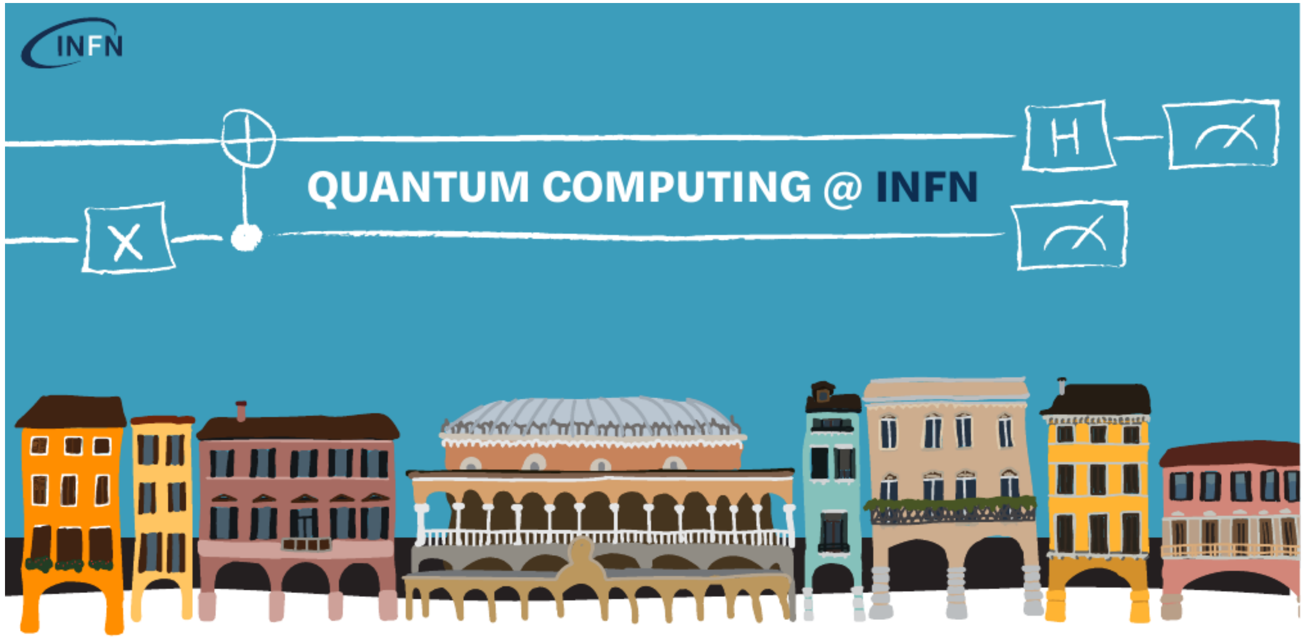
Quantum Computing in experimental HEP
(quant-ph, hep-ph, hep-ex)



Michele Grossi, PhD

Hybrid Quantum Computing Infrastructures and Algorithms Coordinator

CERN
QUANTUM TECHNOLOGY INITIATIVE

Quantum Motivation & Challenge

CERN examples

Discussion

Quantum Motivation & Challenge

CERN examples

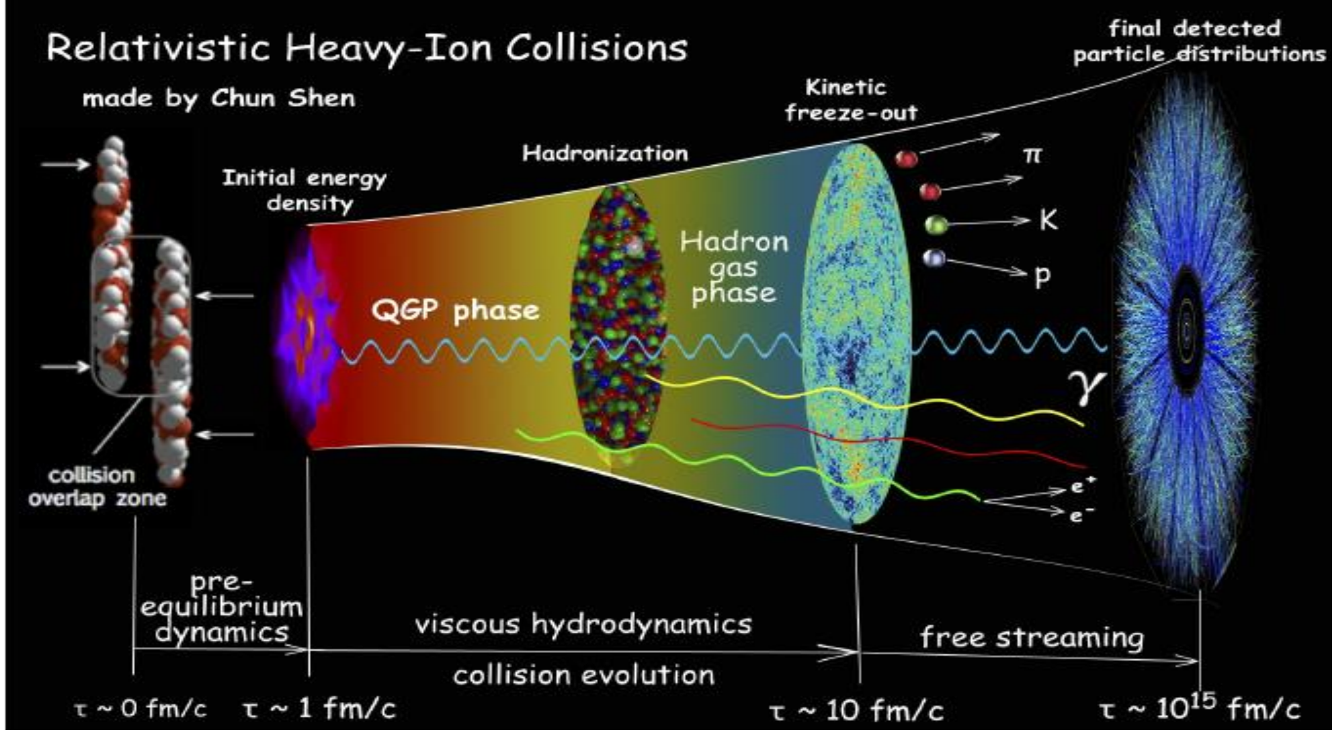
Discussion

Motivation

Theoretical challenge

- Non-zero chemical potential (QCD phase diagram)
- Real time dynamics

  → heavy ion collisions, scattering quenches



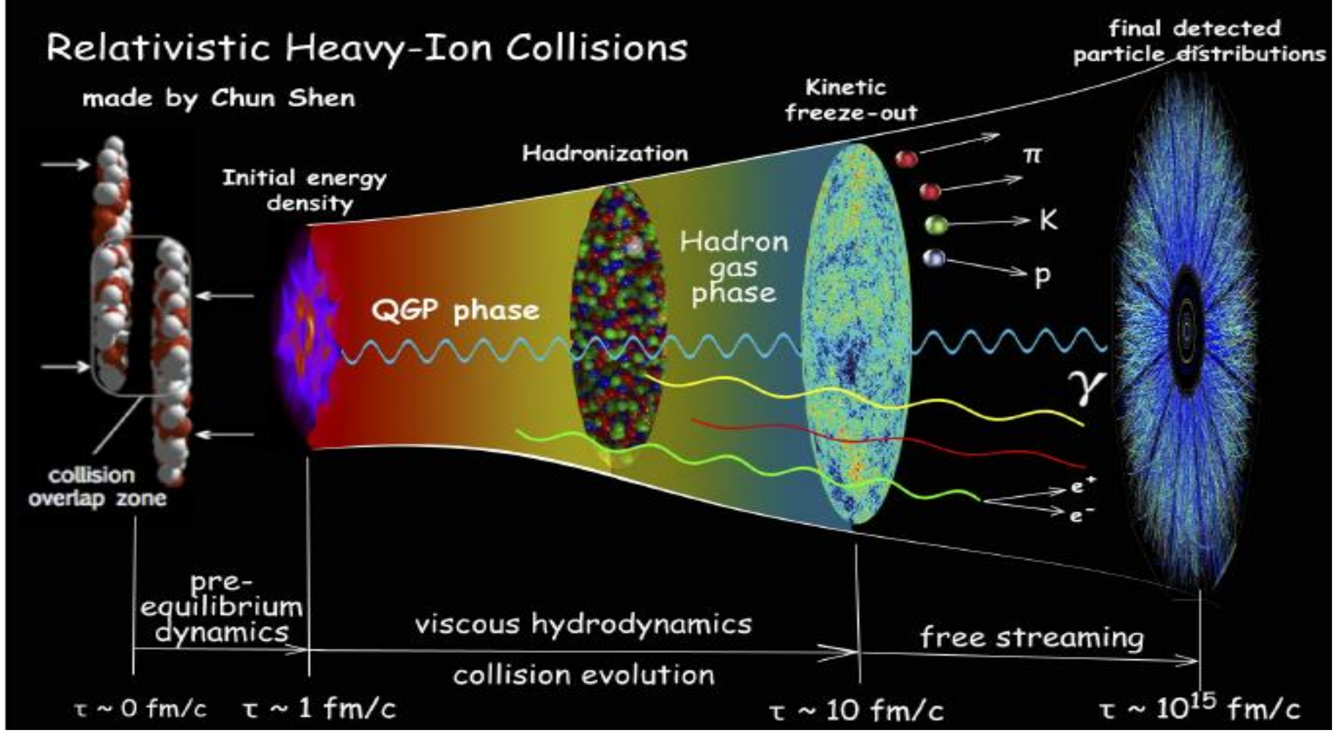
From: 10.1051/epjconf/20159700025
Cartoon of the time evolution of an ultra-relativistic heavy-ion collision

Motivation

Theoretical challenge

- Non-zero chemical potential
- Real time dynamics

  → heavy ion collisions, scattering quenches



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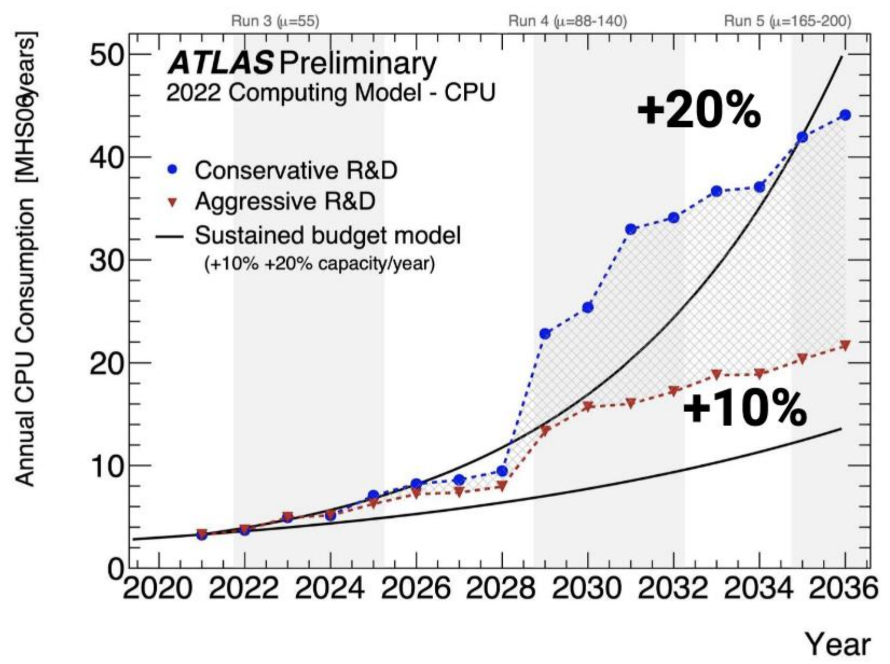
Cartoon of the time evolution of an ultra-relativistic heavy-ion collision



