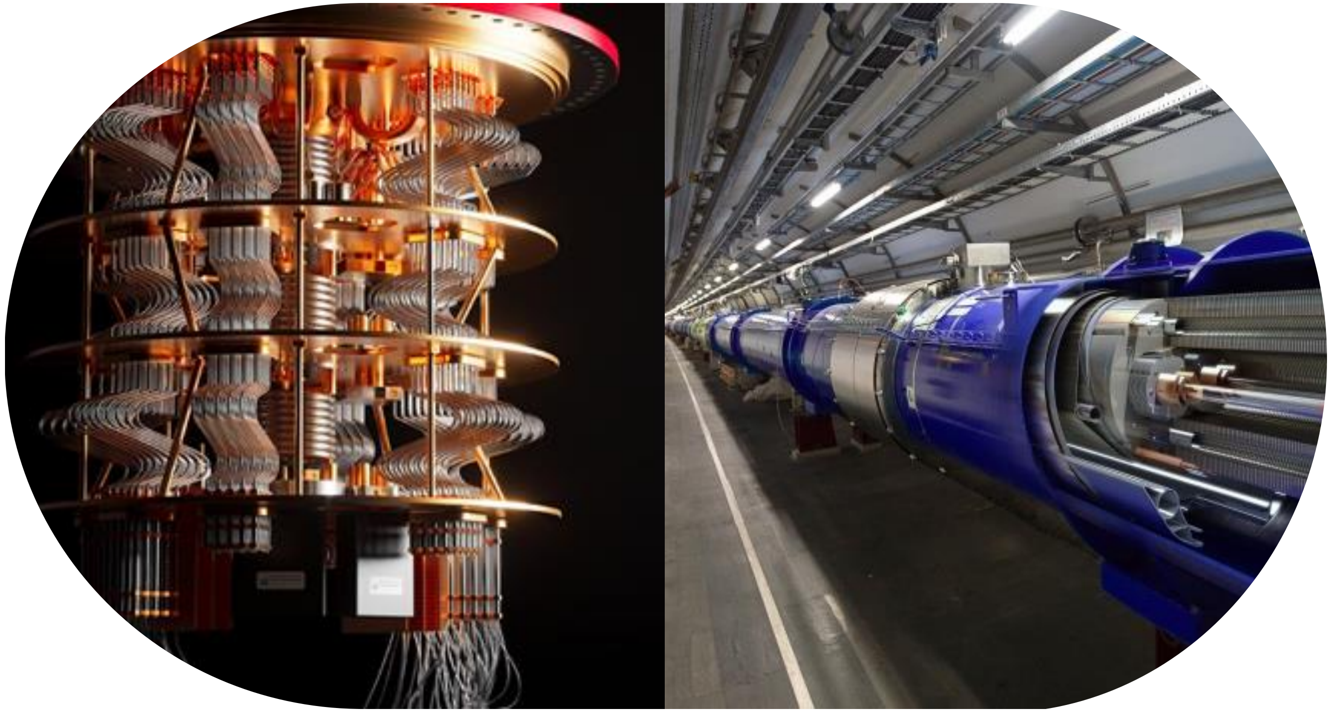
Quantum Machine Learning Integration in the High Energy Physics Pipeline: CERN QTI perspective

Michele Grossi

Hybrid Quantum Computing Infrastructures and Algorithms Coordinator

How does CERN engage in Quantum Technologies?



QT4HEP

Develop technologies required by the CERN scientific programme

Integrate CERN to future quantum infrastructures

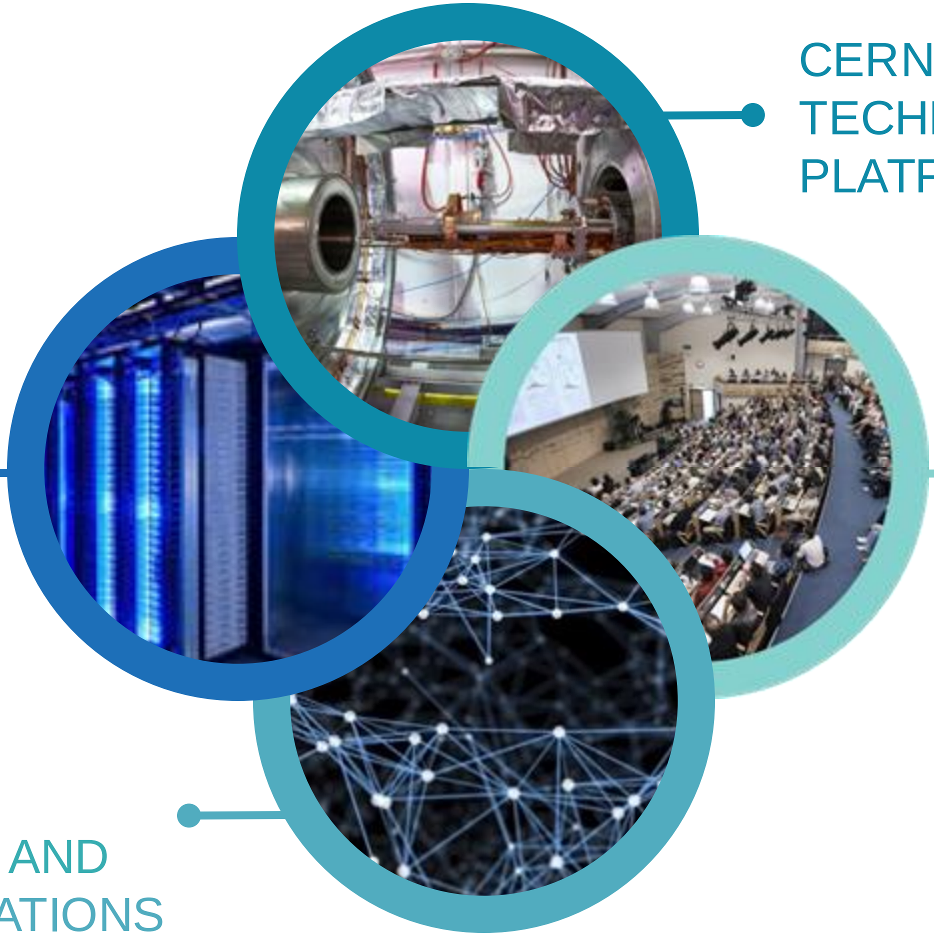
HEP4QT

Extend and share technologies available at CERN

Boost development and adoption of QT beyond CERN

CERN QTI Phase 2

Launched January 2024



CERN QUANTUM TECHNOLOGY PLATFORMS

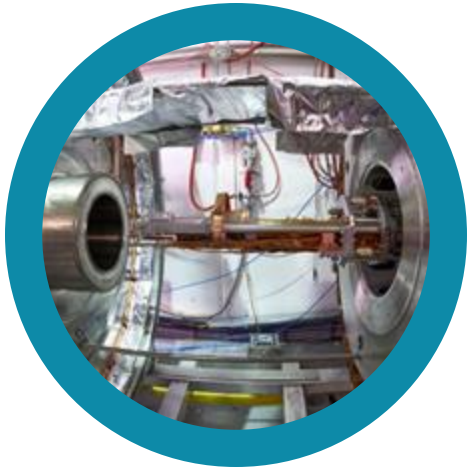
HYBRID QUANTUM COMPUTING AND ALGORITHMS

COLLABORATION FOR IMPACT

QUANTUM NETWORKS AND COMMUNICATIONS

QUANTUM TECHNOLOGY INITIATIVE

A 5 years research plan



CERN QUANTUM TECHNOLOGY PLATFORMS

- Develop quantum sensors to provide new capabilities for particle physics research (dark matter search, axion search, gravitational wave detection…)
- Focus areas: Superconducting RF cavities, hydrogen-like Rydberg ions, and Transition Edge Sensors

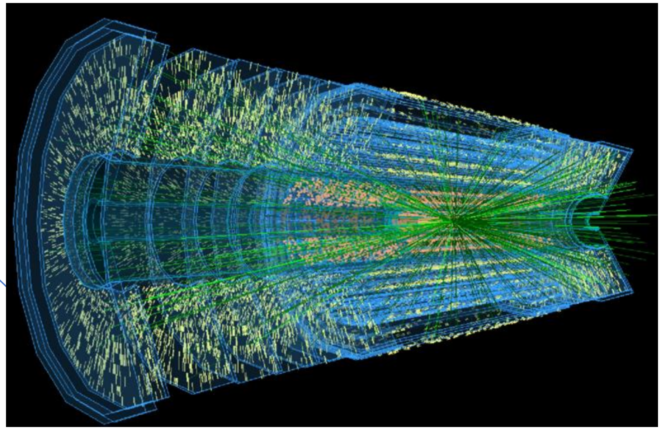
CERN’s broad expertise and experimental facilities in many areas (superconducting materials, magnets, radiation effects, cryogenics, controls etc.) could be useful to support your developments.

