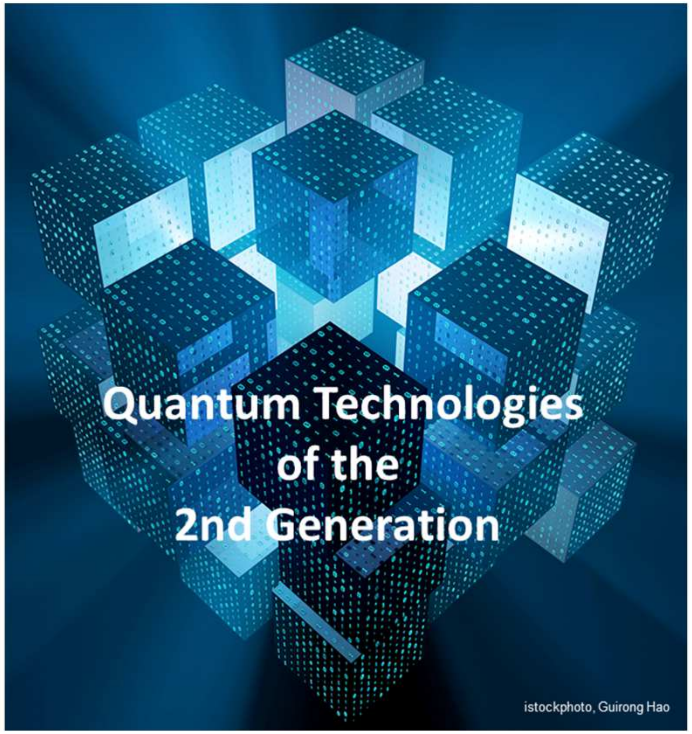
# Quantum Computing
# Quantum Machine Learning
## Status and Prospects



**Prof. Dr. Kerstin Borras**
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DESY Quantum Technology Task Force qt-task-force@desy.de

HELMHOLTZ

DESY. QUANTUM

DESY.

# The Second Quantum Revolution is Transforming the World.

Decoding of Matter with novel methods and tools → get ready today !

**1st Quantum Revolution:**

understand & apply
→ ground-breaking: transistors, lasers etc.

**2nd Quantum Revolution:**

Identify, control, manipulate individual quanta
→ exploit the potential

**Quantum Advantage**:

Improvement versus
the best known conventional method

**Quantum Technologies: Rethinking of our methods**

→ completely different principles
→ pioneering work improves already our classical methods

**→ maximizing our achievable scientific and economic success**

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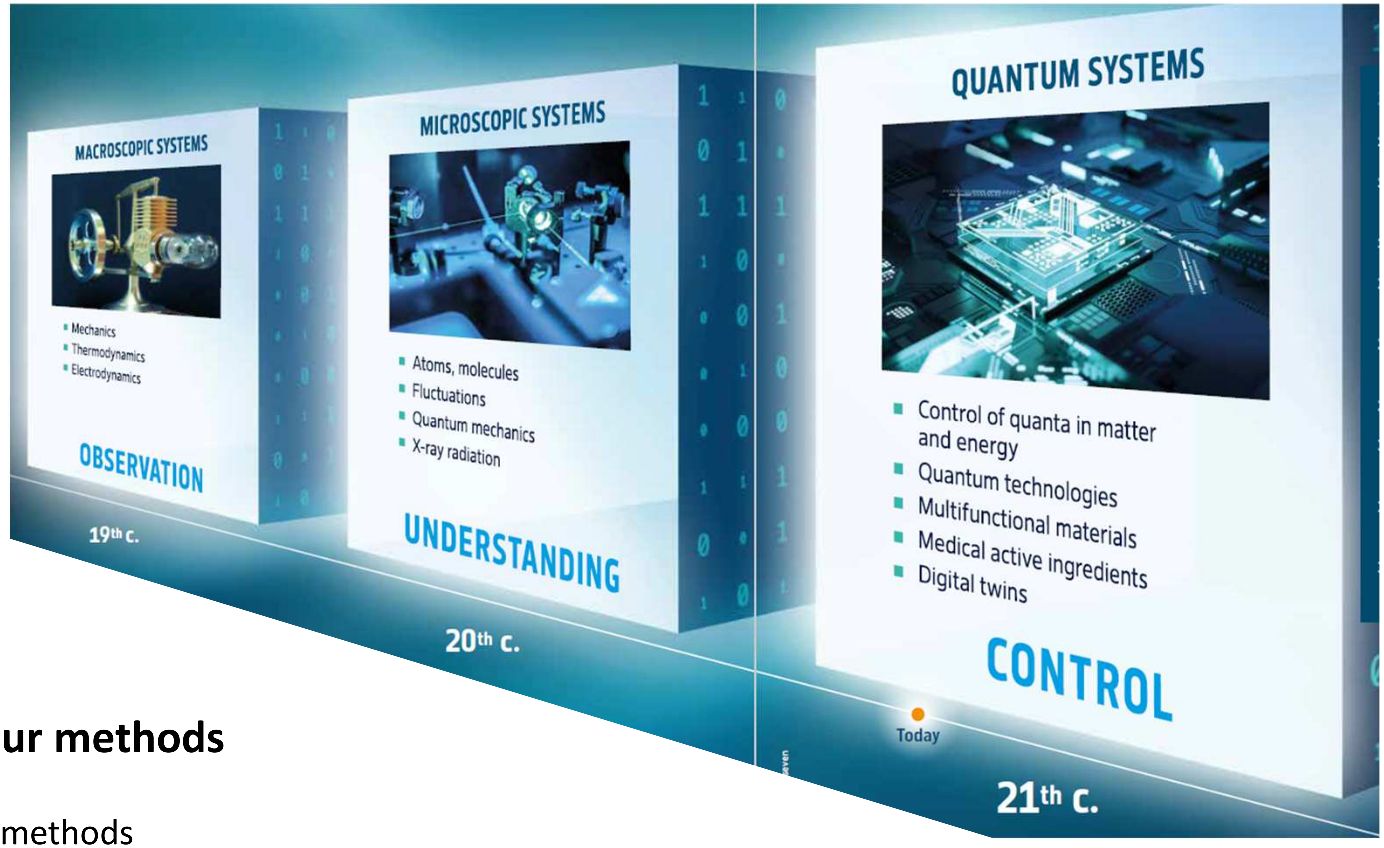

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→ completely different principles
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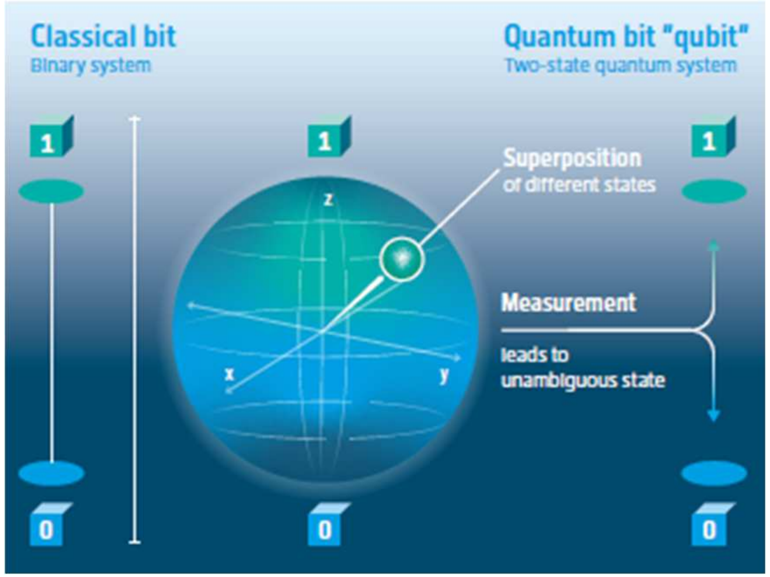
# Quantum Computing is part of our Future.

## Quantum Computing is opening new windows for our science today.



### 2$^{nd}$ Quantum Revolution:

manipulate quantum effects in customized systems and materials

→ expands the useable phase space considerably:

one classical bit turns into a whole Bloch sphere

Example: System of *n* qubits

- → computational basis states of this system are of the form $|x_1, x_2, \ldots x_n\rangle$
- → quantum state is specified by $2^n$ amplitudes
- → *n*=500 → number is larger than the estimated number of atoms in the Universe!
- → storing all these complex numbers is not possible on any conceivable classical computer.

## Quantum Advantage:

For a given problem, the improvement in run time for a quantum computer versus a conventional computer operating the best known conventional algorithm.