From HL-LHC Projections - ATLAS Software and Computing HL-LHC Roadmap

Computing challenge for High-Lumi LHC

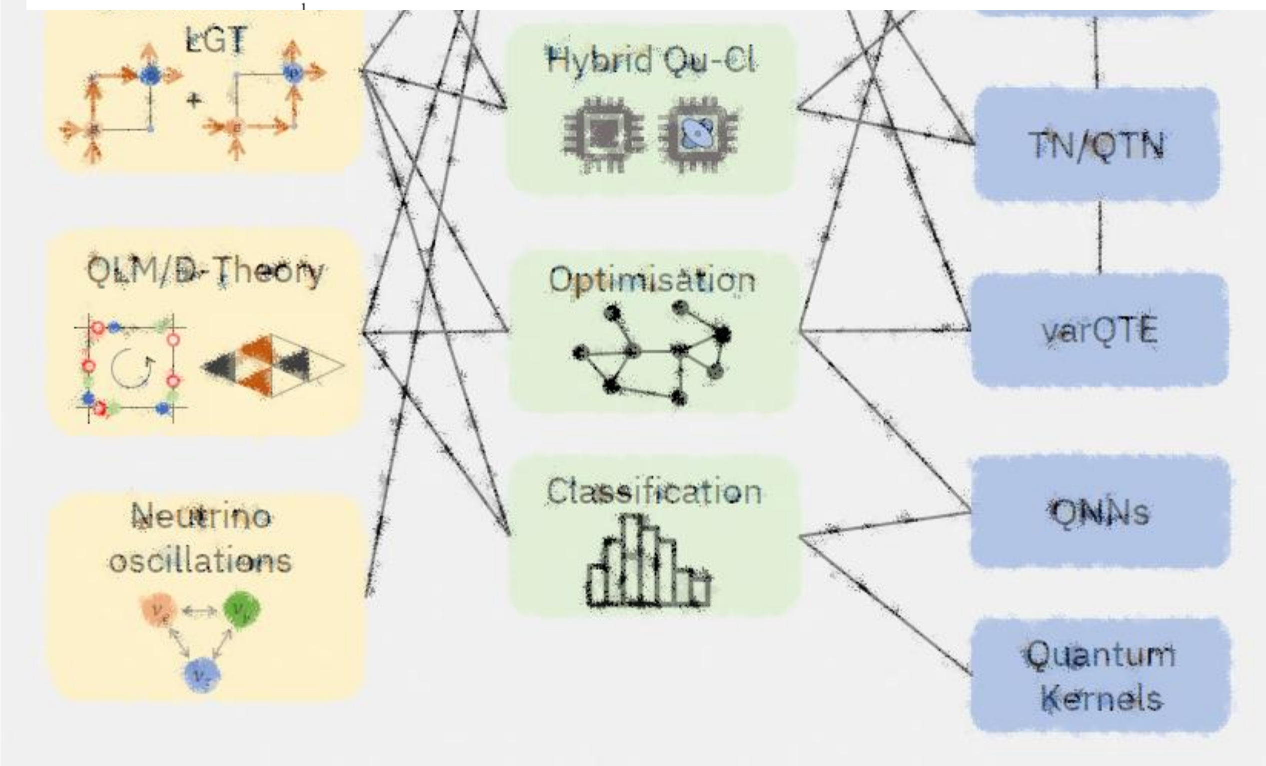
- Simulation and analysis

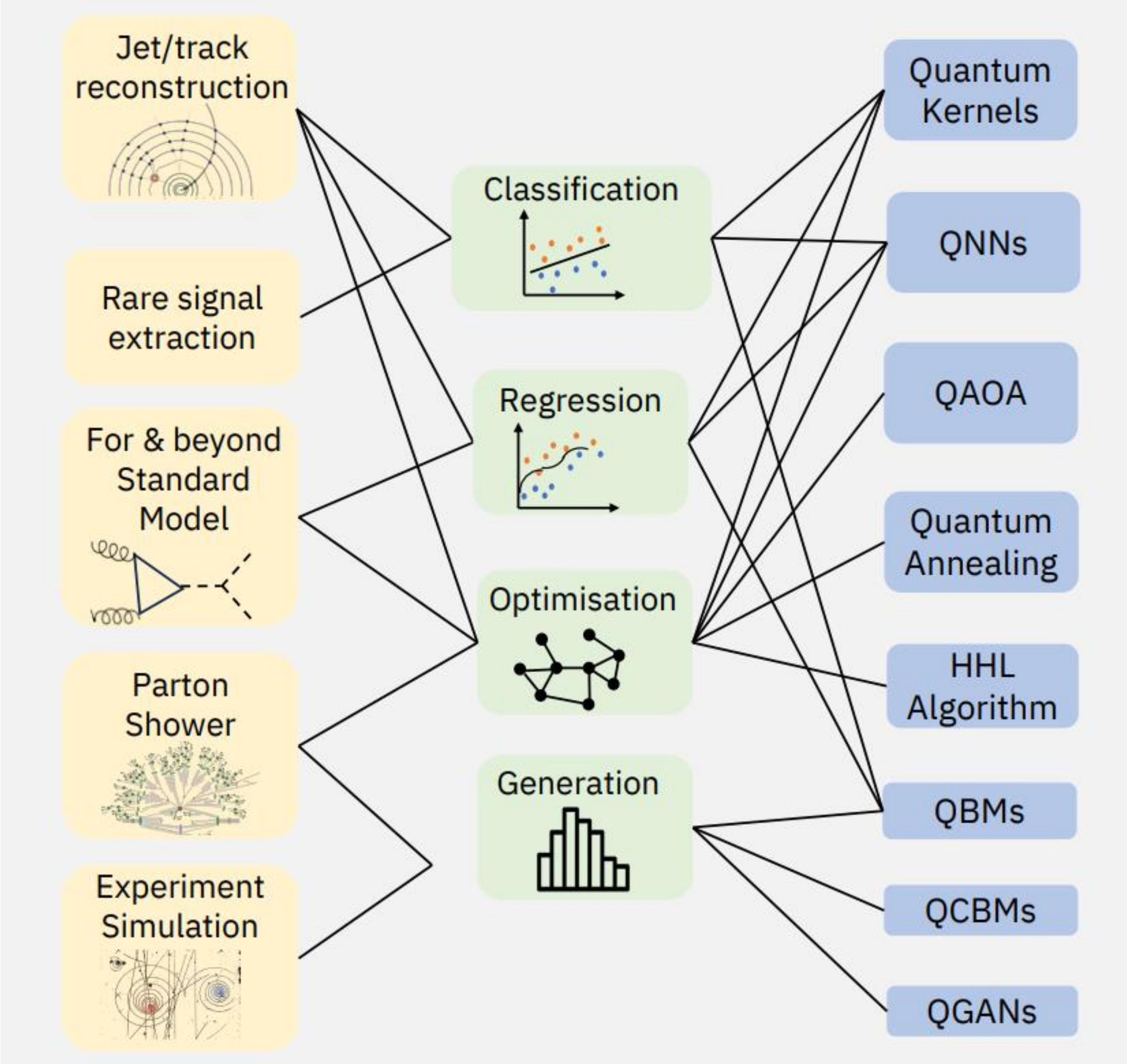
  → need: new technology, algorithms and methods

PRX QUANTUM 5, 037001 (2024)
Roadmap

Quantum Computing for High-Energy Physics: State of the Art and Challenges

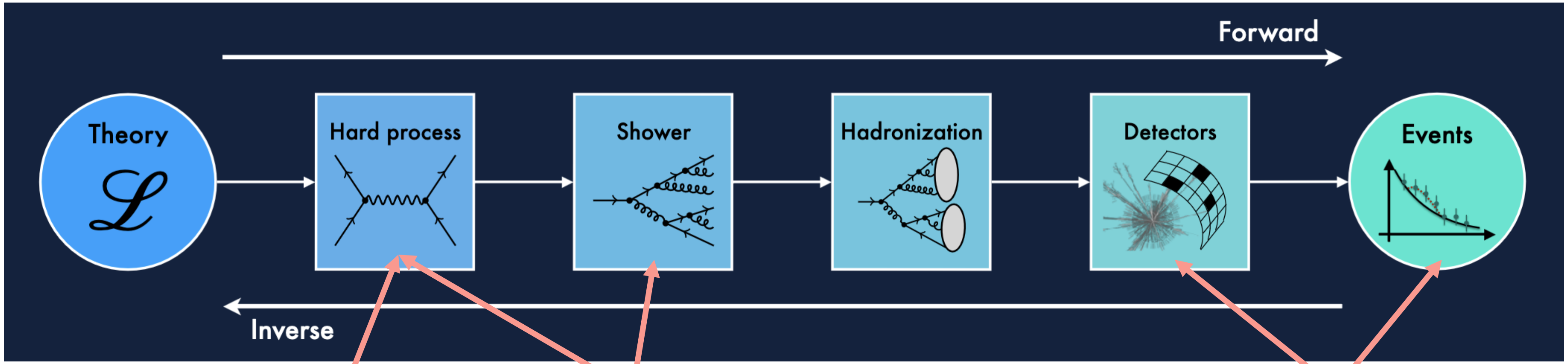
Alberto Di Meglio,[1,*] Karl Jansen,[2,3,†] Ivano Tavernelli,[4,‡] Constantia Alexandrou,[3,5] Srinivasan Arunachalam,[6] Christian W. Bauer,[7] Kerstin Borras,[8,9] Stefano Carrazza,[1,10] Arianna Crippa,[2,11] Vincent Croft,[12] Roland de Putter,[6] Andrea Delgado,[13] Vedran Dunjko,[12] Daniel J. Egger,[4] Elias Fernández-Combarro,[14] Elina Fuchs,[1,15,16] Lena Funcke,[17] Daniel González-Cuadra,[18,19] Michele Grossi,[1] Jad C. Halimeh,[20,21] Zoë Holmes,[22] Stefan Kühn,[2] Denis Lacroix,[23] Randy Lewis,[24] Donatella Lucchesi,[1,25] Miriam Lucio Martinez,[26,27] Federico Meloni,[8] Antonio Mezzacapo,[6] Simone Montangero,[1,25] Lento Nagano,[28] Vincent R. Pascuzzi,[6] Voica Radescu,[29] Enrique Rico Ortega,[30,31,32,33] Alessandro Roggero,[34,35] Julian Schuhmacher,[4] Joao Seixas,[36,37,38] Pietro Silvi,[1,25] Panagiotis Spentzouris,[39] Francesco Tacchino,[4] Kristan Temme,[6] Koji Terashi,[28] Jordi Tura,[12,40] Cenk Tüysüz,[2,11] Sofia Vallecorsa,[1] Uwe-Jens Wiese,[41] Shinjae Yoo,[42] and Jinglei Zhang[43,44]





Are there other indication towards a quantum approach?


