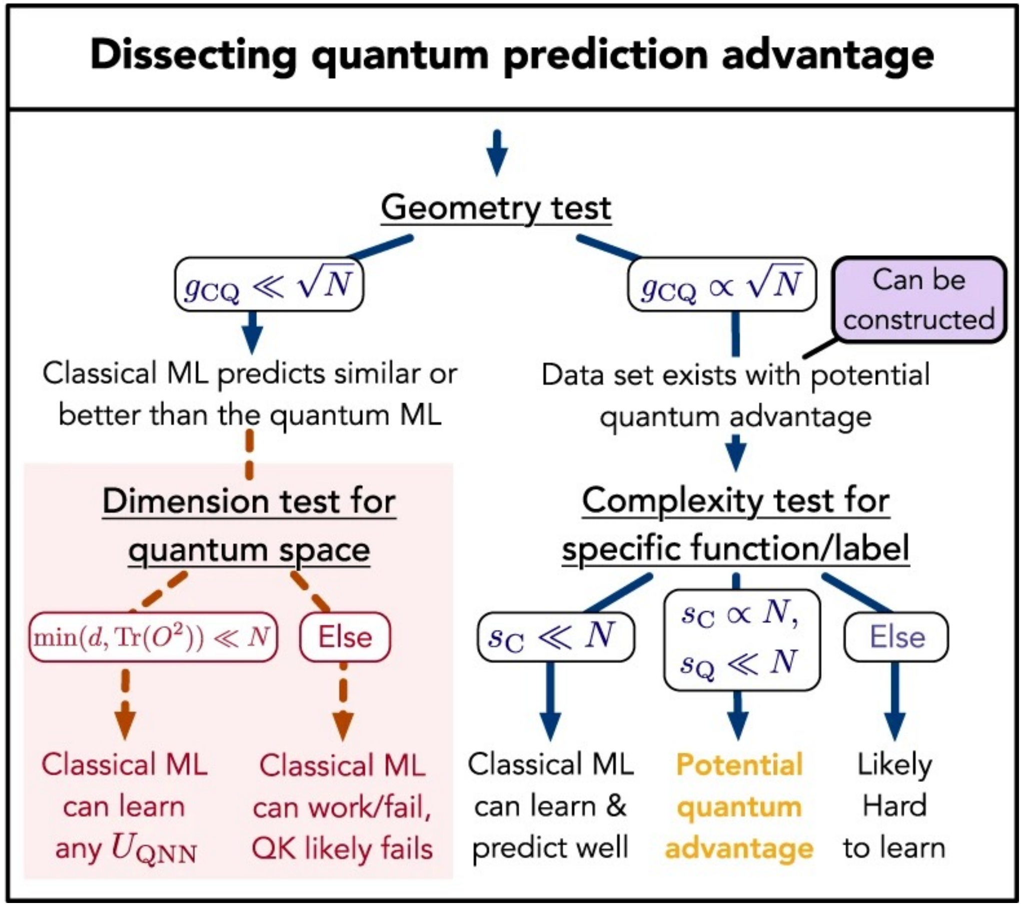
Advantage for QML?

Classical Intractability: quantum algorithm that cannot be efficiently simulated classically[1,2]

- No established recipe for classical data
- Use exponential advantage in Hilbert space, while preserving converge ? (Algorithm **expressivity vs generalization**)

Metrics to evaluate quantum vs classical kernel:

- Geometric difference between quantum and classical kernels
- Model complexity
- Approximate dimension of the quantum feature space
- Propose projected quantum kernels reducing expressivity

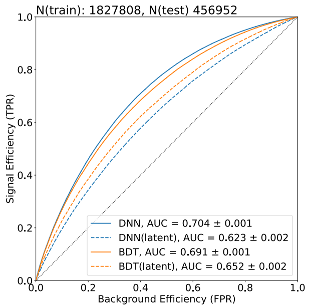


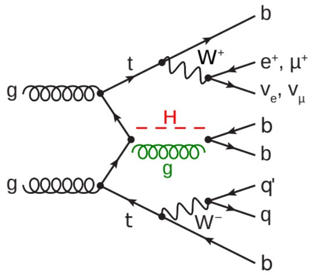
[1]Kübler, Jonas, Simon Buchholz, and Bernhard Schölkopf. "**The inductive bias of quantum kernels**." Advances in Neural Information Processing Systems 34 (2021).
[2] Huang, HY., Broughton, M., Mohseni, M. et al. **Power of data in quantum machine learning**. Nat Commun 12, 2631 (2021). https://doi.org/10.1038/s41467-021-22539-9