HYBRID QUANTUM COMPUTING AND ALGORITHMS

- Integration in the EU and US HPC+QCS infrastructures
- Development of hybrid classic+quantum algorithms for theoretical and experimental physics
- Lead the development of common libraries of quantum algorithms and tools for HEP and other sciences
- Simulation of high dimensional classical / quantum systems
- *Software stacks for quantum devices calibration and control systems*
- *Investigations of distributed quantum computing, resource optimisation, green computing*

HEP Pipeline

Theory

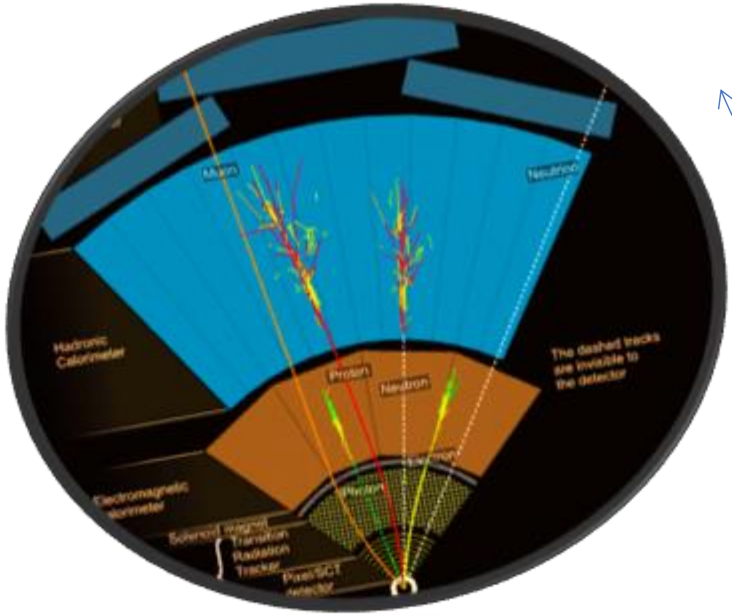


Calculate (differential) cross sections

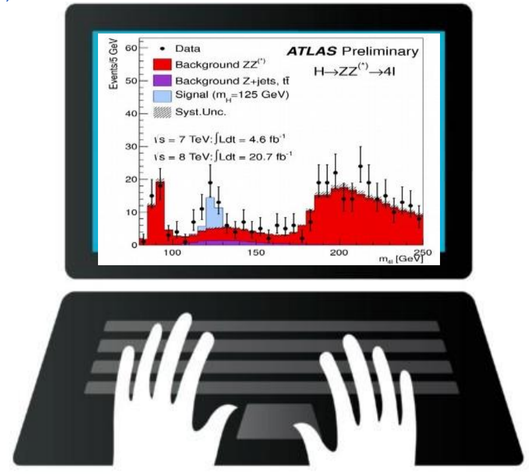
$$d\sigma = \frac{1}{\text{flux}} dx_a dx_b\, f(x_a) f(x_b)\, d\Phi_n \left\langle \, |M_{\lambda,c,\ldots}(p_a, p_b \mid p_1, \ldots, p_n)|^2 \, \right\rangle$$

Data Analysis

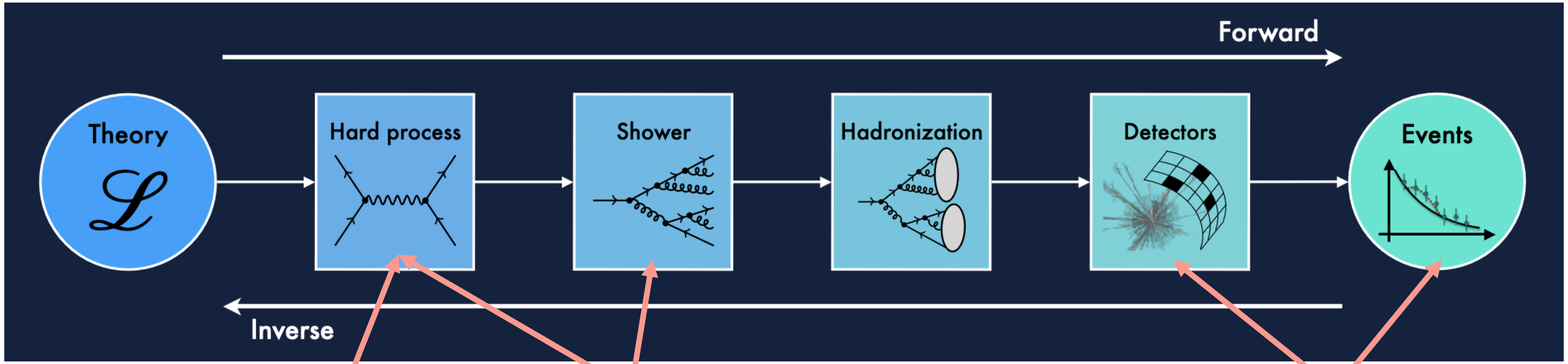
Data Generation



Feature Extraction



Why Quantum Computing for HEP?



interference [2110.10112] *Bell inequalities [2102.11883, 2203.05582]*

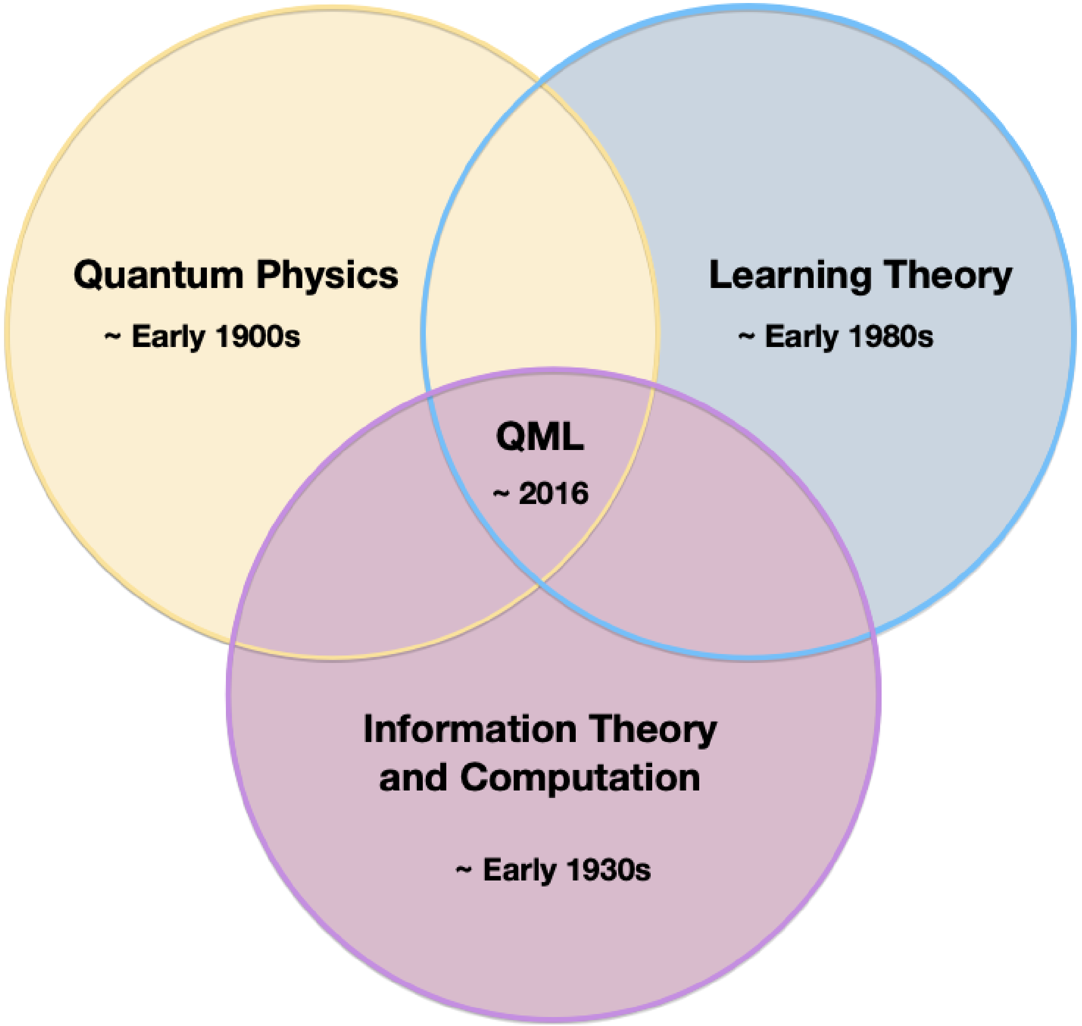
entanglement [1703.02989] *spin correlations [1907.03729]*

Fundamental motivation

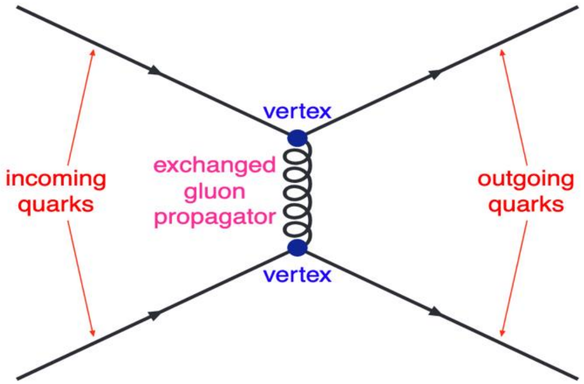
Utilise information and correlations inherent in HEP data.

Exploit "quantum remnants" in data.