→ working on completely different principles than classic technology

**superposition, entanglement, randomization**

→ potential to solve challenges in **Complexity and Big Data**

Exciting times with exponential evolution of novel technologies

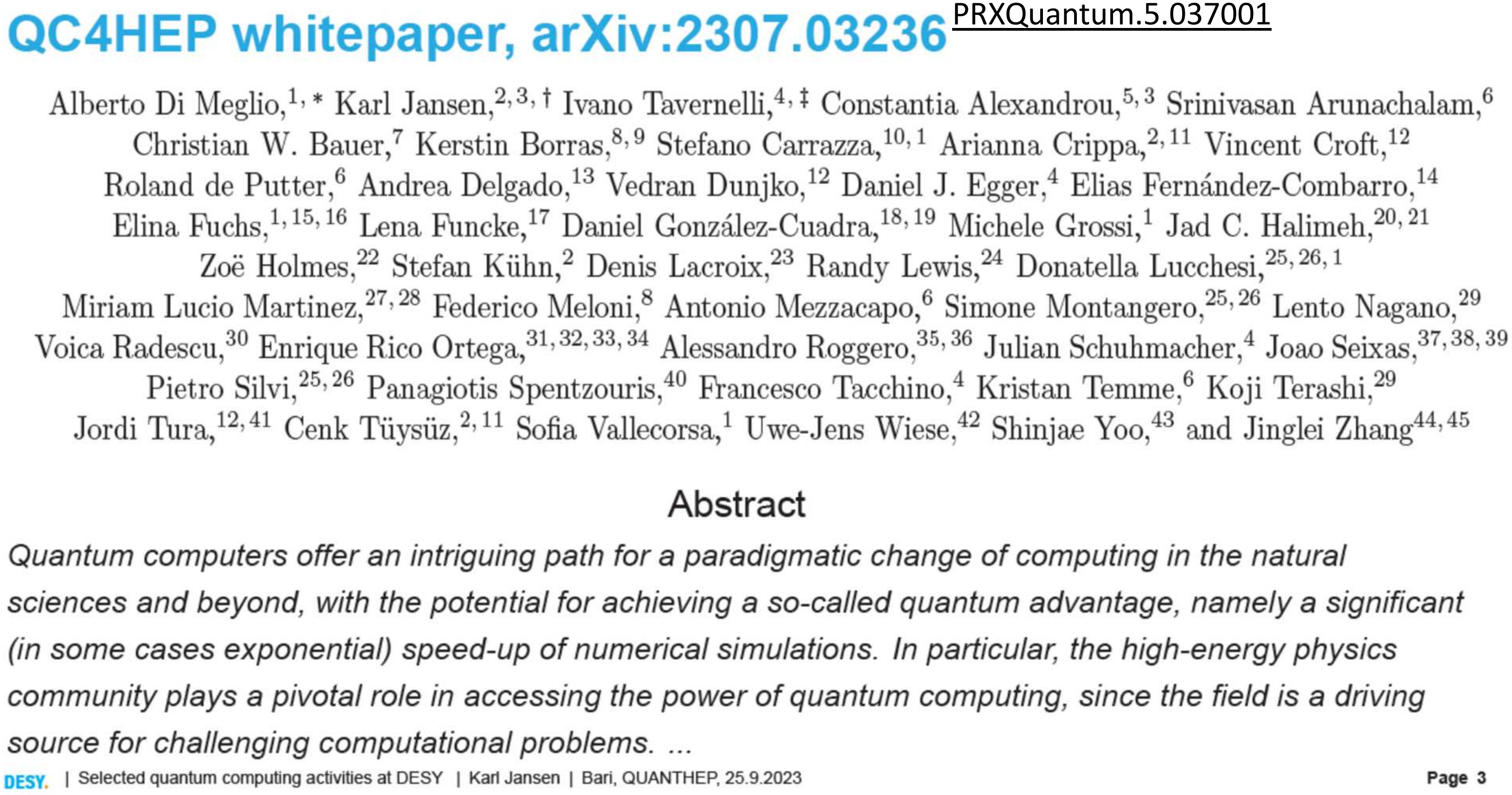
## Quantum Computing demands for a rethinking of our methods

→ pioneering work improves already our classical methods

# Quantum Computing in Particle Physics in Theory and Experiment.

Novel methods and tools for the 100x100 Challenge→ get ready today !

**Published in PRX Quantum:**
https://journals.aps.org/prxquantum/abstract/10.1103/PRXQuantum.5.037001



## QC4HEP whitepaper, arXiv:2307.03236

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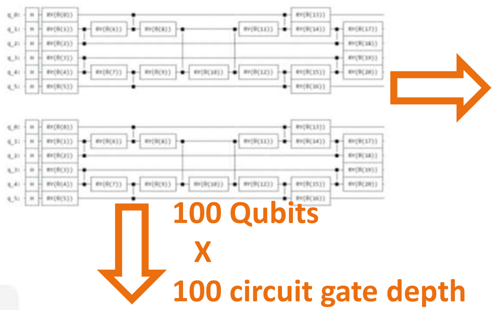
### Abstract

*Quantum computers offer an intriguing path for a paradigmatic change of computing in the natural sciences and beyond, with the potential for achieving a so-called quantum advantage, namely a significant (in some cases exponential) speed-up of numerical simulations. In particular, the high-energy physics community plays a pivotal role in accessing the power of quantum computing, since the field is a driving source for challenging computational problems. ...*

DESY. | Selected quantum computing activities at DESY | Karl Jansen | Bari, QUANTHEP, 25.9.2023 Page 3

