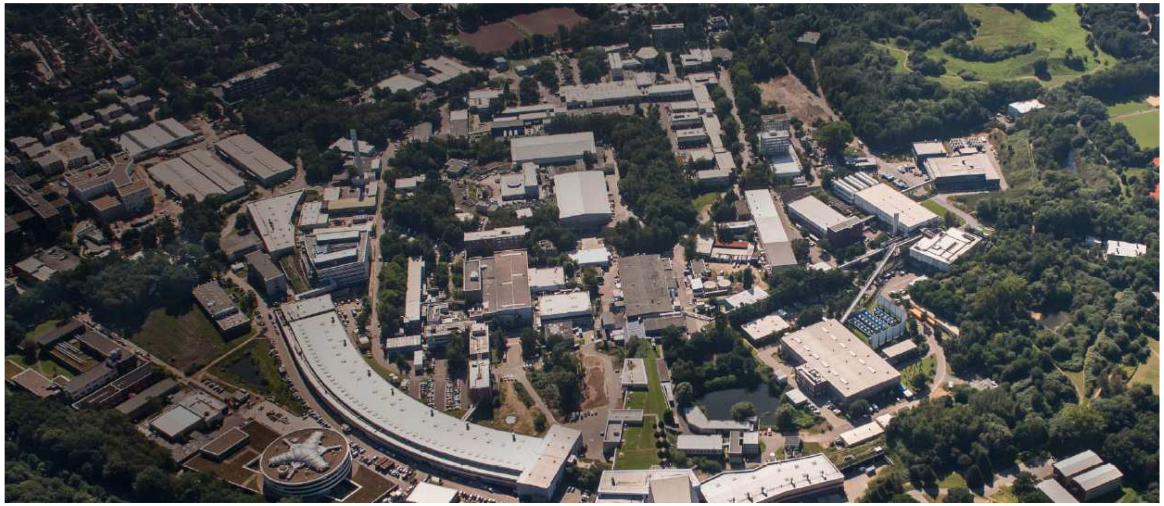


Quantum Technology Applications at DESY.

Prof. Dr. Kerstin Borras
Deutsches Elektronen-Synchrotron DESY and RWTH Aachen University
DESY Quantum Technology Task Force qt-task-force@desy.de

Physics Frontiers with Quantum Science and Technology
9 – 10 Mar 2022, University of Tokyo

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY: A world-leading accelerator laboratory.

Deutsches Elektronen-Synchrotron DESY.

Mission:

- one of the world's leading particle accelerator centres
- investigates the structure and function of matter
- from the interaction of tiny elementary particles and the behavior of novel nanomaterials and vital biomolecules to the great mysteries of the universe.
- develops and builds particle accelerators and detectors as unique research tools
- generating the most intense X-ray radiation in the world, accelerate particles to record energies and open up new windows onto the universe.

Founded 1959 as Germanys national Accelerator Center

More than 2700 employees incl. 1200 scientists in all fields; 650 scientists in the fields of accelerator operation, research and development, more than 3000 visiting scientists from over 40 nations p.a.

Approx. 260 Mio. € base budget plus 100 Mio. € third party funding p.a. (90/10)

Two locations one in Hamburg and one in Zeuthen (in Brandenburg close to Berlin)

DESY is a member of the **Helmholtz Association** Germany's largest scientific association

Quantum Technologies in the Helmholtz Association.

Strategic Roadmap with many contributions from DESY.

Helmholtz Association: DESY's Funding Agency

five primary active research areas

https://www.helmholtz.de/en/research/quantum-technologies/

- **Quantum computing**
- **Simulation, numerical and ML methods**
- **Quantum sensors**
- **Quantum materials and basic research**
- **Quantum communication**

In addition, Helmholtz develops and operates powerful **infrastructures** for researching quantum technologies

https://www.helmholtz.de/fileadmin/user_upload/04_mediathek/21_Quantum_Strategy_Brochure_WEB.pdf

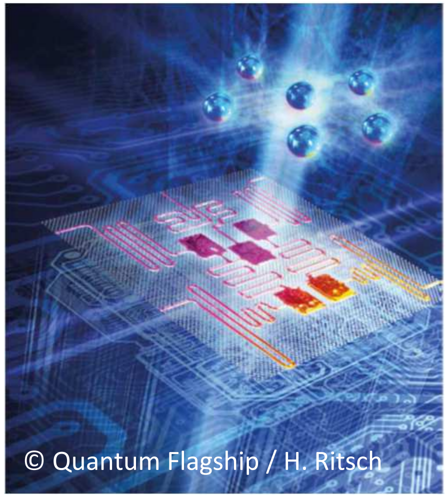
Quantum Technologies at DESY – Strategic Aspects

Introduction

DESY and Campus Partners:

excellent scientific competences and facilities for R&D in QT
crucially complementary to the running research projects
cross-cutting activities like QT are in DESY's DNA

→ unique pole position to drive the evolution and to play a leading role in dedicated QT topics.



Quantum Technology identified as a strategic direction for DESY

→ established a DESY Quantum Technology Task Force.

Three initial pillars for Quantum Technology topics at DESY:

- **Development of quantum computing algorithms for applications**
- **Materials and photonics research and development towards novel quantum devices and a scalable and reliable quantum computer**
- **Quantum sensors as evolving/enabling and also applied technology**

Quantum Technologies at DESY

Overview

DESY. QUANTUM

Overarching Goal: employ novel Quantum Technologies to enhance and enable cutting-edge science in all divisions
→ DESY wide organization connecting inside and to Campus Partners

DESY. QUANTUM

Quantum Technology Applications

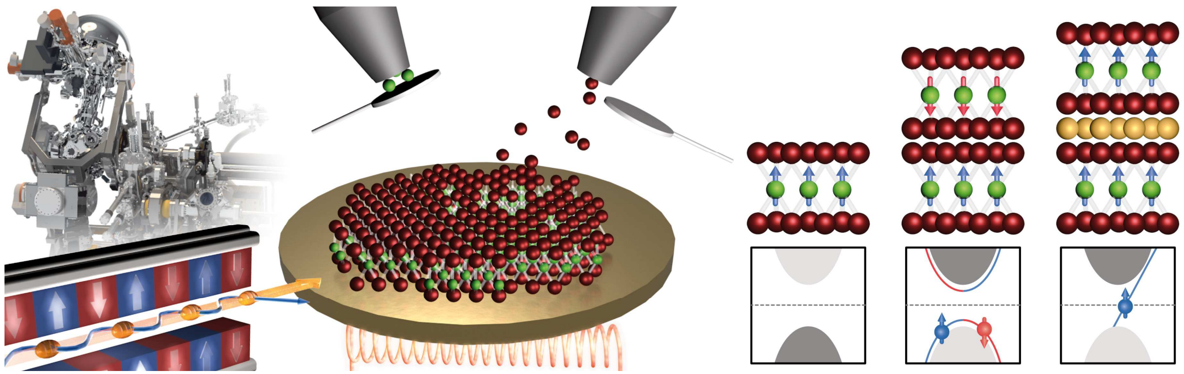
Zeuthen		Hamburg
Quantum Simulations Algorithms & Methods Benchmarking	Knowledge & Technology Transfer	Photon Science for Quantum Materials and for Quantum Devices
Access to Quantum Computers	Training and Education	Quantum Machine Learning Quantum Simulations
Quantum Sensing	Outreach	Quantum Sensing