Quantum Machine Learning (QML)



Theory



$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} + i\bar{\Psi}\not{D}\Psi + h.c. + \Psi_i y_{ij}\Psi_j\Phi + h.c. + |D_\mu\Phi|^2 - V(\Phi)$$

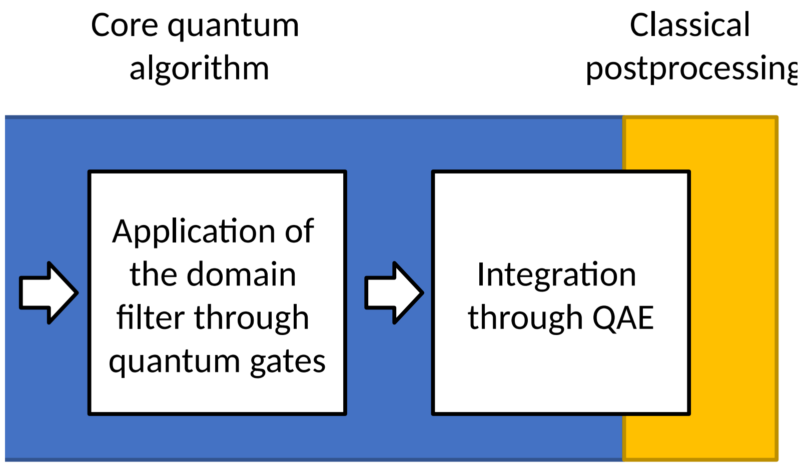
3 billions CPU hours/year
15% is MC integration

phase-space factor *integrand*

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

phase-space cuts

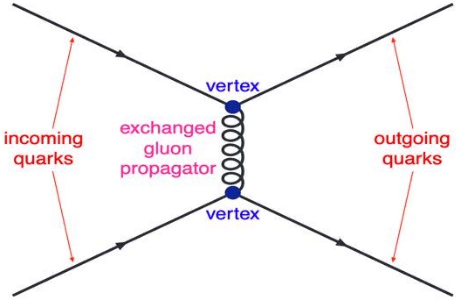
probability distributions/ matrix element



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

With **QAE** the number of call to the algorithm, required to approximate I can be reduced almost quadratically beyond the MC classical bound.

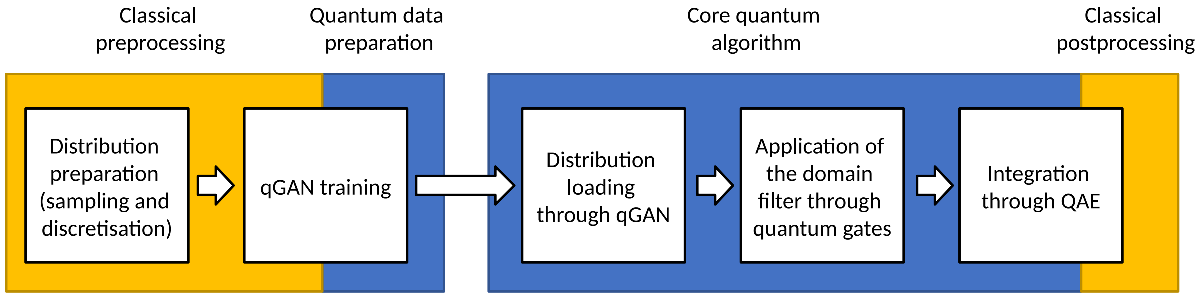
Theory



$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} + i\bar{\Psi}\not{D}\Psi + h.c. + \Psi_i y_{ij}\Psi_j\Phi + h.c. + |D_\mu\Phi|^2 - V(\Phi)$$

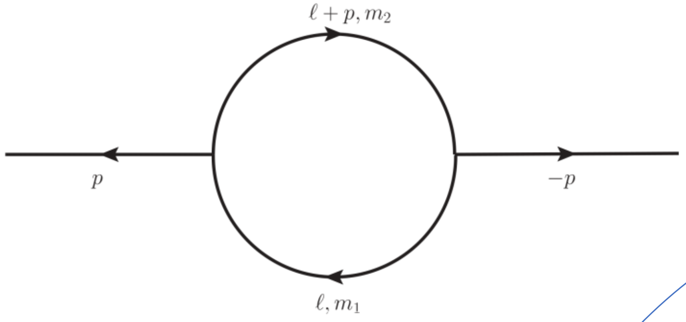
$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

phase-space factor, *matrix element*, *phase-space cuts*

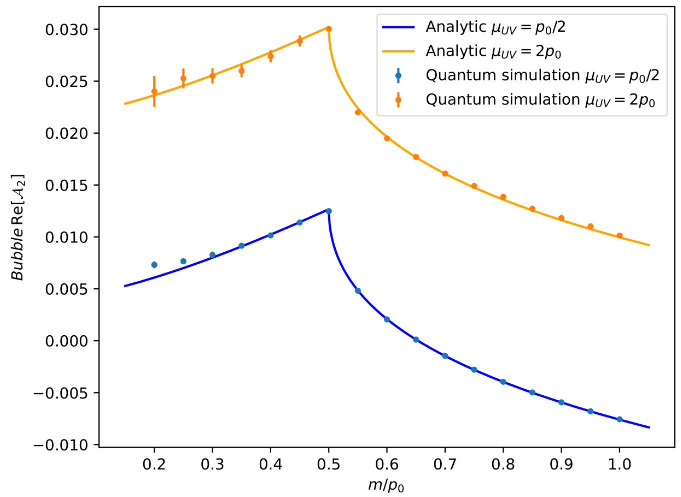


- IQAE: demonstrated speed up
  (Grinko, Gacon, Zoufal, Woerner npj QI 7, 52 (2021))
- QGAN: potential bottleneck for data/function upload
- *Difficult to run on real HW*

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



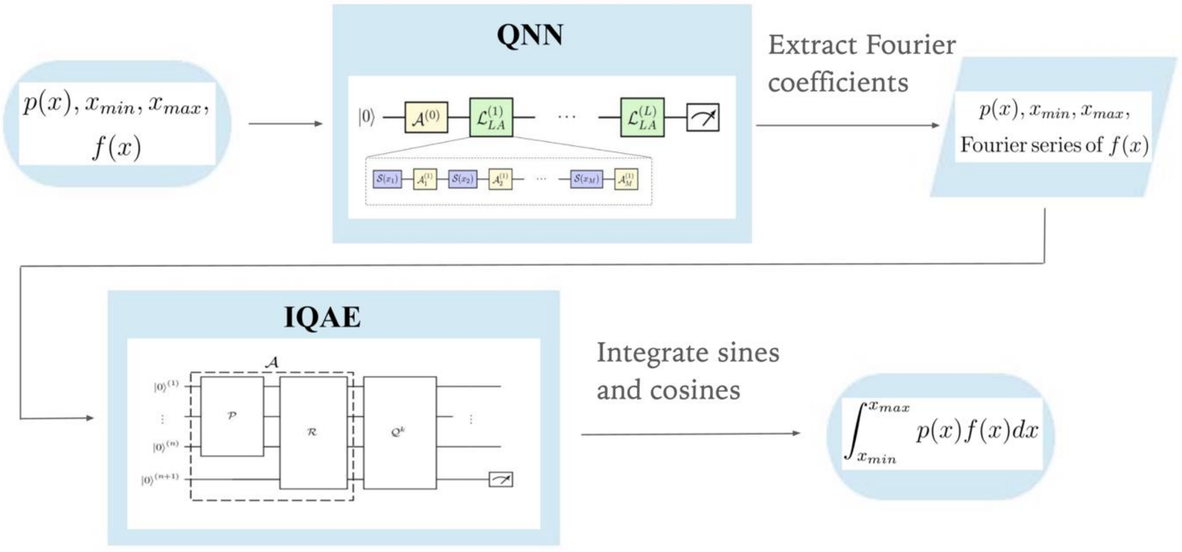
Theory



Loop Feynman integral (Bubble)

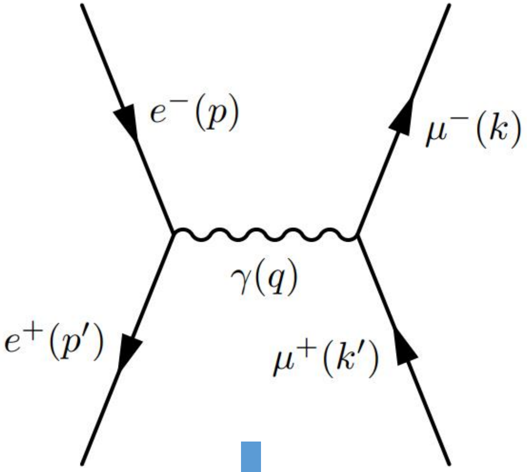
$$\mathcal{A}_2^{(1)}(p, m_1, m_2) = \int_\ell \prod_{i=1}^{2} G_F(q_i) = \int_\ell \frac{1}{(\ell^2 - m_1^2 + \imath 0)\,((\ell + p)^2 - m_2^2 + \imath 0)}$$

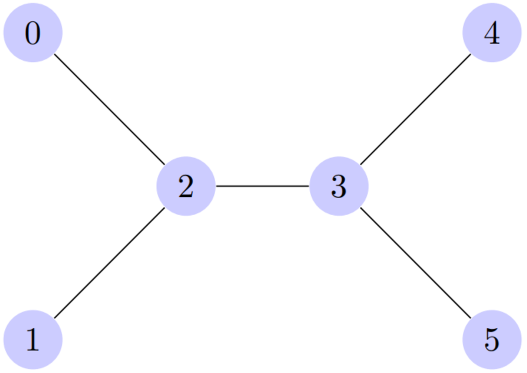
- IQAE: demonstrated speed up
  (Grinko, Gacon, Zoufal, Woerner npj QI 7, 52 (2021))
- Integrate trigonometric functions
- QNN encoding into Fourier series
- **QFIAE** applicable to n-D functions
- Good result (1% error) on HW