Observation of quantum entanglement in top-quark pairs using the ATLAS detector
ATLAS Collaboration
in top−antitop quark events produced at the Large Hadron Collider, using a proton−proton collision data set with
Observation of quantum entanglement in top quark pair production in proton-proton collisions at $\sqrt{s} = 13$ TeV
CMS Collaboration
6 June 2024
Submitted to Reports on Progress in Physics
Abstract: Entanglement is an intrinsic property of quantum mechanics and is predicted to be exhibited in the particles produced at the Large Hadron Collider. A measurement of the extent of entanglement in top quark-antiquark ($t\bar{t}$) events produced in proton-proton collisions at a center-of-mass energy of 13 TeV is performed with the data recorded by the CMS experiment at the CERN LHC in 2016, and corresponding to an integrated luminosity of 36.3 fb^{-1}. The events are selected based on the presence of two leptons with opposite charges and high transverse momentum. An entanglement-sensitive observable D is derived from the top quark spin-dependent parts of the $t\bar{t}$ production density matrix and measured in the region of the $t\bar{t}$ production threshold. Values of $D < -1/3$ are evidence of entanglement and D is observed (expected) to be $-0.480^{+0.026}_{-0.029}$ ($-0.467^{+0.026}_{-0.029}$) at the parton level. With an observed significance of 5.1 standard deviations with respect to the non-entangled hypothesis, this provides observation of quantum mechanical entanglement within $t\bar{t}$ pairs in this phase space. This measurement provides a new probe of quantum mechanics at the highest energies ever produced.
From angular coefficients to quantum observables: a phenomenological appraisal in di-boson systems
arXiv:2409.16731
Michele Grossi,[a] Giovanni Pelliccioli,[b] Alessandro Vicini[c]
Typical entanglement experiment with photons
LHC
eV
KeV
MeV
GeV
TeV



interference [2110.10112]

Bell inequalities [2102.11883, 2203.05582]

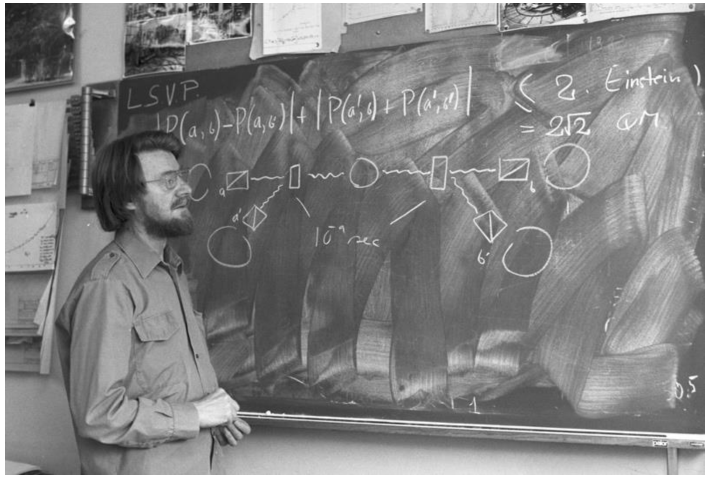
entanglement [1703.02989]

spin correlations [1907.03729]

Fundamental motivation

Utilise information and correlations inherent in HEP data.

Exploit “quantum remnants” in data.

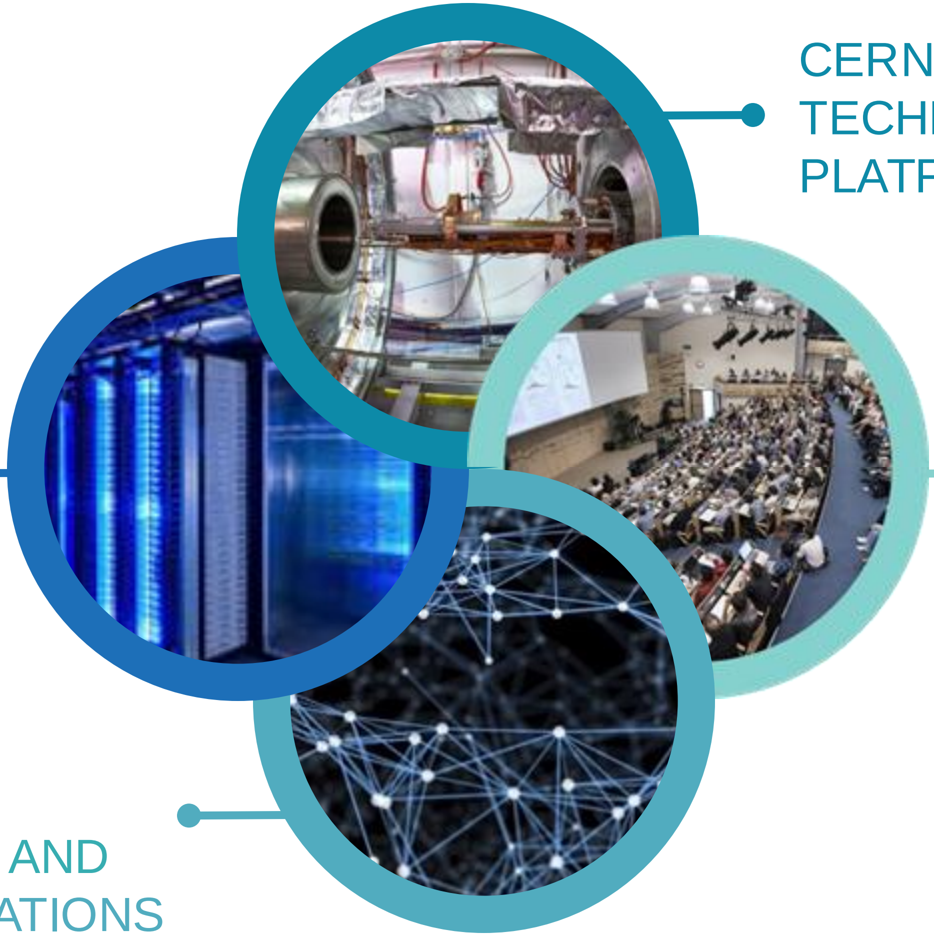


CERN QTI Phase 2

Launched January 2024

CERN QUANTUM TECHNOLOGY PLATFORMS

HYBRID QUANTUM COMPUTING AND ALGORITHMS

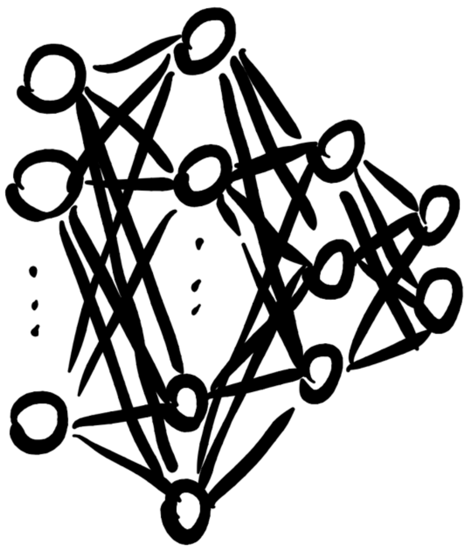


COLLABORATION FOR IMPACT

QUANTUM NETWORKS AND COMMUNICATIONS

A 5 years research plan

From ML to QML: easy?



$\Psi(\vec{x},\vec{\theta}) : \mathbb{R}^{n_{in}} \to \mathbb{R}^{n_{out}}$

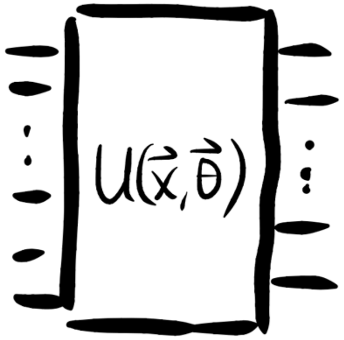
input trainable weights

Classical Neural Network

information

Training (FF)

$|0\rangle^{\otimes n_{in}}$



$|\Psi_{out}(\vec{x},\vec{\theta})\rangle = U(\vec{x},\vec{\theta})|0\rangle^{\otimes n_{in}}$

input trainable weights

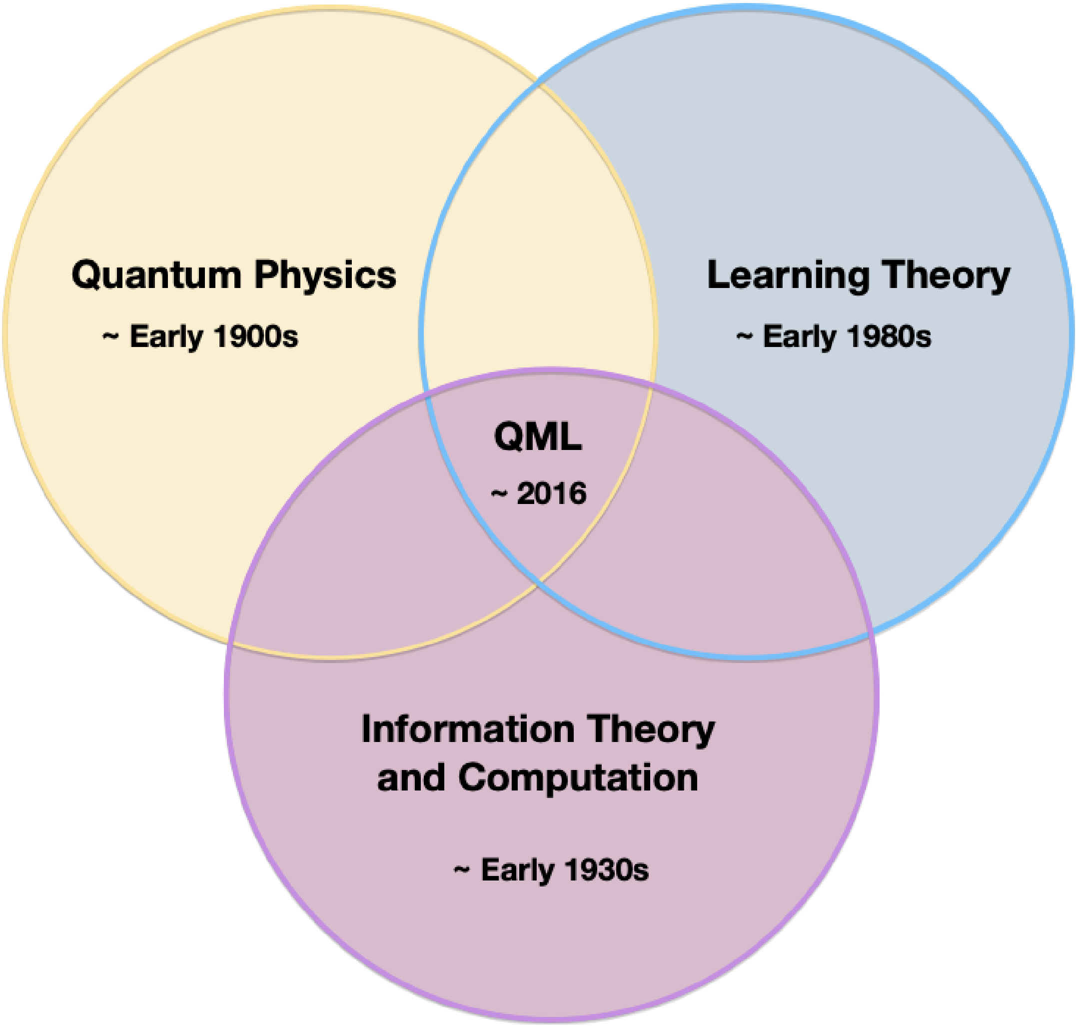
$y(\vec{x},\vec{\theta}) = \langle \Psi_{out}(\vec{x},\vec{\theta}) | \hat{O} | \Psi_{out}(\vec{x},\vec{\theta}) \rangle$

