Quantum Machine Learning for Future Colliders

(Tracking & Q-GAN)

第二届量子计算与高能物理研讨会, March 31, 2023

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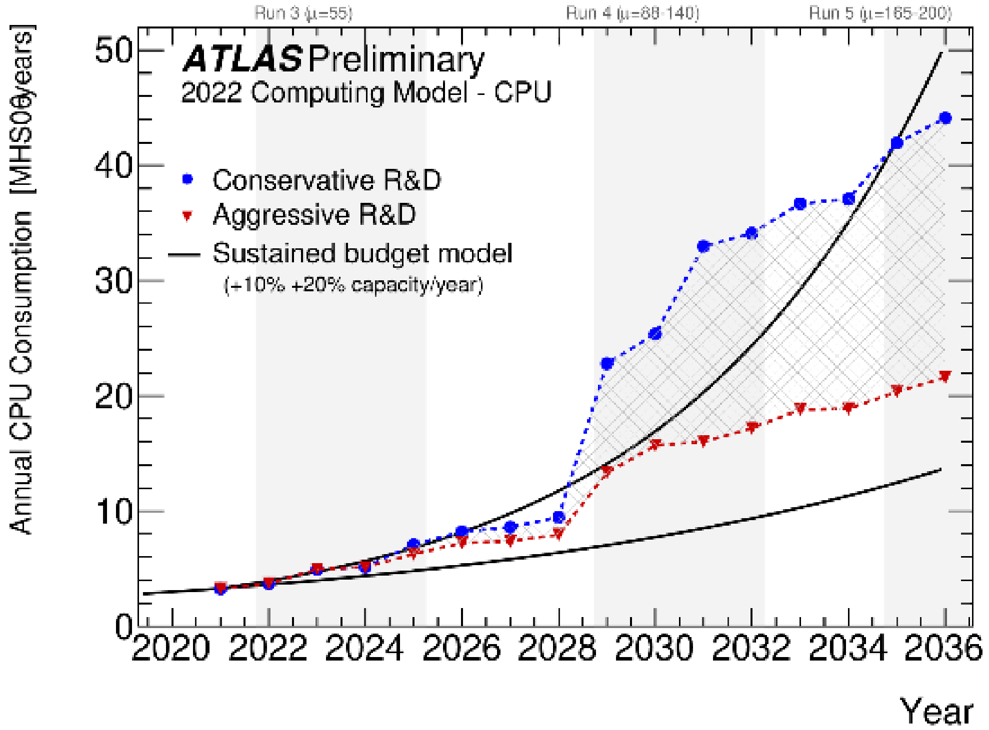
中国科学院高能物理研究所 实验物理中心

High Luminosity LHC & Beyond



- At the HL-LHC, **we will enter the “Exa-byte” era. Annual computing cost will increase by a factor of 10-20**
- **<u>Without various innovations, the experiment will not be able to operate</u>.** The Graphical Processing Units (GPUs) and other state-of-the-art technologies will be the baseline at the HL-LHC.
- **Quantum computing will also likely bring another “leap”.**

- Two of the highly CPU consuming components: **(1) track reconstruction for both data/simulation & (2) simulation of shower development in the calorimeter.**
- Tackling these challenges will also be useful for future colliders, such as CEPC.

Collaborative Projects w/ DESY

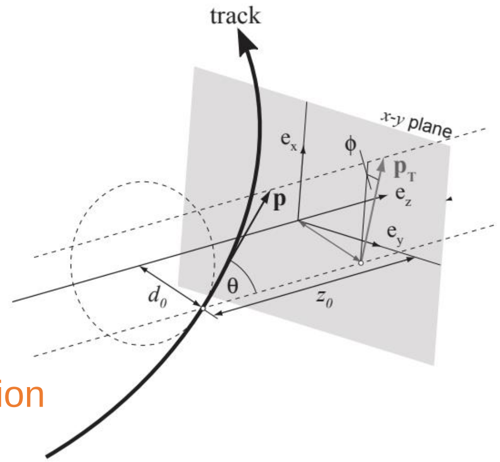
- Visited DESY last month to seek for collaborations on quantum computing.
- **We have agreed to collaborate on two quantum machine learning projects.**

1. **Quantum ML-based (e.g. GNN) tracking**
    - DESY: Federico Meloni et al.
    - From IHEP: Hideki Okawa et al.
    - We may start having "group" meetings in the coming weeks.
2. **Quantum GAN for fast calorimeter simulation**
    - DESY: Kerstin Borras et al.
    - IHEP: Hideki Okawa, Weidong Li, Xiaozhong Huang, Fazhi Qi's future postdoc,
    - BAQIS: Zheng-An Wang, Zhipeng Yang for quafu support

Previous Talk

Tracking

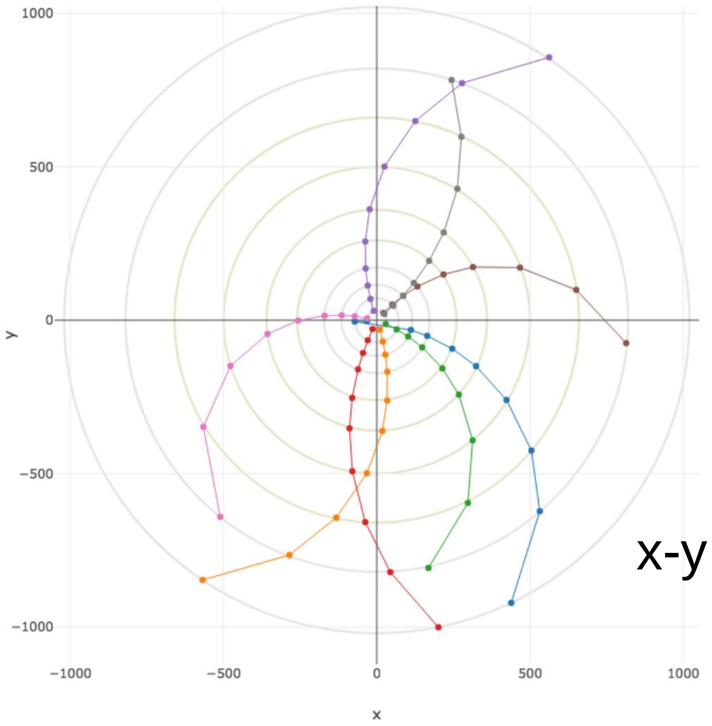
Track Reconstruction



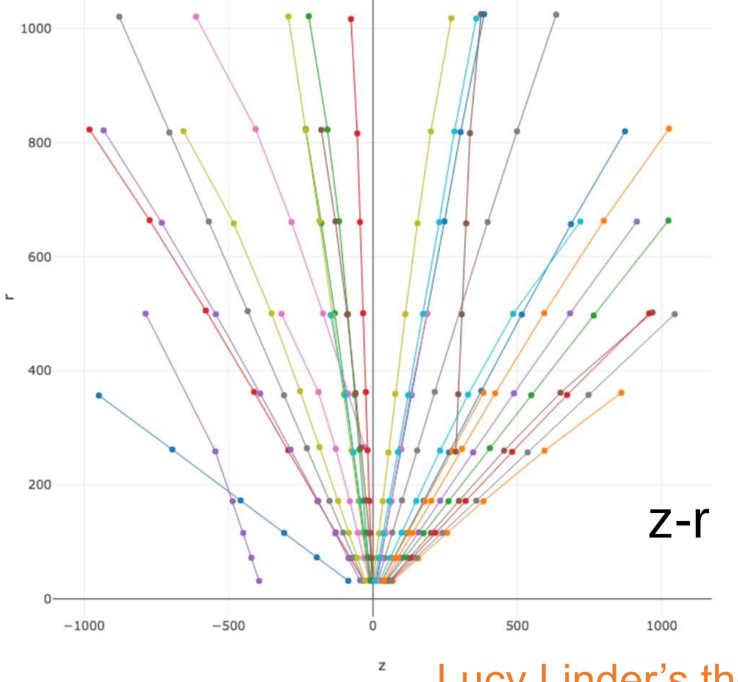
Global track parameters e.g. wrt. perigee

$$\left(d_0, z_0, \phi, \theta, \frac{q}{p}\right)$$

ATLAS Software Documentation



x-y

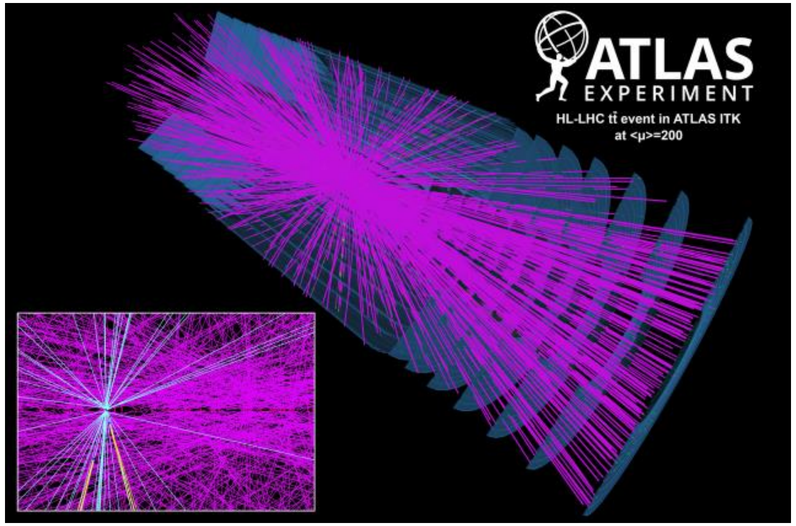


z-r

Lucy Linder's thesis

- Measuring curvature of particle trajectory bent in a magnetic field will provide momentum.
- Particle trajectory (track) will be reconstructed from hits in the silicon detectors (have many irrelevant hits from secondary particles)