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

Jorge J. Martinez de Lejarza, Michele Grossi, Leandro Cieri and German Rodrigo: arXiv: 2305.01686





s-channel

Theory

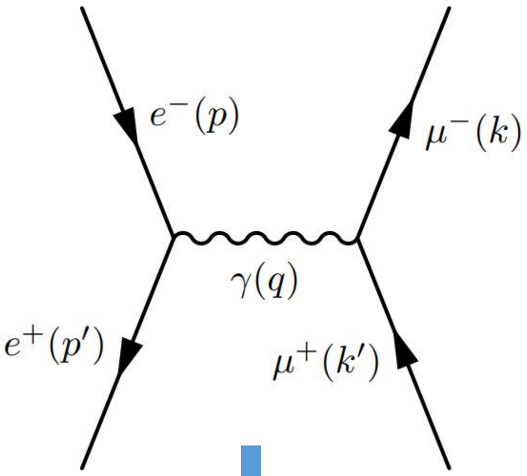
$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} + i\bar{\Psi}\not{D}\Psi + h.c. + \Psi_i y_{ij}\Psi_j\Phi + h.c. + |D_\mu\Phi|^2 - V(\Phi)$$

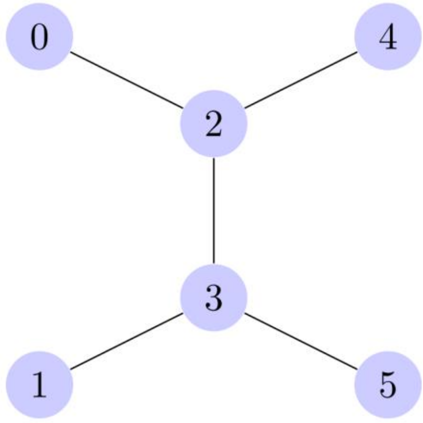
$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

phase-space factor

matrix element

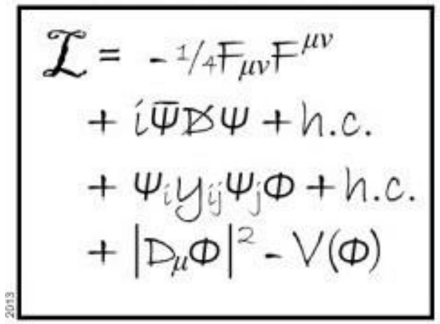
phase-space cuts





t-channel

Theory



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

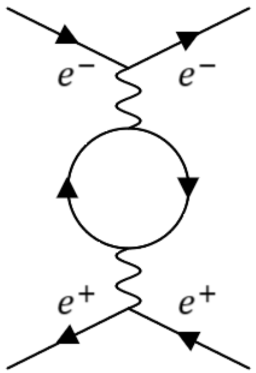
phase-space factor

matrix element

phase-space cuts

- 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

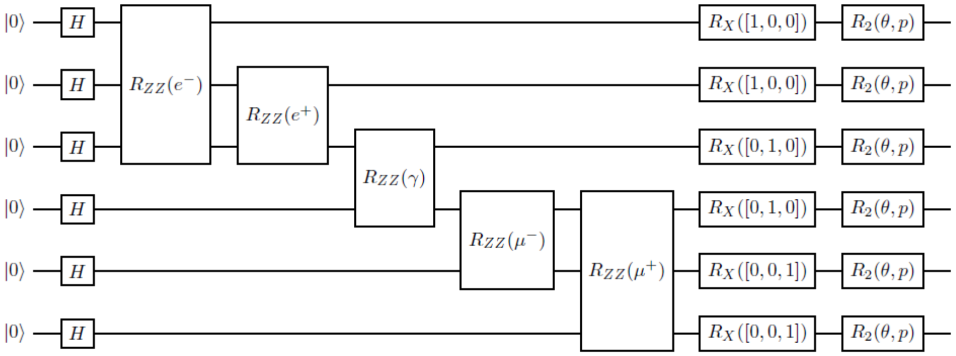


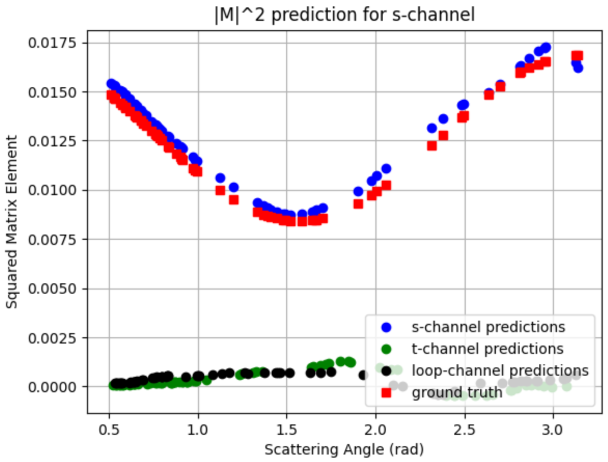
phase-space factor

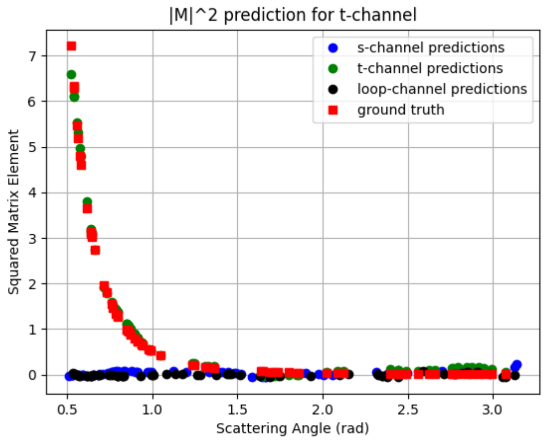
$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

matrix element

phase-space cuts



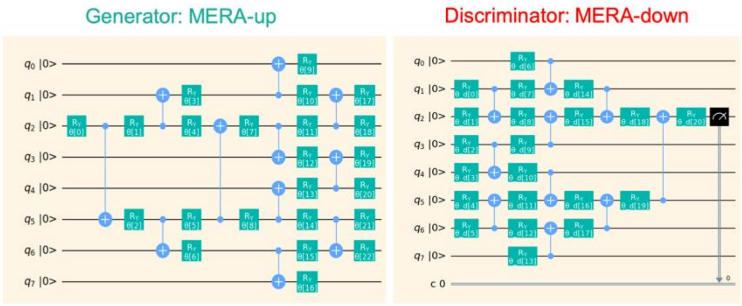


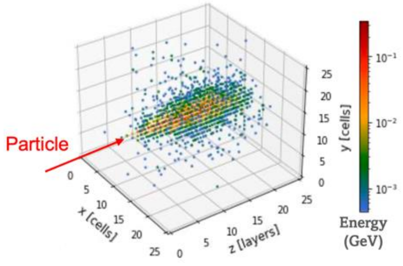


Successful training:

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

F.Rehm et al., **Precise image generation on current noisy quantum computing devices,**
Quantum Sci. Technol. **9** 015009





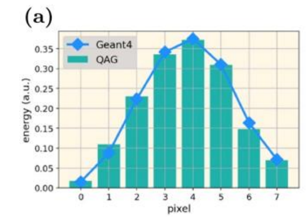
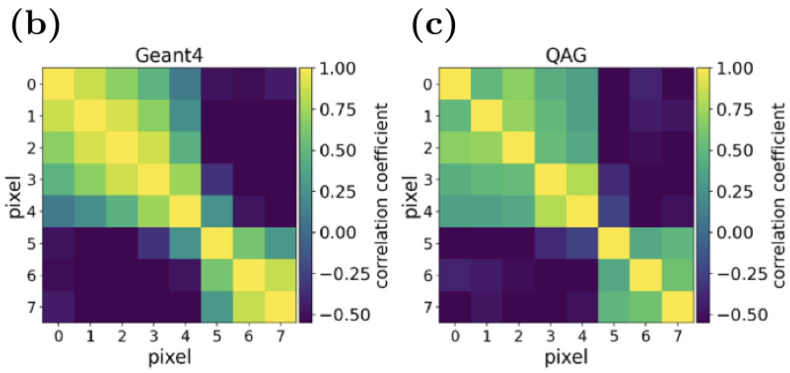
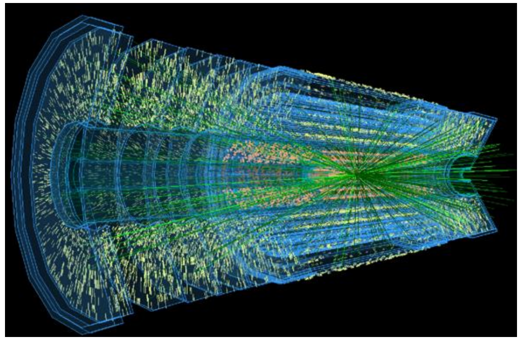


Figure 6. (a) Visualization of the average calorimeter shower shapes. The energy is given in an arbitrary unit (a.u.) due to image downsampling. The pixel-wise correlation plot for (b) Geant4 and (c) the QAG model. The correlation ranges between −1 and 1; a value of 1 indicates a perfect positive correlation.