Parametrized Quantum Circuit

Input at different stage of computation

Unitary operations

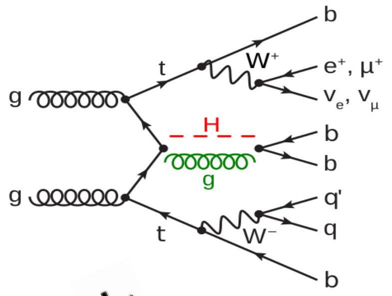
Quantum Machine Learning (QML)



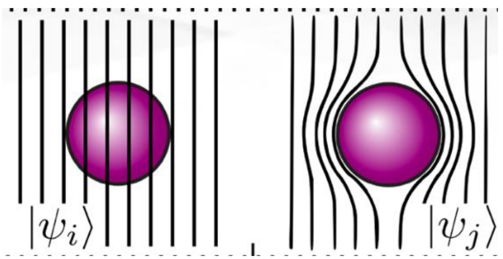
Quantum Circuits for QML

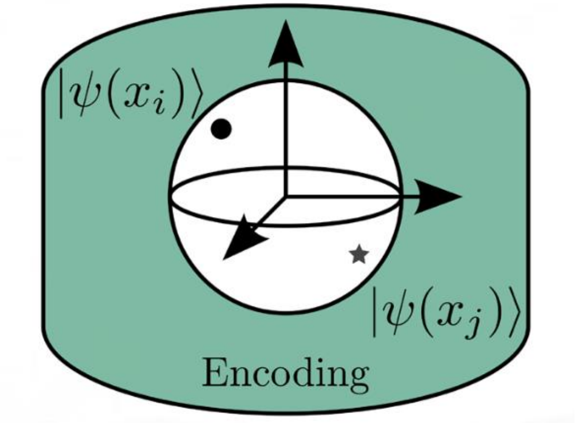
Theoretically: $P(0) = \mathrm{Tr}[|0\rangle\langle 0|\rho]$.
In practice: $P(0) = \frac{N_0}{N}$ with a statistical precision of order $\frac{1}{\sqrt{N}}$

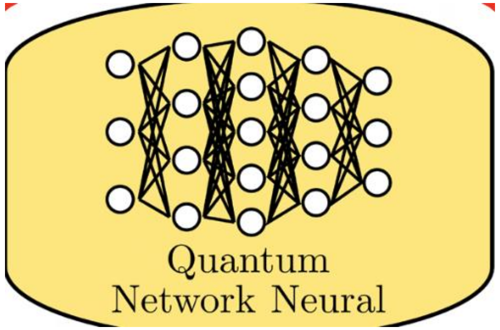
Classical Data



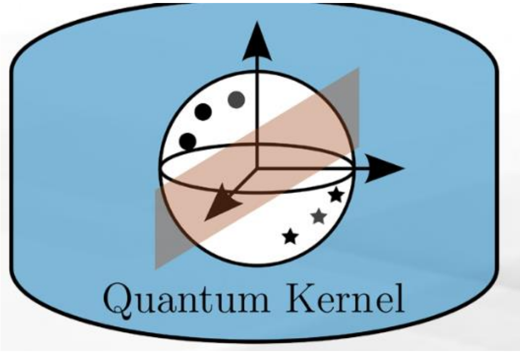
Quantum Data





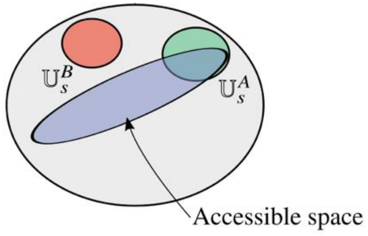


training



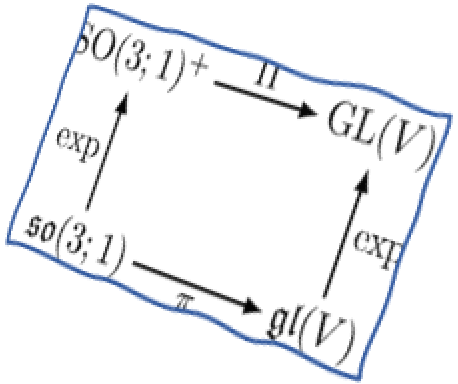
Signal/Background
Paramagnetic/Ferromagnetic
prediction

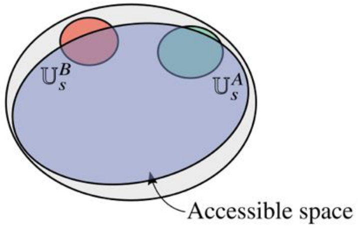
Variational Quantum Algorithms – the Challenge



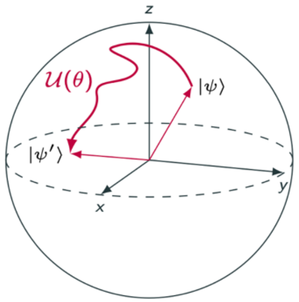
1. **Efficient data handling and data embedding**
2. **Ansatz choice**

   Can we find the most suitable ansatz for the given problem?
   How well can we survey the Hilbert space (SYMMETRY?!)?





3. **Trainability**

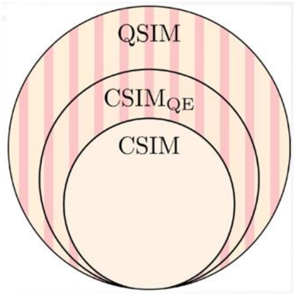


   Can the parameters be updated?

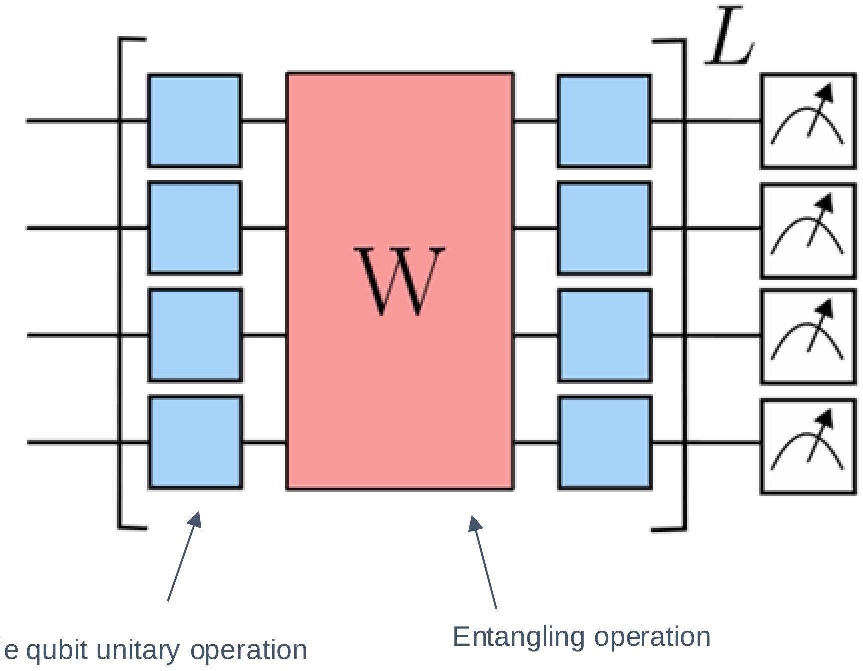
4. **Classical Simulability**

   Are the quantum simulations classically simulable?
   No need for a quantum computer!?

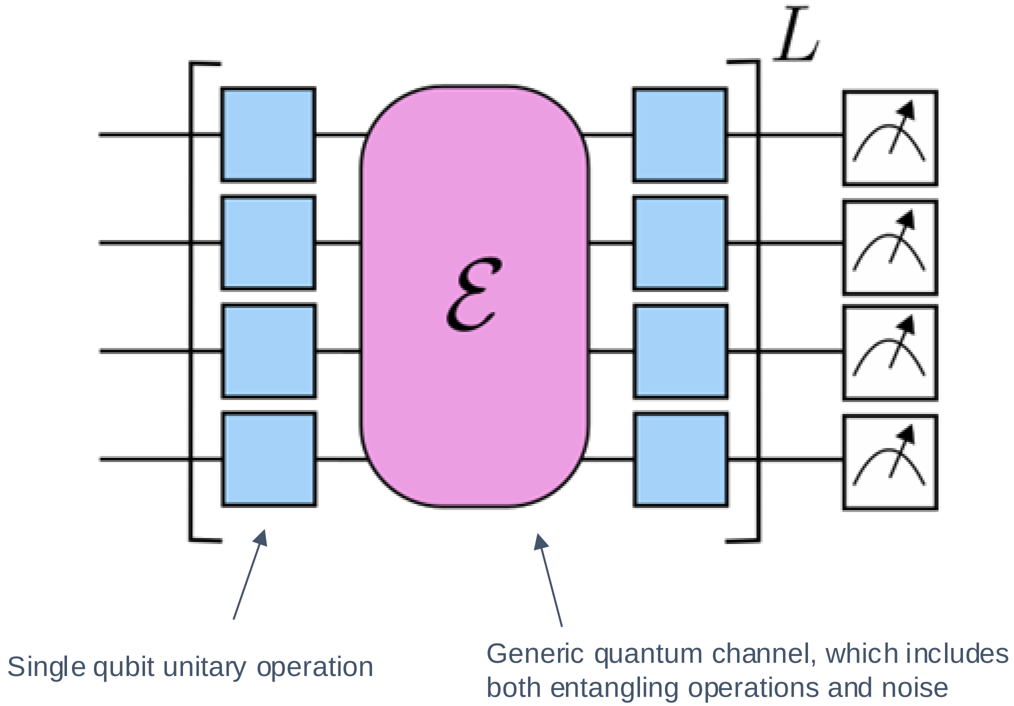
   Just because we can simulate a loss, does not mean it is practical to do so!



