Quantum Machine Learning

Introduction - Examples - Opportunities

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

DESY, IPC Seminar 24 Aug 2021

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Quantum Computing with ML Methods

Heather Gray, CERN Academic Training, https://indico.cern.ch/event/870513/

25

Quantum Machine Learning

- QML lies at the intersection between quantum computing and machine learning
- Usually, we're talking about using quantum computers to analyse classical data
- In many cases, the most promising methods are hybrid classical/quantum approaches
- Both quantum annealers and digital quantum computers have been explored
- Introductory QML textbook
- Recent review article about quantum machine learning in HEP
- Not trying to provide an overview here; rather trying to show examples of studies that have been performed

Don't fall for the hype! - *Frank Zickert*

Hands-On Quantum Machine Learning With Python is your comprehensive guide to get started with **Quantum Machine Learning** - the use of **quantum computing** for the computation of **machine learning** algorithms.

https://www.pyqml.com/

https://iopscience.iop.org/article/10.1088/2632-2153/abc17d/meta

Just try to use it as soon as possible to benefit as soon as possible !

Kerstin Borras

Wide Variety of Opportunities to use QC with ML Methods

Sau Lan Wu, QuantHEP Seminar, https://quanthep.eu/event/quanthep-seminar-sau-lan-wu/

Our program with Quantum Machine Learning

Our Goal:

To perform LHC High Energy Physics analysis with Quantum Machine Learning, to explore and to demonstrate that the potential of quantum computers can be a new computational paradigm for big data analysis in HEP, as a proof of principle

Our present program is to employ the following 3 quantum machine learning methods

1. Variational Quantum Classifier Method
2. Quantum Support Vector Machine Kernel Method
3. Quantum Neural Network Method

to LHC High Energy Physics analysis, for example ttH ($H \rightarrow \gamma\gamma$) and $H \rightarrow \mu\mu$ (two LHC flagship analyses).

Sau Lan Wu (U. Wisconsin) QuantHEP Seminar November 4, 2020 5

Challenges that can be addressed with QML

Introduction

Very diverse challenges can be adressed with Quantum Machine Learning

- Simulation (lattice QCD, parton showers, detector, …)
- Reconstruction (tracking, jet - clustering,…)
- Physics Analyses
- Searches (Grover, …)
- Anomaly Detection, Classifier
- Optimization (scheduling, …)
- ….

An up-to-date collection on quantum algorithms can be found here:
https://quantumalgorithmzoo.org/

Quantum Algorithm Zoo

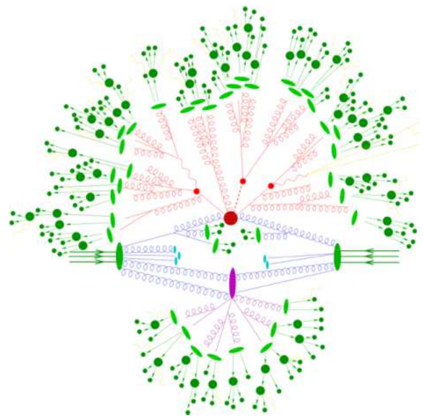
This is a comprehensive catalog of quantum algorithms. If you notice any errors or omissions, please email me at stephen.jordan@microsoft.com. (Alternatively, you may submit a pull request to the repository on github.) Your help is appreciated and will be acknowledged.