Quantum Materials

Find out and cure what causes problems in Quantum Computers and other Quantum Devices

- **From fundamental understanding of quantum phenomena in materials to the development of tailor-made materials for quantum technology devices, including innovative qubit systems.**

- **DESY light sources: uniquely powerful quantum tools - PETRA IV: ultimate multi-D quantum microscope**
  - **Precision spectroscopy on quantum materials and devices**
    study novel, complex quantum materials and devices with high resolution and highly selective X-ray spectroscopies
    → understand the atomic and electronic structure and connect to the functional properties
  - **Ultrafast spectroscopy on quantum materials** → assess couplings and decoherence mechanisms
    employed to study quantum materials at FLASH and EuXFEL
    → insights to coupling strengths and mechanisms of decoherence mechanisms
  - **X-ray quantum optics**
    employ nuclear resonant scattering
    to extend quantum optics to the hard X-ray range
    → explore the vastly different coupling strengths, photon energies, material parameters
    → improve the generalizability of underlying theories
    → potentially discover novel applications that require exotic parameter sets.



Quantum Materials Analytics Lab (under consideration)

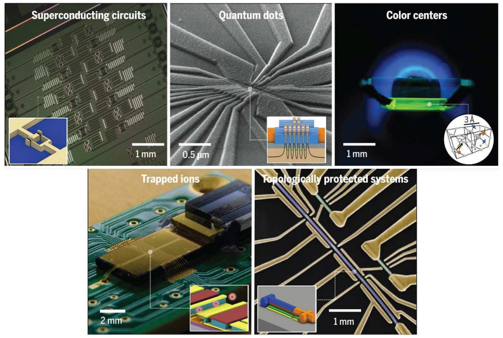
Fast-reaction materials analytics laboratory.

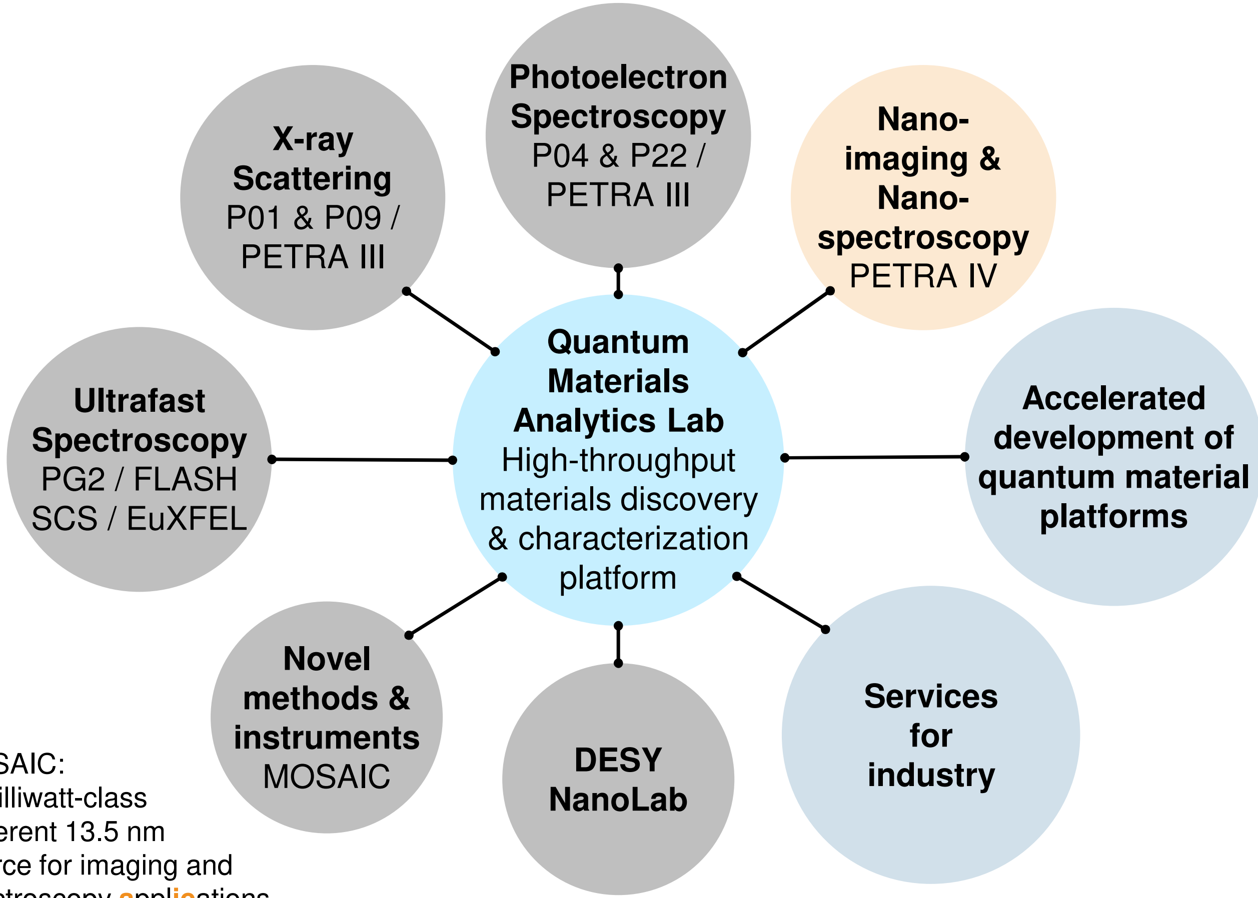
REVIEW de Leon *et al.*, *Science* **372**, eabb2823 (2021)

QUANTUM COMPUTING

Materials challenges and opportunities for quantum computing hardware

First, understanding the microscopic mechanisms that lead to noise, loss, and decoherence is crucial. This would be accelerated by developing **high-throughput methods** for correlating qubit measurement with **direct materials spectroscopy and characterization**.
Second, relatively few material platforms for solid-state QIP have been explored thus far, and the discovery of a new platform is often serendipitous. It is thus important to develop **materials discovery pipelines** that exploit directed, rational material searches in concert with **high-throughput characterization approaches** aimed at rapid screening for properties relevant to QIP.