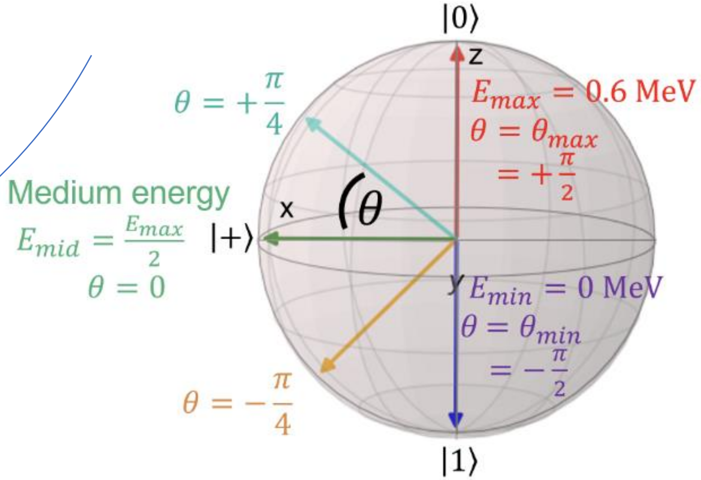




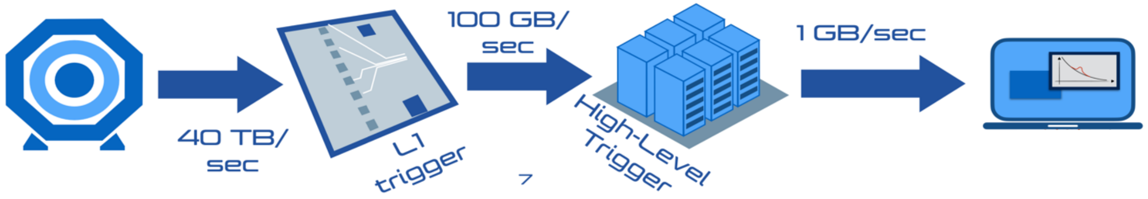
Data Generation

- Quantum angle generator (QAG): a full quantum machine learning model designed to generate accurate images on current quantum devices

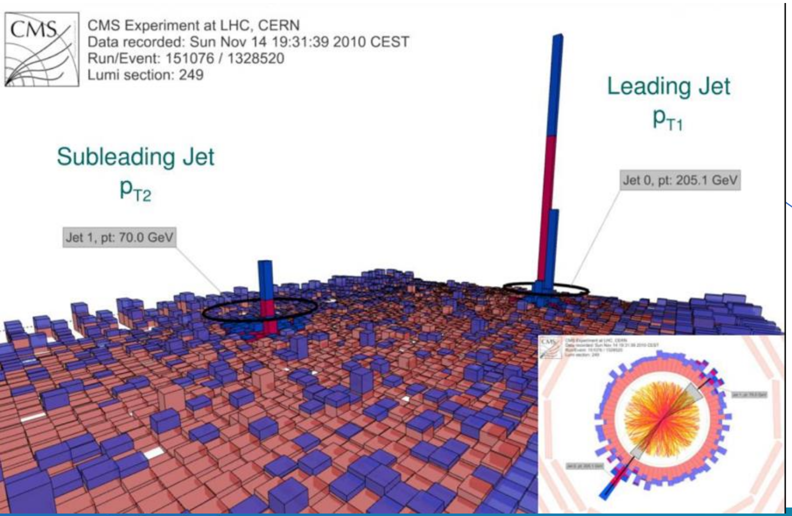
- Reproduces average values, AND, complex pixel-wise correlations

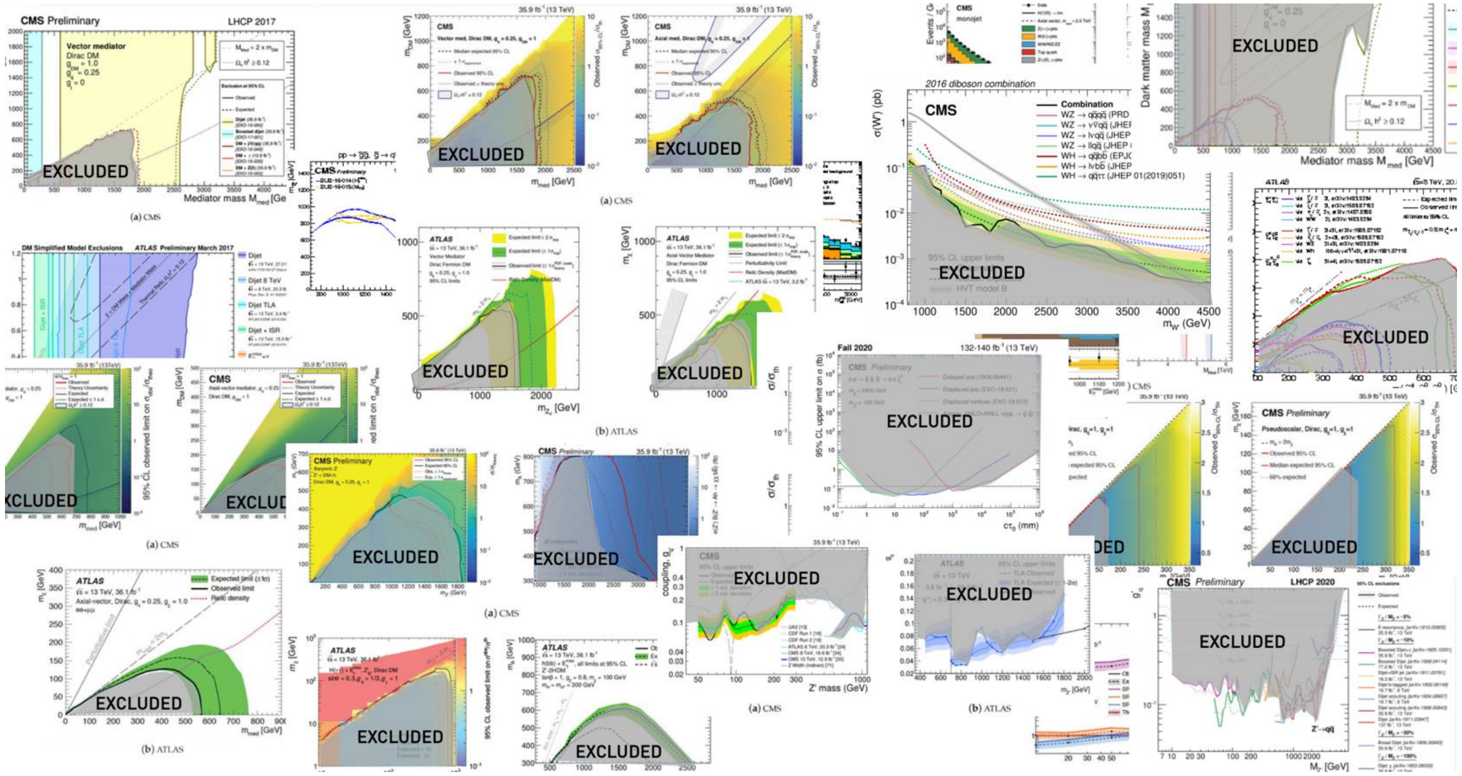


Where is NEW PHYSICS?
Are we using the right data?



Data Analysis





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

What if you do not know the signal or where to look for new-physics ?

Data Analysis

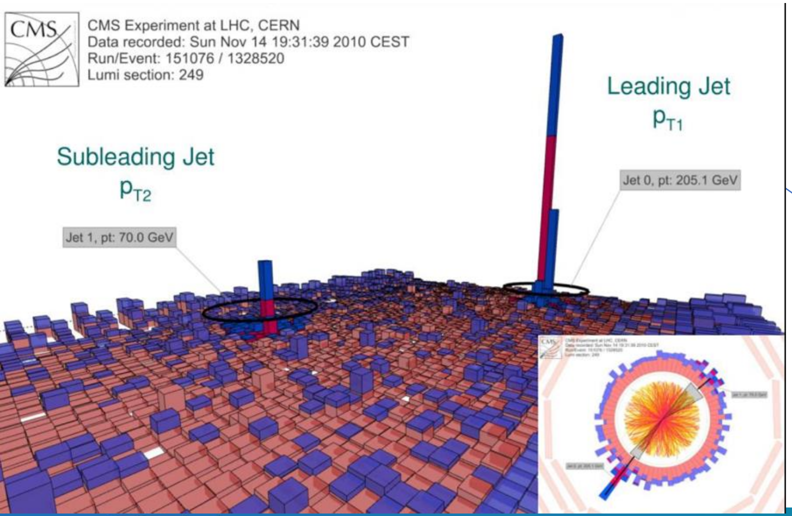
Re-embracing the scientific method:
starts gathering information about nature

… our baseline is the SM (from 1970!) → let's change the approach

Rather than specifying a signal hypothesis upfront, we could start looking at our data

Based on what we see (e.g., clustering alike objects) we could formulate a signal hypothesis