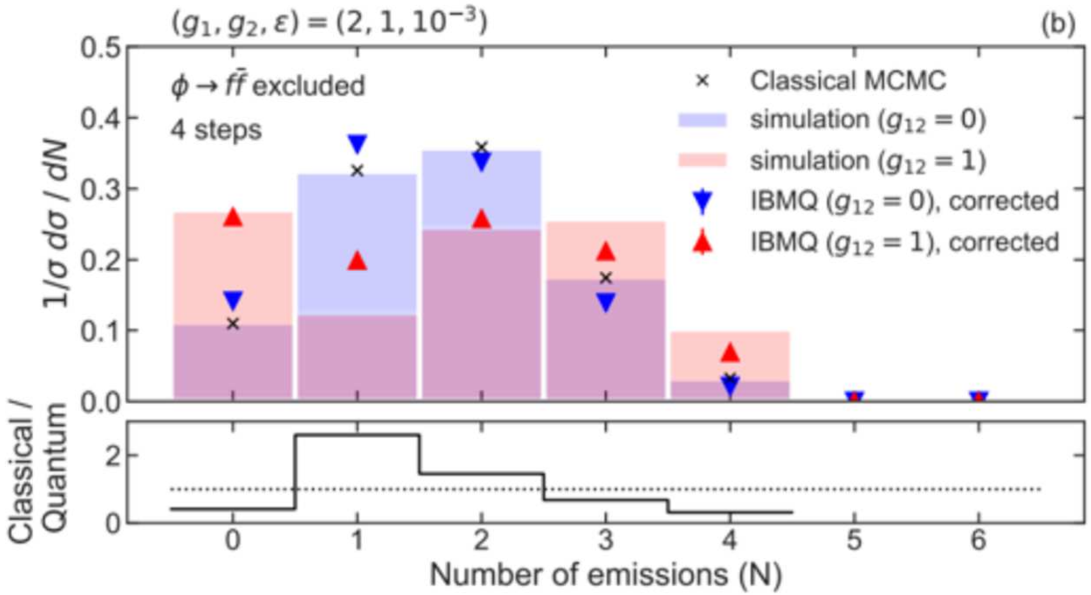
Algebraic and Number Theoretic Algorithms

Algorithm: Factoring
Speedup: Superpolynomial
Description: Given an n-bit integer, find the prime factorization. The quantum algorithm of Peter Shor solves this in $\widetilde{O}(n^3)$ time [82,125]. The fastest known classical algorithm for integer factorization is the general number field sieve, which is believed to run in time $2^{\widetilde{O}(n^{1/3})}$. The best rigorously proven upper bound on the classical complexity of factoring is $O(2^{n/4+o(1)})$ via the Pollard-Strassen algorithm [252, 362]. Shor's factoring algorithm breaks RSA public-key encryption and the closely related quantum algorithms for discrete logarithms break the DSA and ECDSA digital signature schemes and the Diffie-Hellman key-exchange protocol. A quantum algorithm even faster than Shor's for the special case of factoring “semiprimes”, which are widely used in cryptography, is given in [271].

Hadronic Structure, Fragmentation, Parton Shower

C. Bauer, W. de Jong, B. Nachman, D. Provasoli - 1904.03196 [quant-ph]





A quantum algorithm for high energy physics simulations

Christian W. Bauer, Wibe A. de Jong, Benjamin Nachman, Davide Provasoli, arXiv:1904.03196 [hep-ph]

$$\mathcal{L} = \bar{f}_1(i\partial\!\!\!/ + m_1)f_1 + \bar{f}_2(i\partial\!\!\!/ + m_2)f_2 + (\partial_\mu\phi)^2 + g_1\bar{f}_1 f_1\phi + g_2\bar{f}_2 f_2\phi + g_{12}\left[\bar{f}_1 f_2 + \bar{f}_2 f_1\right]\phi\,.$$

Deeply inelastic scattering structure functions on a hybrid quantum computer

Niklas Mueller,* Andrey Tarasov,† and Raju Venugopalan‡
Physics Department, Brookhaven National Laboratory, Bldg. 510A, Upton, NY 11973, USA
(Dated: August 21, 2019)

Parton Physics on a Quantum Computer

Henry Lamm,[1,*] Scott Lawrence,[1,†] and Yukari Yamauchi[1,‡]
(NuQS Collaboration)
[1]*Department of Physics, University of Maryland, College Park, Maryland 20742, USA*
(Dated: February 18, 2020)

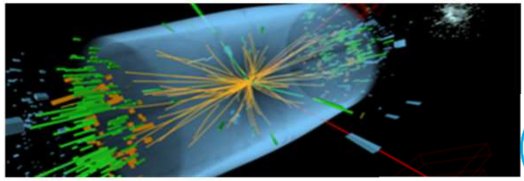
Quantum Generative Adversarial Network (GAN)