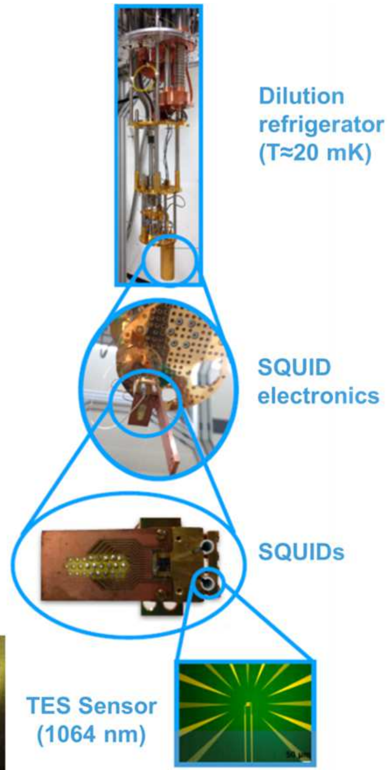


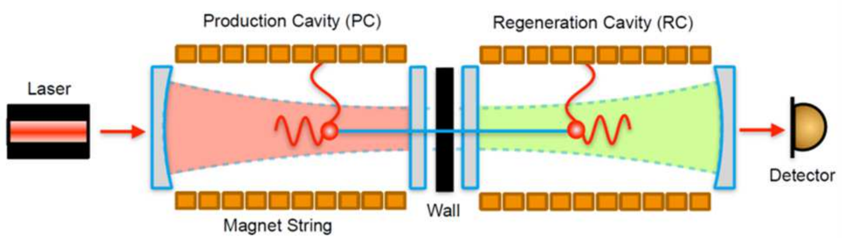
MOSAIC:
A **m**illiwatt-class co**h**erent 13.5 nm **s**ource for imaging and spectroscopy appl**ic**ations

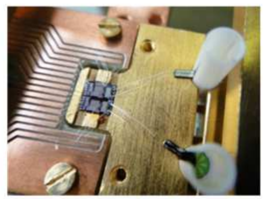
Quantum Sensing

Enabling technology for novel experiments and operation

- **Explore, develop and apply quantum sensors and electronics in particle and astro-particle physics experiments and beyond** (see also talk from Michael Doser)
- **Evolving and enabling technology → part of genuine detector R&D**
- **Applied in already operating experiments like ALPS II**
  (axion-like dark matter particles in a Light-shining-through-walls setup)
  - Transition Edge Sensor (TES):operating in the superconducting transition region
  - Detection challenge:
    Single 1064 nm photon detection: extremely low dark counts required
    Extremely low rates (about 10-5 s-1, i.e. 10-24 W)
  - TES quantum sensing up and running at DESY
    noise reduction successful; resolution of ≈10% for 1064 nm photons
    extremely low intrinsic dark counts; < 7.7*10-6 s-1 photon-like events (<1/day)







DESY. QUANTUM in Zeuthen CQTA Center for Quantum Technology Applications

Special focus on Quantum Computing Applications

- **Innovation-Funding from the state of Brandenburg:**
- **up to 15 Million Euros over 5 years**
- **Focus topics**
  - provide access to quantum computer hardware
  - develop applications and use cases
  - enable quantum simulations
  - benchmark, tests and verification of emerging hardware platforms
  - provide training in quantum computing
  - make new generation "quantum ready"

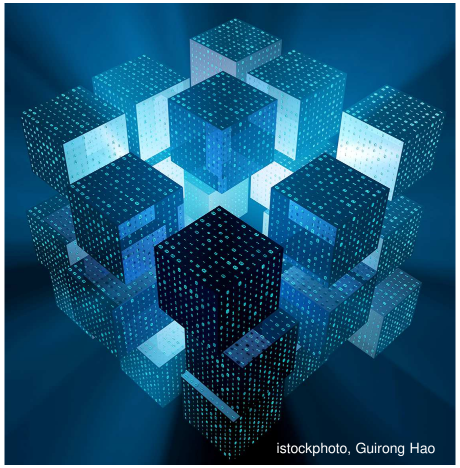
DESY. QUANTUM

Quantum Technology Applications

Zeuthen		Hamburg
Quantum Simulations Algorithms & Methods Benchmarking	Knowledge & Technology Transfer	Photon Science for Quantum Materials and for Quantum Devices
Access to Quantum Computers	Training and Education	Quantum Machine Learning Quantum Simulations
Quantum Sensing	Outreach	Quantum Sensing

Quantum Computing in Particle Physics and beyond

Pilot Projects in Quantum Computing



- Quantum Computers have the potential to solve problems that cannot be addressed with classical computers.
- **Develop algorithms and methods**
  - Calculations in Lattice Gauge Theory with Variational Quantum Simulation (VQS)
    → novel results for complex theoretical problems
    → frequently demanded by companies (IBM) to test their novel devices
  - Application to various models in high energy and condensed matter physics and others (flight gate assignment (together with DLR))
  - Error mitigation in Quantum Computer Calculations
  - Optimize Dimensional Expressivity of Quantum Gate Circuits → lower noise
  - Quantum Machine Learning for experiment simulation and reconstruction

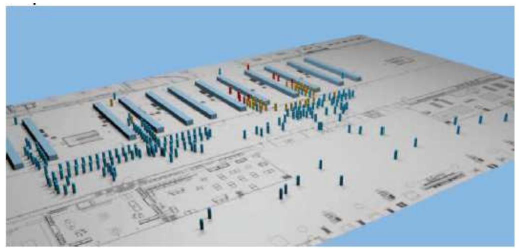
Logistic: Example for Variational Quantum Simulation