What about noise? Non-unitary QML



Add noise



The presence of noise is often overlooked in such analyses

→ Symmetry breaking in geometric quantum machine learning in the presence of noise

[MG et al. PRX Quantum 5, 030314]

→ Estimates of loss function concentration in noisy parametrized quantum circuits

[G. Crognaletti., GM, et al – arXiv:2410.01893]

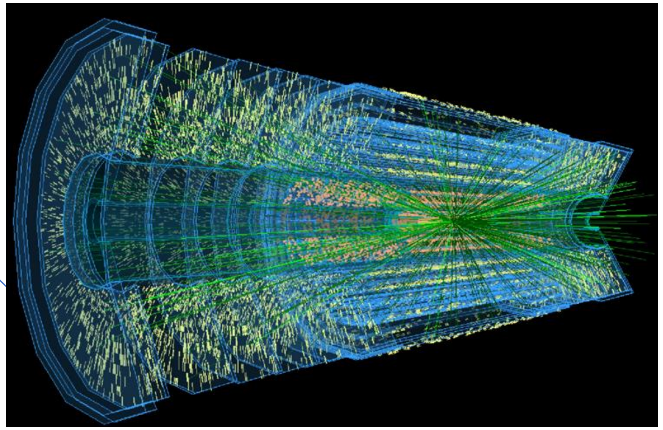
Quantum Motivation & Challenge

CERN examples

Discussion

HEP Pipeline

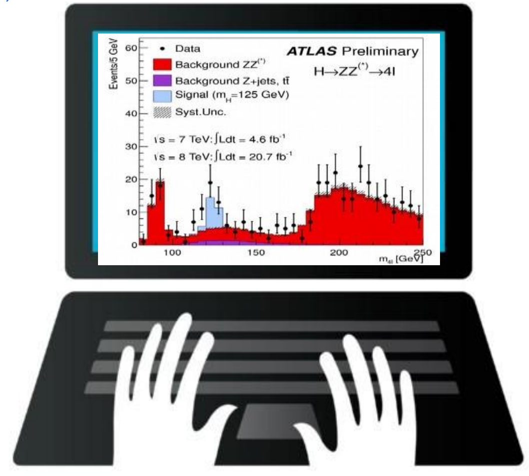
Theory



Calculate (differential) cross sections

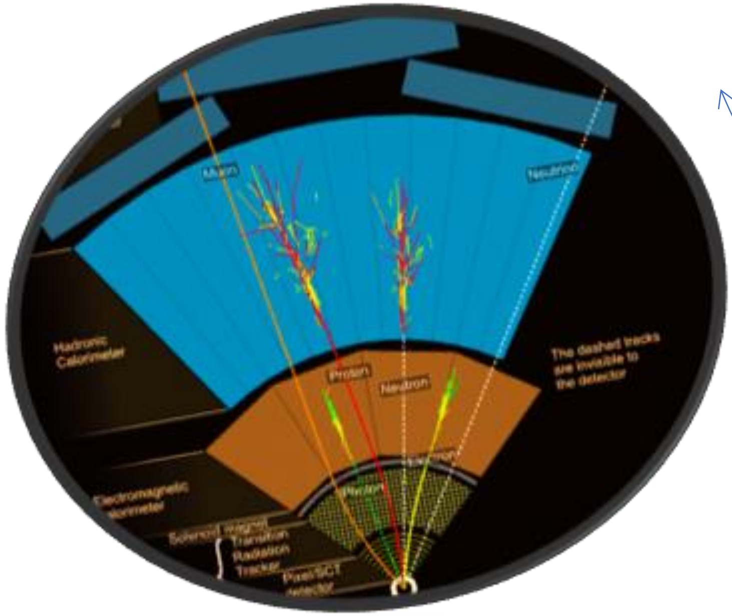
$$d\sigma = \frac{1}{\text{flux}} dx_a dx_b\, f(x_a) f(x_b)\, d\Phi_n \left\langle \, |M_{\lambda,c,\ldots}(p_a, p_b \,|\, p_1, \ldots, p_n)|^2 \, \right\rangle$$

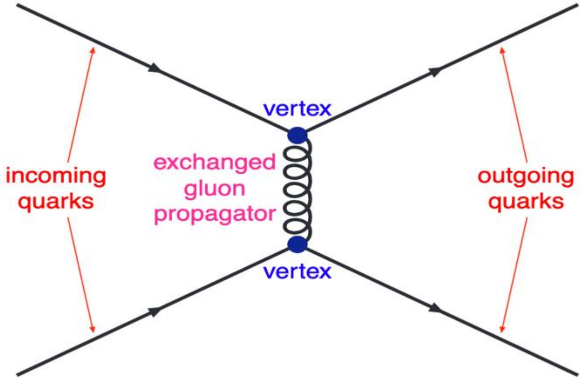
Data Generation



Feature Extraction

Data Analysis





Theory

3 billions CPU hours/year
15% is MC integration

phase-space factor

integrand

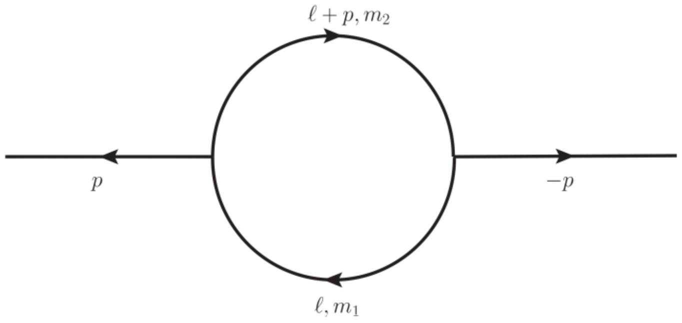
$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

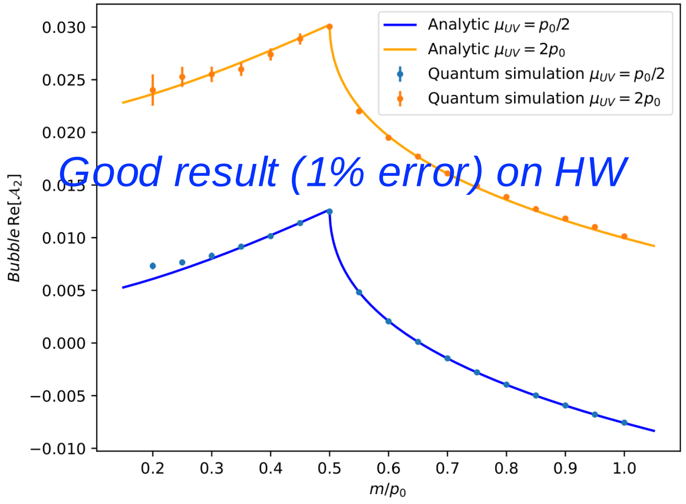
phase-space cuts

probability distributions/
matrix element

Agliardi, Grossi, Pellen, Prati "**Quantum integration of elementary particle processes**." https://doi.org/10.1016/j.physletb.2022.137228

Theory

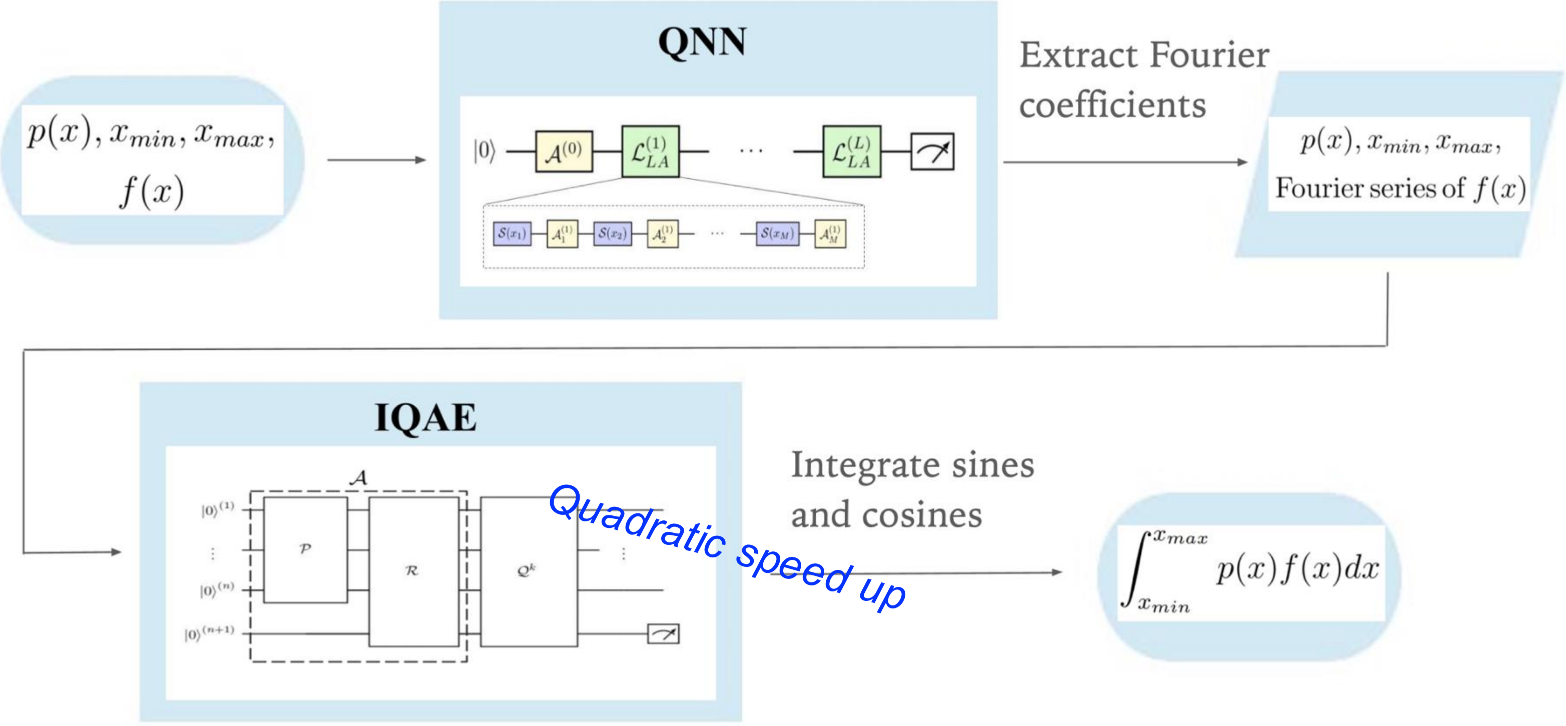




Good result (1% error) on HW

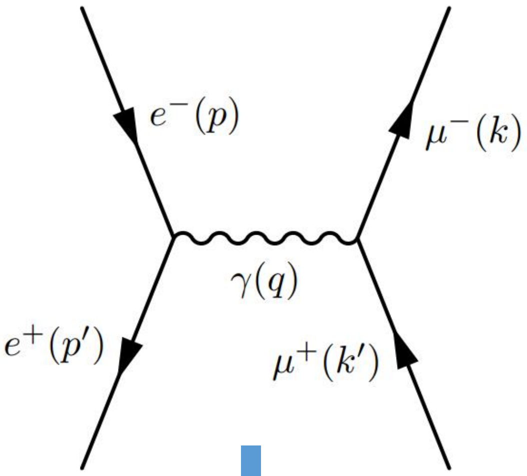
Loop Feynman integral (Bubble)