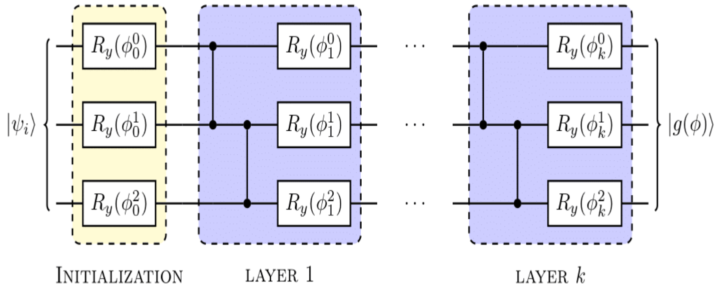
Quantum Machine Learning as Tool for fast and precise Simulations

https://www.nature.com/articles/s41534-019-0223-2

Complex MC simulation needed (digital twins) for LHC experiments

- Computational needs are beyond projected computational resources of HL-LHC
- Urgent need for new methods of fast simulation





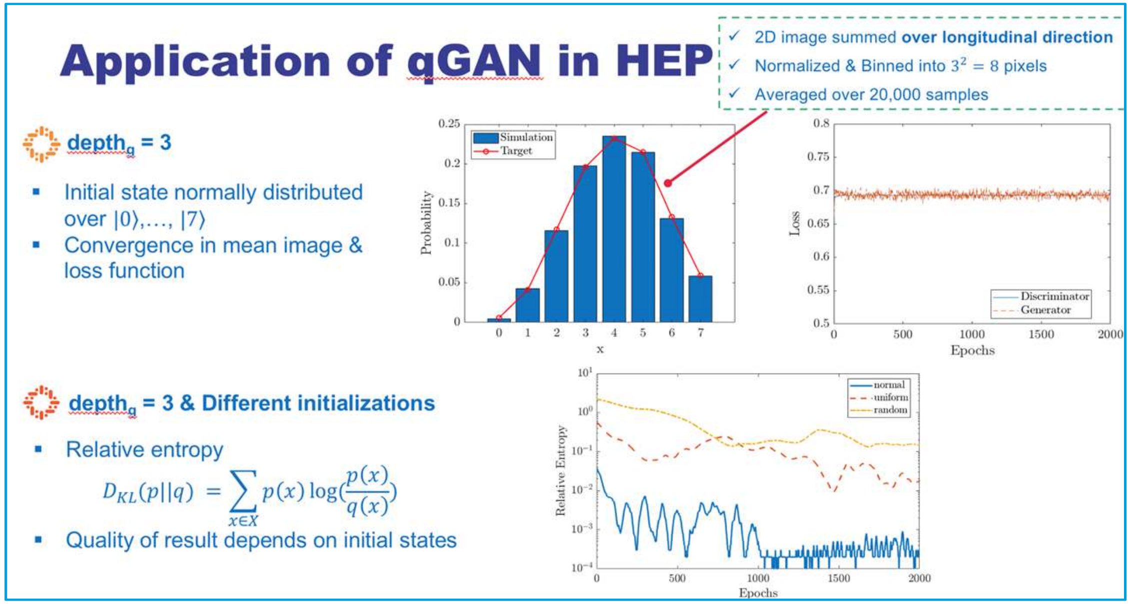
IBM/ETH Zürich suggested a Hybrid algorithm

- Quantum Generator + Classical Discriminator
  - proposed for discrete prob. distribution

Deep Learning allows to replace iterative simulation by Deep Neural Nets (typical approach: GAN)

- Even larger gain with Quantum Algorithms ⟹ **qGAN**
- Ongoing cooperation between DESY-CERN (1 Gentner Student)

Calorimeter application needs continuous probability → new approaches have to be developed



Material thanks to Su Yeon Chang (EPFL, CERN openlab) https://indico.cern.ch/event/852553/contributions/4057624/attachments/2127835/3582797/QGAN.pdf

Quantum GANs - Towards more complexity

Quantum Machine Learning as Tool for fast and precise Simulations

RWTH AACHEN UNIVERSITY

CERN openlab

Quantum Machine Learning for HEP Detector Simulations

GRID 2021

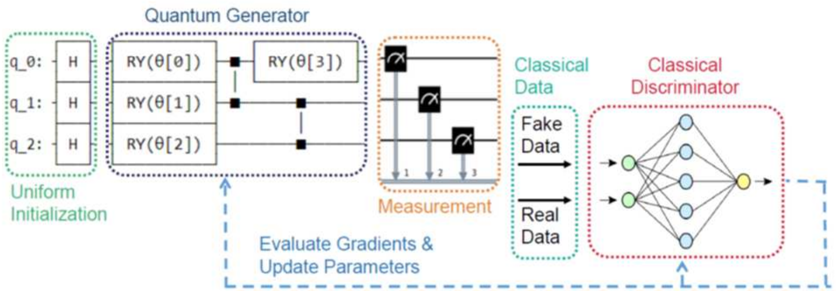
Florian Rehm [CERN openlab, RWTH Aachen]