Track Reconstruction at LHC & HL-LHC



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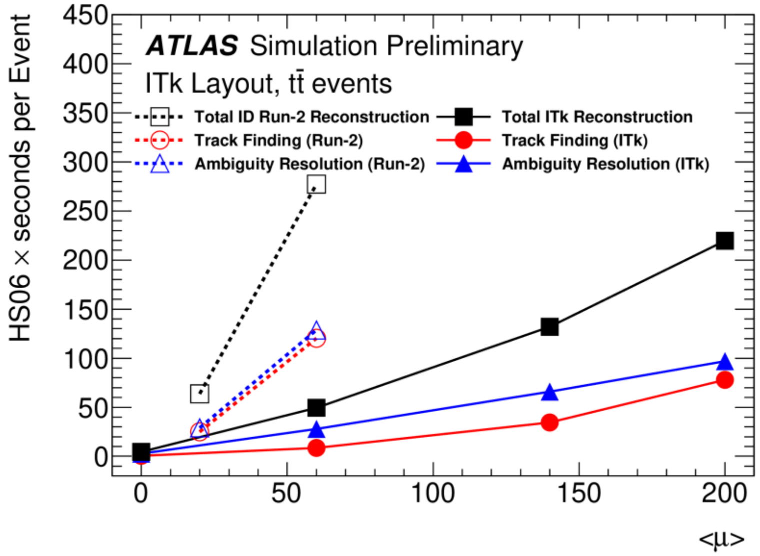
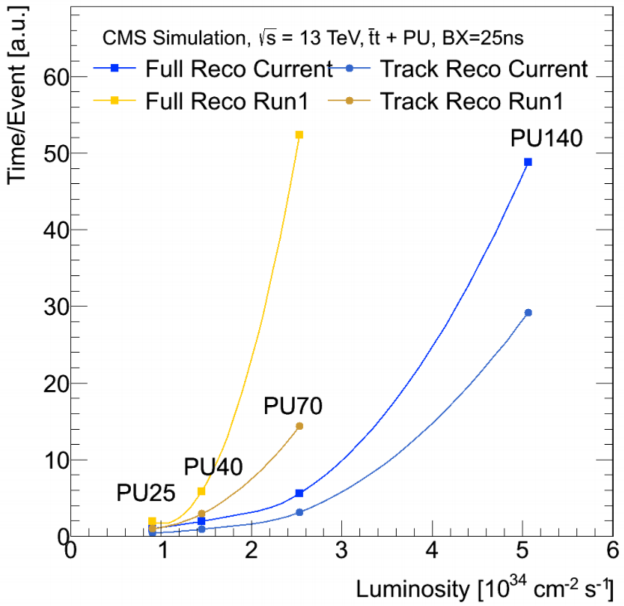


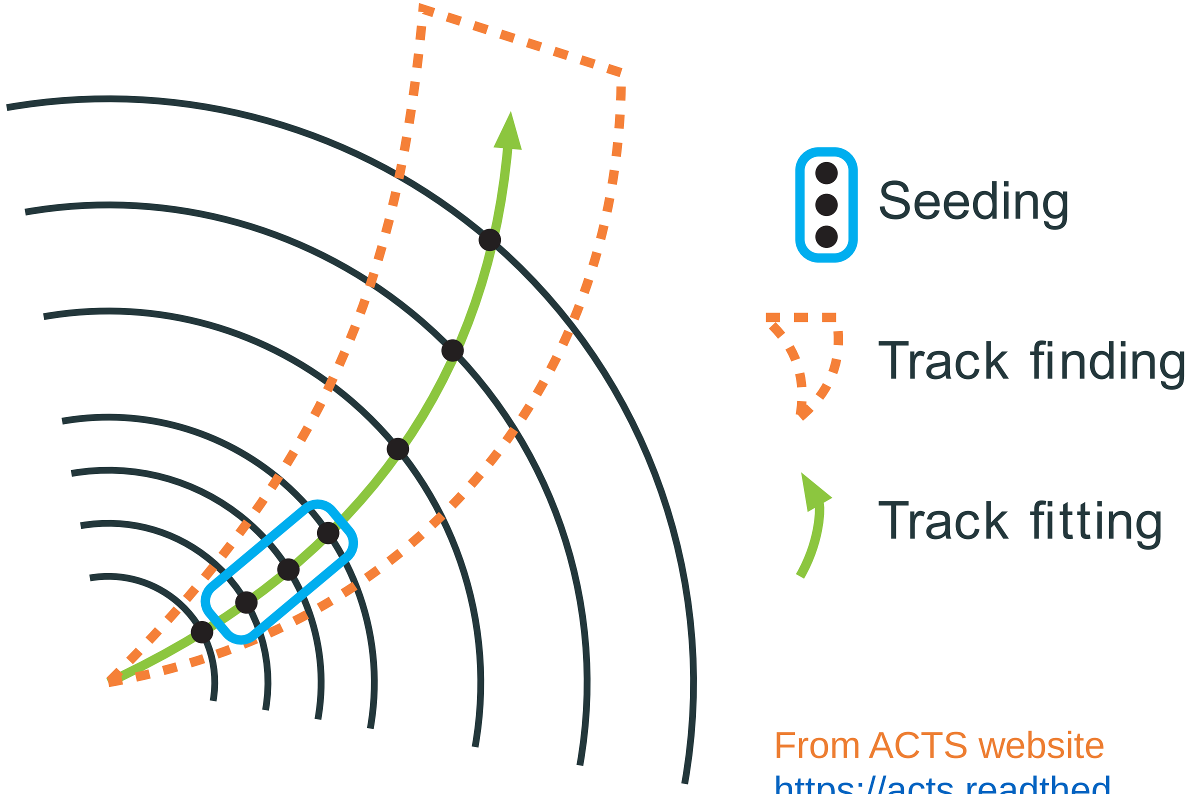
https://cds.cern.ch/record/1966040



	Run 1	Run 2	HL-LHC
μ	21	40	150-200
Tracks	~280	~600	~7-10k

- At the HL-LHC, additional interactions per bunch crossing becomes exceedingly high & **CPU time blows up with more pileup**.
- GPU & ML-based approaches are considered as a baseline, but quantum may play an important role.

Classical Benchmark: Kalman Filter

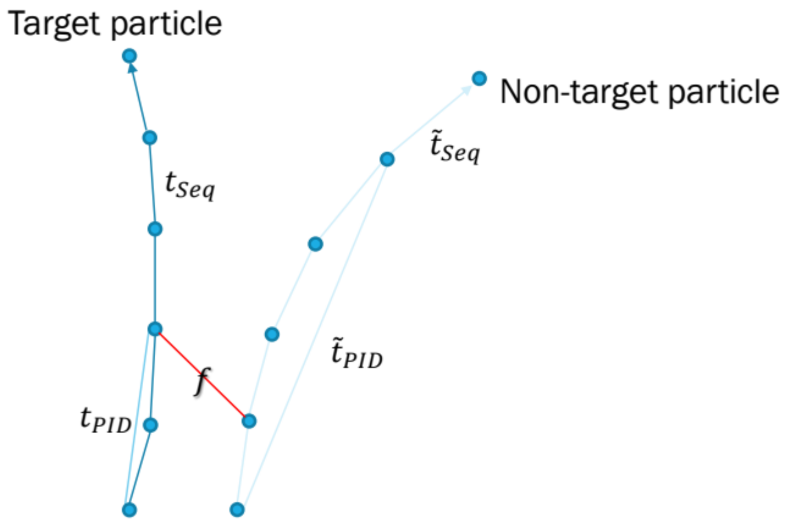


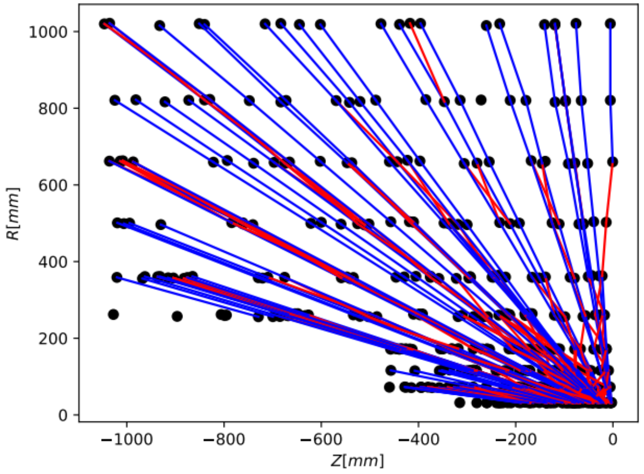
From ACTS website https://acts.readthedocs.io