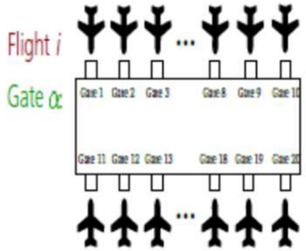
DESY's Pioneers in Quantum Computing

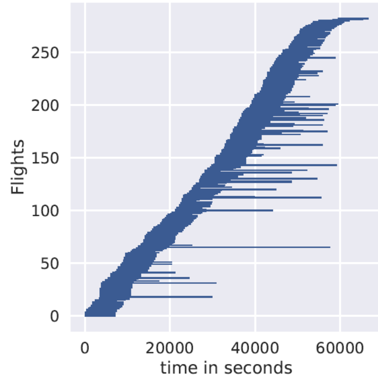
- **VQS can be applied to many different problems.**
- **Logistics Optimization: flight gate assignment (with DLR)**
  - Classical optimization problem
  - Find shortest path between connecting flights
    - different incoming and outgoing flights
    - need to be assigned to gates
    - find optimal assignment
  - Mathematical description (analogue of energy)

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

  - Task: find lowest energy ⇔ shortest path
  - **Same mathematical description for problems in traffic, logistics, aerospace, ... tracking in particle physics**







Example for Error Mitigation in VQS

Increase the Reliability for Quantum Computing Calculations

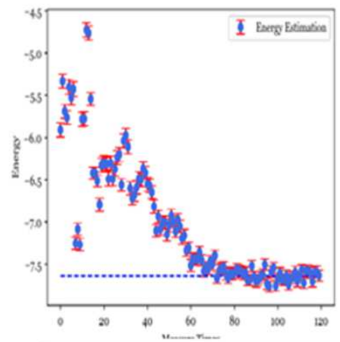
➢ **Model in Condensed Matter Physics: 1-Dimensional Heisenberg model**

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

- Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

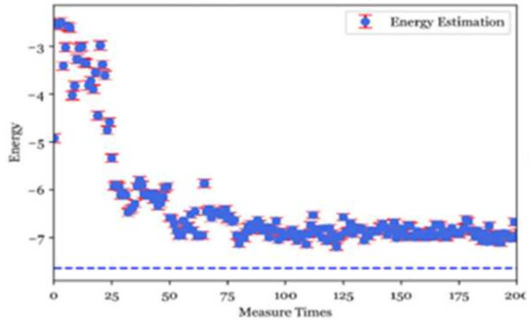
- nearest neighbor interaction,
  tensor products
- Hamiltonian expressed in Pauli matrices
  → suitable for quantum computer
- shows phase transitions, critical behavior,
  non-trivial spectrum

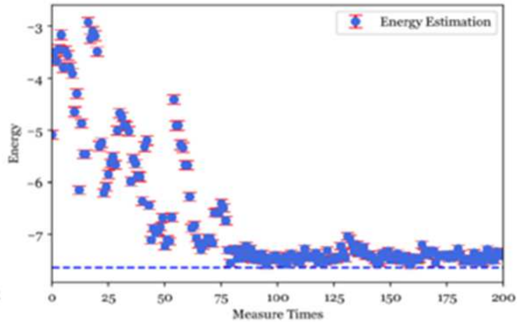


no noise:
reaching exact result very fast

full noise
cannot find
ground state

corrected
ok !



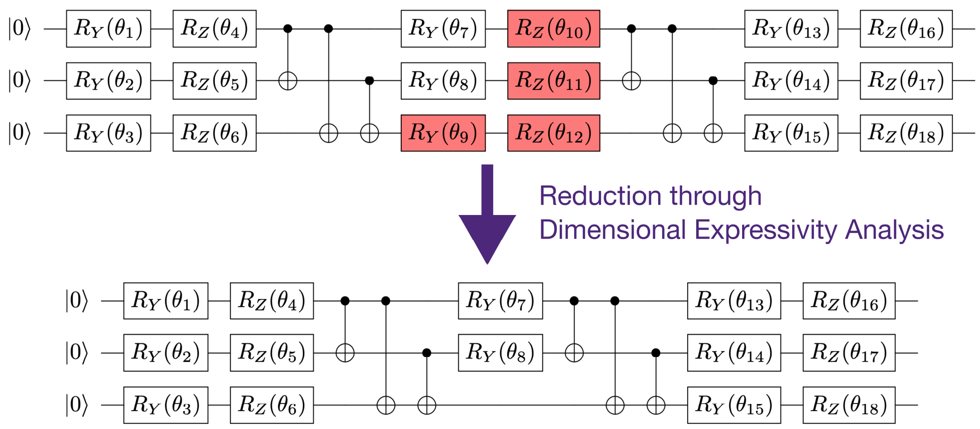


Measurement Error Mitigation in Quantum Computers Through Classical Bit-Flip Correction
L. Funcke, T. Hartung, S.Kühn, P. Stornati, X. Wang, K.Jansen, arxiv:2007.03663, under review in Phys. Rev. D

Optimize Dimensional Expressivity of an Quantum Gate Circuit

Less gates → less noise.

- **Gate Operations are a source of noise in QC calculations.**
- **Develop algorithms and methods for Dimensional Expressivity Analysis**
  - generate as many/complicated states as possible with fewest number of gates
  - for non-parametric gates: algebraic techniques (commutator rules) to minimize gate count (no decrease in expressivity)
  - parametric gates: algebraic techniques become difficult (groups have infinitely many generators)
  - need a metric of expressivity



Dimensional Expressivity Analysis of Quantum Circuits
L. Funcke, T. Hartung, S. Kühn, P. Stornati, K.Jansen,
Quantum 5 (2021) 422

Quantum Machine Learning

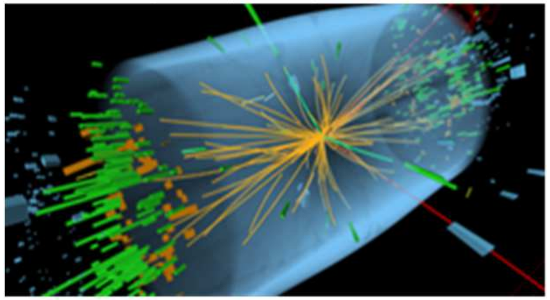
Early examples in Experimental Particle Physics

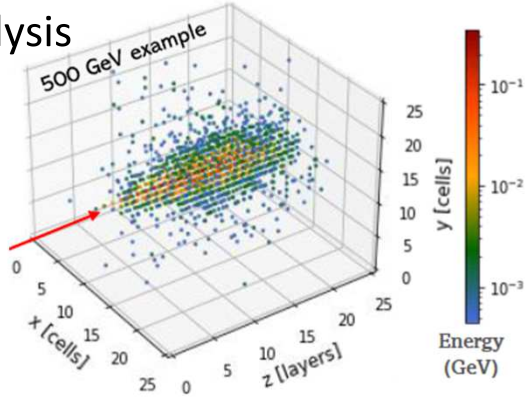
- **Quantum Maschine Learning lies at the intersection of Quantum Computing and Maschine Learning**