F. Di Marcantonio et al., The Role of Data in Projected Quantum Kernels: the Higgs Boson Discrimination.

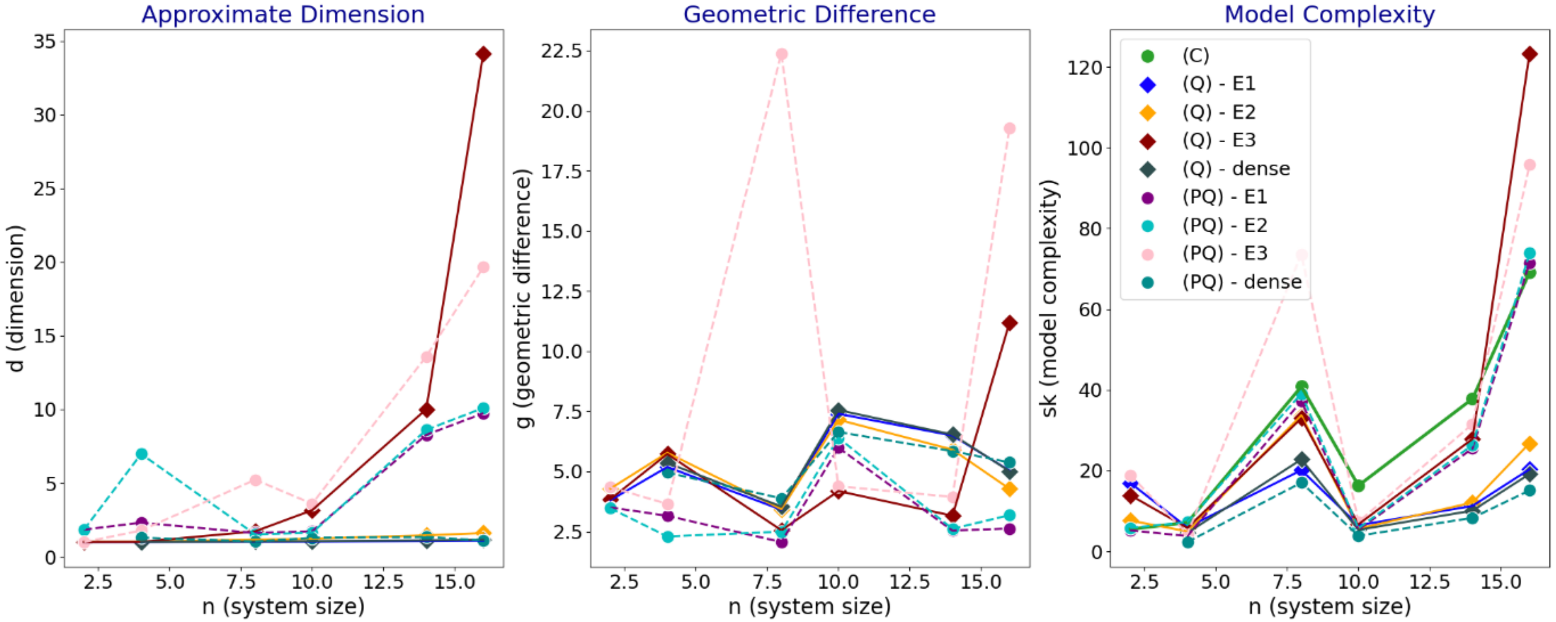
Analize the performance of quantum kernels

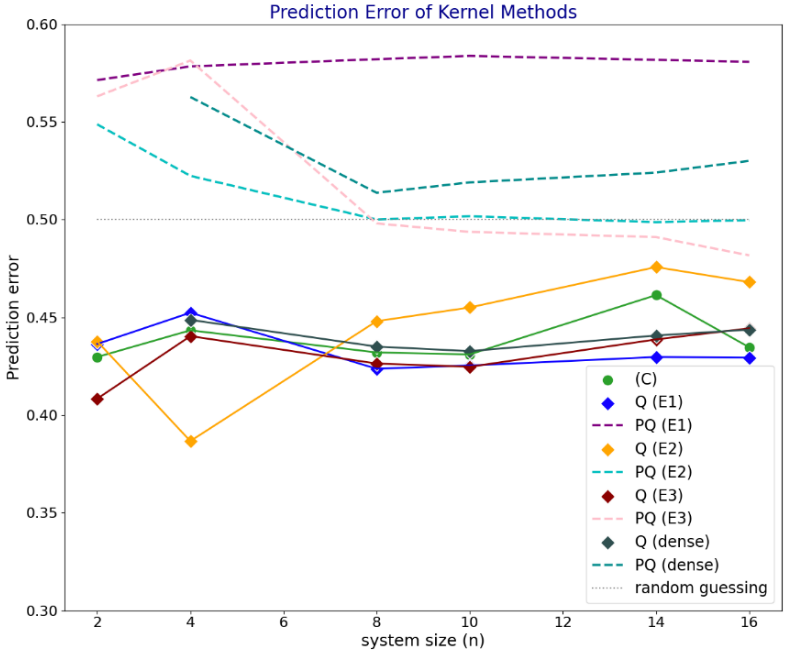
- Focus on **H(tbb) classification**
- quantum kernels keep data in low-dimensional Hilbert spaces
- model complexity increases with the number of qubits for all ML models.
- Model complexity are similar (sometimes below classical models)
- Projected kernels don’t help





V. Belis, EPJ Web of Conferences 251, 03070 (2021)





^{6}Li Ground state preparation
with the Variational Quantum Eigensolver (VQE)

Variational principle:

$$E_0 \leq \frac{\langle\psi(\theta)| H |\psi(\theta)\rangle}{\langle\psi(\theta)|\psi(\theta)\rangle}.$$

We are looking for a state which minimize the expectation value of H_0.

6Li nuclei with an 4He inert core (12 orbitals in the shell model):

$$H = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2}\sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l,$$

Unitary Coupled Clusters (UCC) ansatz

$$|\psi(\boldsymbol{\theta})\rangle = e^{i(\hat{T}(\boldsymbol{\theta}) - \hat{T}^\dagger(\boldsymbol{\theta}))} |\psi_0\rangle.$$

Hartree Fock solution

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$$

Cluster operators

$$\hat{T}_1 = \sum_{i \in \mathrm{virt}; \alpha \in \mathrm{occ}} \theta_i^\alpha \hat{a}_i^\dagger \hat{a}_\alpha$$