→ QCD dijet events

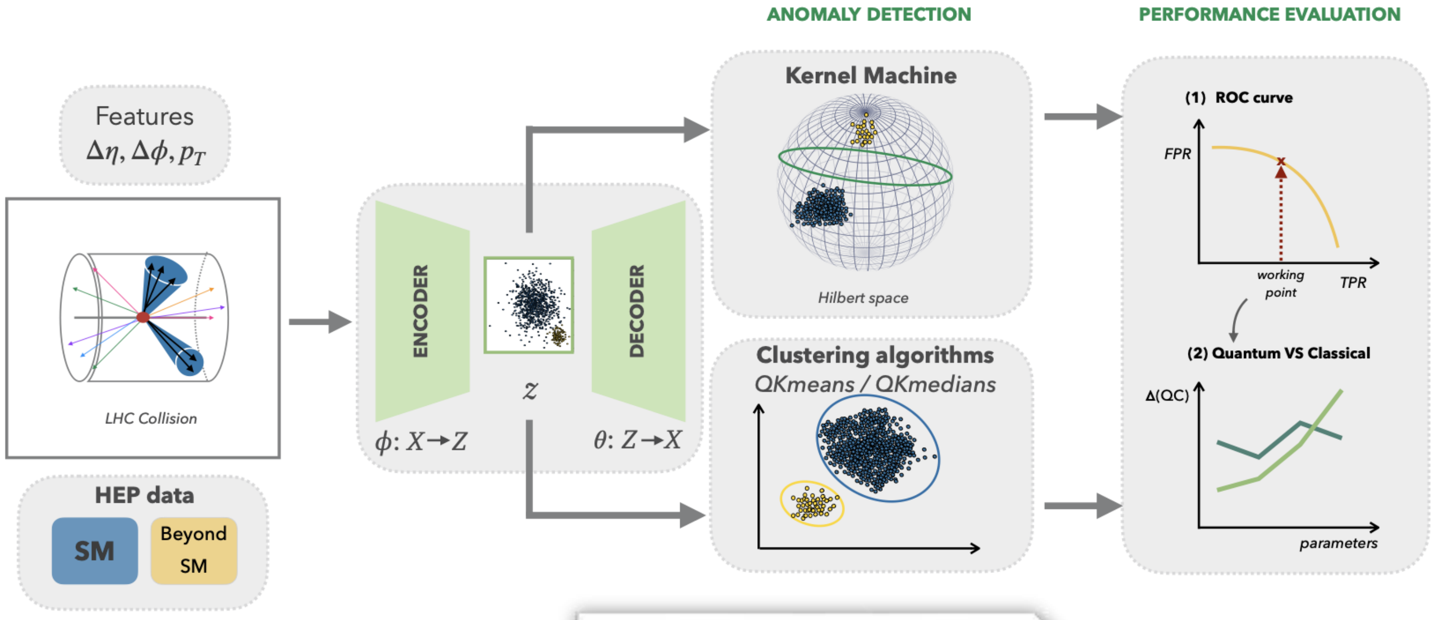


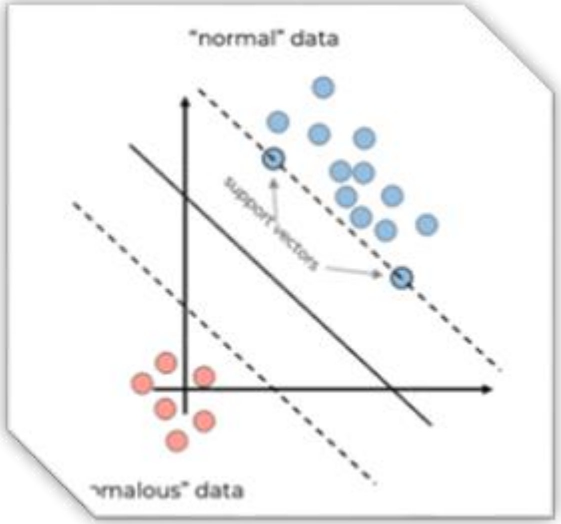
$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} + i\bar{\Psi}\not{D}\Psi + h.c. + \Psi_i y_{ij}\Psi_j\Phi + h.c. + |D_\mu\Phi|^2 - V(\Phi)$$

2013

Quantum Anomaly Detection

Data Analysis

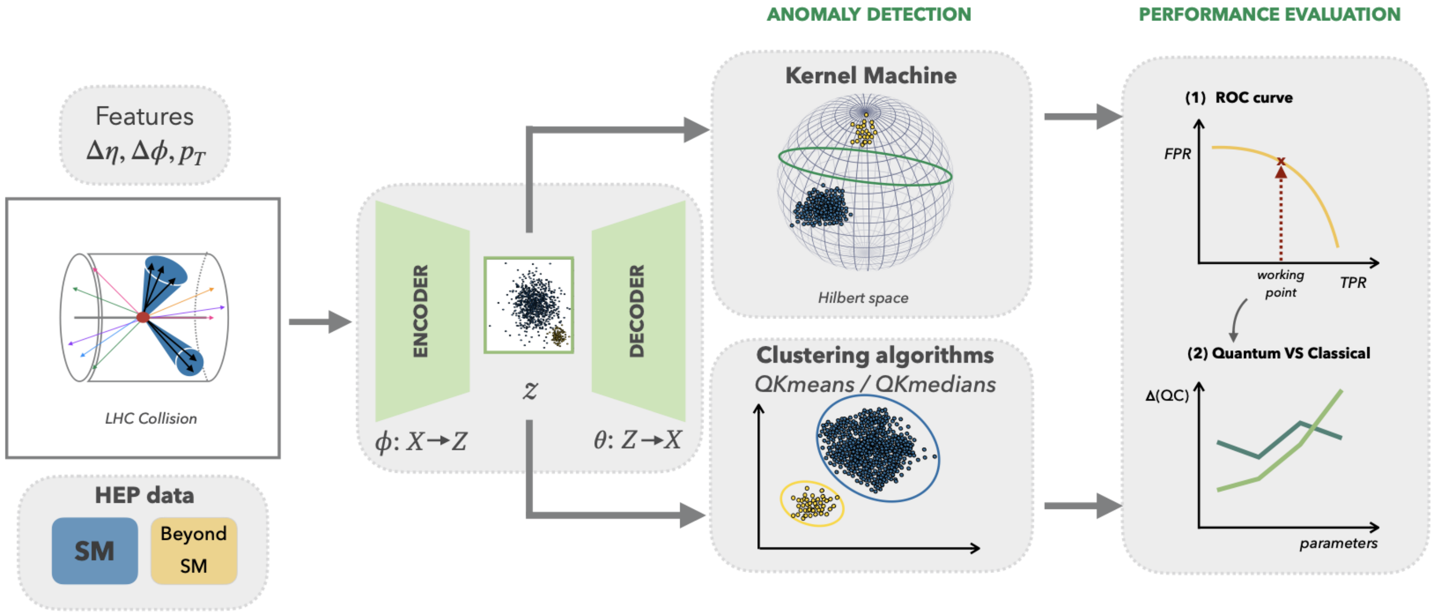


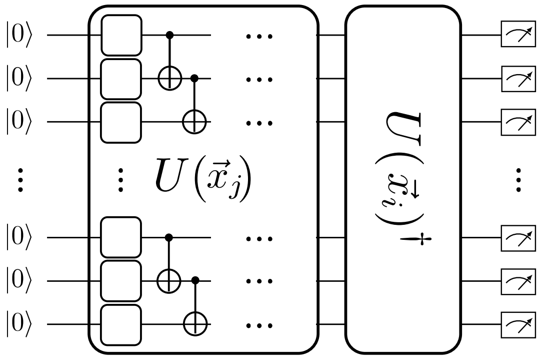


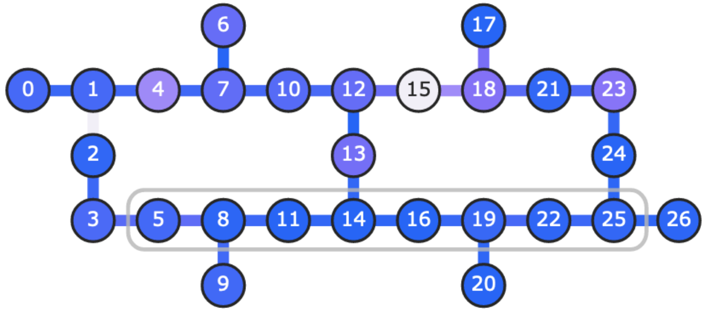
Quantum Anomaly Detection

[Belis V., GM, et al – *arXiv:2301.10780*](https://arxiv.org/abs/2301.10780)