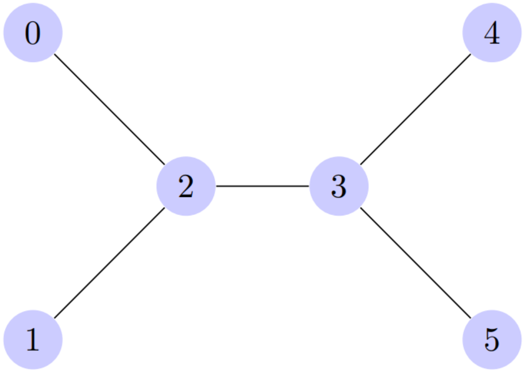
$$\mathcal{A}_2^{(1)}(p, m_1, m_2) = \int_\ell \prod_{i=1}^{2} G_F(q_i) = \int_\ell \frac{1}{(\ell^2 - m_1^2 + \imath 0)\left((\ell + p)^2 - m_2^2 + \imath 0\right)}$$



Quadratic speed up

PhysRevD.110.074031 *- Martinez de Lejarza, GM., et al.*
Loop Feynman integration on a quantum computer





s-channel

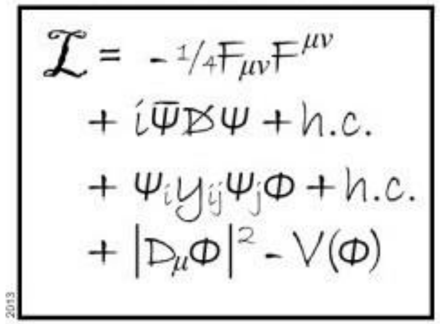
Theory

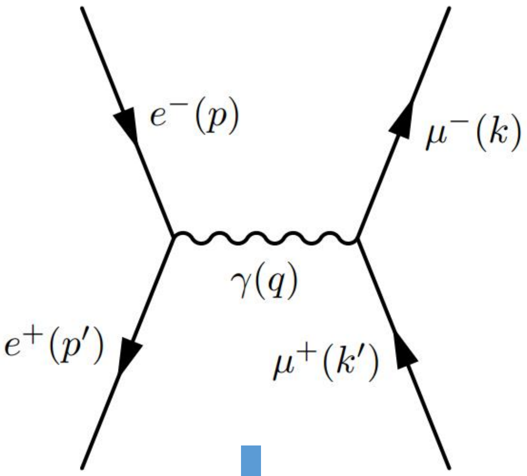
phase-space factor

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

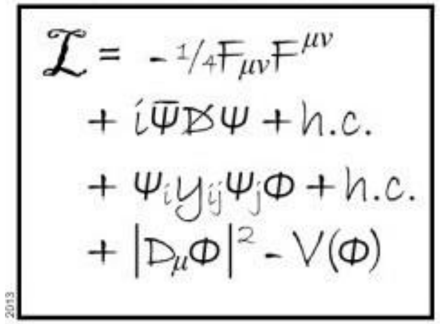
matrix element

phase-space cuts





Theory

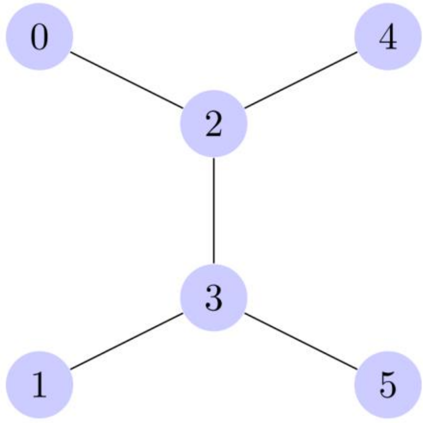


phase-space factor

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

matrix element

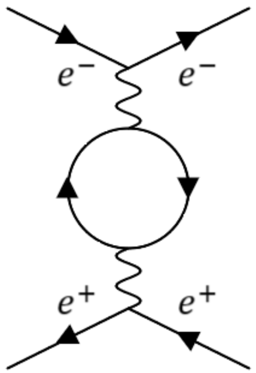
phase-space cuts



t-channel

- Build **a quantum supervised model** that can distinguish (C) and compute (R) the scattering amplitude squared for related Feynman diagrams LO QED process
- Topology encoded in the adjacency matrix of the graph
- Particles (m,Q,S) encoded in the edges
- Time flow (initial state, interaction vertex, final state) encoded in the vertices

Theory

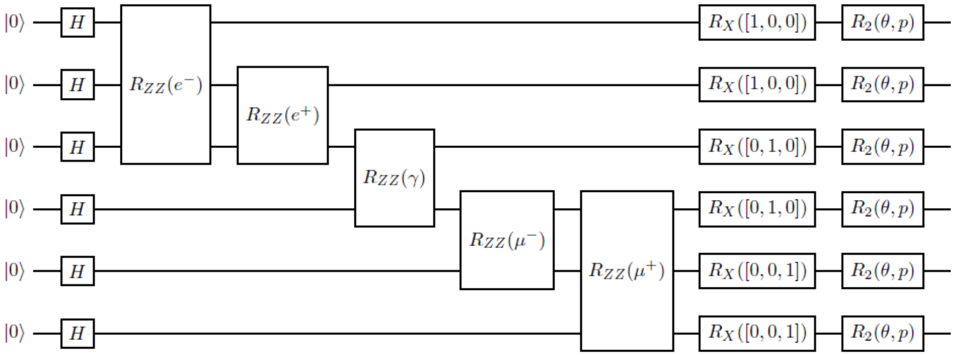


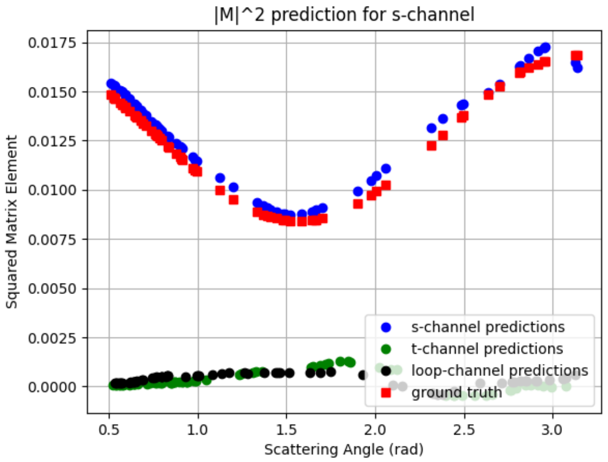
phase-space factor

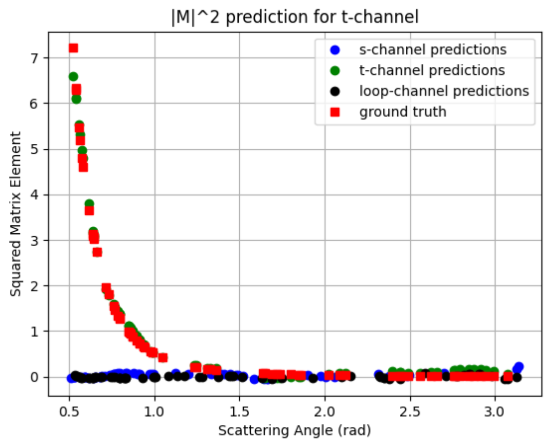
$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

matrix element

phase-space cuts

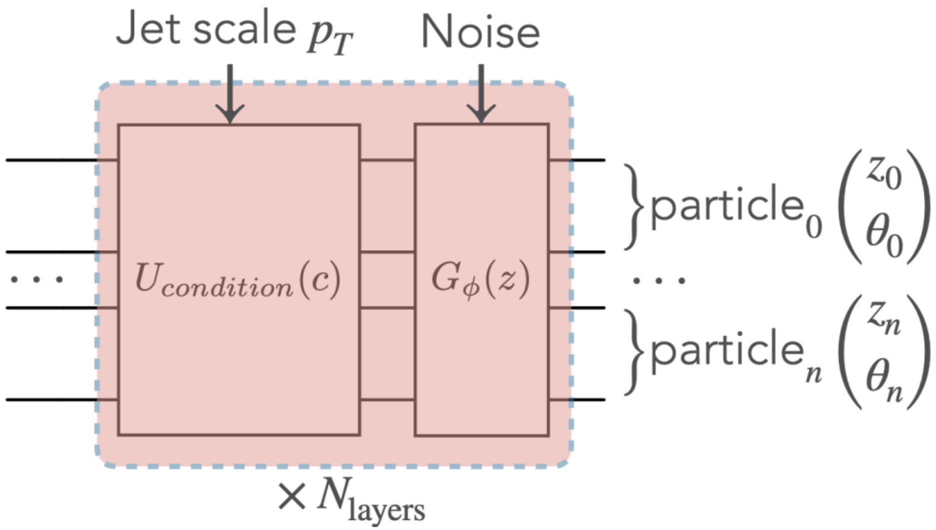




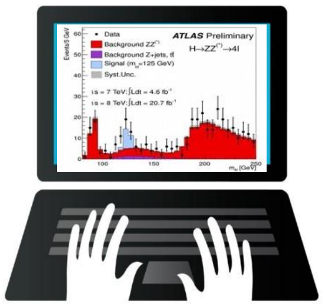


Successful training:

- Is able to learn several diagrams at the same time
- Can learn diagrams with same topology but different particles
- Task difficult with classic approaches



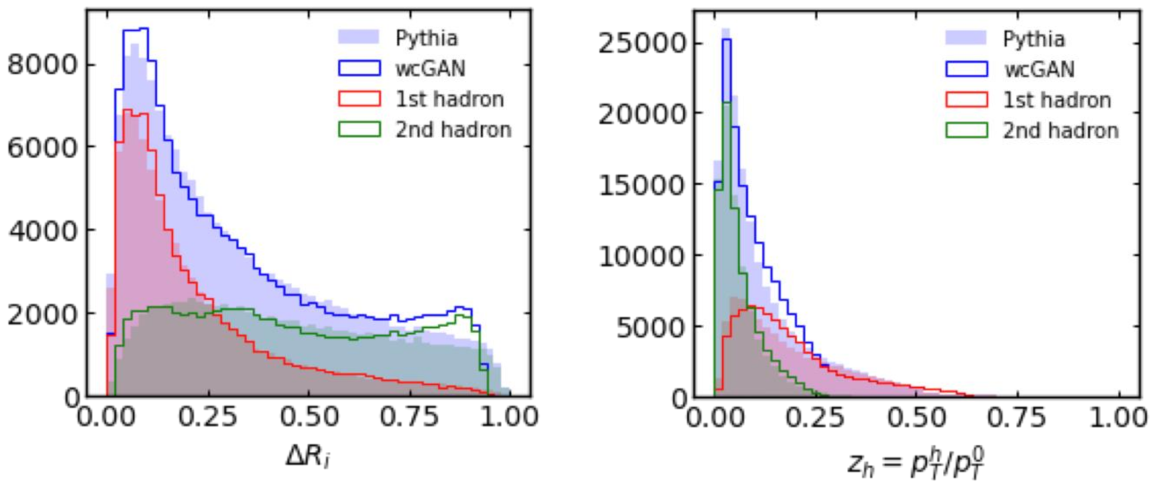
- Each jet constituent represented by two features:
  1. Momentum fraction $z_i = p_T^i / p_T^{jet}$
  2. Angle with reference to the jet axis $\theta_i = \Delta R_i / R$
- qubit → 1 feature: $\mathbf{x}_{\text{fake}} = \{\langle\sigma_Z^0\rangle, \langle\sigma_Z^1\rangle, \ldots, \langle\sigma_Z^n\rangle\}$
- Style-based approach: The noise is inserted in every gate:$R_{x,y,z} \to R_{x,y,z}(w \cdot z + b)$

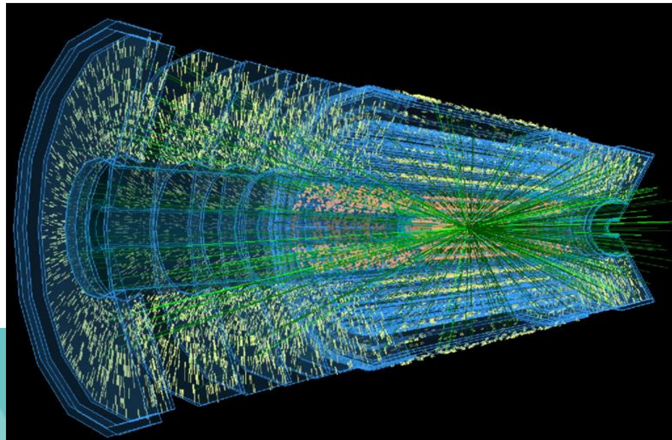


Style-based Hybrid QGAN

The Quantum GAN trained on Z+jets events generated by Pythia8.