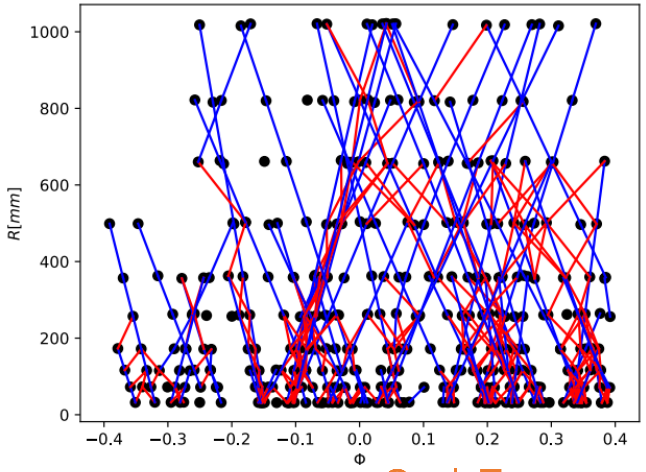
- In high energy collider experiments, Kalman Filter technique (e.g. implemented in A Common Tracking Software [ACTS]) has been often used as a standard algorithm.
- Seeding from the inner layers, extrapolated to predict the next hit & iterated to find the best quality combination.

Graph Neural Network

Daniel Murnane

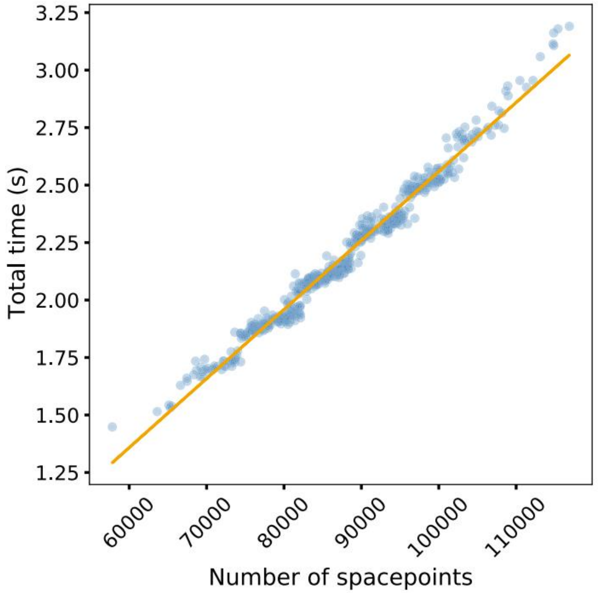






Cenk Tueysuez

- Active developments on the ML approach, especially using the graph neural network (GNN).
- Silicon hits can be regarded as **"nodes"** & connected segments as **"edges"**
- Computing time scales linearly with # of tracks

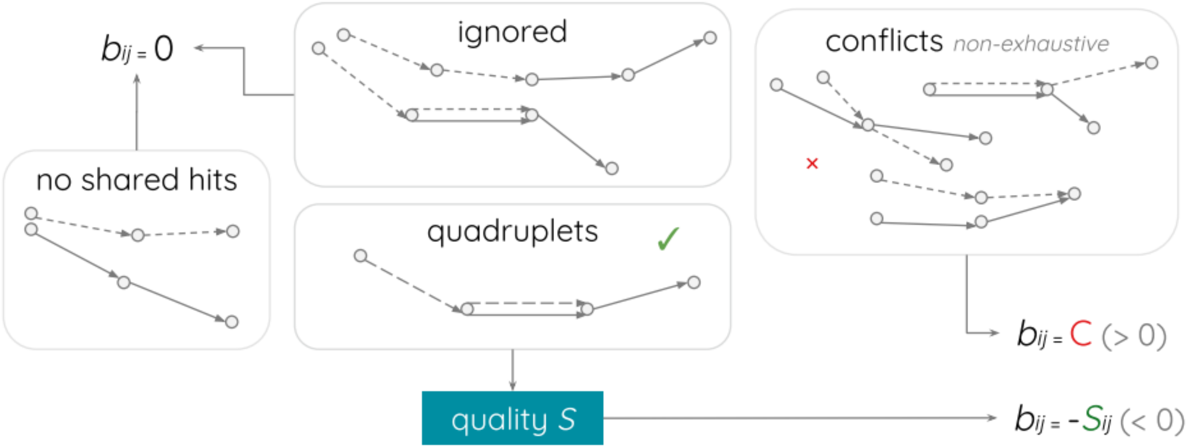


Quantum Approach: QUBO

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

F. Bapst et al. Comp. Soft. Big Sci. 4 (2019) 1.

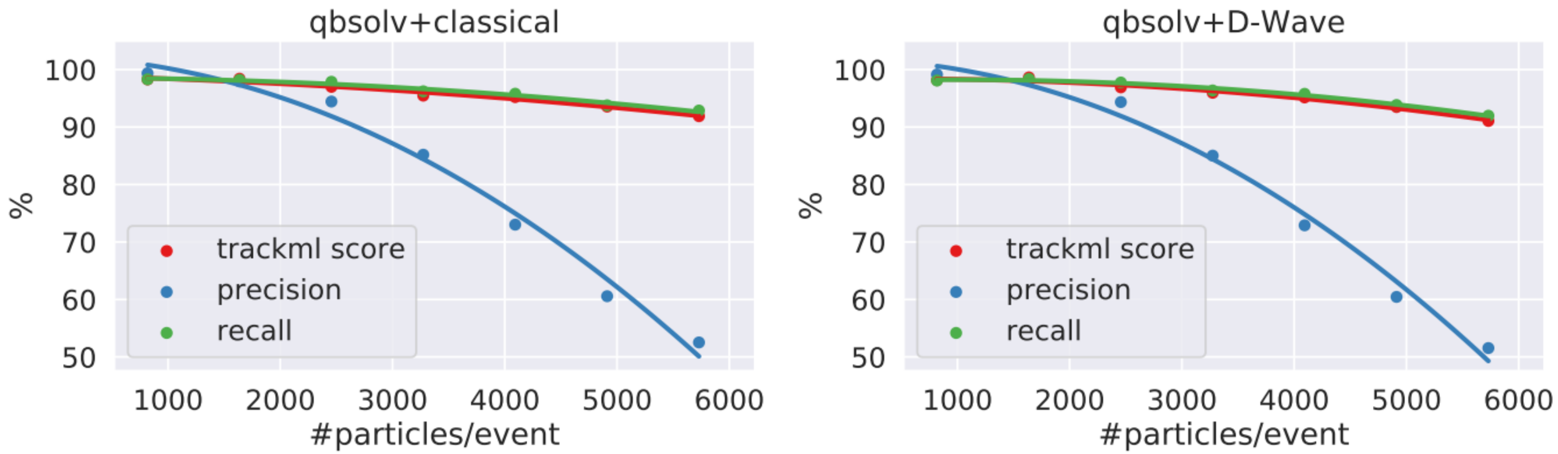
b_{ij} = 0 (if no shared hit)
= 1 (if conflict)
= $-S_{ij}$ (if two hits are shared)



- Triplets (segments w/ 3 hits) are formed from doublets (segments w/ 2 hits).
- Triplets are used to reconstruct tracks & can be regarded as a **quadratic unconstrained binary optimization (QUBO)** problem.
- Minimizing QUBO is equivalent to searching for the ground state of the Hamiltonian.