# Quantum Computing in Particle Physics in Theory and Experiment.

## Novel methods and tools for the 100x100 Challenge→ get ready today !

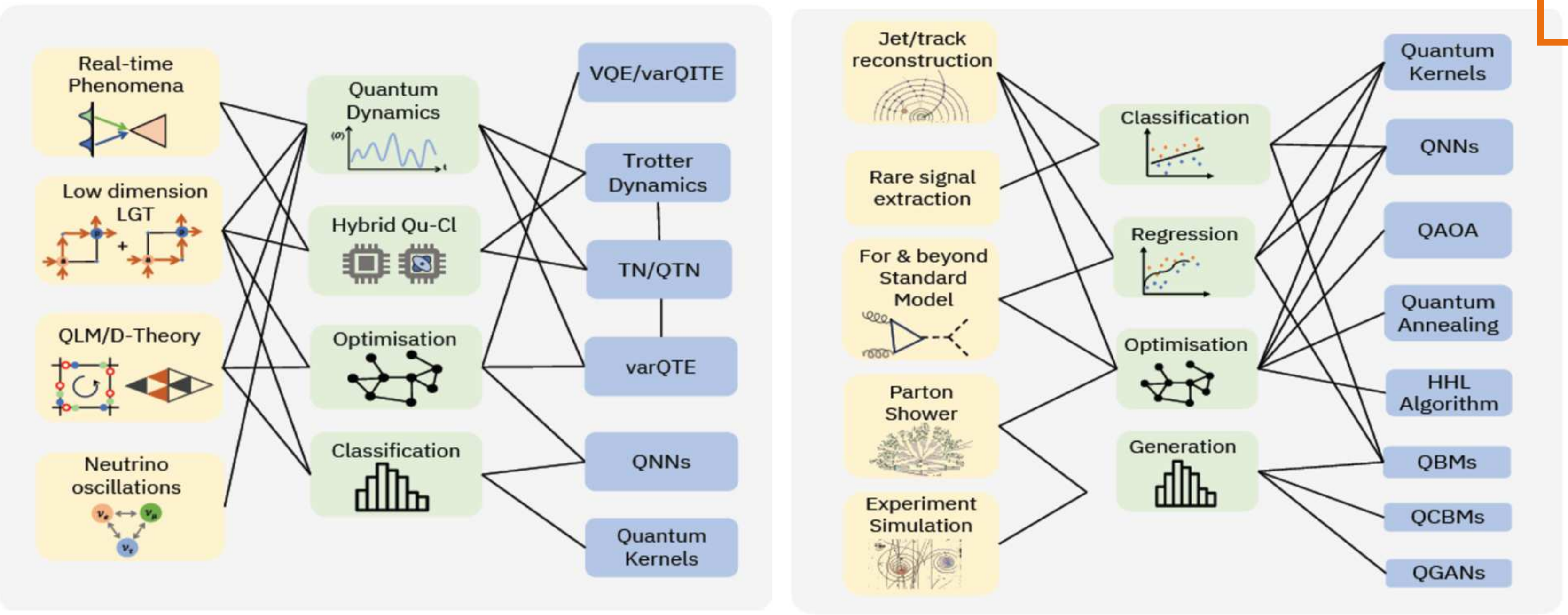


100 Qubits
X
100 circuit gate depth

Roadmap in Particle Physics Applications for the 100 x 100 Challenge

Theory | Experiment

Application | Category | Algorithm | Application | Category | Algorithm

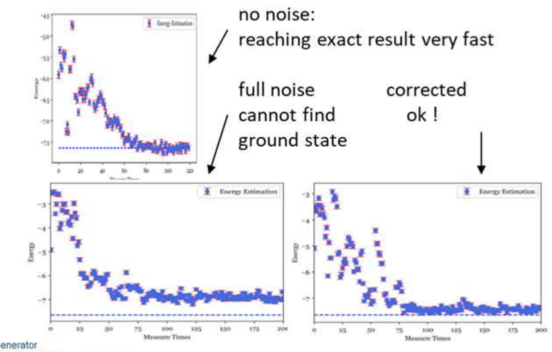


**Published in PRX Quantum:**
https://journals.aps.org/prxquantum/abstract/10.1103/PRXQuantum.5.037001

# Quantum Computing Activities at DESY

## Quantum Computing will be part of our future

**Quantum Computers have the potential to solve problems that cannot be addressed with classical computers**

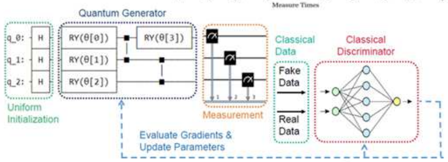


no noise:
reaching exact result very fast

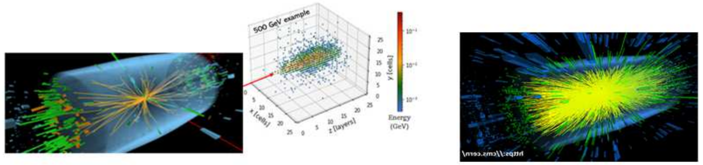
full noise
cannot find
ground state

corrected
ok !

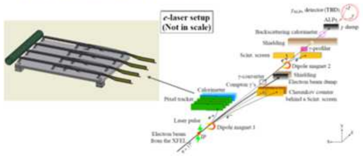
- **Develop algorithms and methods in Theoretical Particle Physics**
  - Calculations in theory → novel unique results &benchmark novel devices
  - Applications in particle physics similar to other logistics problems (optimization of flight gate assignment)
  - Error mitigation in QC calculations
  - Optimization of Quantum Gate Circuits (to reduce noise)

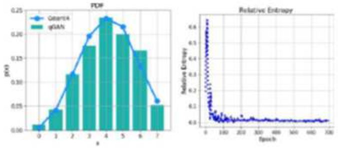


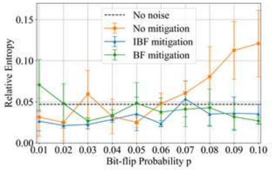
- **Quantum Machine Learning (usually in hybrid mode)**
  **Develop machine learning and tensor network methods for QC**
  - Simulations for detectors at LHC (CERN), IBM
  - Tracking for LUXE (DESY), IBM
  - Particle identification at Belle II (KEK, Japan), Annealer
  - EFT Fits to find New Physics (Annealer)



LUXE EXPERIMENT SETUP



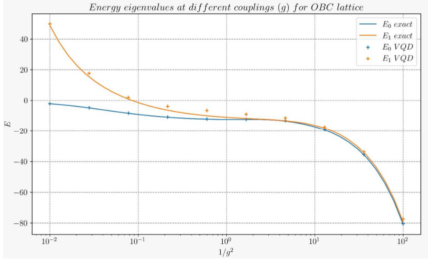




# Quantum Computing: From Theory towards Applications

## From QED in 2+1 dimensions to Flight Gate Assignments

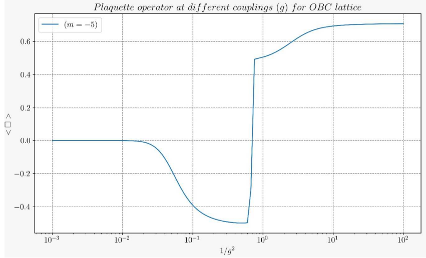
- Variational Quantum Simulations (VQS) for QED



Particle Mass

$\Delta = E_1 - E_0$

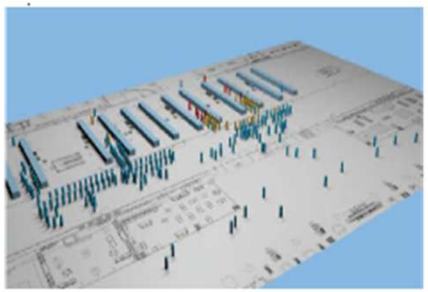
→ physical quantity

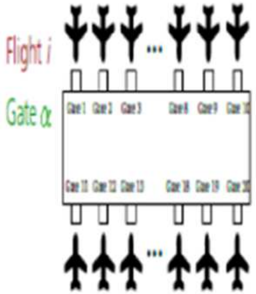


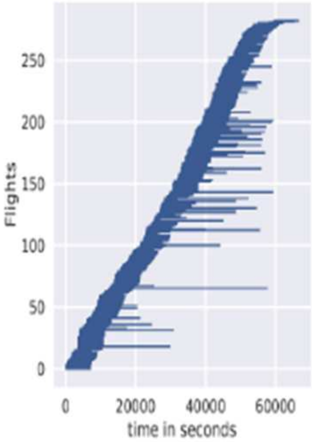
Detecting a phase transition
at negative mass
→ **not possible with MC methods**

*Clemente G. et al, Strategies for the Determination of the Running Coupling of (2+1)-dimensional QED with Quantum Computing, https://arxiv.org/abs/2206.12454*

- Very similar approach for
  **Flight Gate Assignment Optimization**
  find lowest energy ⇔ shortest path
  same mathematics for problems in
  traffic, logistics, aerospace, ...







Theoretical optimization:
Y. Chai, L. Funcke, T. Hartung, S. Kühn, T. Stollenwerk, P. Stornati, K. Jansen, arXiv:2302.11595
Hardware Runs:
Y. Chai, E. Epifanovsky, K. Jansen, A. Kaushik, S. Kühn, arxiv:2309.09686

$$H = \sum_{j=1}^{n} Q_{jj}\sigma_j^z + \sum_{\substack{j,k=1 \\ j<k}}^{n} Q_{jk}\sigma_j^z \otimes \sigma_k^z$$

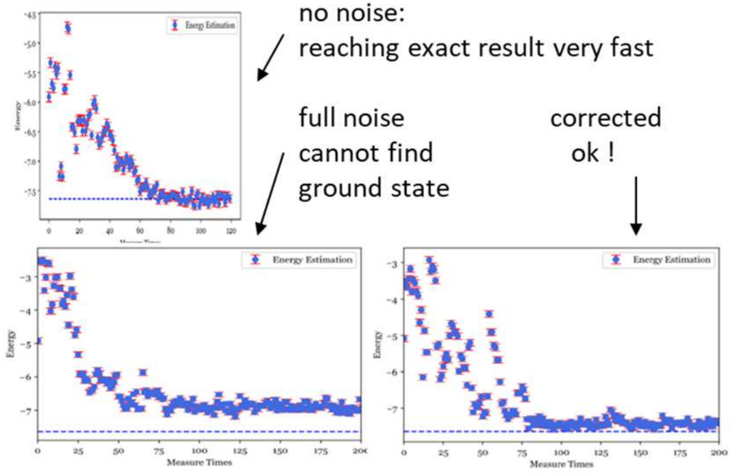
# Methods for reliable Quantum Computing Calculations

## Increase the Reliability for Quantum Computing Calculations

$$H = \sum_{i=1}^{N} \beta \left[\sigma_x(i)\sigma_x(i+1) + \sigma_y(i)\sigma_y(i+1) + \sigma_z(i)\sigma_z(i+1)\right] + J\sigma_z(i)$$

- **Example for Error Mitigation** in Variational Quantum Simulation **VQS**
  - Model in Condensed Matter Physics:
    1-Dimensional Heisenberg model, very prone to QC errors
    **Cured by own developed error mitigation methods**

*Funcke L. et al, Measurement Error Mitigation in Quantum Computers Through Classical Bit-Flip Correction, arxiv:2007.03663, Phys. Rev. A 105, 062404*



no noise:
reaching exact result very fast

full noise
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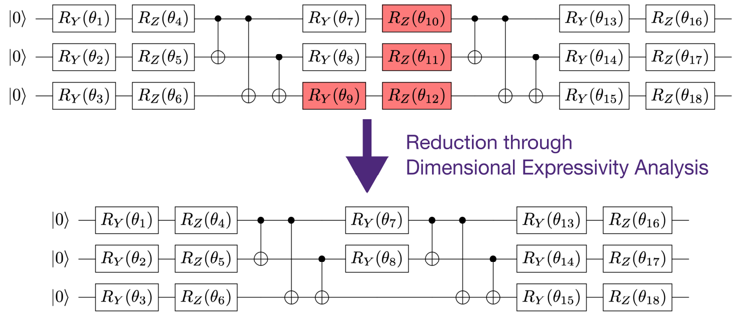
corrected
ok !