Sofia Vallecorsa [CERN openlab], Kerstin Borras [DESY, RWTH Aachen], Dirk Krücker [DESY]

Hybrid qGAN

Quantum Generative Adversarial Networks

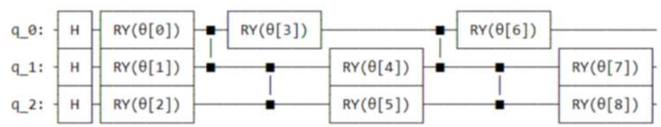
- Hybrid quantum – classical ansatz



1D Quantum Generator Circuit

- Only 1D 8-pixel images
  - 3 qubits ($2^3 = 8$) in quantum generator circuit
    - 8 quantum states: $|000\rangle$, $|001\rangle$, $|010\rangle$, $|011\rangle$, $|100\rangle$, $|101\rangle$, $|110\rangle$, $|111\rangle$
- Modified a Qiskit qGAN model developed by IBM

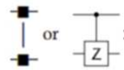
Quantum Generator Circuit:



Gates:

$$\boxed{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$R_y(\theta) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$



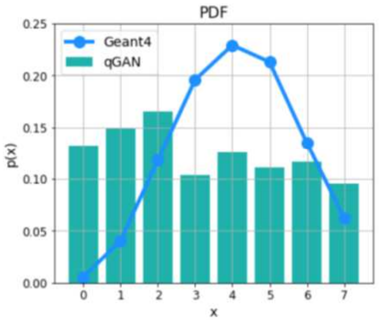
$$= CZ = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Quantum GANs - Towards more complexity

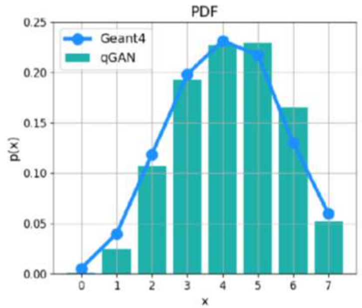
Quantum Machine Learning as Tool for fast and precise Simulations

1D Quantum Simulator

Without Noise



Uniform Initialization

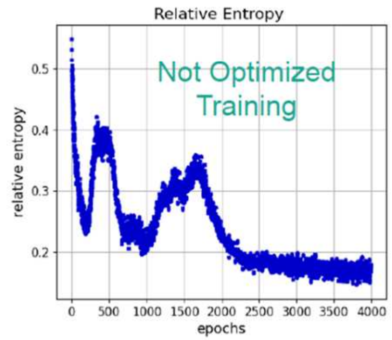


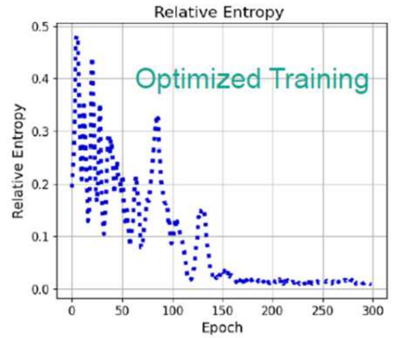
Trained Model

→ Good results

Optimize Training

- Training time ~ 1 day for 3000 epochs
  - → speeding training up
- Hyperparameter optimizations:
  - Higher learning rate
  - Implement exponential learning rate decay
  - Different generator and discriminator learning rate
  - Train discriminator more often than generator
- Results:
  - **10x speed up** in training time
    → Only ~300 epochs instead of > 3000





CERN openlab

Florian Rehm - GRID 2021

Quantum GANs - Towards more complexity - Noise

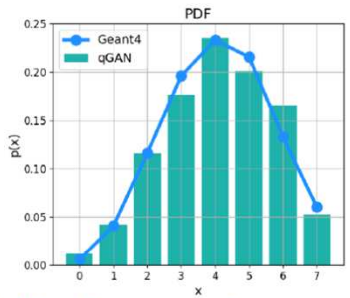
Quantum Machine Learning as Tool for fast and precise Simulations