  → usually employed to analyze classical data in a hybrid mode

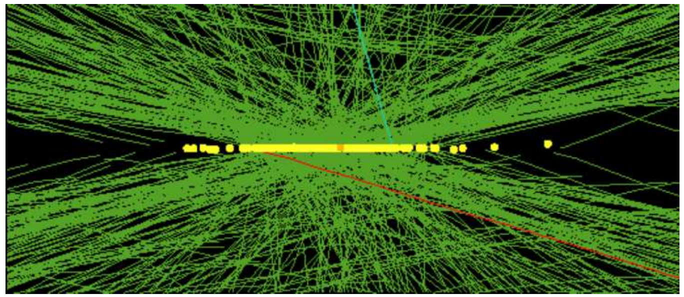
  - High Luminosity LHC (>2029) needs vast amount of simulations with 200 pile-up events, GRID Computing, Big Data Analysis

LHC (~20 pile-up events)





LHC (~140 pile-up events)

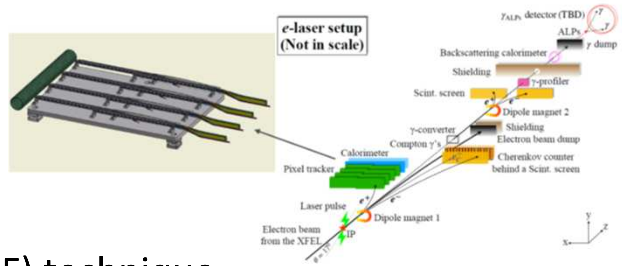


- **Develop machine learning and tensor network methods for QC**
  - Quantum GAN (Quantum Generative Adversarial Network) simulations for detectors (CERN Openlab with joint Gentner PhD Student)
  - Tracking with Quantum Computers for LUXE and ATLAS

Track Reconstruction with Quantum Computers at LUXE

L.Funcke,T.Hartung,B.Heinemann,K.Jansen,A.Kropf,S.Kühn,F.Meloni,D.Spataro,C.Tüysüz,Y.C.Yap **https://arxiv.org/abs/2202.06874**

LUXE EXPERIMENT SETUP



- **LUXE** (Laser Und XFEL Experiment)
  - study QED in the strong-field regime where it becomes non-perturbative
  - use European XFEL electron beam and high-power laser
- **Develop Quantum tracking algorithms and compare to others**
  - **Convential** benchmark: ACTS-based tracking with combinatorial Kalman Filter (CKF) technique.
  - Graph Neural Network (**GNN**): constructed from doublets, all nodes of consecutive layers are connected, and only the ones that satisfy pre-selection cuts are kept.
  - Quantum Approach: Triplets are identified to form tracks by expressing the problem as a quadratic unconstrained binary optimisation (QUBO), problem similar to https://doi.org/ 10.1007/s41781-019-0032-5.
    Minimising the QUBO is equivalent to finding the ground state of the Hamiltonian:

$$O(a,b,T) = \underbrace{\sum_{i=1}^{N} a_i T_i}_{\text{Quality of triplets}} + \underbrace{\sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j}_{\text{Compatibility between triplet pairs}} \quad T_i, T_j \in \{0,1\}$$

a_i quantify the quality of the triplets.
b_{ij} quantify the compatibility between triplet pairs.

$$b_{ij} = \begin{cases} 0, & \text{if no shared hit} \\ +1, & \text{if in conflict} \\ -S(T_i, T_j), & \text{if two hits are shared} \end{cases}$$

QUBO can be mapped to Ising Hamiltonian and solved using Variational Quantum Eigensolver (VQE)

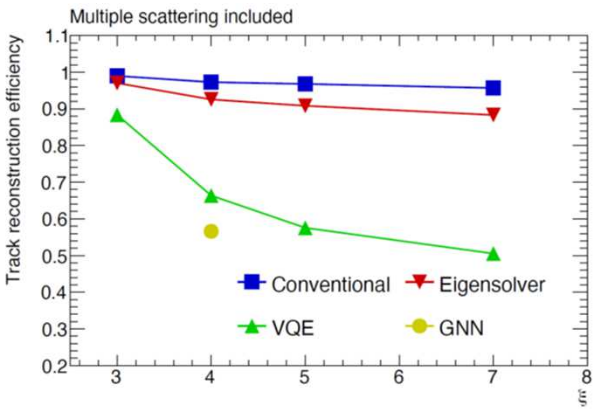
$$\mathcal{H} = -\sum_{n=1}^{N} \sigma_n^x \sigma_{n+1}^x - \alpha \sum_{n=1}^{N} \sigma_n^x$$

Two sets of results:

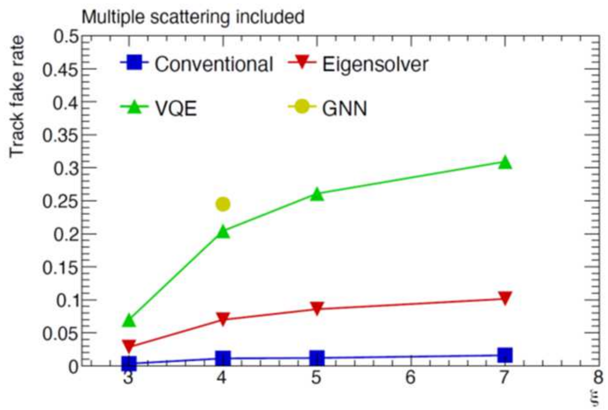
- Exact solution using matrix diagonalisation (NumPy **Eigensolver**) for benchmarking
- **VQE** (without QC noise) using one choice of Ansatz and optimiser

Track Reconstruction with Quantum Computers at LUXE

L.Funcke,T.Hartung,B.Heinemann,K.Jansen,A.Kropf,S.Kühn,F.Meloni,D.Spataro,C.Tüysüz,Y.C.Yap https://arxiv.org/abs/2202.06874



Track reconstruction efficiency as a function of the field intensity parameter ξ



Track fake rate as a function of the field intensity parameter ξ

Very preliminary results , For example GNN is limited by the training dataset size

→ system with quantum approach and classical benchmarks is working

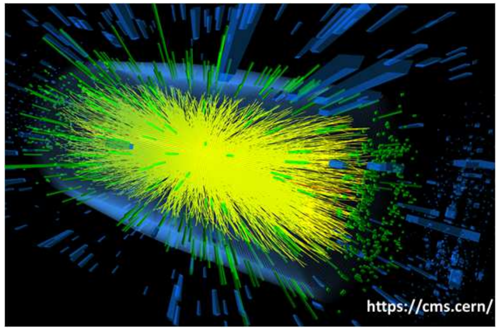
→ conventional tracking shows the performance that can be realistically achieved