- **Optimize Dimensional Expressivity of a Quantum Gate Circuit**
  - Gate Operations are erroneus
  - Develop methods for Dimensional Expressivity Analysis
    **Generate as many/complicated states as possible**
    **with fewest number of gates**

*Funcke L. et al, Dimensional Expressivity Analysis of Quantum Circuits Quantum 5 (2021) 422*



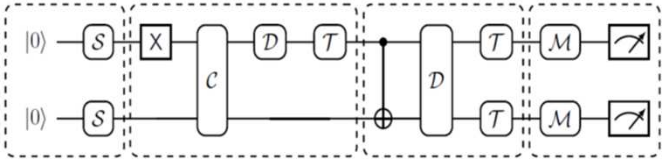
Reduction through
Dimensional Expressivity Analysis

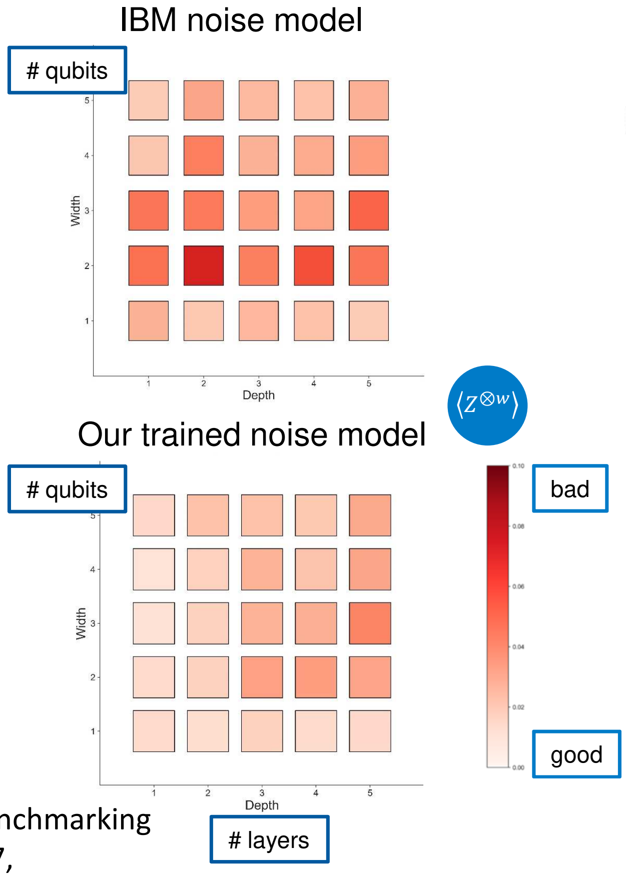
# Software engineering for Noise Model Benchmarks

## Increase the Reliability for Quantum Computing Calculations

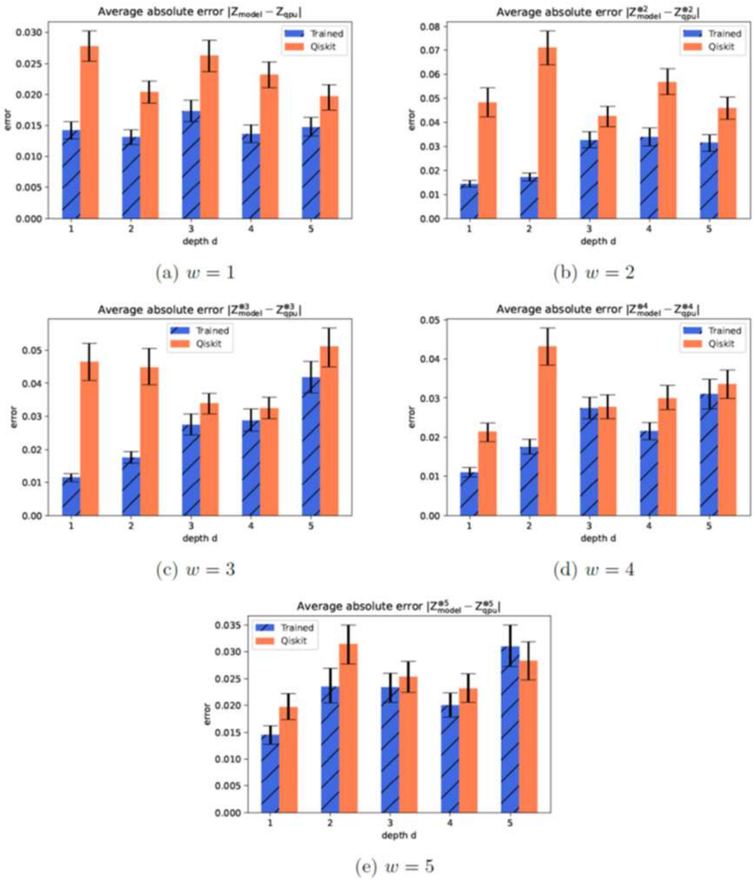
- **Software Engineering Models for Error Mitigation**
  - Systematic approach to train error models with Machine Learning and perform benchmarks for quantum computing applications

| symbol | error | parameters | number of parameters |
|---|---|---|---|
| $\mathcal{S}$ | state preparation | $p_{\text{sp}}(q)$ | $N$ |
| $\mathcal{D}$ | depolarization | $\lambda_g(q)$ | $4N-1$ |
| $\mathcal{C}$ | crosstalk | $\phi_g(q)$ | $2N$ |
| $\mathcal{T}$ | thermal relaxation | $T_{1,2}(q)$ | $2N$ |
| $\mathcal{M}$ | measurement | $p_{0\to1}(q)$,<br>$p_{1\to0}(q)$ | $2N$ |
| total | | | $11N-1$ |




IBM noise model

Our trained noise model



(a) $w = 1$ (b) $w = 2$

(c) $w = 3$ (d) $w = 4$

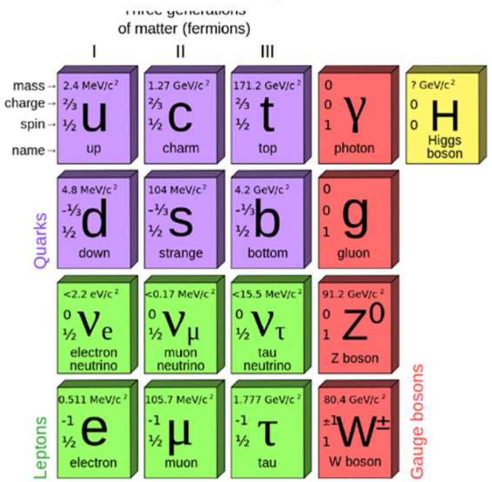
(e) $w = 5$

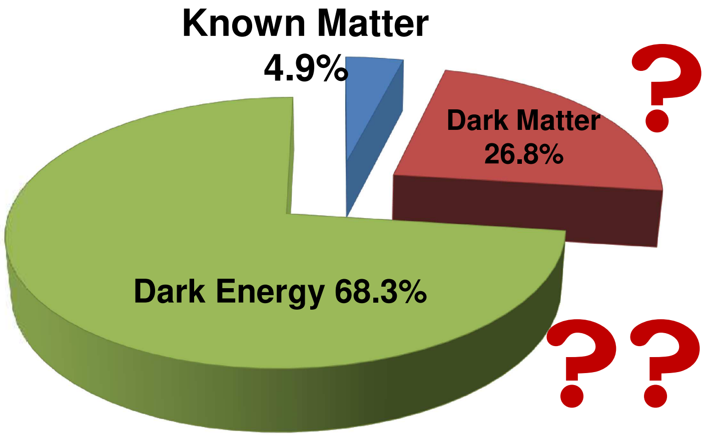
Weber, T. et al (2023) "Construction and volumetric benchmarking of quantum computing noise models", arXiv:2306.08427, IOPScience Physica Scripta, Volume 99, Number 6

# Particle Physics: What is our Universe made of ?

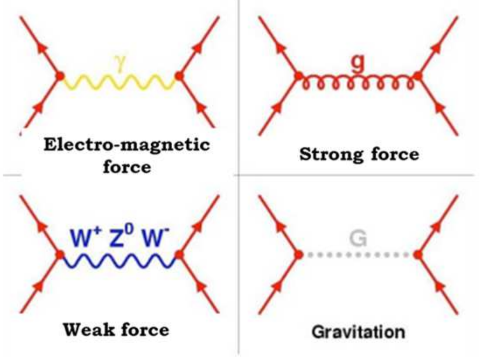
## What are our elementary particles and their interaction to build matter and our Universe

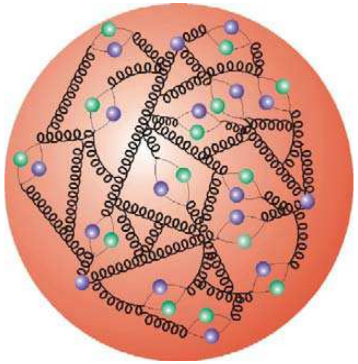
Fundamental particles:





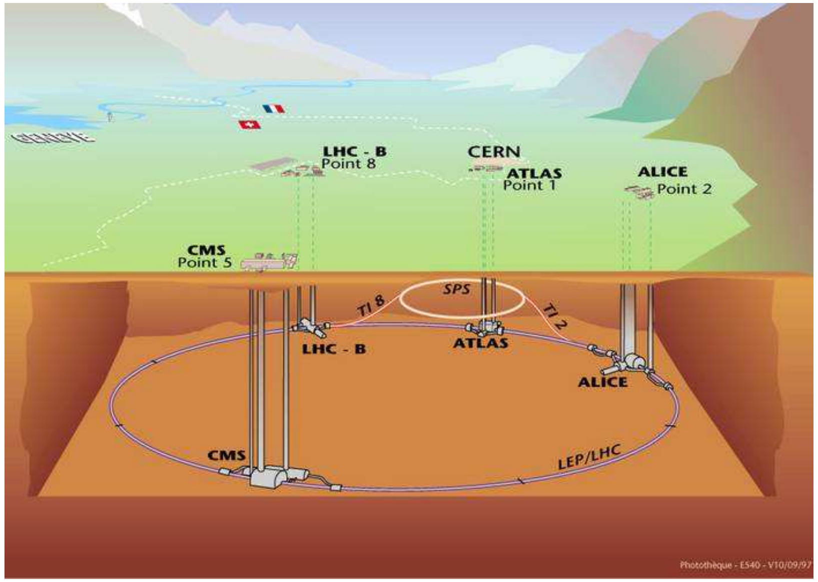
Four fundamental forces:





Proton

### Proton-Proton Collisions at the LHC



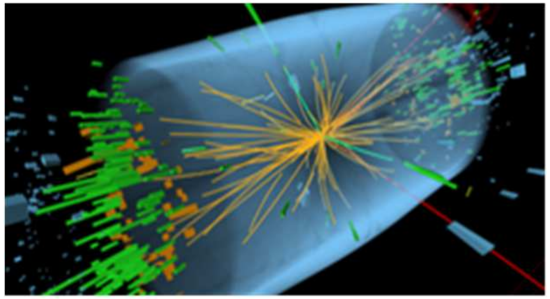
# Quantum Machine Learning for Detector Simulations in Particle Physics

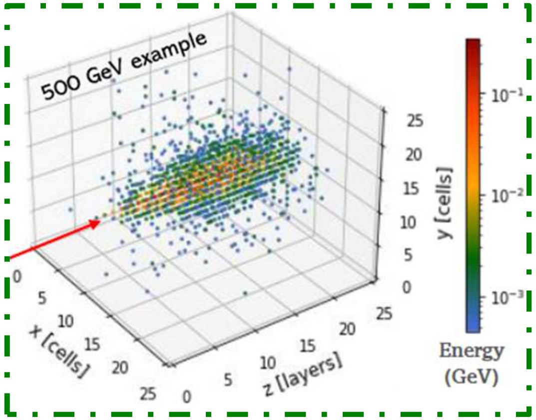
## Early examples in Experimental Particle Physics

- **Quantum Machine Learning lies at the intersection of Quantum Computing and Machine Learning**
  - High Luminosity LHC (>2029) needs vast amount of simulations with 200 overlaid events, Big Data Analysis

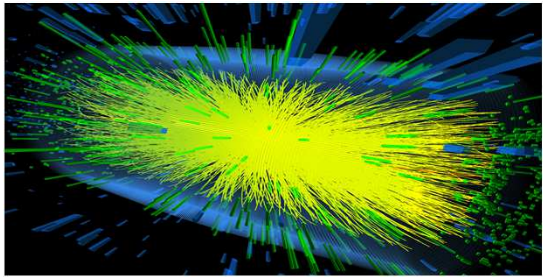
5D images of particle showers
in a calorimeter to measure
the energy of the incoming particle
5D = X,Y,Z, energy, time.

LHC (~20 pile-up events)





LHC (~200 pile-up events)



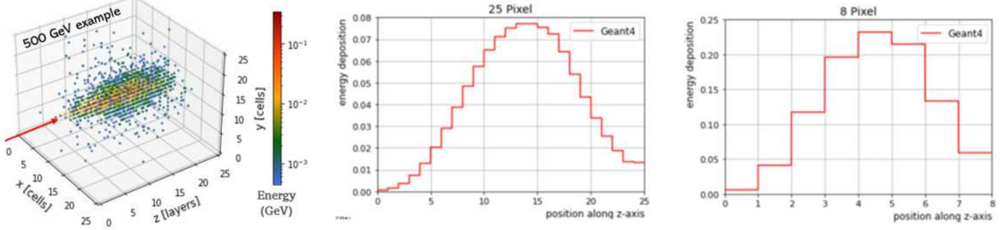
- **Develop machine learning methods for Quantum Computing**
  - Q-GAN (Quantum Generative Adversarial Network) simulations for detectors (CERN Openlab with joint BMBF Gentner PhD Student)

# Hybrid Q-GAN in One Dimension

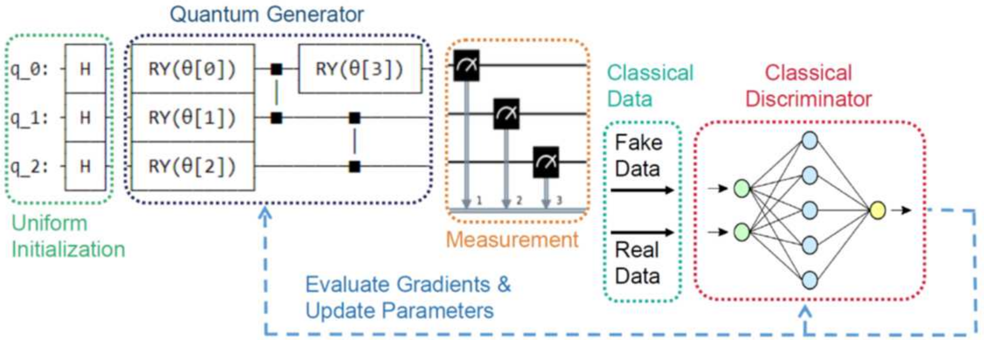
## Quantum Generative Adversarial Network

BMBF
NiQ

- **Down sample 3D shower image → 8 pixels → 3 qubits**



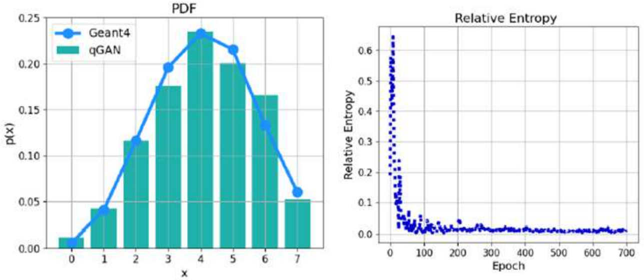
8 quantum states:
|000⟩, |001⟩, |010⟩, |011⟩,
|100⟩, |101⟩, |110⟩, |111⟩



- **Use hybrid approach: quantum + classical**

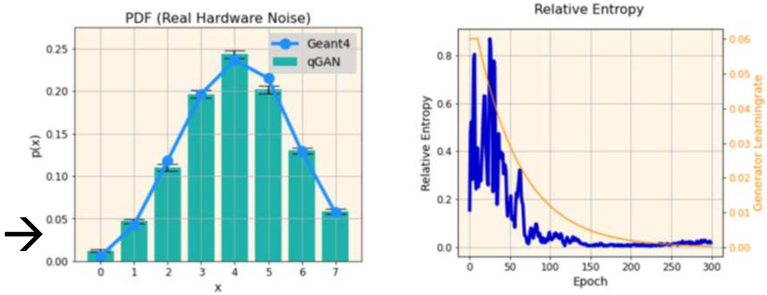
- **Employ a Qiskit Q-GAN model developed by IBM***

**Q-GAN simulations in one dimension (with noise)**



← readout noise

**full noise**
real hardware →



* https://qiskit.org/documentation/machine-learning/tutorials/04_qgans_for_loading_random_distributions.html

# Full Quantum Angle Generator (QAG)

## Less parameters for complex data and robustness against noise

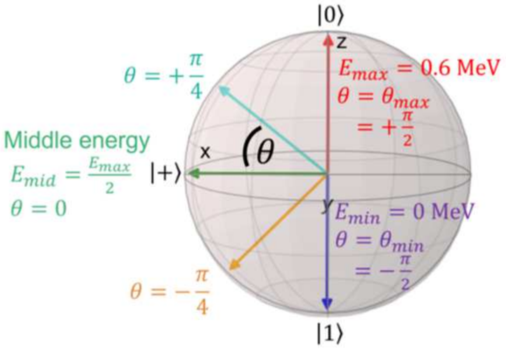
The Quantum Angle Generator (QAG):
represents a full quantum model

Utilizes angle encoding (instead of amplitude encoding).
→ multiple individual images with pixel energies

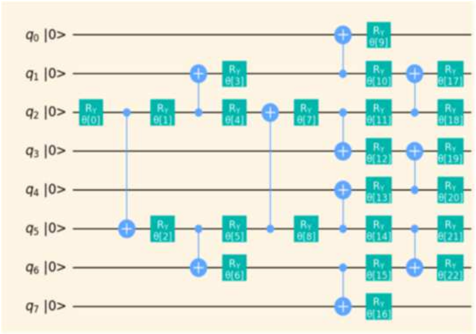
Trained by objective functions (MMD, Corr) + a new quantum circuit:
→ lightweight training
→ trainable on real quantum devices

Identify the best circuit with the lowest number of parameters,
the best expressibility and the best entanglement capability.