Single fermionic excitation terms

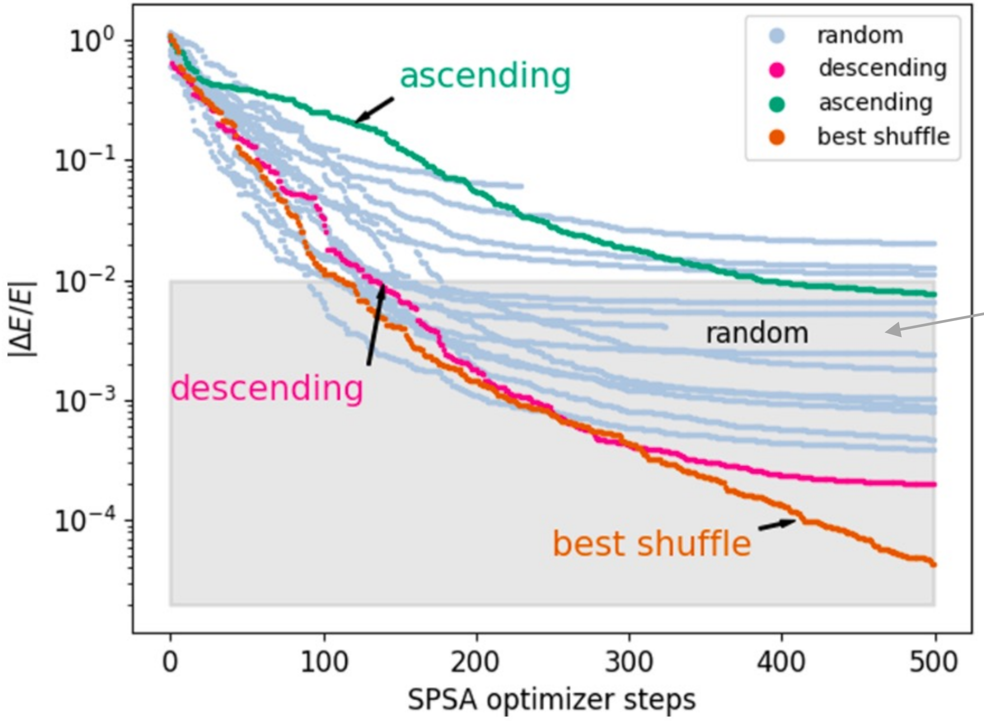
$$\hat{T}_2 = \sum_{i,j \in \mathrm{virt}; \alpha,\beta \in \mathrm{occ}} \theta_{ij}^{\alpha\beta} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_\alpha \hat{a}_\beta.$$

Double fermionic excitation terms

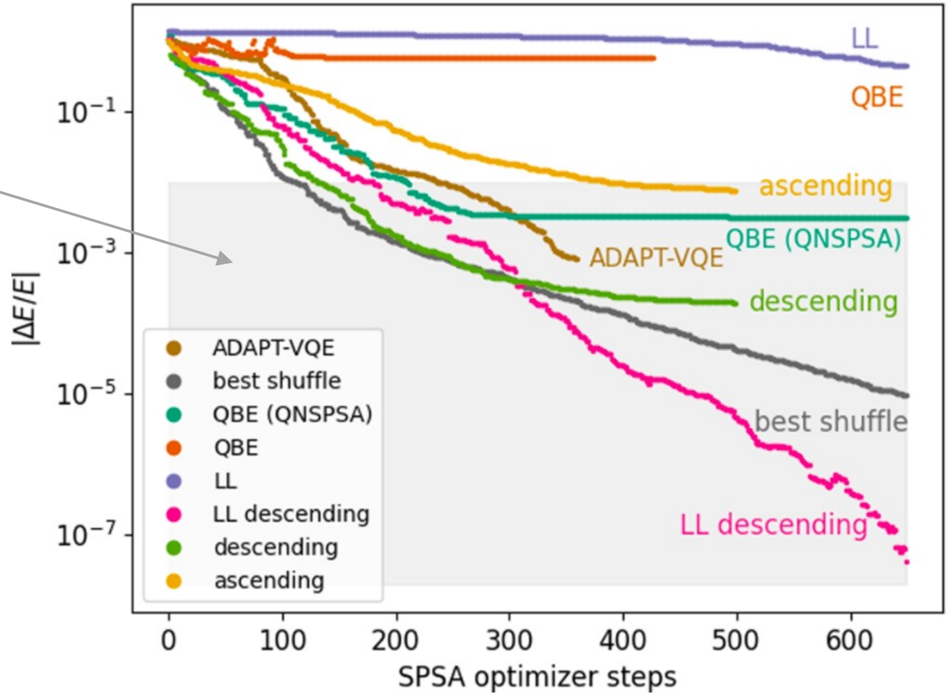
Comparison of different ansatz

The effect of shuffling the fermionic excitations operators. We should order them in descending order of magnitude (of the corresponding term in the hamiltoninan).

Best approach: train the ansatz recursvily in descending order.
Qubit Based Excitation UCC: adapted to NISQ devices



1% barrier needed for most applications



Kiss et al., *Phys. Rev. C* **106**, 034325 (2022)

Perspective

The CERN QTI is studying impact of Quantum Technologies in High Energy Physics:

- Some **preliminary hints** of advantage
- So far.. we can do «**as good as classical methods**». In many cases, limitations are hardware-related
- Need more **robust studies** to estimate **performance** and drive **model development**

We are now formulating a **longer term research plan**

- Identify cases where quantum approach could be **more effective** than classical algorithms**...**
- Study performance **beyond near-term hardware**
- **…**

QT4HEP conference
CERN, 1- 4 November 2022

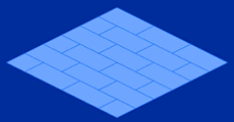
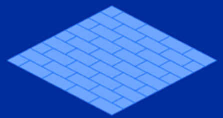
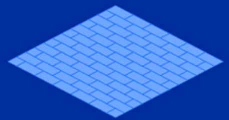
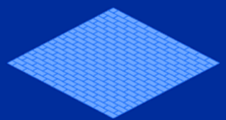
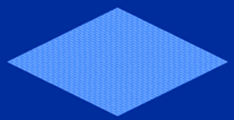
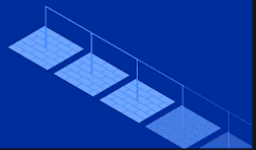
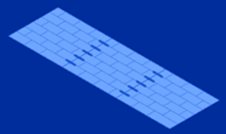
More information:
https://indico.cern.ch/event/1190278

Thanks!