Quantum Annealing Approach

- Quantum annealer is a natural machine to search for the ground state of a Hamiltonian. D-Wave currently provides 5000+ qubit service (7440 qubits may be available in 2023-2024).
- Pros: High number of qubits available (though its concept fundamentally different from gate-based machines).
- Cons: Limited options to access the actual computer.
- Simulator studies can be pursued at the IHEP platform



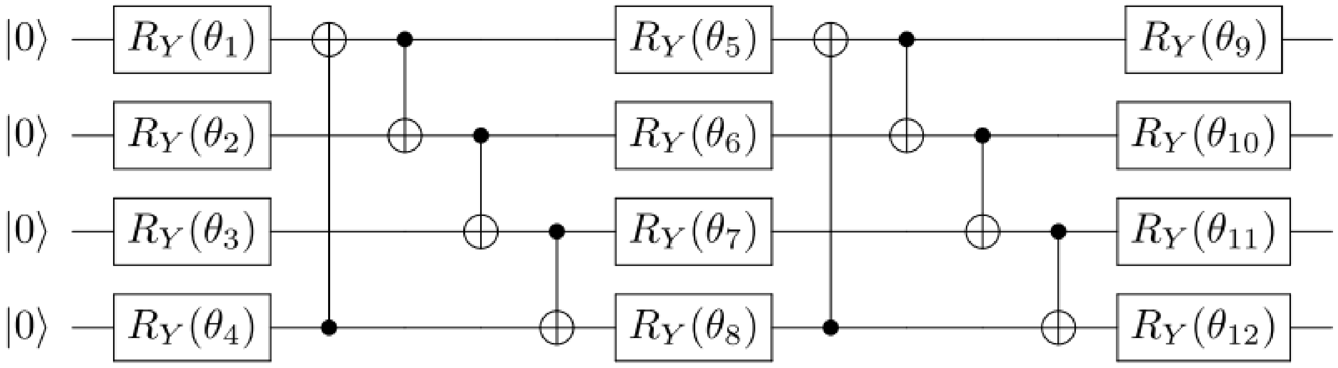
F. Bapst et al. Comp. Soft. Big Sci. 4 (2019) 1.

- Previous studies w/ 1000-qubit machine show that efficiency is almost stable w/ # of particles, but purity degrades.
- Simulator provides consistent results w/ hardware

QUBO w/ VQE

- QUBO can be mapped to Ising Hamiltonian and be solved using Variational Quantum Eigensolver (VQE). → Can run on quantum-gate computers.

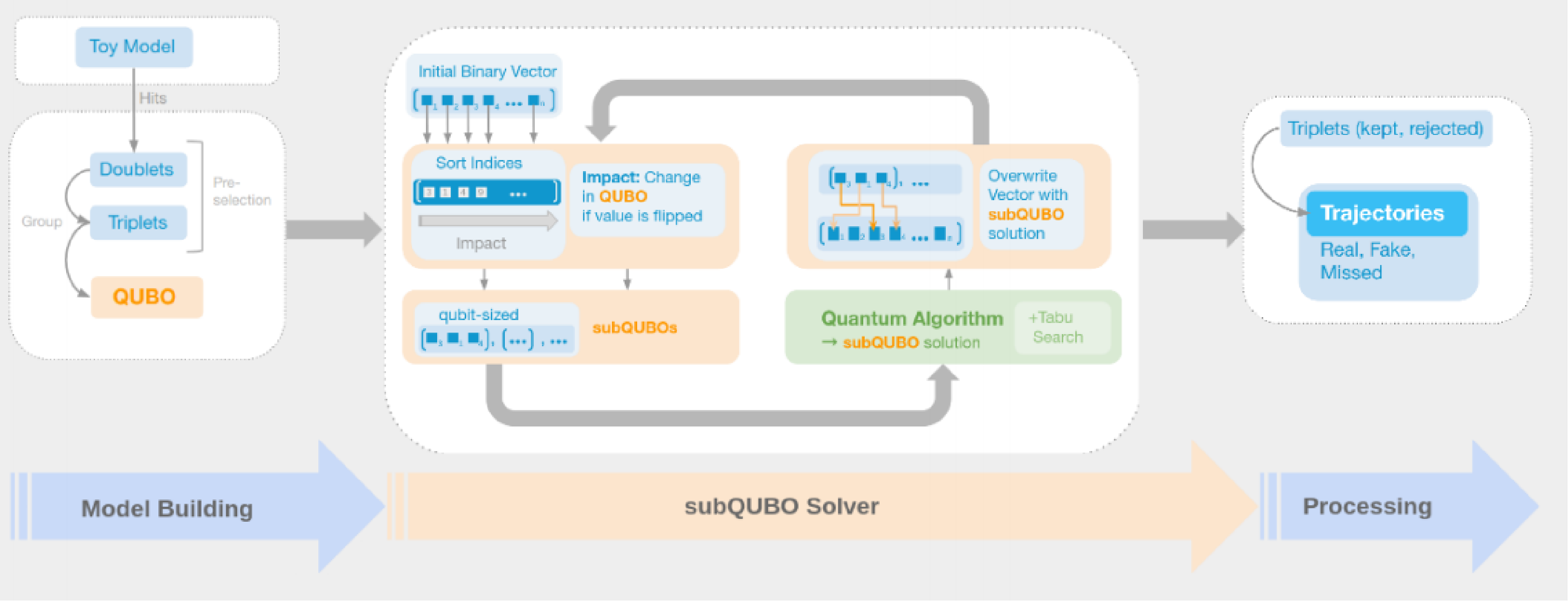
$$\mathcal{H} = -\sum_{n=1}^{N}\sum_{m<n} \bar{b}_{nm}\sigma^x_n\sigma^x_m - \sum_{n=1}^{N}\bar{a}_n\sigma^x_n$$



- TwoLocal ansatz w/ R_Y gates & circular CNOT entangling pattern were considered in L.Funcke et al., https://arxiv.org/abs/2202.06874

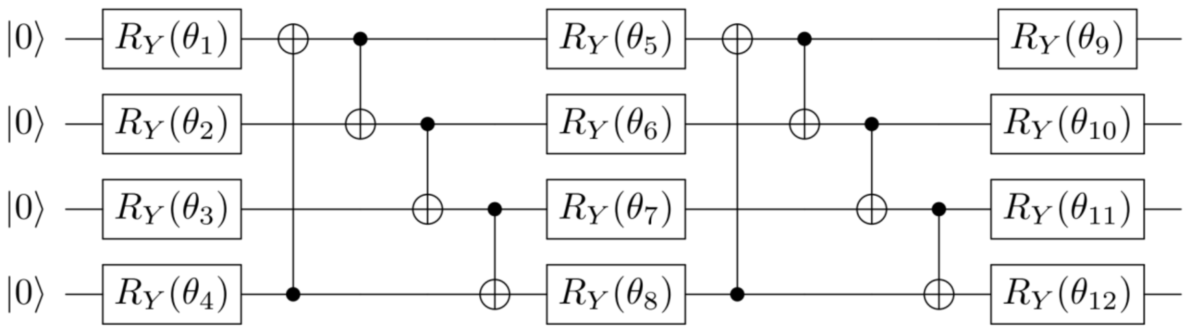
Sub-QUBOs

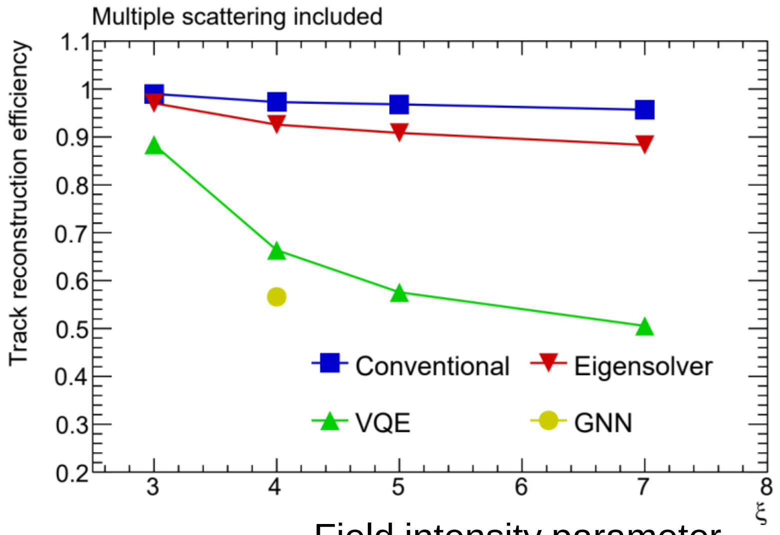
- Number of required qubits is determined by the number of triplet candidates → Obviously cannot cover the full QUBO in the NISQ era
- QUBO is split into sub-QUBOs of size N (N=7 in arXiv:2202.06874)

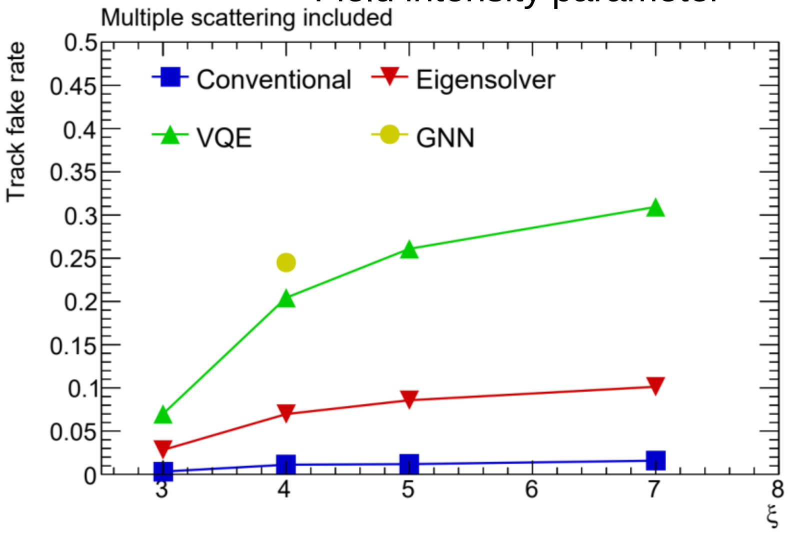


L.Funcke, T.Hartung, B.Heinemann, K.Jansen, A.Kropf, S.Kühn, F.Meloni, D.Spataro,C.Tüysüz,Y.C.Yap, https://arxiv.org/abs/2202.06874