Angle Encoding



Best Circuit



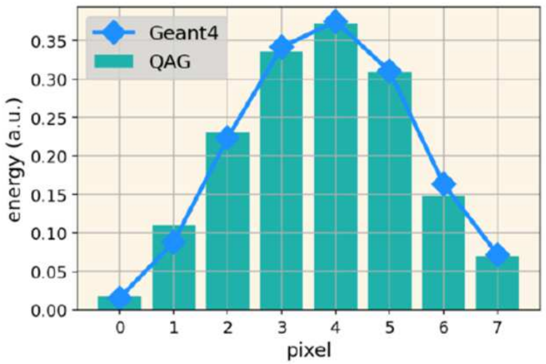
*Rehm, F. et al. Precise Image Generation on Current Noisy Quantum Computing Devices.*
*IOP Quantum Science and Technology* https://doi.org/10.1088/2058-9565/ad0389. *PhD Thesis RWTH Aachen more details* http://doi.org/10.18154/RWTH-2023-09302

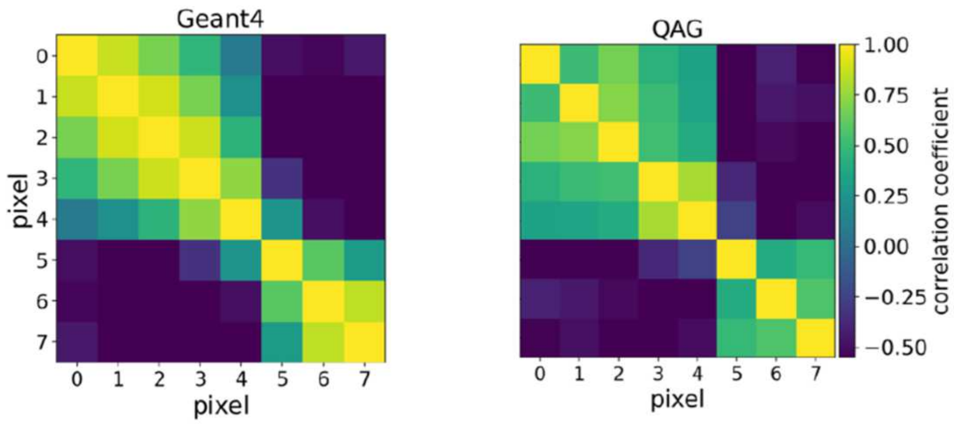
# Quantum Angle Generator: Model Accuracy

## Less parameters for complex data and robustness against noise

The Quantum Angle Generator (QAG) achieves

good accuracy in the shower profiles and reproduces the correlations





**→ The QAG model learns complex image correlations due to highly entangled qubits in the quantum circuit.**

*Rehm, F. et al. Precise Image Generation on Current Noisy Quantum Computing Devices.*
*IOP Quantum Science and Technology* https://doi.org/10.1088/2058-9565/ad0389. *PhD Thesis RWTH Aachen more details* http://doi.org/10.18154/RWTH-2023-09302

# Quantum Angle Generator: Noise Robustness

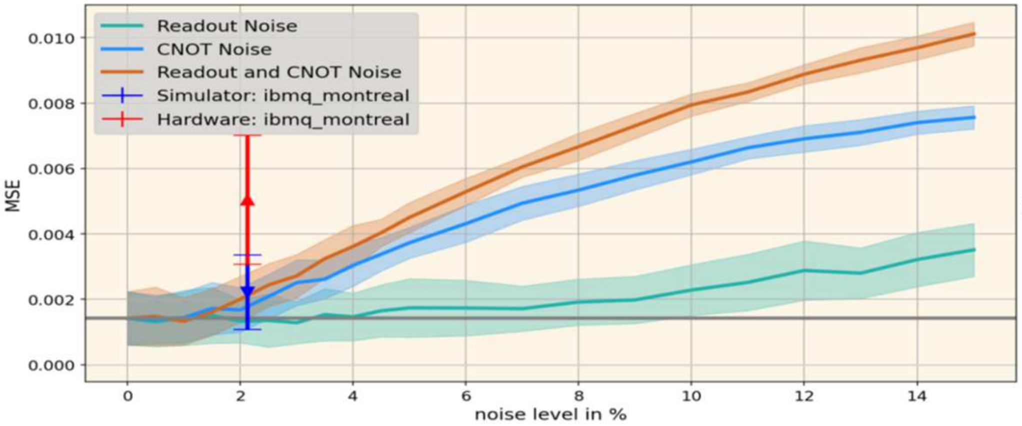
## Less parameters for complex data and robustness against noise

BMBF
NiQ

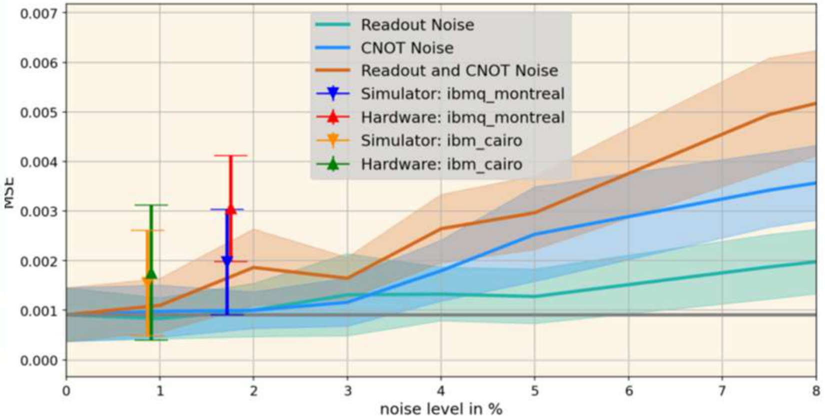
Noise studies to test the robustness of the QAG model against noise:

- in inference and in training
- on quantum simulator:
  - simulated noise up to different (same) levels: readout / gate / readout + gate
  - real hardware noise (in different mixture) as given by IBM
- on real quantum devices:
  - ibmq_montreal
  - ibm_cairo

Noise in Inference



Noise in Training



**Readout + Gate Noise**
**Gate Noise**
**Readout Noise**

**▼ HW Sim M**
**▲ HW M**

**▼ HW Sim M**
**▲ HW C**

*Rehm, F. et al. Precise Image Generation on Current Noisy Quantum Computing Devices. IOP Quantum Science and Technology* https://doi.org/10.1088/2058-9565/ad0389.

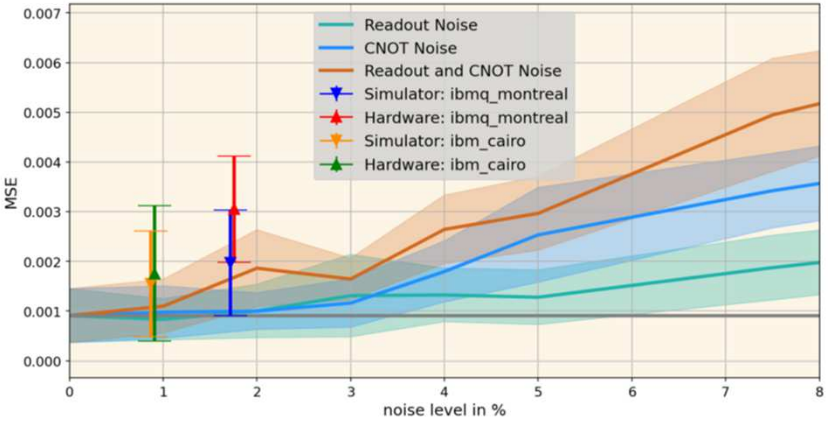
*PhD Thesis of F.Rehm with details* http://doi.org/10.18154/RWTH-2023-09302