1D qGAN with Noise

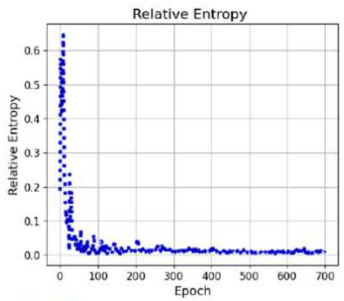
Readout Noise Only

- We applied readout noise to the qubit measurements
  - Noise model from IBMq belem quantum computer

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



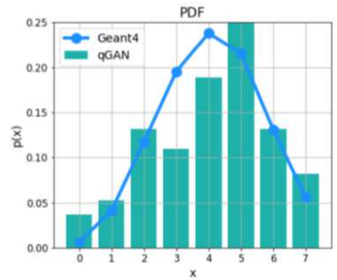
→ No decrease in accuracy



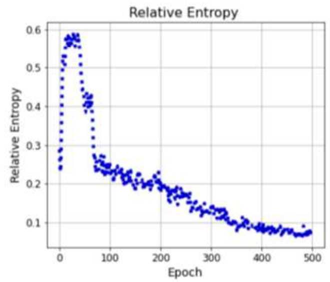
→ Fast convergence

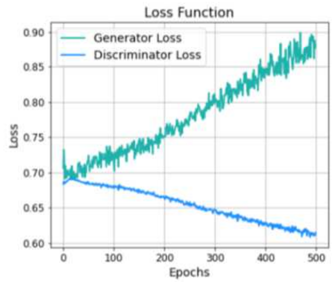
Full Noise Model

- We applied noise to the qubit gates (readout noise + gate level noise)
  - Noise model from IBMq belem quantum computer
  - Average gate level noise: 4.32%