→ room for improvement for other tracking methods

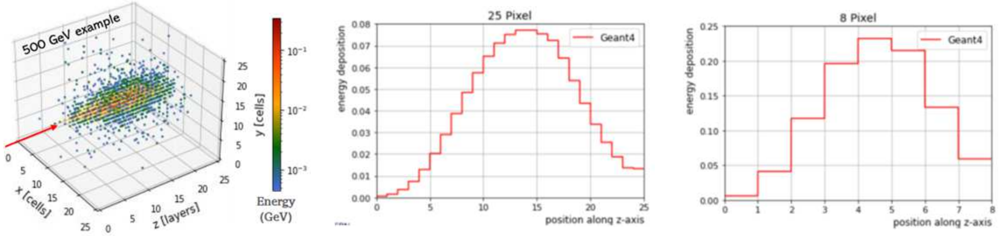
→ further optimization studies in progress.

Quantum GANs in One Dimension

Quantum Generative Adversarial Network

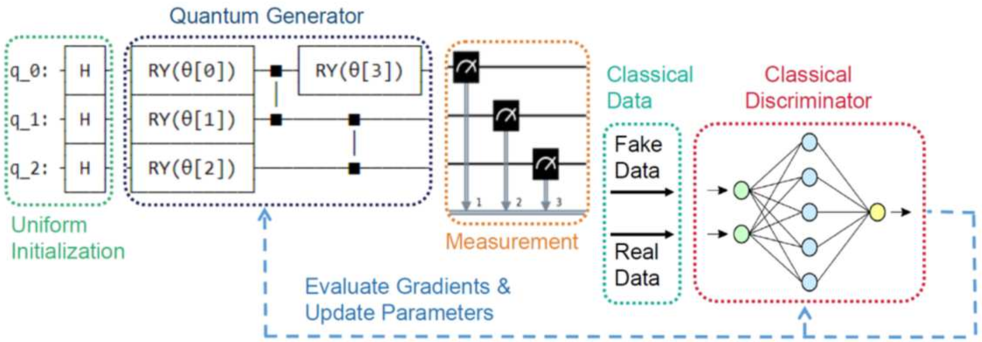


- **Down sample 3D shower image → 8 pixels → 3 qubits**

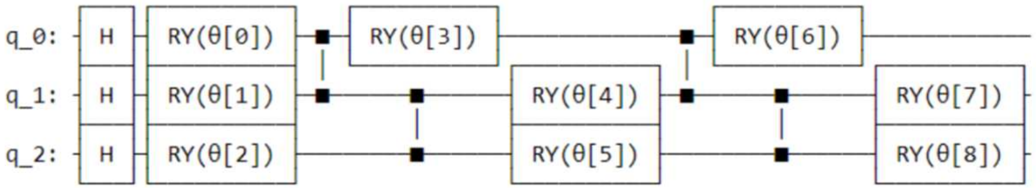


8 quantum states:
|000⟩, |001⟩, |010⟩, |011⟩,
|100⟩, |101⟩, |110⟩, |111⟩

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



- **Employ a Quiskit qGAN model developed by IBM***



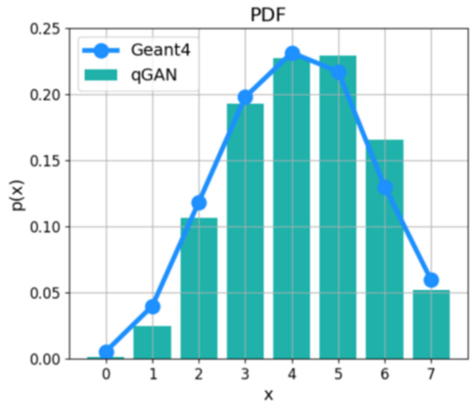
Initial work by CERN Openlab et al:
Quantum Generative Adversarial Networks in a Continuous-Variable Architecture to Simulate High Energy Physics Detectors:
arXiv:2101.11132 [quant-ph]
Dual-Parameterized Quantum Circuit GAN Model in High Energy Physics
EPJ Web of Conferences 251, 03050 (2021)

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

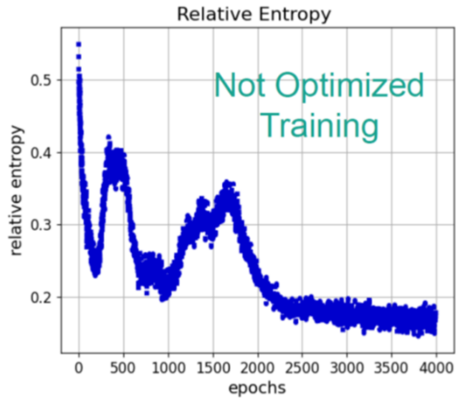
Quantum GAN in One Dimension without Noise

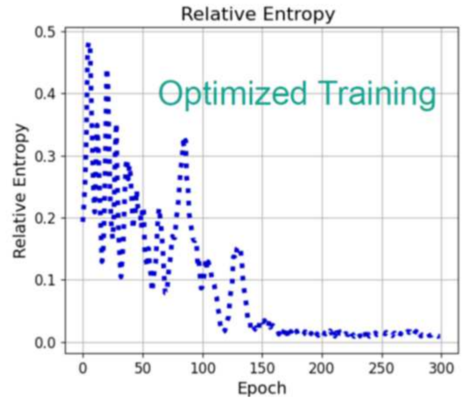
F. Rehm, S. Vallecorsa, K. Borras, D. Krücker http://symsim.jinr.ru/grid2021/363-368-paper-67.pdf

Uniform Initialization



Trained Model





- training time ~ 1 day for 3000 epochs → speed up training
- hyperparameter optimizations:
  - higher learning rate
  - implement exponential learning rate decay
  - different generator and discriminator learning rate
  - train discriminator more often than generator
- **Result:**

  10x speed up in training time → need only ~300 epochs instead of > 3000

CERN openlab DESY.