Previous Results from LUXE







- Tracking successfully ran w/ quantum & classical benchmarks
- Classical GNN performance is limited by the training dataset size
- Room for improvement for both GNN & quantum tracking (optimization ongoing)

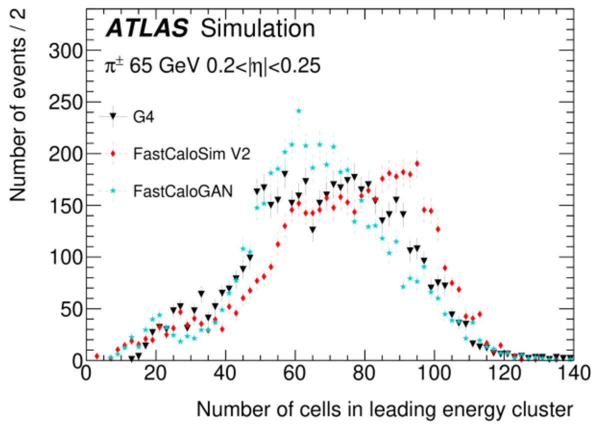
Near Future Plans

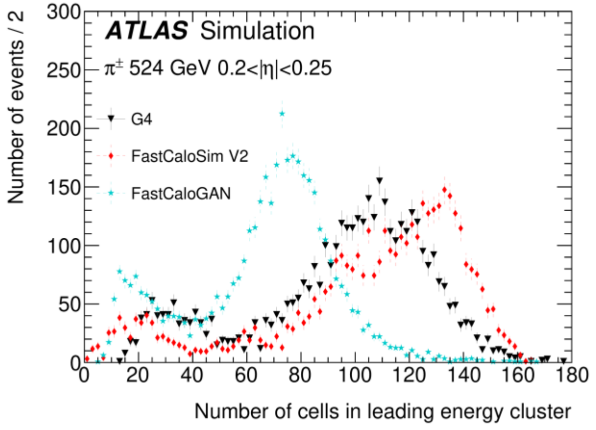
- We definitely need high-qubit machines for tracking studies
  → We are interested in quafu (in particular,136-qubit machine)
  - Currently discussing the test circuit & dataset. Should be available pretty soon.
  - Then we will start implementing on quafu.
- Try on publicly available tracking sample or HL-LHC/CEPC simulation.
  - Gang Li suggested to use Delphes for the 4^{th} detector concept
- (Also consider quantum annealers?)
- Try quantum GNN as well as look into new algorithms

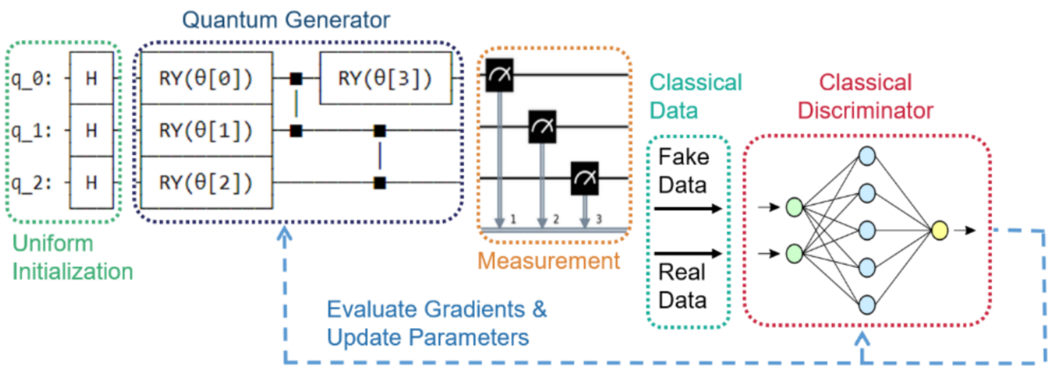
Q-GAN

Quantum GAN

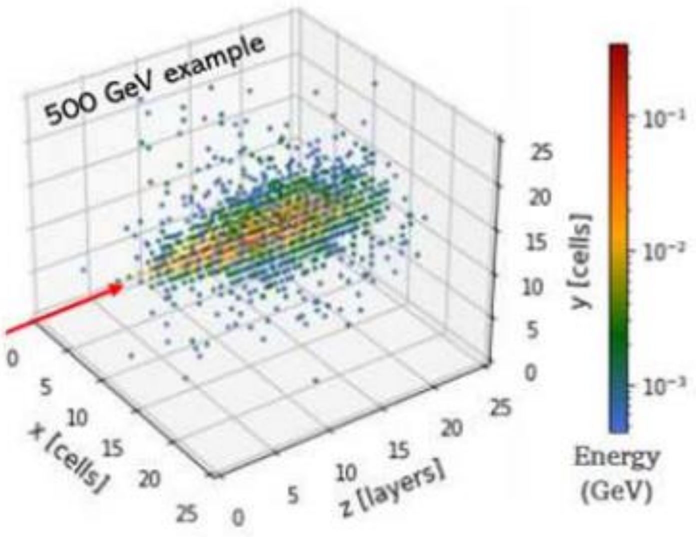
- HL-LHC will require enormous computing resource. **Already in Run 2, ~40% of the CPU is consumed by MC simulation.** (Complicated accordion geometry in EM calo)
  - e.g. 80% of the total simulation time taken by the shower development in the calo for ttbar events.
- Classical GAN is partially used in fast sim (Atlfast3), but is still time consuming
  → Quantum GAN may be able to reduce the training time & improve the accuracy.
- Currently testing two approaches: (1) hybrid of quantum generator & classical discriminator (→for NISQ era), (2) full quantum version of generator & discriminator