Sofia.Vallecorsa@cern.ch

Development Roadmap | Executed by IBM / On target

IBM **Quantum**

	2019	2020	2021	2022	2023	2024	2025	Beyond 2026
	Run quantum circuits on the IBM cloud	Demonstrate and prototype quantum algorithms and applications	Run quantum programs 100x faster with Qiskit Runtime	Bring dynamic circuits to Qiskit Runtime to unlock more computations	Enhancing applications with elastic computing and parallelization of Qiskit Runtime	Improve accuracy of Qiskit Runtime with scalable error mitigation	Scale quantum applications with circuit knitting toolbox controlling Qiskit Runtime	Increase accuracy and speed of quantum workflows with integration of error correction into Qiskit Runtime
Model Developers					Prototype quantum software applications →		Quantum software applications Machine learning | Natural science | Optimization	
Algorithm Developers		Quantum algorithm and application modules Machine learning | Natural science | Optimization			Quantum Serverless	Intelligent orchestration	Circuit Knitting Toolbox	Circuit libraries
Kernel Developers	Circuits		Qiskit Runtime	Dynamic circuits	Threaded primitives	Error suppression and mitigation		Error correction
System Modularity	Falcon 27 qubits 	Hummingbird 65 qubits 	Eagle 127 qubits 	Osprey 433 qubits 	Condor 1,121 qubits 	Flamingo 1,386+ qubits 	Kookaburra 4,158+ qubits 	Scaling to 10K-100K qubits with classical and quantum communication
					Heron 133 qubits x p 	Crossbill 408 qubits 		

CERN QTI Roadmap:

- Di Meglio, Alberto, Doser, Michael, Frisch, Benjamin, Grabowska, Dorota, Pierini, Maurizio, & Vallecorsa, Sofia. (2022). CERN Quantum Technology Initiative Strategy and Roadmap (1.0_Rev3). Zenodo. https://doi.org/10.5281/zenodo.5846455

Snowmass:

- Humble, Travis S., et al. "Snowmass White Paper: Quantum Computing Systems and Software for High-energy Physics Research." *arXiv preprint arXiv:2203.07091* (2022).
- Delgado, Andrea, et al. "Quantum Computing for Data Analysis in High-Energy Physics." *arXiv preprint arXiv:2203.08805* (2022)

Review article :

- Gray, Heather M., and Koji Terashi. "Quantum Computing Applications in Future Colliders." *Frontiers in Physics* (2022): 473.

Quantum Theory

pQCD and Standard Model : collider physics

Heavy Ion:
quark gluon plasma, heavy ion collisions, …

Lattice:
theory inputs for nuclear and particle physics, first principle calculations,…

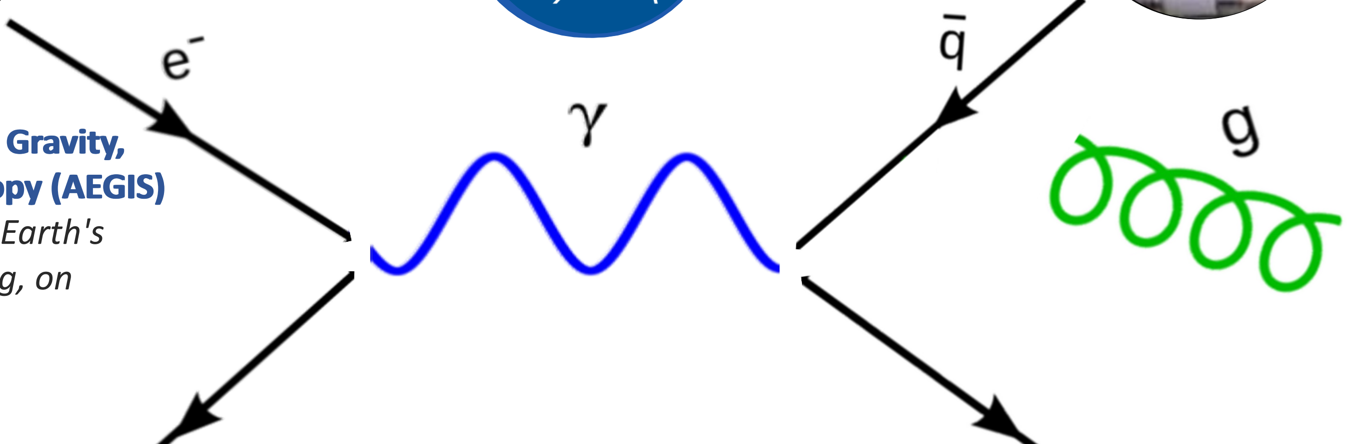
BSM :
dark matter model building, new physics, BSM explanation of experimental anomalies

Strings/QFT:
quantum gravity, string theory, …

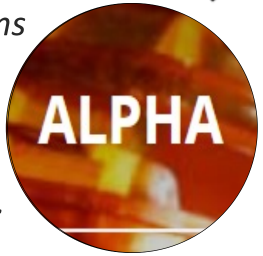
Cosmo, AstroParticle:
properties and evolution of the early universe, dark sector,…

Non-LHC Experiments

Antihydrogen Experiment: Gravity, Interferometry, Spectroscopy (AEGIS)
direct measurement of the Earth's gravitational acceleration, g, on antihydrogen.



ALPHA (successor of ATHENA)
makes, captures and studies atoms of antihydrogen and compares these with hydrogen atoms.