→ Lower accuracy

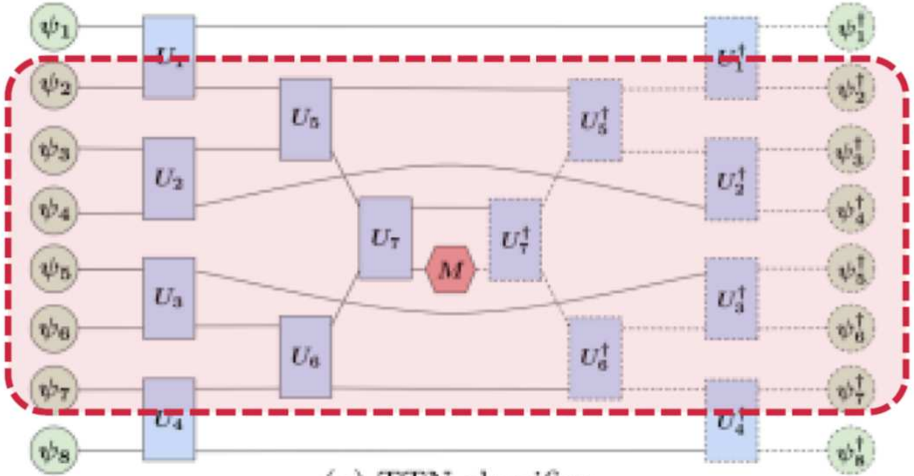




→ Non-converging losses

Quantum GANs - Towards more complexity - Dimensions

Quantum Machine Learning as Tool for fast and precise Simulations



(a) TTN classifier

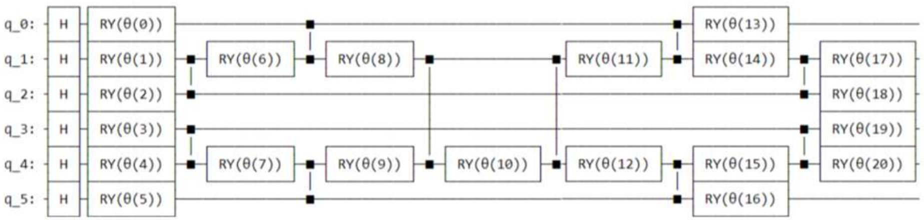
8 x 8 = 64 pixels $= 2^6$

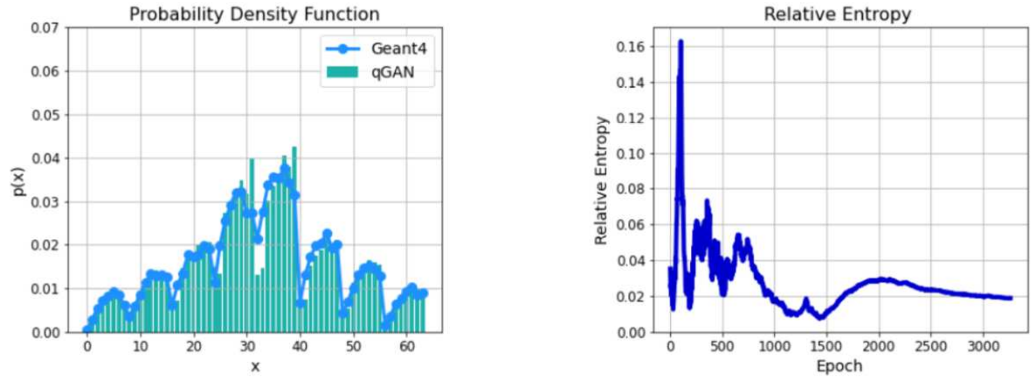
Only 6 qubits

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

2D Quantum Generator Circuit

Tree Tensor Network Architecture

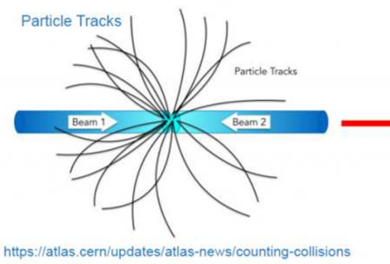


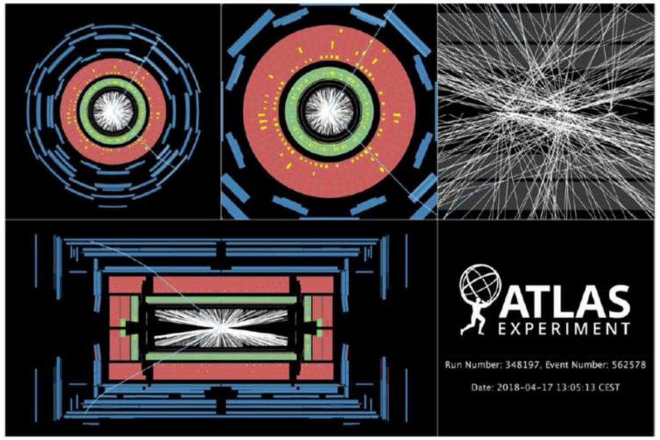


Trained Model

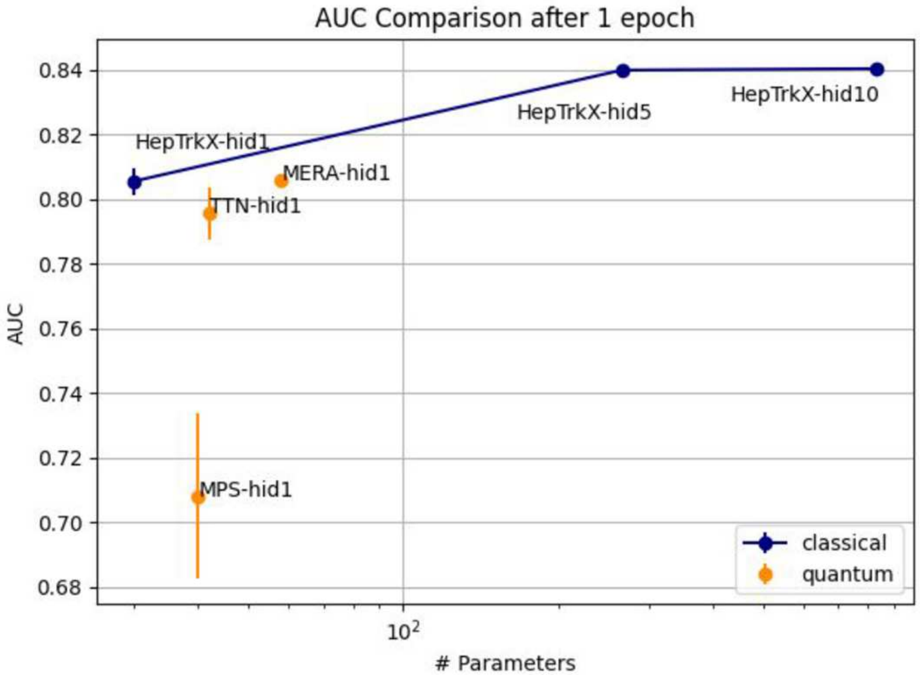
Quantum Graph Neural Networks for Particle Physics and beyond