Data Analysis



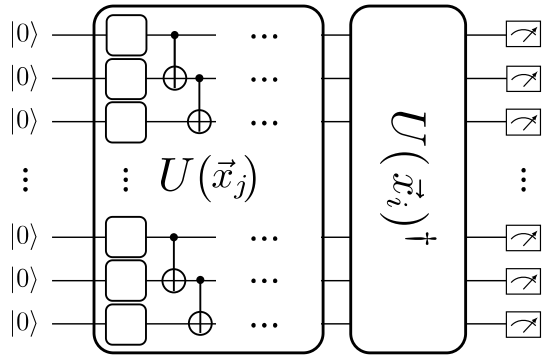


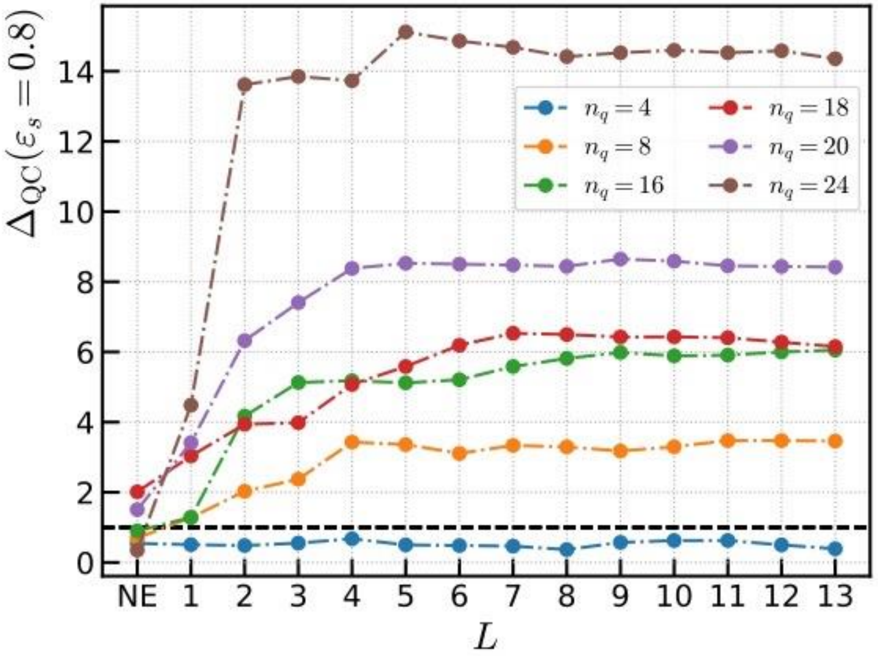


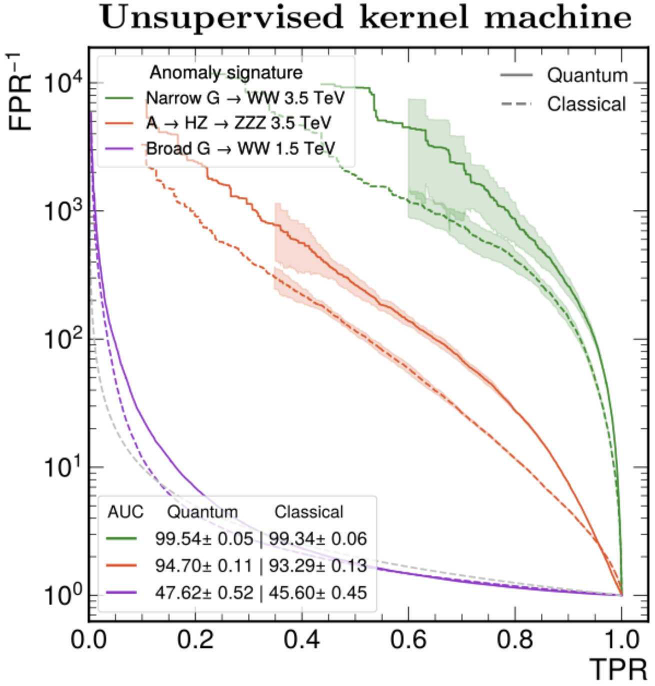
Quantum Anomaly Detection

[Belis V., GM, et al – *arXiv:2301.10780*](#)

Data Analysis







QC research directions in HEP

QC4HEP working group

- Quantum computing could be **revolutionary in HEP**
- To go beyond the hype we need **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?
  - Can we reduce **the impact of data reduction techniques**?
- Experimental data is shaped by physics laws
  - Can we leverage them to build better algorithms?

PRX QUANTUM **5**, 037001 (2024)

Roadmap

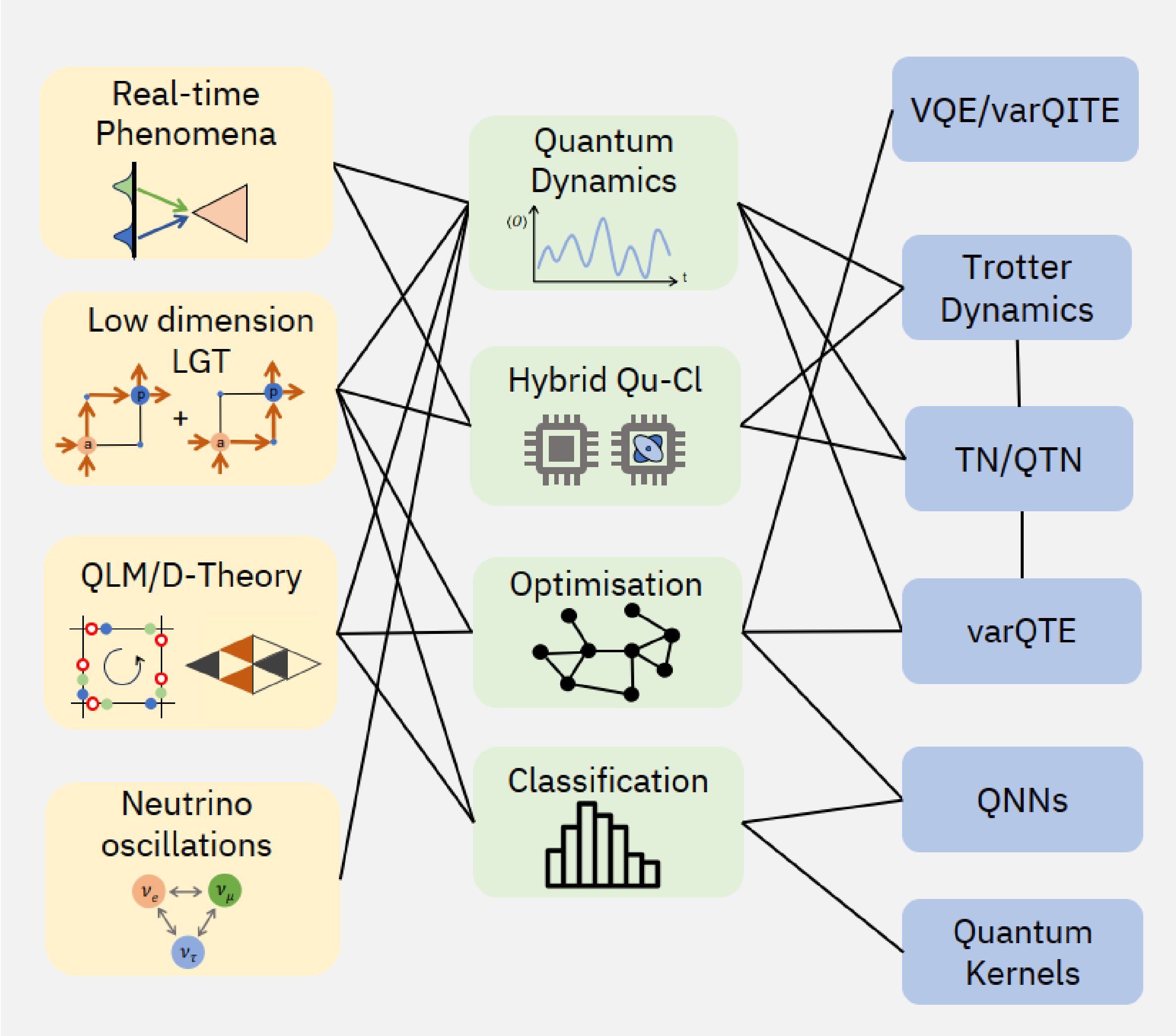
Quantum Computing for High-Energy Physics: State of the Art and Challenges