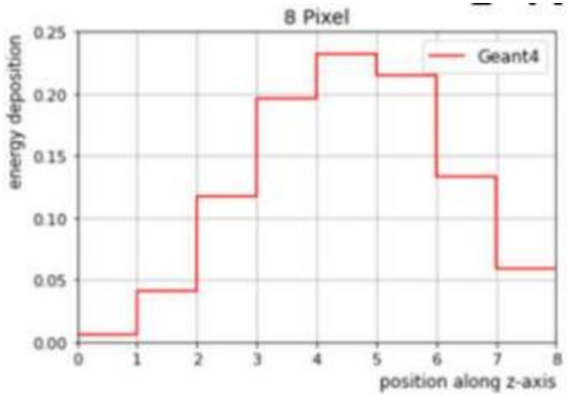


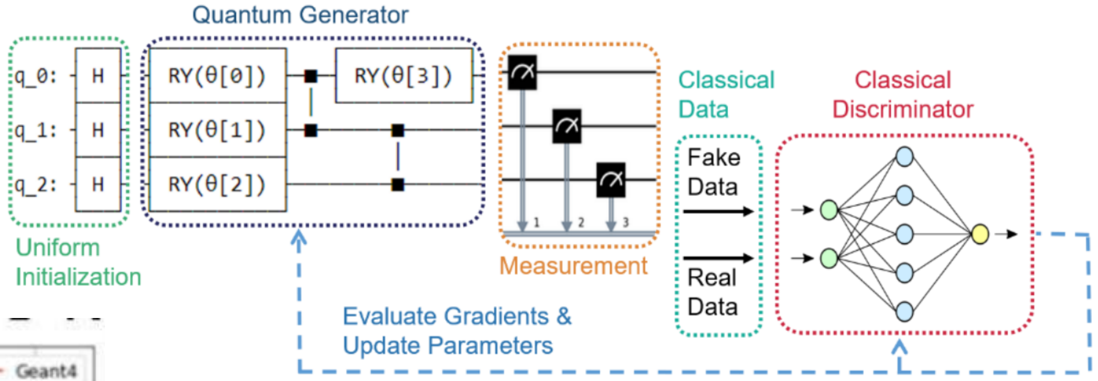


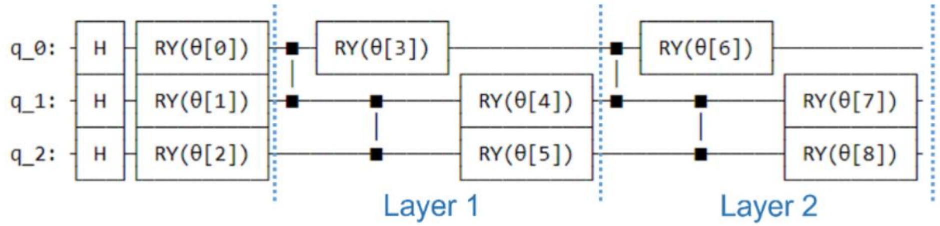


Previous Studies





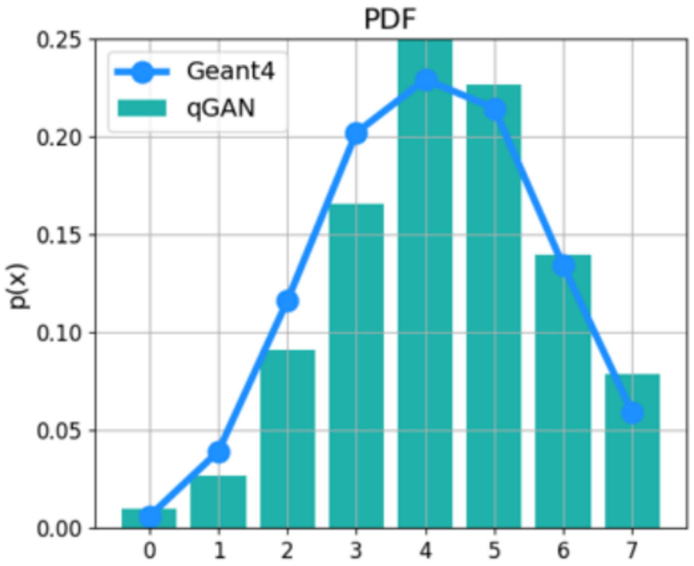


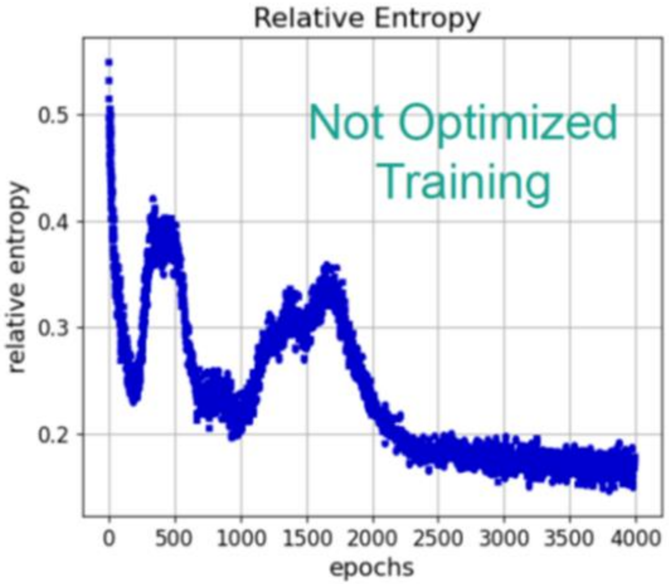


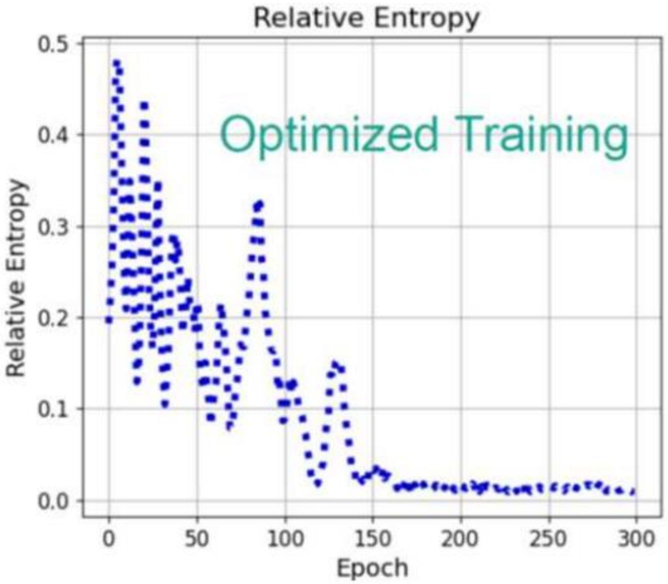
- <u>**Final goal is to generate highly granular 3D energy distributions**</u>, but they have been simplified to coarse 1D or 2D distributions due to the limited number of qubits as well as to develop algorithms starting from simple cases.
- So far, DESY has mostly worked on simulation-based studies using qiskit.

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

Quantum GAN w/o Noise (Simulator)







- Training time ~ 1 day for 3000 epochs
- Hyperparameter optimizations: higher learning rate, implement exponential learning rate decay, different generator and discriminator learning rates, train discriminator more often than generator
- Led to 10 times speed up in training → ~300 epochs is sufficient

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

Quantum GAN w/ Noise (Simulator)

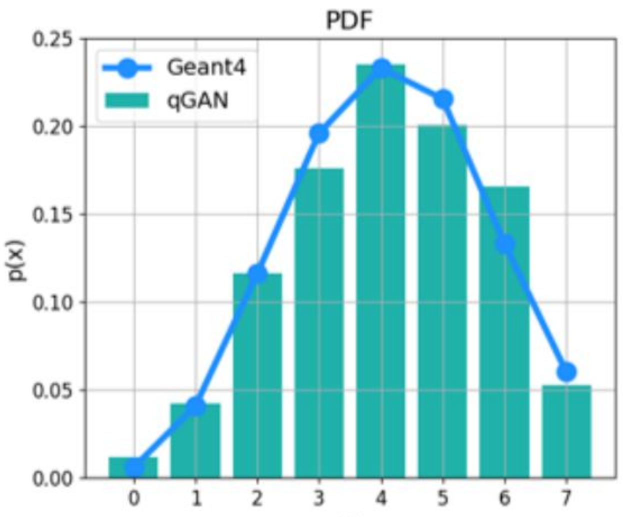
- Two noise conditions considered
  1. Readout noise only (IBMq belem model)

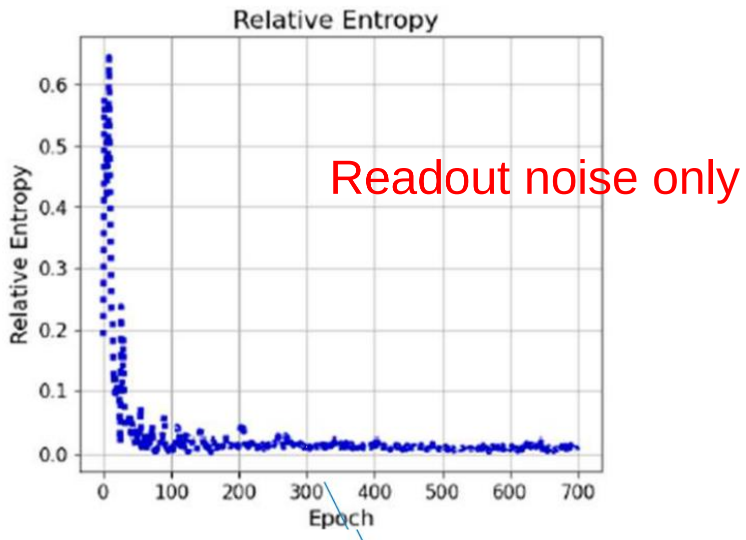
Qubit Number:	0	1	2
Readout Error:	3.6%	4.7%	9.6%

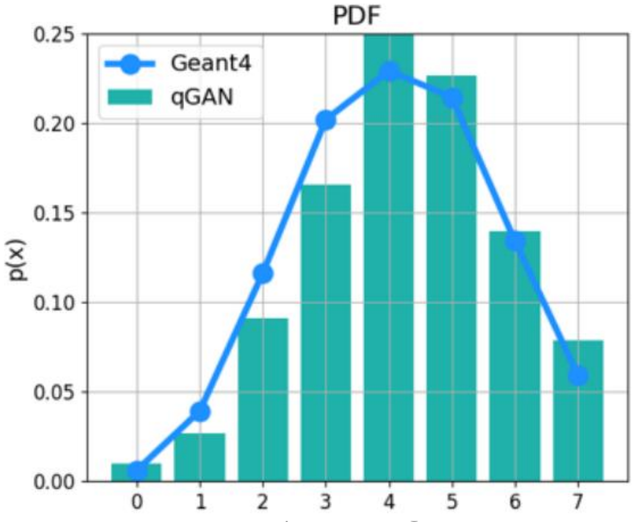
  2. Readout + gate noise

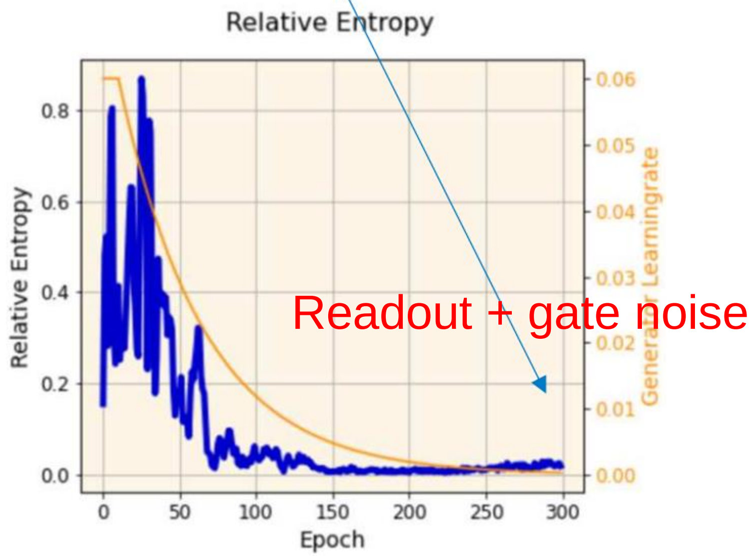
Qubit Number	0	1	2	Average
Readout Error	2.34%	2.66%	2.05%	**2.35%**
CX-gate Error	1.11%		1.75%	**1.43%**