Quantum Machine Learning for Particle Tracking and Flight Tracking





AUC: Area Under ROC, a measure of accuracy for different thresholds. AUC = 1.0 means perfect score.



Results:

- A comparison with Hep.TrkX after a single epoch shows that the QGNN model performs similarly.
- Better AUC possibly achievable by future improvements:
  better hardware, more qubits, more training time
  ….

Material thanks to Cenk Tüysüz (METU,CERN openlab) https://indico.cern.ch/event/852553/contributions/4057625/attachments/2127652/3582465/IML_2020_cenk_tuysuz.pdf

Wide Variety of Opportunities to use QC with ML Methods

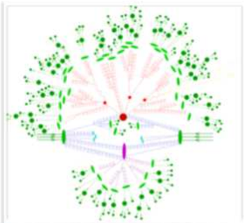
Heather Gray, CERN Academic Training, https://indico.cern.ch/event/870513/

Outline for Today

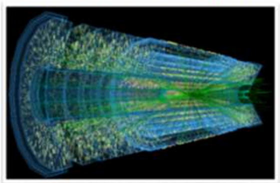
- **Applications** of quantum computing in **HEP**
  - Simulation
    - Parton shower correlations
    - Lattice QCD
  - Reconstruction
    - Particle tracking
  - Analysis
    - Higgs analyses
    - SUSY search

Progress has been very rapid here…
Relying on a mix of published and unpublished results
My apologies to anyone who's work I've left out or don't do justice to

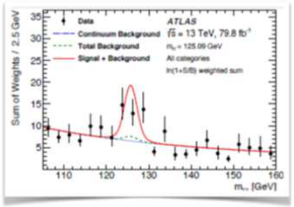
Simulation



Reconstruction



Analysis



5

Track reconstruction studies

- Quantum Annealing x 2
- Quantum Associative Memory
- Quantum Hough Transform
- Quantum Graph Neural Network

41

Incomplete list of other studies for HEP

- Quantum gate optimization for scientific applications: https://arxiv.org/pdf/2102.10008.pdf
- Simulating collider physics on QC: https://arxiv.org/pdf/2102.05044.pdf
- Vertexing with QA: https://arxiv.org/pdf/1903.08879.pdf
- QA for jet clustering: https://journals.aps.org/prd/abstract/10.1103/PhysRevD.101.094015
- Unfolding with QA: https://link.springer.com/article/10.1007/JHEP11(2019)128
- Unfolding to mitigate readout errors: https://www.nature.com/articles/s41534-020-00309-7

Quantum Technology at DLR

DLR general:
Ca. 8000 people,
50 institutes, 26 sites

QuantumTech DLR:

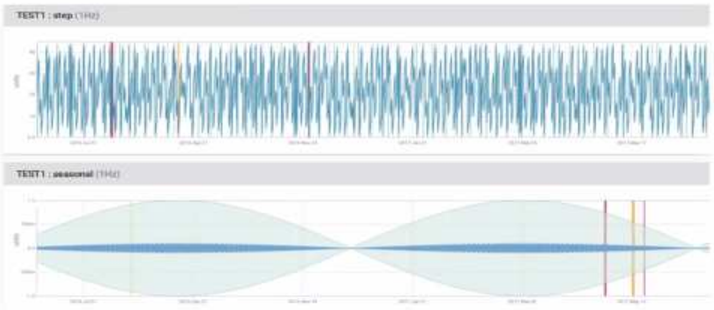
- DLR-QT (Ulm) Quantum Technologies
- DLR-SI (Hannover)
  Satellite Geodesy & Inertial Sensing
- DLR-SC (Köln)
  Simulation & S/W TechLab
- DLR-TT (Stuttgart)
  Technical Thermodynamics
- DLR-KN (Oberpfaffenhofen)
  Communications & Navigation
- DLR-MF (Oberpfaffenhofen)
  Remote Sensing
- ...
- DLR-RB (Oberpfaffenhofen)
  German Space Operations Center