Data Generation

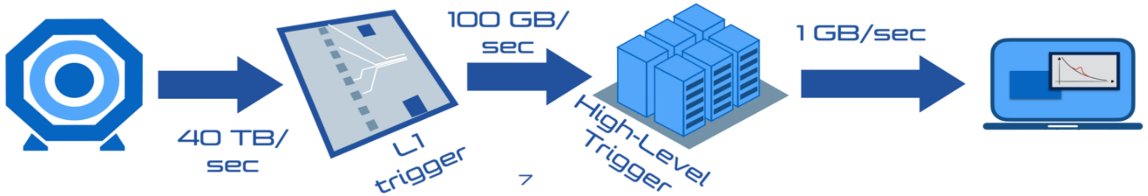




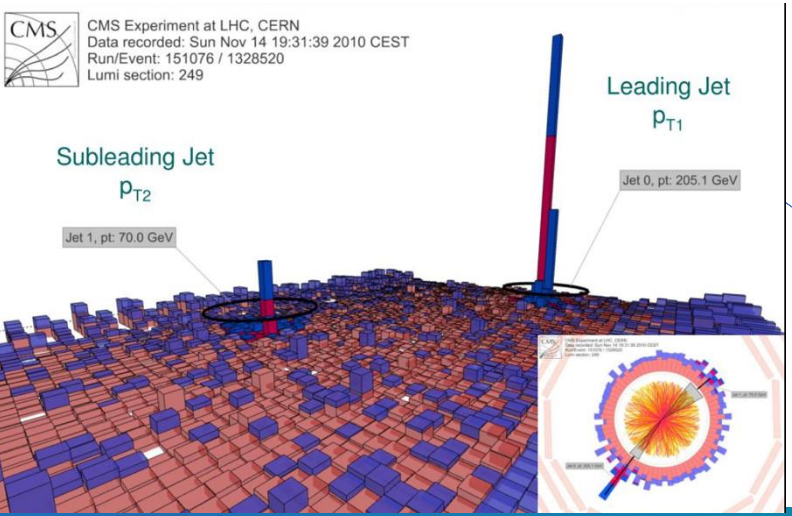
The Quantum GAN captures the distributions of the first and second emissions, reproduce their dependence with the jet scale

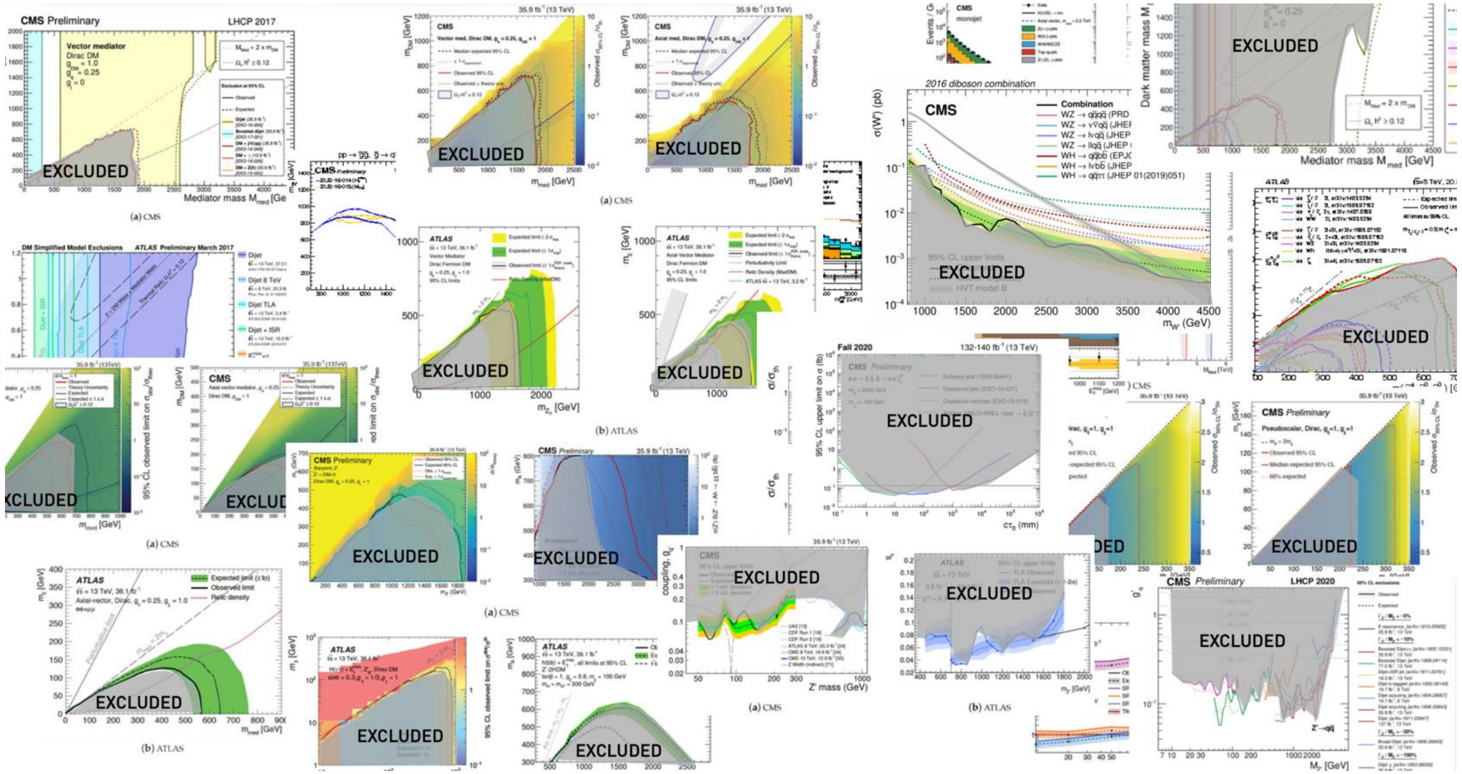
MG, Y. Haddad, V. Croft, C. Tusyz in preparation

Where is NEW PHYSICS?
Are we using the right data?



Data Analysis

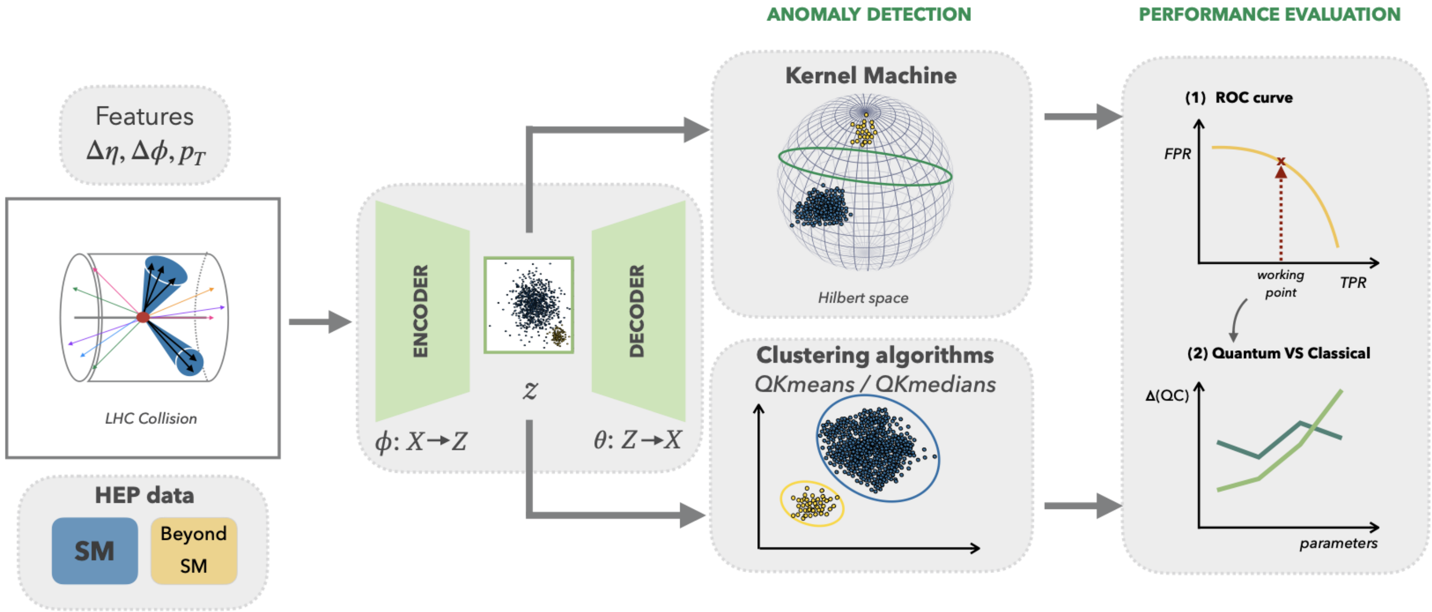


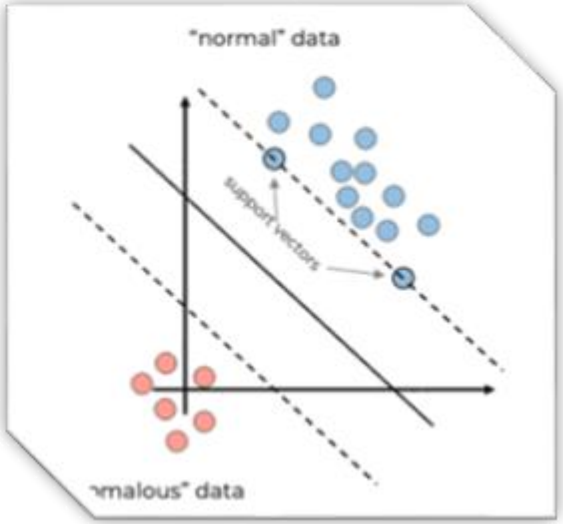


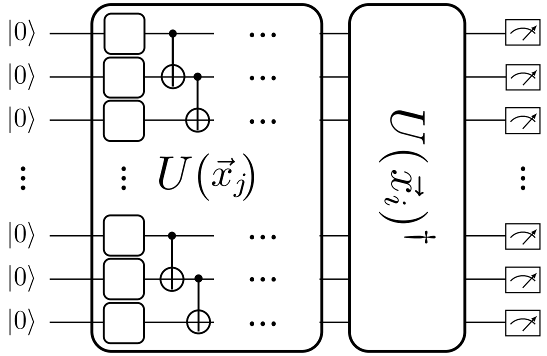
Quantum Anomaly Detection

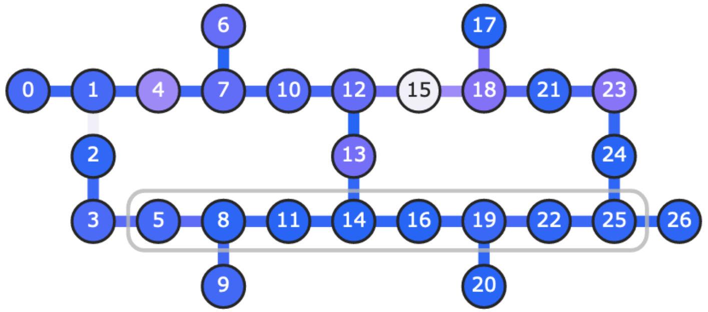
Belis V., GM, et al – *COMMSPHYS-23-1149C*