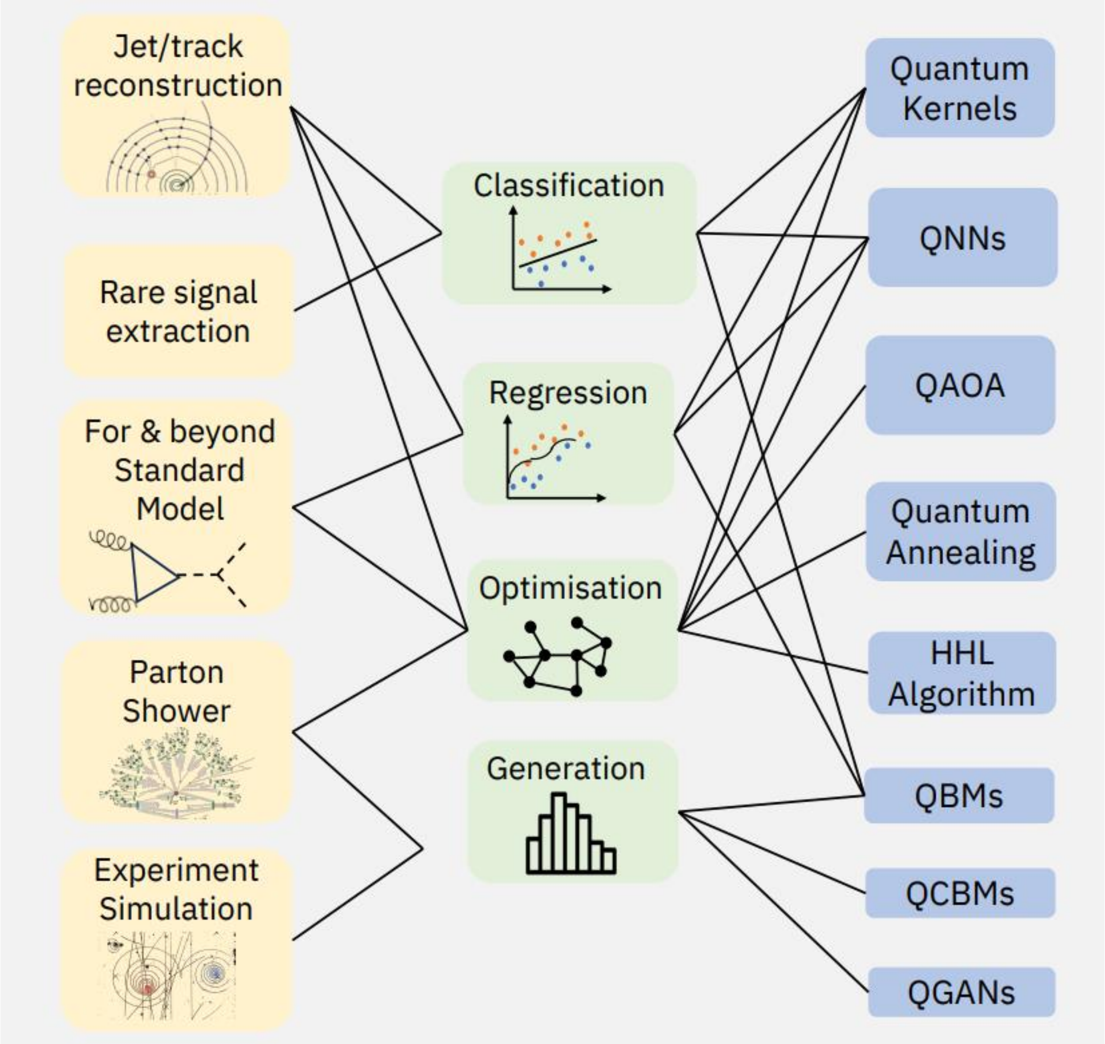
Alberto Di Meglio,[1,*] Karl Jansen,[2,3,†] Ivano Tavernelli,[4,‡] Constantia Alexandrou,[3,5] Srinivasan Arunachalam,[6] Christian W. Bauer,[7] Kerstin Borras,[8,9] Stefano Carrazza,[1,10] Arianna Crippa,[2,11] Vincent Croft,[12] Roland de Putter,[6] Andrea Delgado,[13] Vedran Dunjko,[12] Daniel J. 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]

[1] *European Organization for Nuclear Research (CERN), 1211 Geneva, Switzerland*
[2] *CQTA, Deutsches Elektronen-Synchrotron DESY, Platanenallee 6, 15738 Zeuthen, Germany*
[3] *Computation-based Science and Technology Research Center, The Cyprus Institute, 20 Konstantinou Kavafi Street, CY-2121 Nicosia, Cyprus*
[4] *IBM Research Europe — Zurich, 8803 Rüschlikon, Switzerland*
[5] *Department of Physics, University of Cyprus, PO Box 20537, CY-1678 Nicosia, Cyprus*
[6] *IBM Quantum, IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA*
[7] *Physics Division Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Mailstop 50A5104, Berkeley, California, USA*
[8] *Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany*
[9] *RWTH Aachen University, Templergraben 55, 52062 Aachen, Germany*
[10] *TIF Lab, Dipartimento di Fisica, Università degli Studi di Milano and INFN Sezione di Milano, Milan, Italy*
[11] *Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany*
[12] *⟨aQa^L⟩ Applied Quantum Algorithms – Leiden, Leiden, Netherlands*
[13] *Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[14] *Department of Computer Science, Facultad de Ciencias, University of Oviedo, 33007 Asturias, Spain*
[15] *Institute of Theoretical Physics, Leibniz University Hannover, 30167 Hanover, Germany*
[16] *Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany*
[17] *Transdisciplinary Research Area "Building Blocks of Matter and Fundamental Interactions" (TRA Matter) and Helmholtz Institute for Radiation and Nuclear Physics (HISKP), University of Bonn, Nußallee 14–16, 53115 Bonn, Germany*
[18] *Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria*
[19] *Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria*
[20] *Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Munich, Germany*
[21] *Munich Center for Quantum Science and Technology, Munich, Germany*
[22] *Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland*
[23] *CNRS/IN2P3, IJCLab, Paris-Saclay University, 91405 Orsay, France*
[24] *Department of Physics and Astronomy, York University, Toronto, Ontario M3J 1P3, Canada*
[25] *INFN—Sezione di Padova, Via Marzolo 8, 35131 Padua, Italy*
[26] *Nikhef—National Institute for Subatomic Physics, Science Park 105, 1098 XG Amsterdam, Netherlands*

*Contact author: alberto.di.meglio@cern.ch
†Contact author: karl.jansen@desy.de
‡Contact author: ita@zurich.ibm.com

Methods and applications





Phase Detection with Anomaly Detection

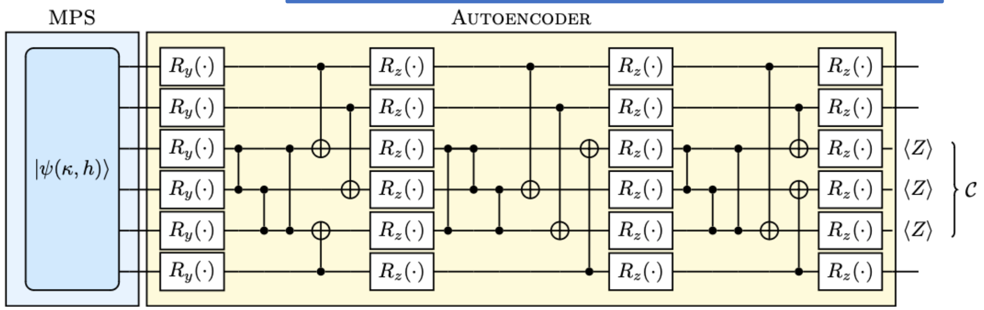
Compression: $|\psi\rangle \rightarrow \underbrace{|\phi\rangle}_{N-k} \otimes |0\rangle^{k}$

$$\mathcal{U}(\vec{\theta})|\psi\rangle^{N} = |0\rangle^{\otimes K} \otimes |\phi\rangle^{N-K}$$

- Quantum equivalent of an Autoencoder to learn an effective unitary operation capable of compressing all the information in the Pauli-Z expectation values of a subset of the qubits

- Minimization of the loss function

$$\mathcal{C} = \frac{1}{2}\sum_{j \in q_T}(1 - \langle \sigma_j^z \rangle),$$



- *All anomaly detection models were trained to compress the point (κ, h) = (0, 0) of the Hamiltonian*
- *Training: single state selected to achieve compression*
- *Cost is assigned to compressed state allowing the outline of all phases*

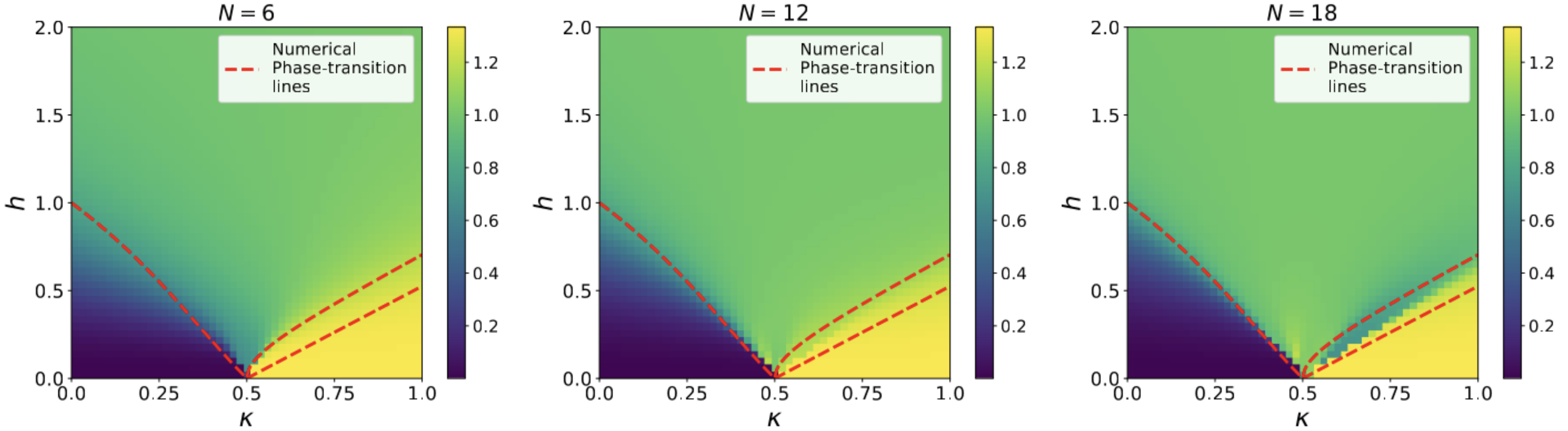


FIG. 13: Compression Scores $\mathcal{C}$ of the AD circuits trained on the $(\kappa, h) = (0, 0)$ point of the ANNNI model phase diagram at different system sizes N: 6 (left), 12 (middle), and 18 (right). The scores are showcased as a function of the interaction strength ratio ($\kappa = -J_2/J_1$) and the external magnetic field ($h = B/J_1$). Lower compression scores indicate better disentanglement of trash qubits from others, as defined by eq. 2.

Exploring the Phase Diagram of the quantum one-dimensional ANNNI model
https://arxiv.org/abs/2402.11022

QT4HEP 2025 - save the date

CERN

QUANTUM TECHNOLOGY INITIATIVE