# Quantum Angle Generator: Learning Noise !

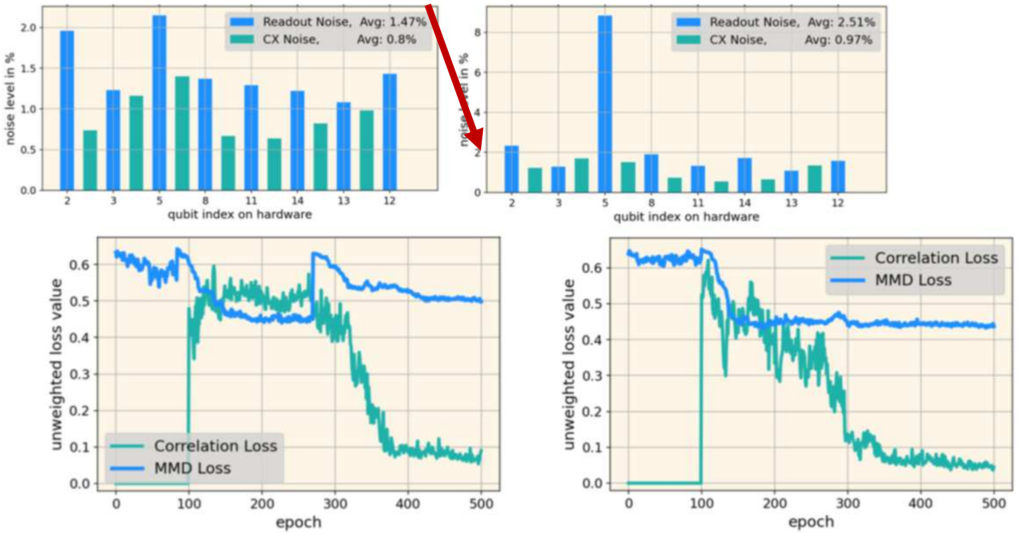
## Less parameters for complex data and robustness against noise

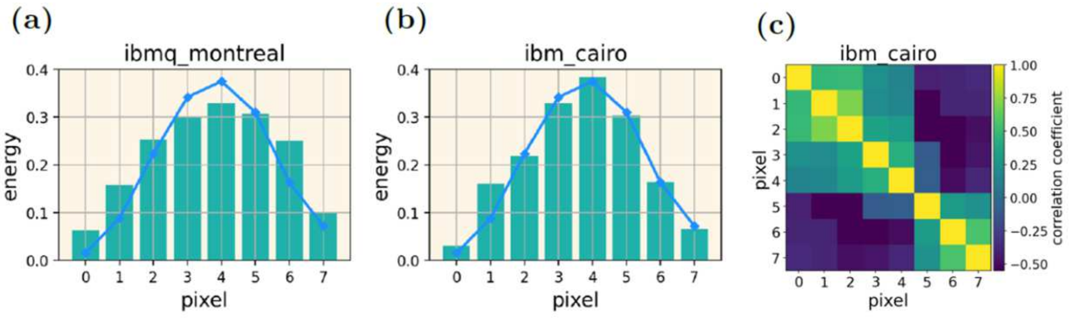
BMBF
NiQ

Noise in Trainng



Calibration change during training





- **Noise in training + inference leads to better accuracy.**
- **Quantum Neural Networks can adapt to changing error enviroment and learn the noise condition**
  **→ robustness against and employing noise !**

*Rehm, F. et al. Precise Image Generation on Current Noisy Quantum Computing Devices.*
*IOP Quantum Science and Technology* https://doi.org/10.1088/2058-9565/ad0389.

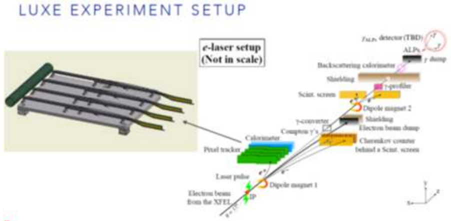
*PhD Thesis of F.Rehm with details*
http://doi.org/10.18154/RWTH-2023-09302

# Quantum Computing for Classical Optimization Problems

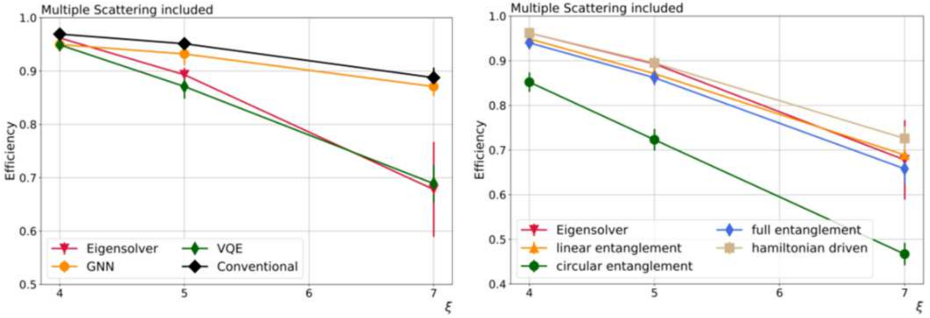
## From Tracking to Logistics

- ➢ **Tracking at the LUXE Experiment @ DESY**

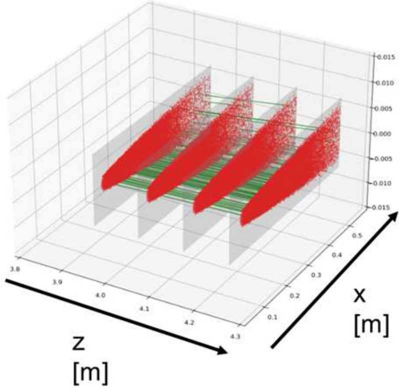
**Q-GNN and VQE for**
**particle tracking**
**in the LUXE Experiment**
(Laser Und XFEL Experiment)
**study of the influence of entanglement**



*First paper 2109.12636*
*Second paper: Crippa A. et al, Quantum algorithms for charged particle track reconstruction in the LUXE experiment, https://arxiv.org/abs/2304.01690*

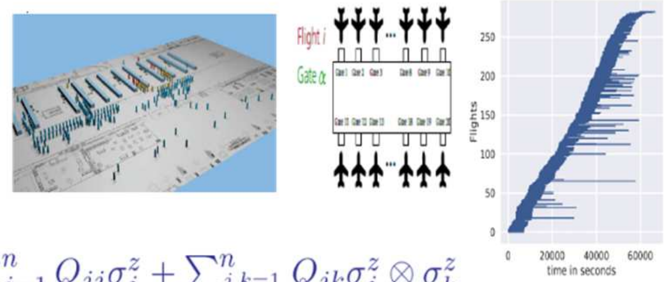


Efficiency as a function of the field intensity ξ



**Particle tracking**

Observe particles through their interaction with detectors
→ Need to single out each particle's trajectory from a cloud of hits



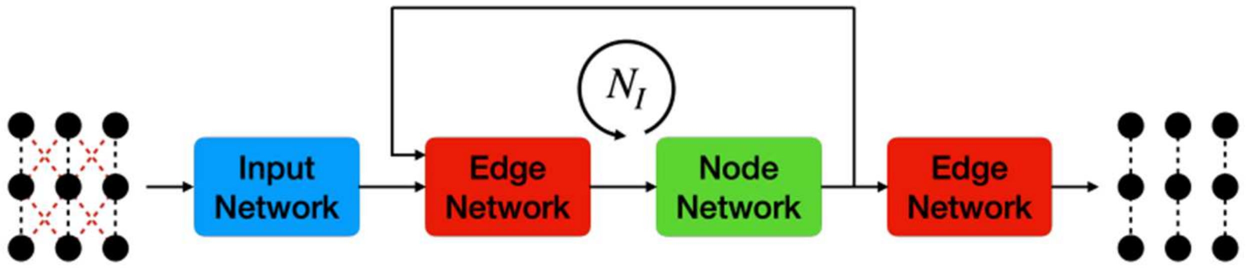
$$H = \sum_{j=1}^{n} Q_{jj}\sigma_j^z + \sum_{\substack{j,k=1 \\ j<k}}^{n} Q_{jk}\sigma_j^z \otimes \sigma_k^z$$

**Flight Gate Assignment**

find lowest energy ⇔ shortest path
Same mathematics for problems in traffic, logistics, aerospace, ...