CERN Neutrino Platform
CERN's undertaking to foster and contribute to fundamental research in neutrino physics at particle accelerators worldwide

Atomic Spectroscopy And Collisions Using Slow Antiprotons
studies the fundamental symmetries between matter and antimatter by precision spectroscopy of atoms containing an antiproton.

Antiproton Trap
compares protons with their antimatter equivalents.

CERN Axion Solar Telescope
search for hypothetical "axions", proposed to explain why there is a subtle difference between matter and antimatter.

Theory and Simulation

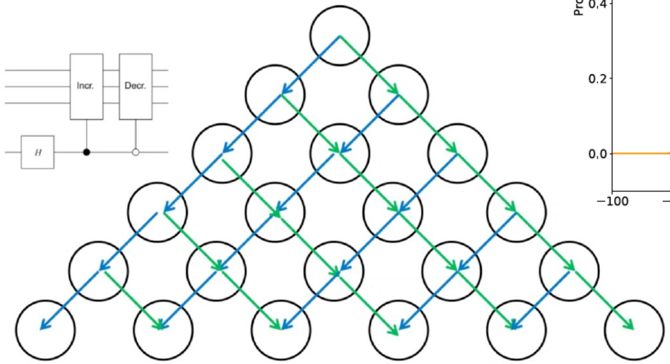
Quantum Field Theory. Ex. Sign problems in particle theory

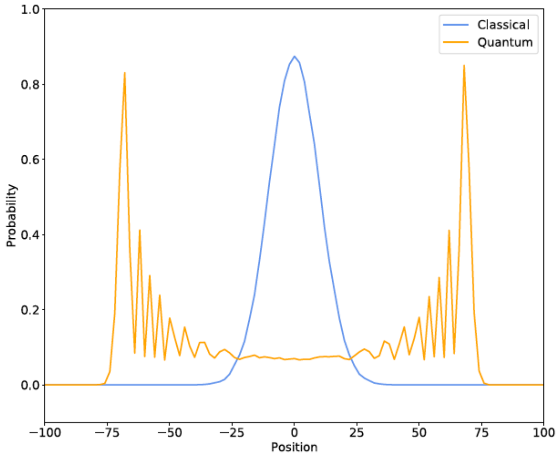
- Dynamical Simulations of Lattice Gauge Theories
- Finite-Density Nuclear Matter
- Challenges related to digitization and truncation of filed representation (on a finite number of quantum states) and redundancy in the Hilbert space[1]

Cross section integration as quantum amplitude estimation[3]

Event generation with quantum generative models or direct simulation

Parton showering as quantum random walk[2]





[1] D. Grabowska's presentation at the CERN QTI workshop (https://indico.cern.ch/event/1098355)
[2] A quantum walk approach to simulating parton showers Khadeejah Bepari, Sarah Malik, Michael Spannowsky, Simon Williams arxiv:2109.13975 and presentation at the CERN QTI workshop (https://indico.cern.ch/event/1098355)
[3]Agliardi, Gabriele, et al. "**Quantum integration of elementary particle processes**." *arXiv preprint arXiv:2201.01547* (2022)

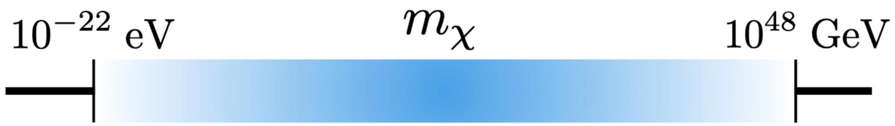
Quantum sensing

Change of quantum state caused by the interaction with an external system:

- **transition between superconducting and normal-conducting**
- **transition of an atom from one state to another**
- **change of resonant frequency of a system (quantized)**

quantum sensors & particle physics: what are we talking about?