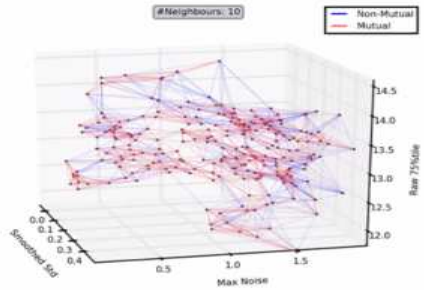
DLR

Quantum Computing at DLR

Example from DLR

Quantumalgorithms in Satellite operations:
QuATHMoS: Anomaly detection via QuantumMachineLearning





Telemetry data is represented in a feature vector space. A model is trained by nominal data. Outliers are detected to point out anomalies.

Applicable Quantum Algorithms

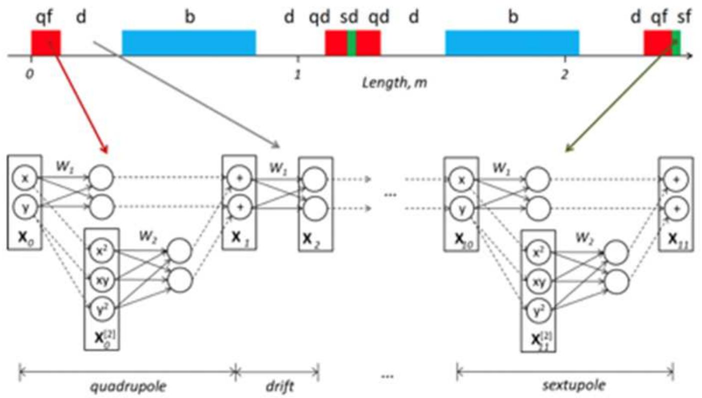
- Quantum Principle Component Analysis
- Quantum Support Vector Machines

Challenge: How to get telemetry data to the quantum computer?

DLR

QC Opportunities from the Particle Accelerators Perspective

Quantum algorithms in particle beam dynamics and ML



To be noted:
Our current interest within the M mission is to leverage ML and HPC for design, operation and automation of (electron) accelerator facilities.

- Example application: regularization techniques for training of DNNs for control and modelling of accelerators based on QUBO
- Open question for R&D: beam dynamics simulations: classical many-body systems on quantum computers?
  Synergies with FH/FS/AP

Y. Cao et al. Quantum algorithm and circuit design solving the Poisson equation, NJP 15 2013

Prospects for Quantum Computing at DESY

A Division-Wide Activity including Campus Partners

Center for Quantum Technology Applications CQTA

Zeuthen

Quantum Simulations
Algorithms & Methods
Benchmarking

Access to Quantum Computers

Quantum Sensing

Transfer
Training and Education
Outreach

Hamburg

Photon Science
for Quantum Materials and
for Quantum Devices

Quantum Machine Learning
Quantum Simulations

Quantum Sensing

The CQTA will help **us all** to get started in time to benefit as soon as possible.

Lively field with extremely rapid evolution !

Many opportunities for enabling novel technology for our science!

The imminent future

Several PhD students and few PostDocs are starting now and until next year with different funding sources (InnoPool, MSCA Co-Fund…)
→ nice opportunity to join, get training and start with small prototypes
→ get quantum-fit.

Zeuthen received the approval for major funding (15 Mio € in 5 y) for building a Laboratory for Quantum Computing Applications.

One BMBF short proposal for a user network to investigate and mitigate noise has been approved to submit a full proposal.

One short proposal in the framework of QuantHEP has been approved to submit a full proposal.

One ERC grant will be submitted for Quantum Annealing

Campus:
One BMBF short proposal for a hub can move on,
DLR & ITT in discussion, DLR received 740 Mio € to enable Industry (80%) and to do QC research (20%).

Within Helmholtz more funding opportunities will show up.

Any
Questions ?

DESY QT Taskforce reachable via **qt-task-force@desy.de**

Interested ? → Sign-up in this common email list **quantum-technologies@desy.de**