# Quantum Graph Neural Network

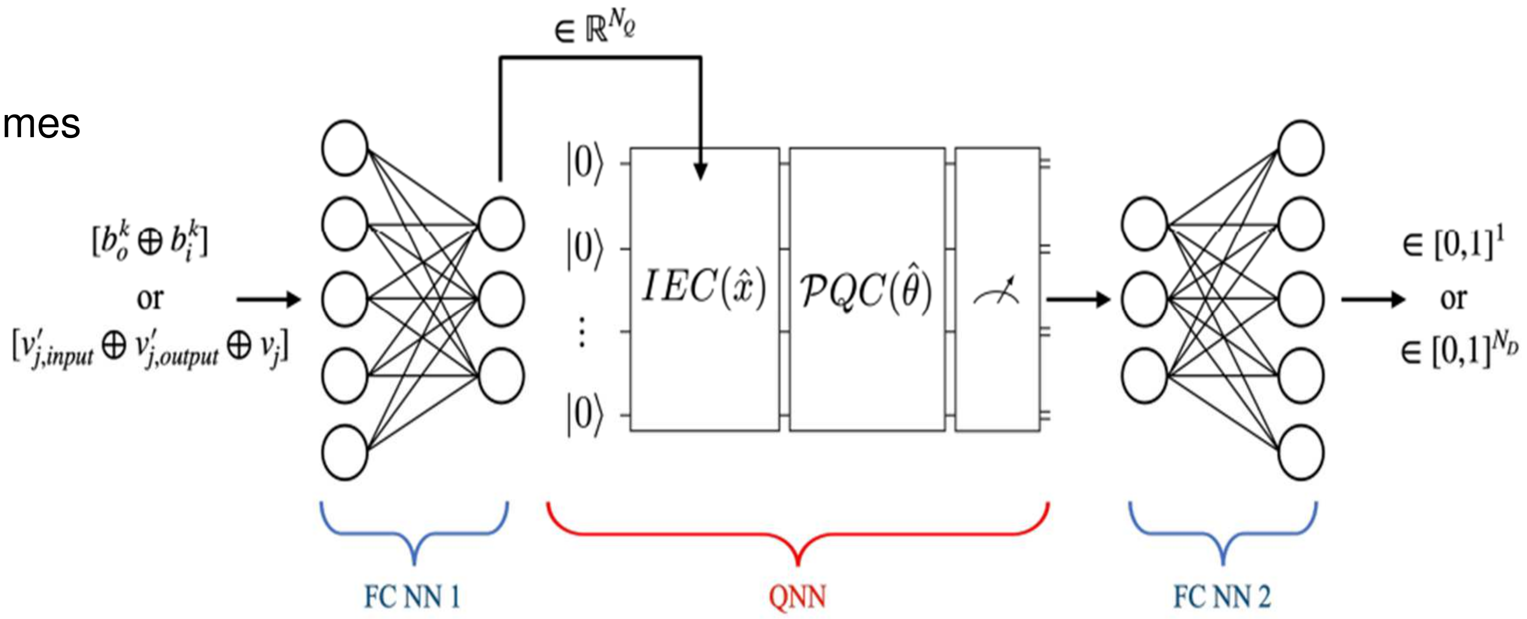
*First paper 2109.12636*
*Second paper: Crippa A. et al, Quantum algorithms for charged particle track reconstruction in the LUXE experiment, https://arxiv.org/abs/2304.01690*



Input network encodes information (10 hidden features)

Edge and node nets applied 4 times (as many as the tracker layers)

Retain edges with scores above fixed threshold



# Algorithmic performance

## Based on ideal classical simulations of quantum circuits

*First paper 2109.12636*

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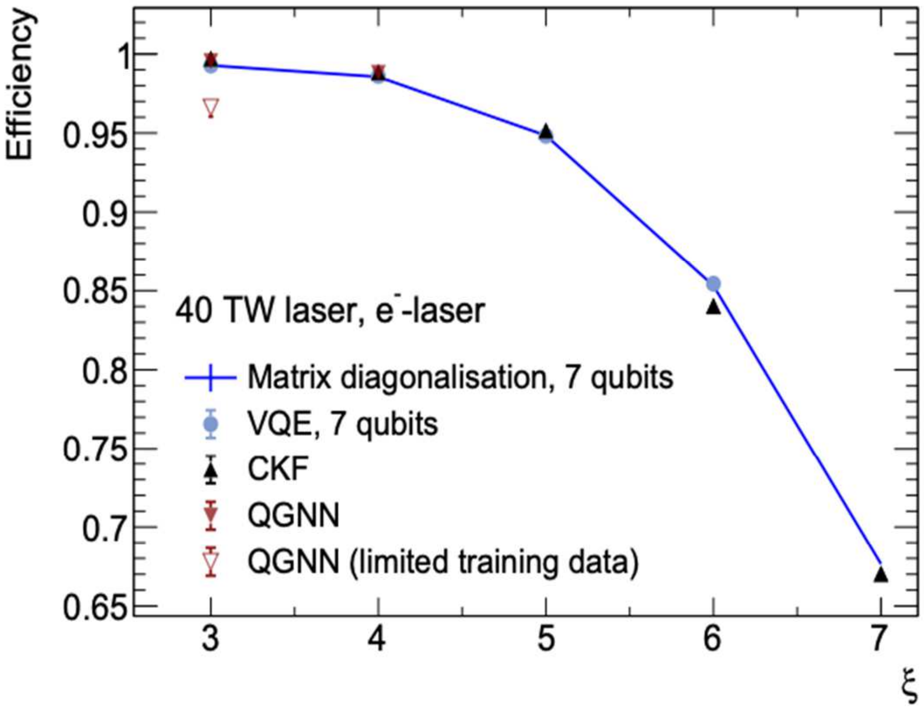
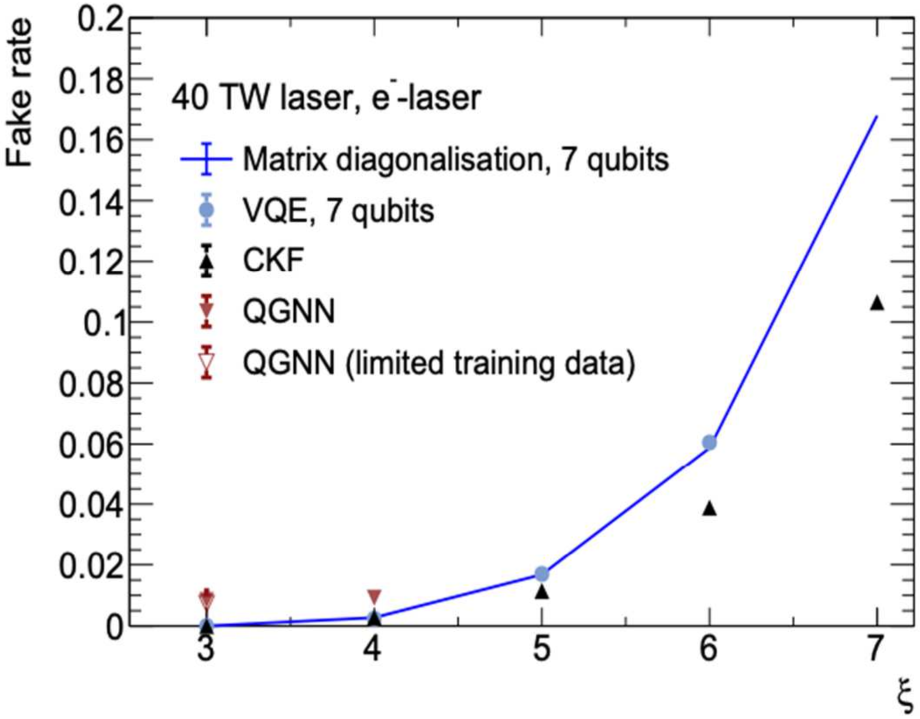




**Excellent performance, in line with state-of-the-art classical tracking**

→ Quantum algorithms have higher efficiency but ~2x fakes

Not all methods available for each value of $\xi$ (due to computational limitations)

Performed also tests with quantum hardware (ibm_nairobi)

$$\text{Efficiency} = \frac{N^{\text{matched}}_{\text{tracks}}}{N^{\text{generated}}_{\text{tracks}}}$$

$$\text{Fake rate} = \frac{N^{\text{fake}}_{\text{tracks}}}{N^{\text{reconstructed}}_{\text{tracks}}}$$

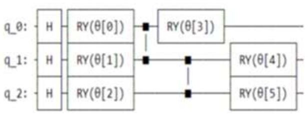
# Some Key Questions for the Future

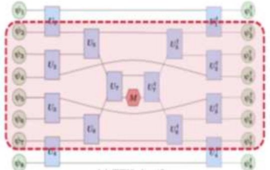
## Challenges and Opportunities in Quantum Computing

**How can we profit from the higher encoding potential given by qubits?**

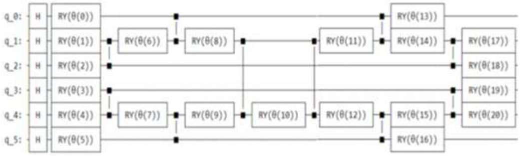
**How can quantum algorithms enable timing inclusion ($4^+$D-tracking / 5 D-calorimetry?**

**How can we profit from different entanglements of qubits?**





(a) TTN classifier



**How can we use quantum devices to solve complex fitting problems?**

### QFitter for measurement combinations

Quantum annealing-based method for fitting EFT coefficients to experimental measurements

2207.10088

**How can we use quantum devices to solve complex problems in theory calculations, simulation, reconstruction, correlations, anomalies, tomography…**

**How can we profit from the need to limit I/O by extracting features ?**

**How can we profit from the unique access to different Quantum Technology Computers?**

**Any**

**Questions ?**

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