Axions, ALP's, DM & non-DM UL-particle searches



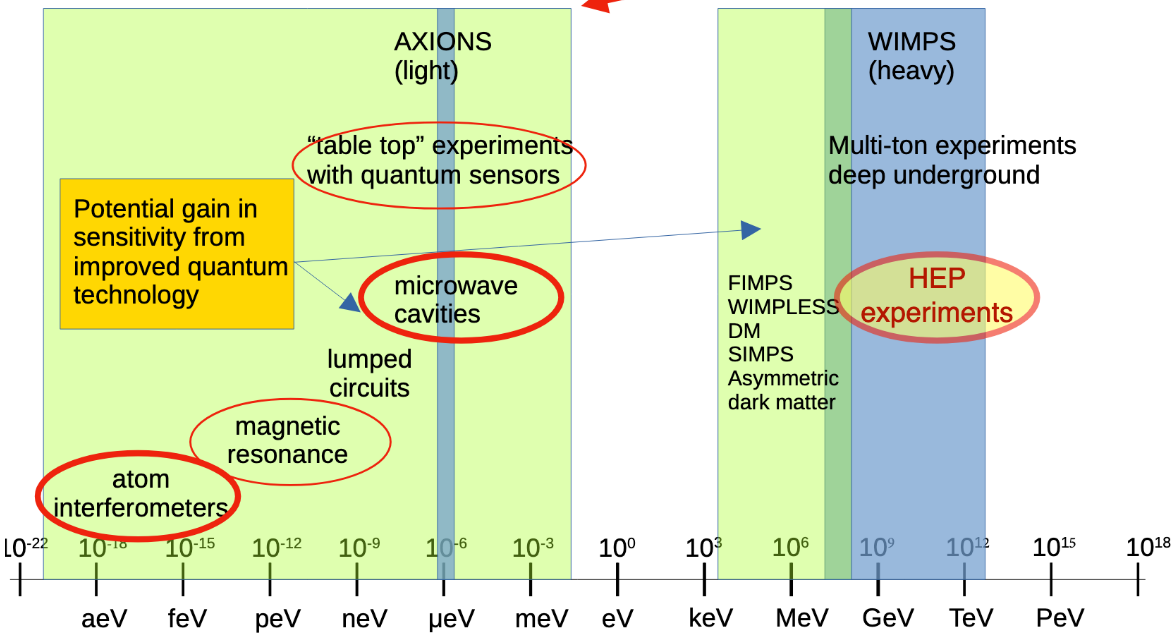
cavity size = axion size

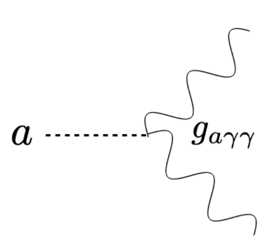
axion mass = unknown

$$F \sim g_{a\gamma}^2 m_A^2 B^4 V^2 T_{sys}^{-2} G^4 Q,$$

system noise temperature

cryo-amplifiers JJPA



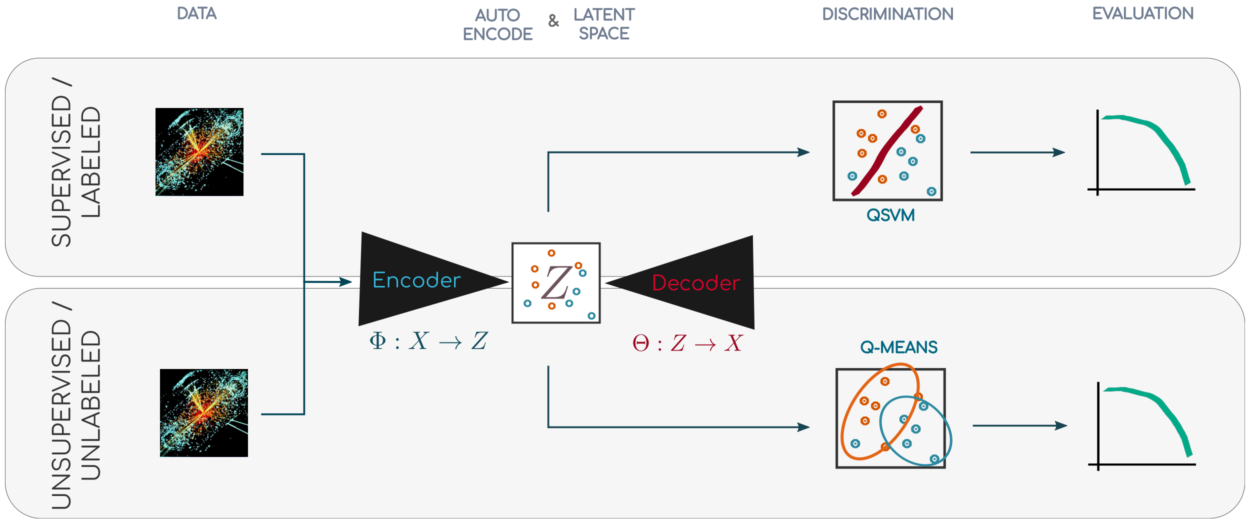


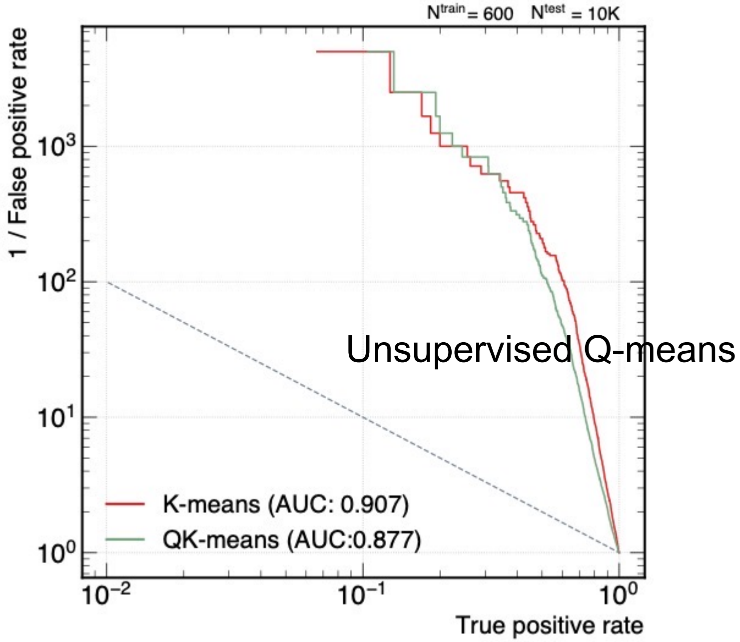
(but not only…)

Kinga Wozniak, **Unsupervised clsutering for a Randall–Sundrum Graviton at 3.5TeV narrow resonance, 5th IML workshop, May 2022**

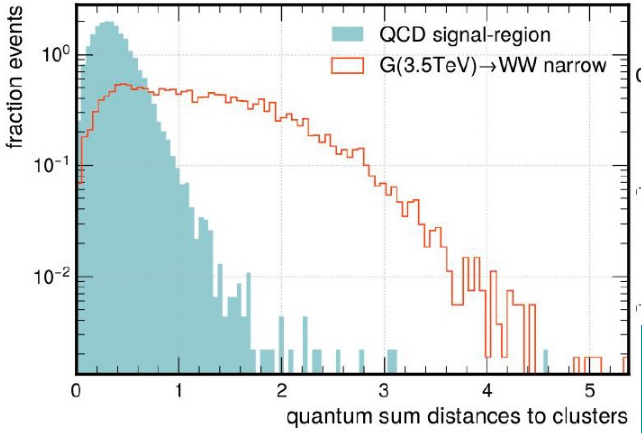
Hybrid setup for anomaly detection

Di-jet events ($\Delta\varphi$, $\Delta\eta$, p_T). Train AE on **QCD sidebands**.
Train classifiers on **signal region**.