- No decrease in accuracy & fast convergence for both



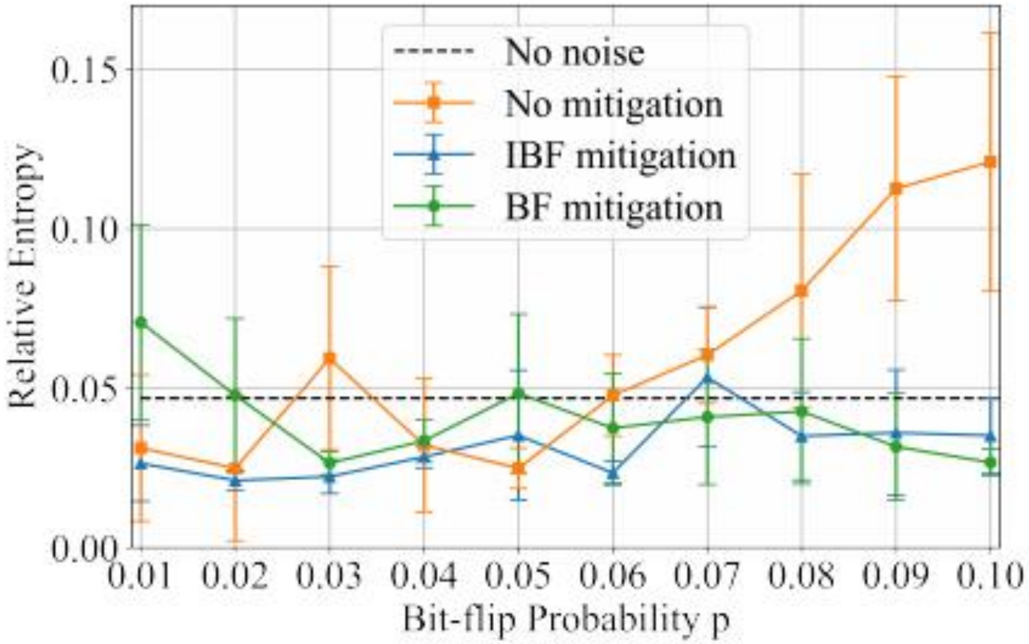


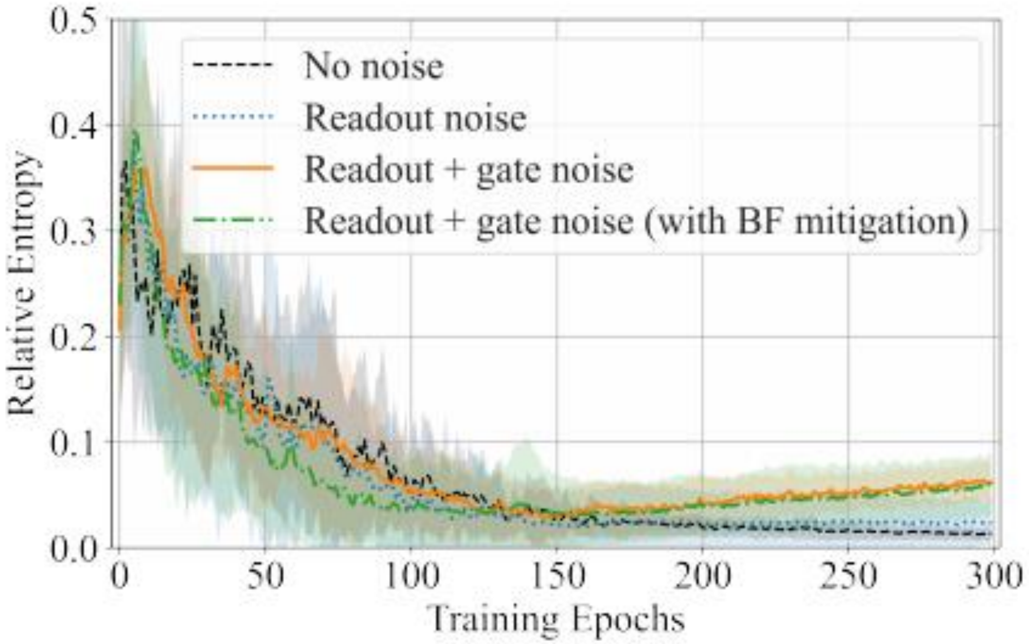




K.Borras,S.Y.Chang,L.Funcke,M.Grossi,T.Hartung,K.Jansen,
D.Kruecker,S.Kühn,F.Rehm, C.Tüysüz,S.Vallecorsa https://arxiv.org/abs/2203.01007

Noise Mitigation Studies





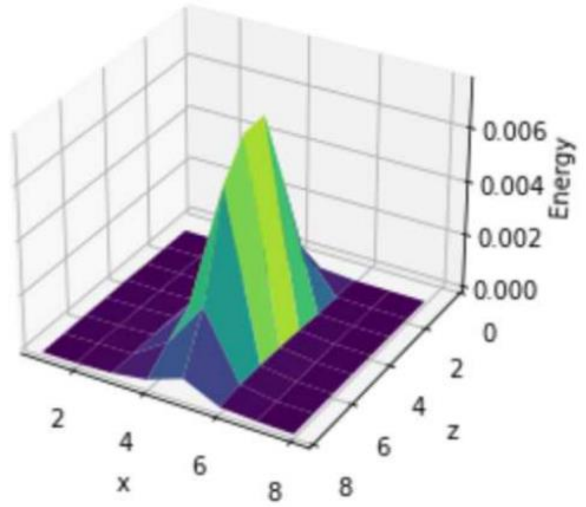
- Two noise mitigation techniques considered (1) bit-flip (BF) [M is 2^nx2^n matrix] & (2) independent bit-flip (IBF) [M is tensor product of each M_N; assumes uncorrelated multi-qubit readout errors]
- Converges well w/ readout errors only, but two-qubit gate errors prevents convergence

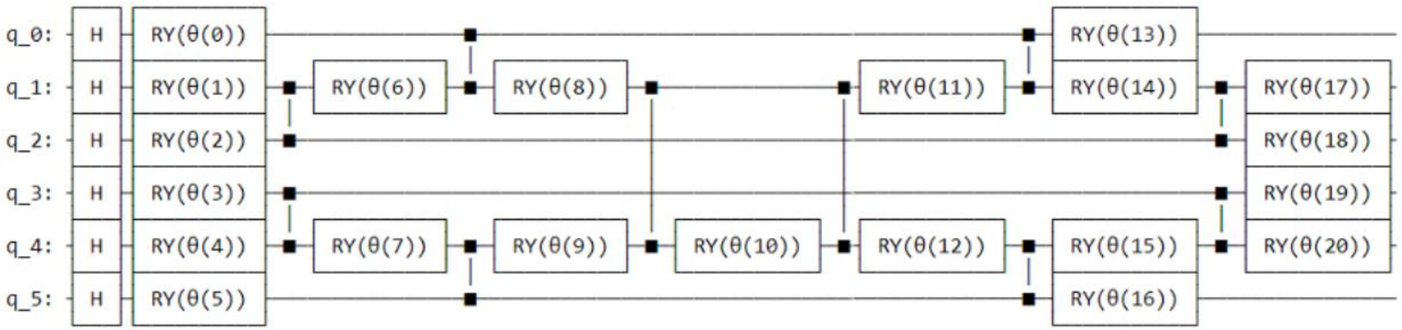
$$M = \begin{bmatrix} 1 - p_{01} & p_{10} \\ p_{01} & 1 - p_{10} \end{bmatrix}$$

p_{01}, p_{10}: bit-flip probability

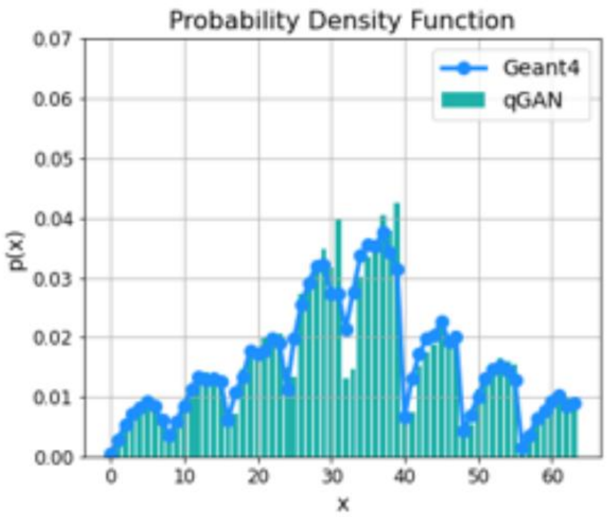
F. Rehm, S. Vallecorsa, K. Borras, D. Krücker
http://symsim.jinr.ru/grid2021/363-368-paper-67.pdf