QUANTUM MACHINE LEARNING FOR HEP DETECTOR SIMULATIONS

Proceedings of the 9th International Conference "Distributed Computing and Grid Technologies in Science and Education" (GRID'2021), Dubna, Russia, July 5-9, 2021 http://symsim.jinr.ru/grid2021/363-368-paper-67.pdf

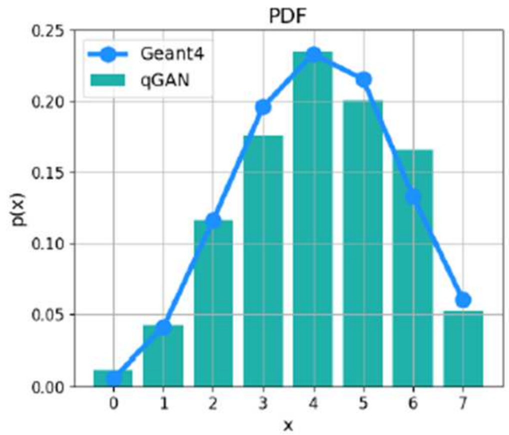
Quantum GAN in One Dimension with Noise

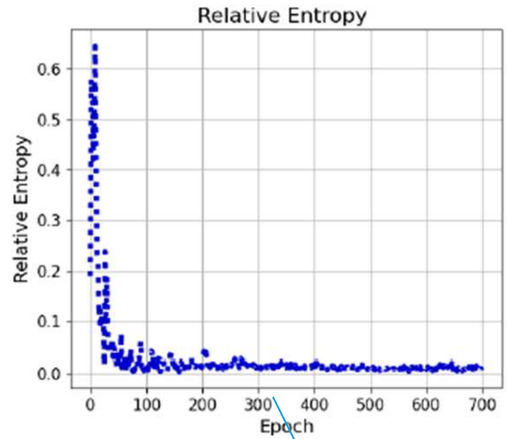
F. Rehm, S. Vallecorsa, K. Borras, D. Krücker http://symsim.jinr.ru/grid2021/363-368-paper-67.pdf

➢ Apply Readout Noise (model IBMq belem)

Qubit Number:	0	1	2
Readout Error:	3.6%	4.7%	9.6%

no decrease in accuracy
fast convergence

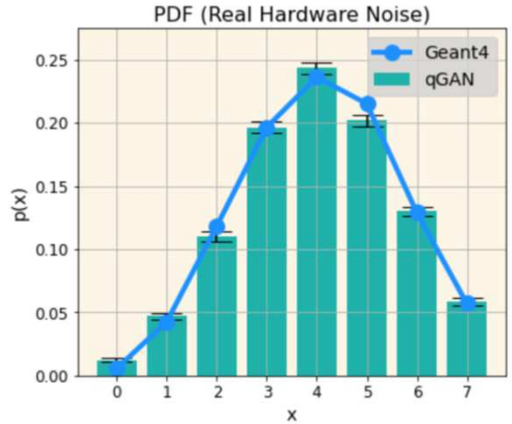


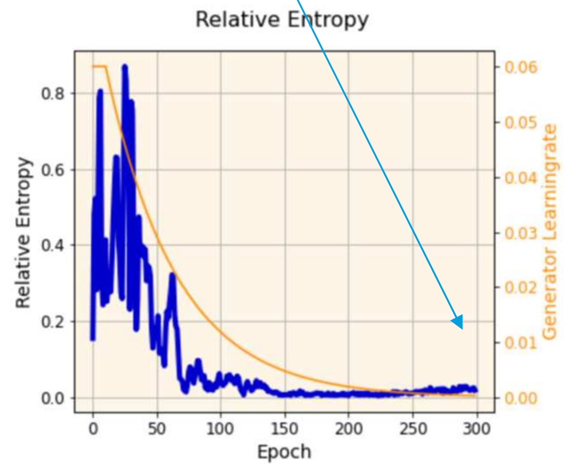


➢ Apply Full Noise (model IBMq manila)

Qubit Number	0	1	2	Average
Readout Error	2.34%	2.66%	2.05%	**2.35%**
CX-gate Error	1.11%		1.75%	**1.43%**

no decrease in accuracy
fast convergence



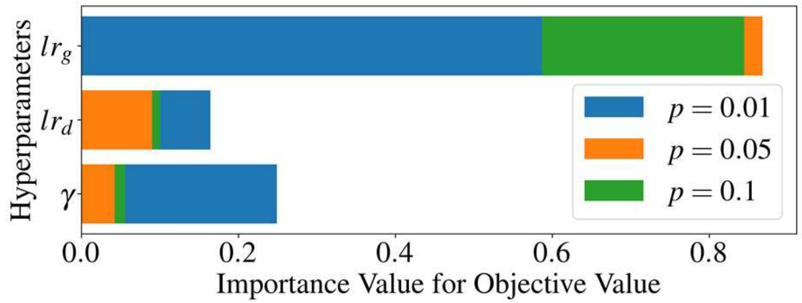


Impact of quantum noise on the training of Quantum GANs

K.Borras,S.Y.Chang,L.Funcke,M.Grossi,T.Hartung,K.Jansen, D.Kruecker,S.Kühn,F.Rehm, C.Tüysüz,S.Vallecorsa

https://arxiv.org/abs/2203.01007

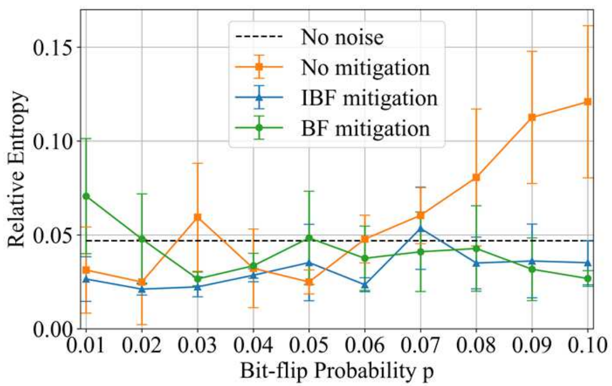
Detailed studies with noise and noise mitigation



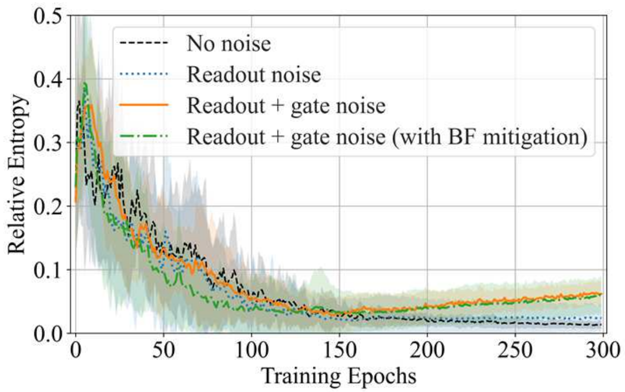
- **Importance of hyperparameters for different values of the bit-flip probability, p = {0.01, 0.05, 0.1}**
  - generator learning rate lrg, discriminator learning rate lrd, exponential decay rate γ for the learning layers