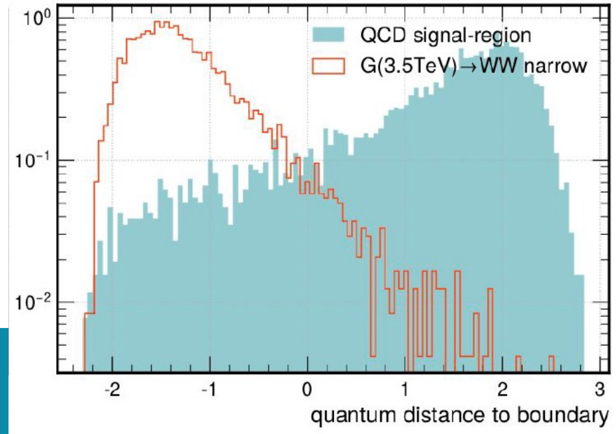


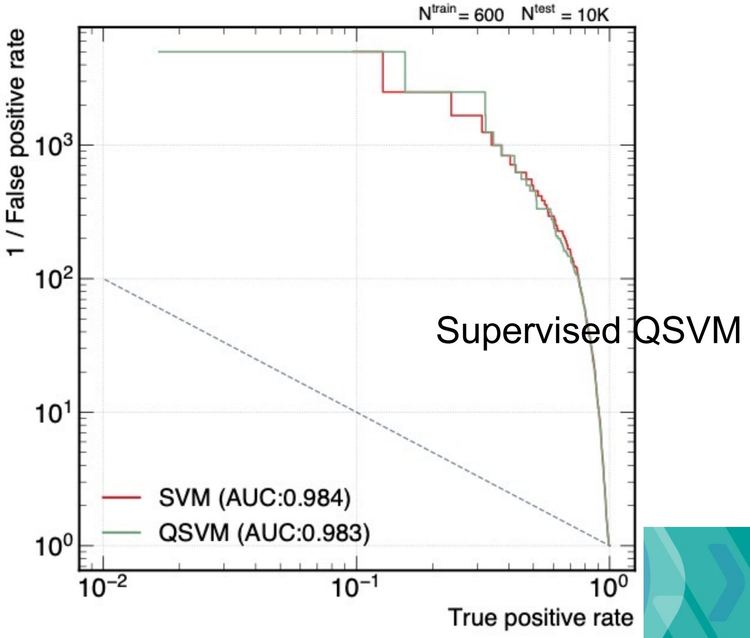


Unsupervised Q-means

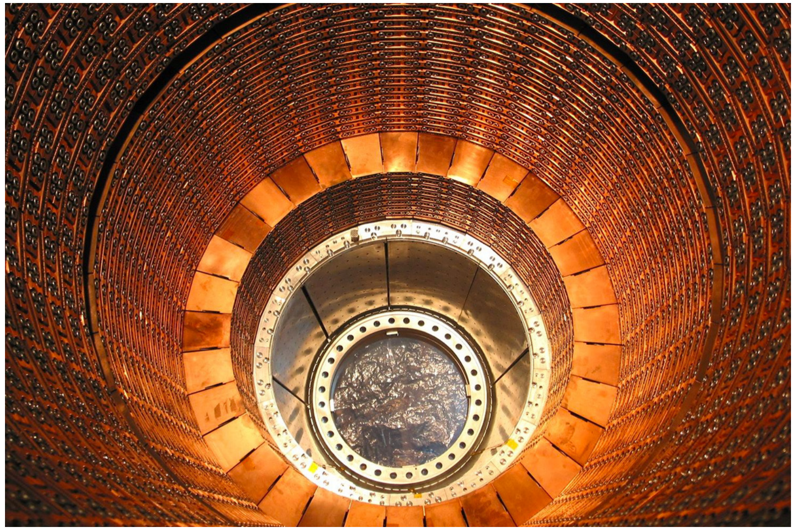


Supervised QSVM





Quantum Sensing for High-Energy Physics



Scope

High-Energy Physics, particle tracking, calorimetry, identification in HEP detectors

Strategy

Quantum “priming” of detectors before measurement, signal enhancement by laser excitation, quantum effects due to size, cryogenics