Data Analysis





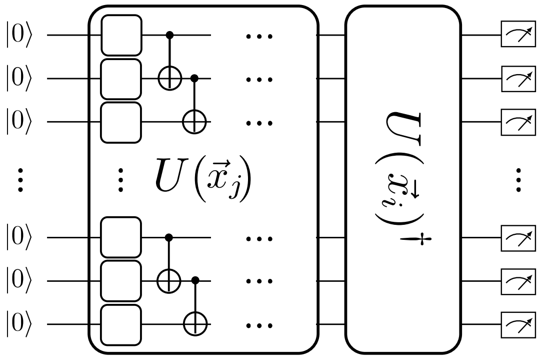


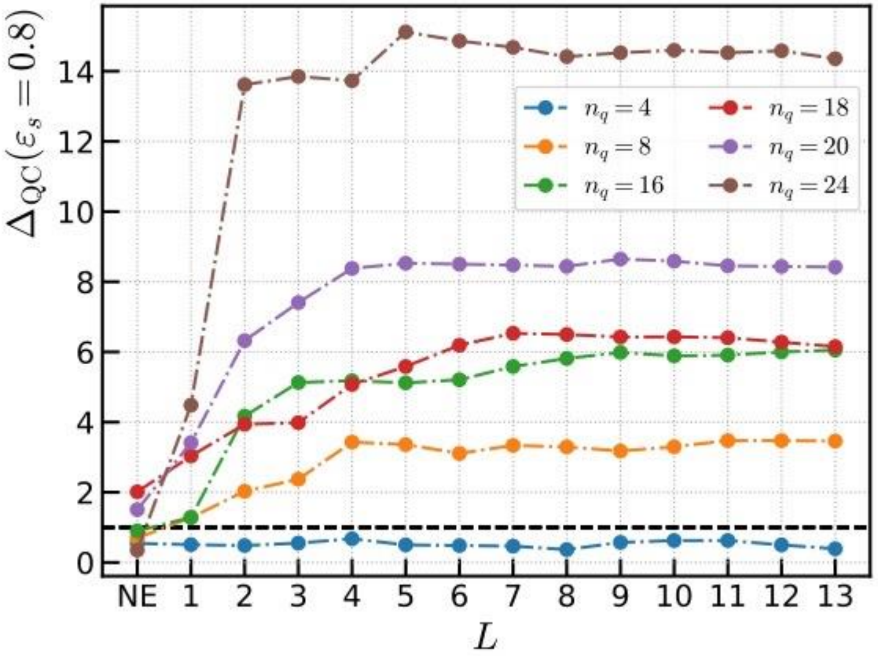


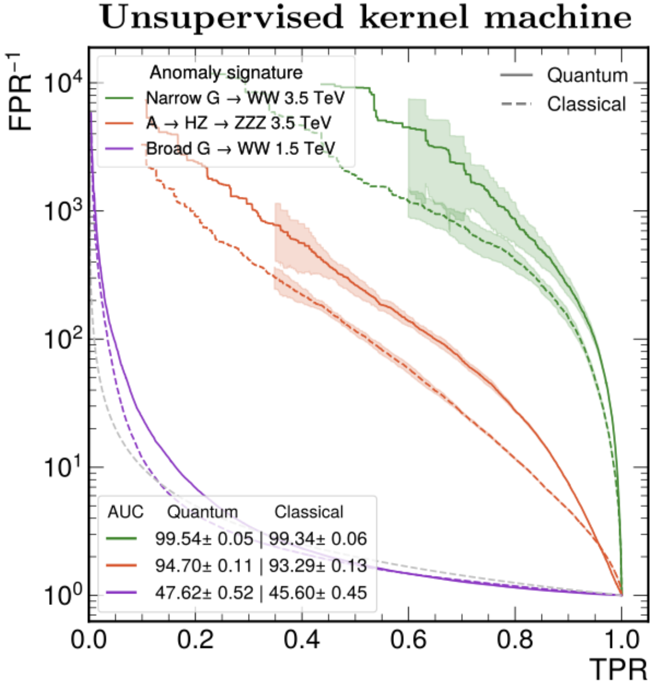
Quantum Anomaly Detection

[Belis V., GM, et al – *COMMSPHYS-23-1149C*]

Data Analysis







Quantum Motivation & Challenge

CERN examples

Discussion

QC research directions in HEP

QC4HEP working group

Concrete challenges

- What are the most promising applications?
- How to **define performance metrics** and validate results?

Experimental data has high dimensionality

- Can we train **Quantum Machine Learning** algorithms effectively?

Experimental data is shaped by physics laws

- Can we leverage them to build better algorithms?
- Can we train the loss on a classical device, and sample on quantum (GENERATIVE MODELs)
- Quantum Error Mitigation is the way, waiting for scalable ERROR CORRECTION

PRX QUANTUM 5, 037001 (2024)

Roadmap

Quantum Computing for High-Energy Physics: State of the Art and Challenges

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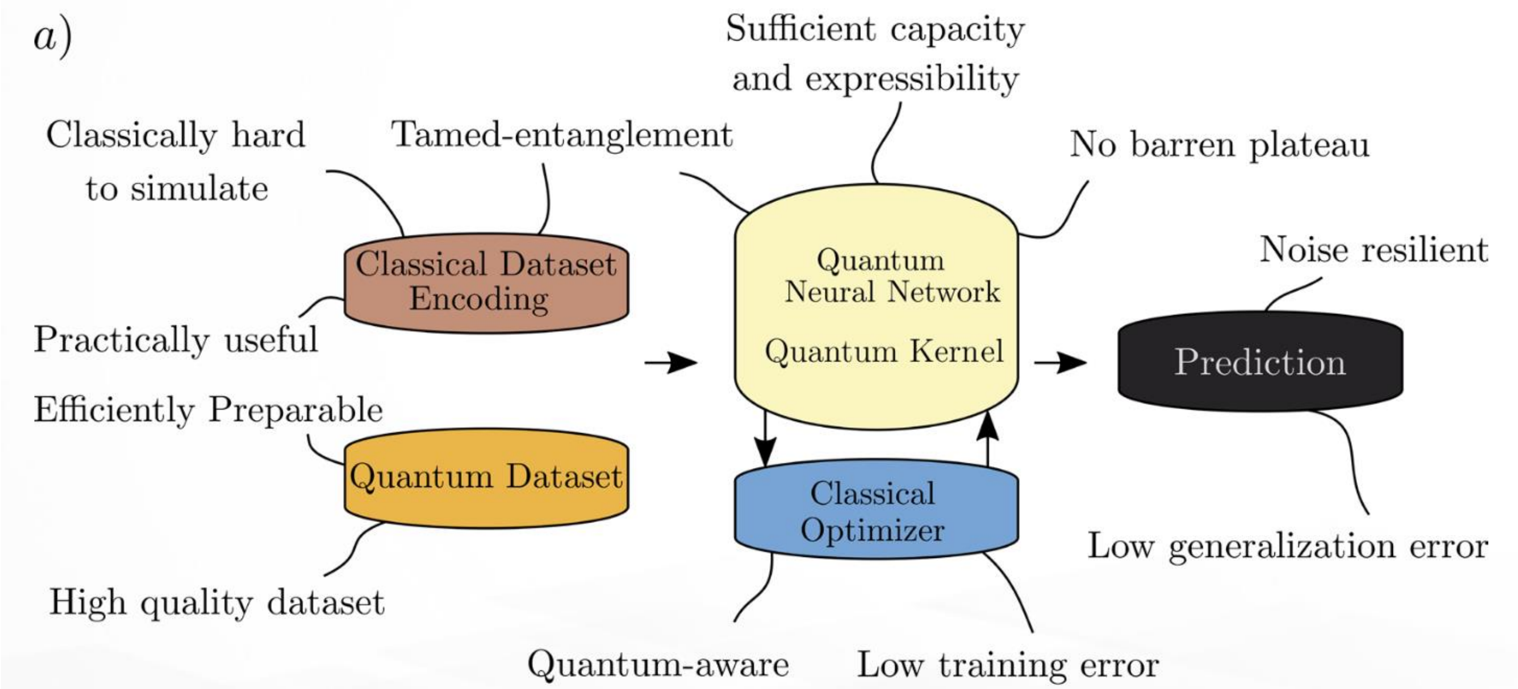
NISQ → ISQ

Variational Quantum Algorithms – Summary

- VQA can't be trusted any more than classical machine learning
- VQA requires linear algebra and python
- Some success has been achieved for small problem sizes (N< 30 qubits)
- We do not yet have the hardware required to test these algorithms at scale



Perspective*: Challenges and opportunities in quantum machine learning,* M. Cerezo, et al., Nature Comp. Sc., 2, 567 (2022).

Quantum Algorithms – Summary

Conventional quantum algorithms

→ come with provable guarantees

→ require significant knowledge of quantum information, group theory, physics, etc.

Query complexity: classical versus quantum

	Determ. machine (worst case)	Quantum computer
Deutsch	2	1
Deutsch–Jozsa	$2^n/2+1$	1
Bernstein–Vazirani	n	1
Grover	2^n-1	$O(\sqrt{2^n})$
Simon	$2^n/2+1$	$O(n)$
Period finding	$O(r)$	$O(1)$

Conclusion

NISQ → ISQ

- Complexity & learning theory mostly gives us insights into **worst-case behavior**

  → ML: Learning theory predicted deep neural networks to not be trainable

  → Optimization: The travelling salesperson problem is NP-complete. An instance with 85900 cities was solved in 2006. Exponential complexity does not imply infeasibility
- **Benchmarking** can help us to understand the behavior on specific instances
- We need to make a comparison of **computational cost** - may lead to poly advantages!
- Change the goal: quantum advantage will be unlikely in many cases **BUT** we can identify promising paths for **hybrid computational advantages**
- We can train the loss on a classical device, and sample on quantum (GENERATIVE MODELs)

  → larger devices for high-quality data?
- What's the role of data?
- Community goal is bridging the gap between near-term and fault-tolerant quantum machine learning

QT4HEP 2025 - save the date