  → generator learning rate lrg has the highest impact → demonstrates the difficulty of training the quantum generator

- **Results without and with two different error mitigation methods**



Error mitigation plays a crucial role for qGAN training in the presence of the large readout errors on current NISQ devices

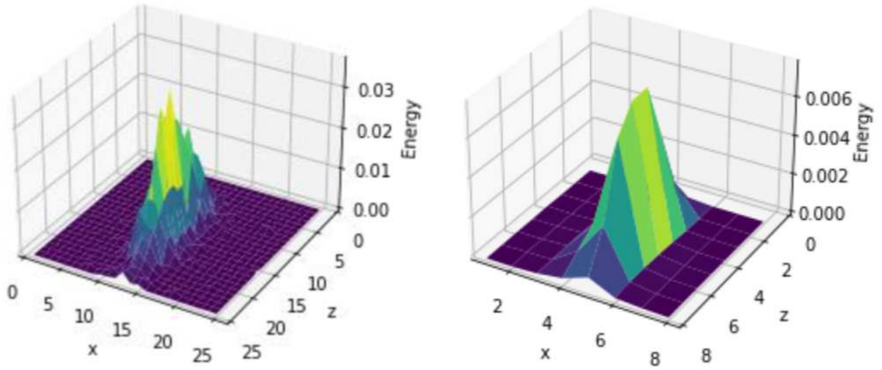


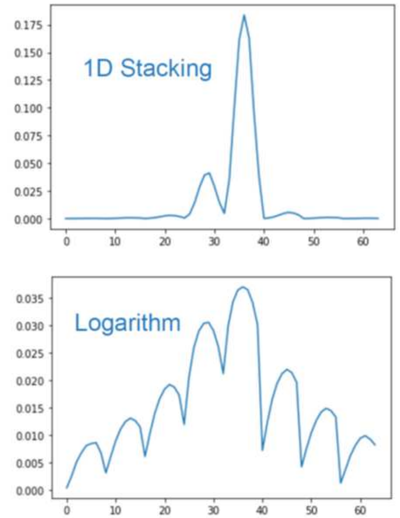
Average values quickly converge in the noise-free and readout-error only cases, but do not seem to converge when including two-qubit gate errors → reveal the critical effect of two-qubit gate errors on qGAN training with current NISQ devices.

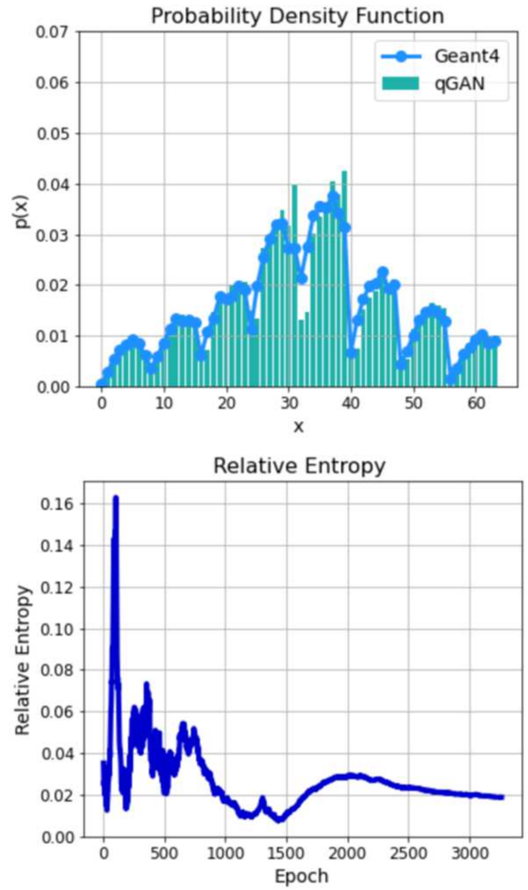
Quantum GAN in Two Dimensions

Early examples in Experimental Particle Physics

➢ **Down sample → 8x8 pixels → 6 qubits**

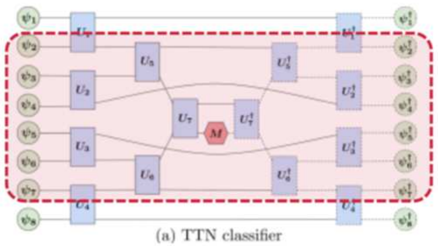


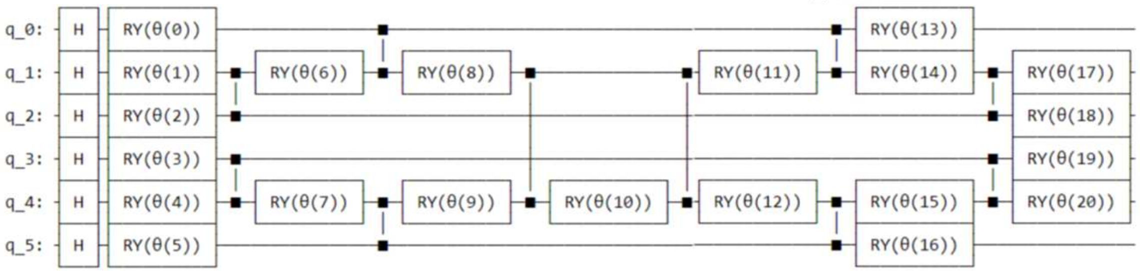




➢ **Adapt Tree Tensor Network**

Grant, E., Benedetti, M., Cao, S.*et al.*
Hierarchical quantum classifiers.
*npjQuantum Inf***4,**65 (2018).
https://doi.org/10.1038/s41534-018-0116-9





Summary

DESY's Competence in Quantum Technology

DESY develops a large variety of Quantum Computing Applications:
VQS, Quantum-ML in simulation and reconstruction and more:

- useful for particle physics, condensed matter as well as optimization problems and simulations and reconstruction of detectors and arbitrary events
- algorithms can be generalized towards many interdisciplinary areas (logistic, scheduling and more)

DESY develops methods for efficient Quantum Computing:

- error mitigation, expressivity optimization, benchmark tests for QC hardware

DESY employs its unique photon source facilities:

- understand the working of Quantum Materials, shape and design tailor-made materials for Quantum devices like qubits and sensors

DESY studies and develops Quantum Sensors:

- apply and operate Quantum Sensors in new experiments, evolve and enable unprecedented precision for novel experiments to answer fundamental questions.

Interested in collaboration? Please get in touch with us: DESY QT Taskforce **qt-task-force@desy.de**

Any

Questions ?