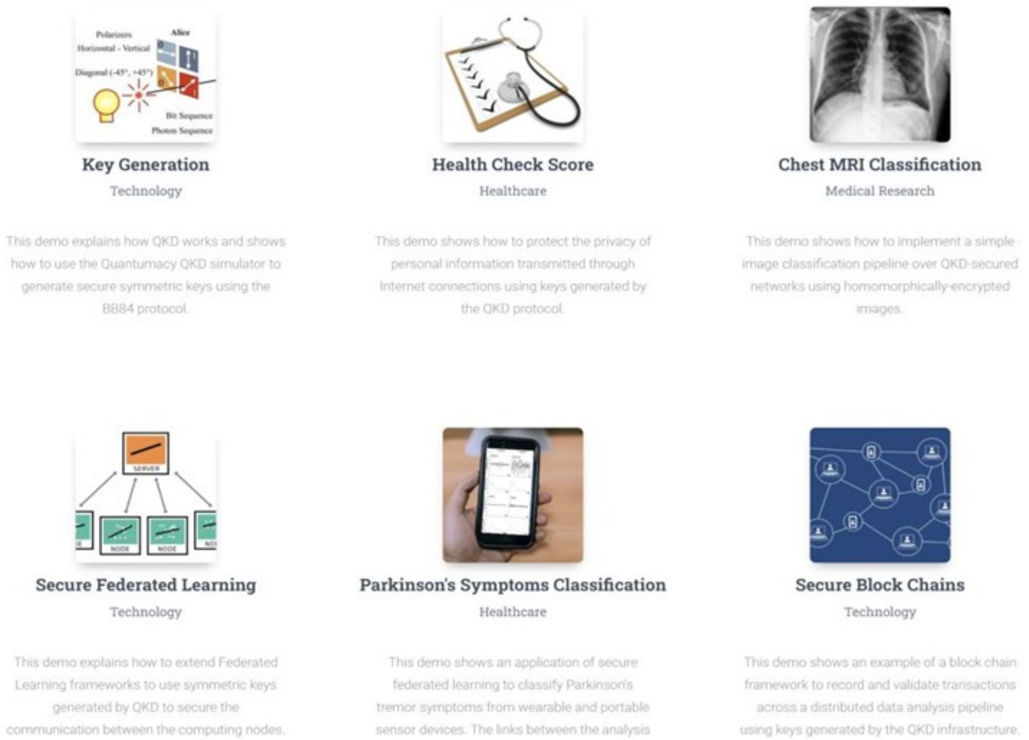
Applications

Chromatic particle trackers composed of arrays of nanodots of varying size, nanocrystals (eg. XPbBr3) as scintillator or charged particle tracking for HEP detectors
Calorimeters and low-energy single-particle (photons, mip’s, ions,...) detectors made of arrays of nanowires (SNSPD)
2D-structures (graphene) for gaseous detector signal amplification, synergies with atomic and quantum optics experiment control/DAQ

Quantum Communication

QUANTUMACY

OPEN QKD



Presented at openQKD General Assembly in Paris

Jose Cabrero-Holgueras & Gabriele Morello

Model Convergence and Barren Plateau

Given the size of the Hilbert space a compromise between **expressivity**, **convergence** and **generalization** performance is needed.

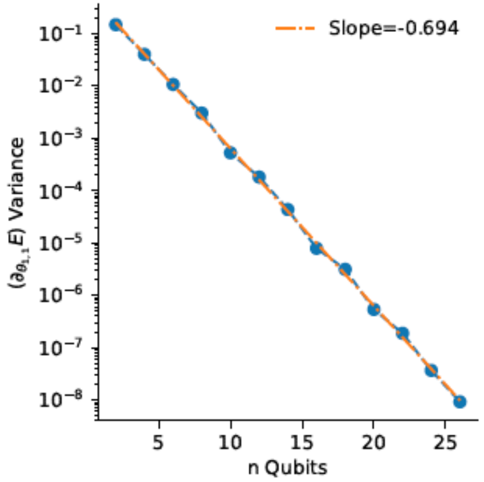
Classical gradients **vanish exponentially** with the number of layers (J. McClean *et al.*, arXiv:1803.11173)

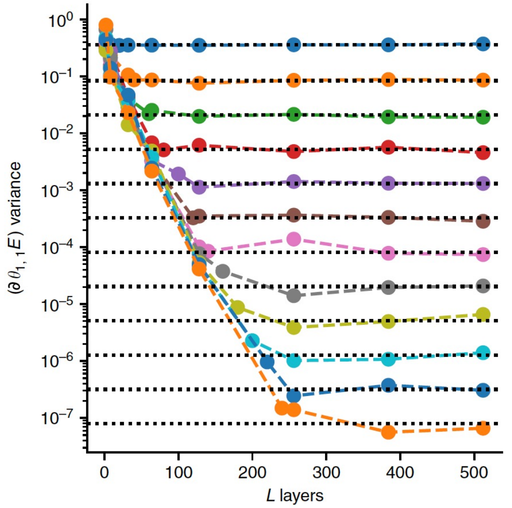
- Convergence still possible if gradients consistent between batches.

Quantum gradient decay exponentially in the number of qubits

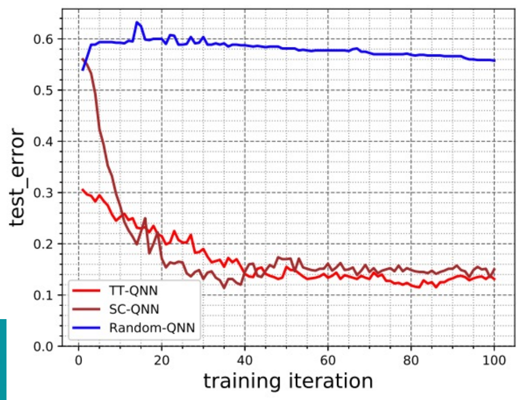
- Random circuit initialization
- Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
- Ansatz choice: TTN, CNN (Zhang *et al.*, arXiv:2011.06258, A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011.)
- Noise induced barren plateau (Wang, S *et al.*, Nat Commun 12, 6961 (2021))

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

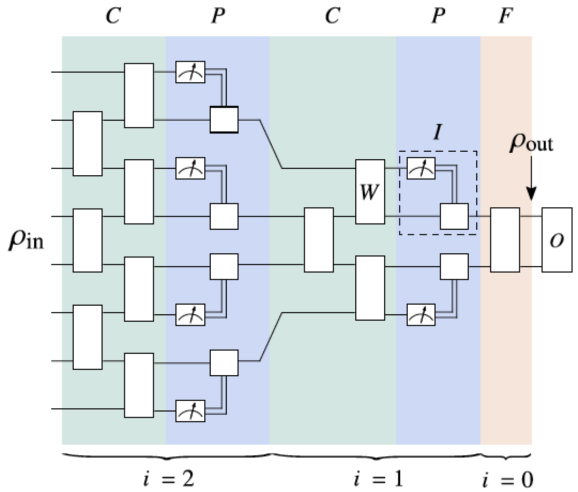




TTN for MNIST classification (8 qubits), Zhang *et al.*, arXiv:2011.06258



QCNN: A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011



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