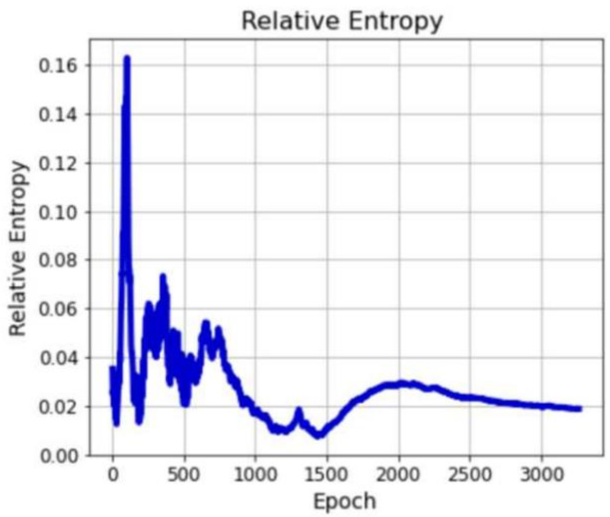
Quantum GAN in 2D (Simulator)





- Down sample to 8x8 pixels → 6 qubits
- Tree Tensor Network classifier considered
- Training lasted for over 6000 epochs (> 5 days) & is unstable





Near Future Plans for Quantum GAN

- Use a common dataset (CLIC) for DESY/IHEP collaboration → i.e. independent from ATLAS/CMS etc.
- Cope w/ gate noise → needs further investigations
- Need to proceed step by step from simplified cases (1D→2D→3D).
- After all, the final target is highly granular 3D distributions.
  → Interested in high-qubit machines (e.g. quafu)
  - Zheng-An Wang (BAQIS) is currently helping us to implement Q-GAN in quafu
- Also check full quantum GAN in addition to quantum-classical hybrid? (maybe long-term?)

Summary

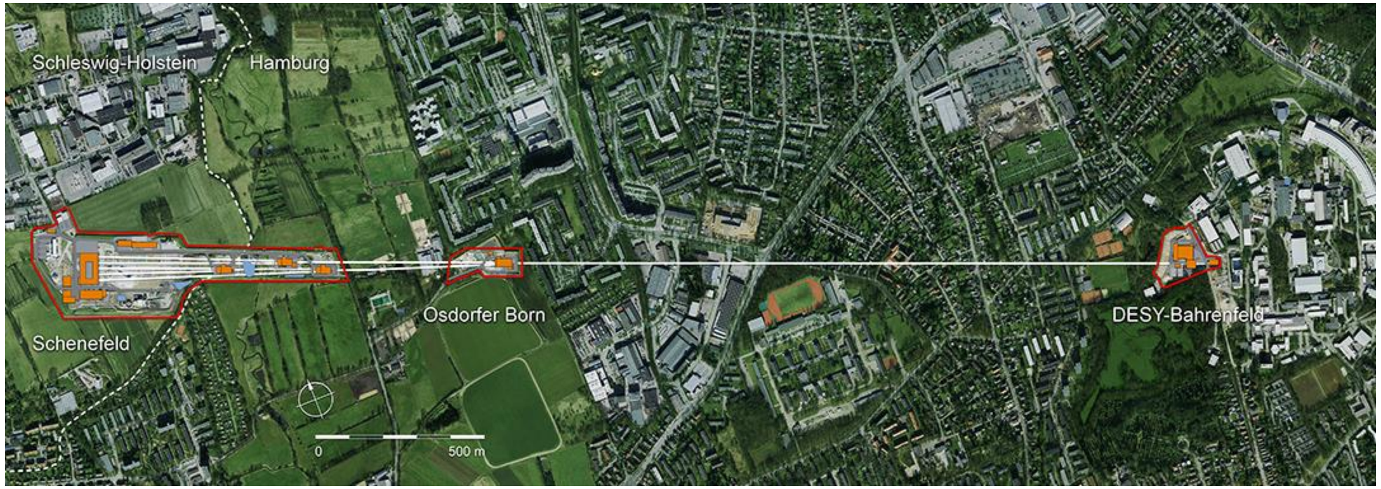
- Presented some previous studies on the quantum tracking & GAN in high energy physics (especially those relevant for our research plans).
- Two collaborative projects with DESY are ramping up.
- Quafu implementation under way.
- It would be really interesting to iterate on the actual high qubit machines & could be a unique opportunity in China.

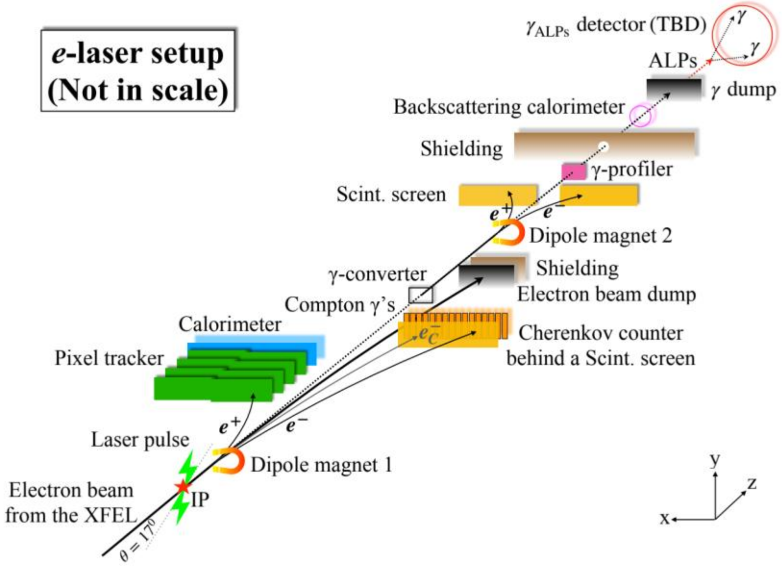
Backup

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 (Laser Und XFEL Experiment)
  - QED studies under the strong-field regime (i.e. non-perturbative)
  - Exploits European XFEL electron beam and high-power laser





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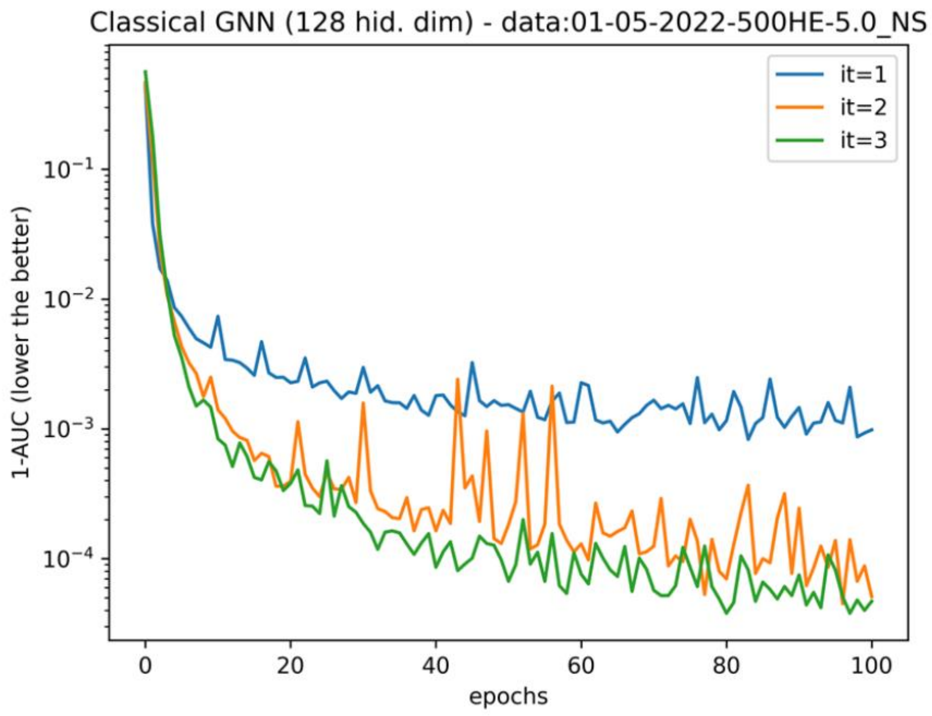
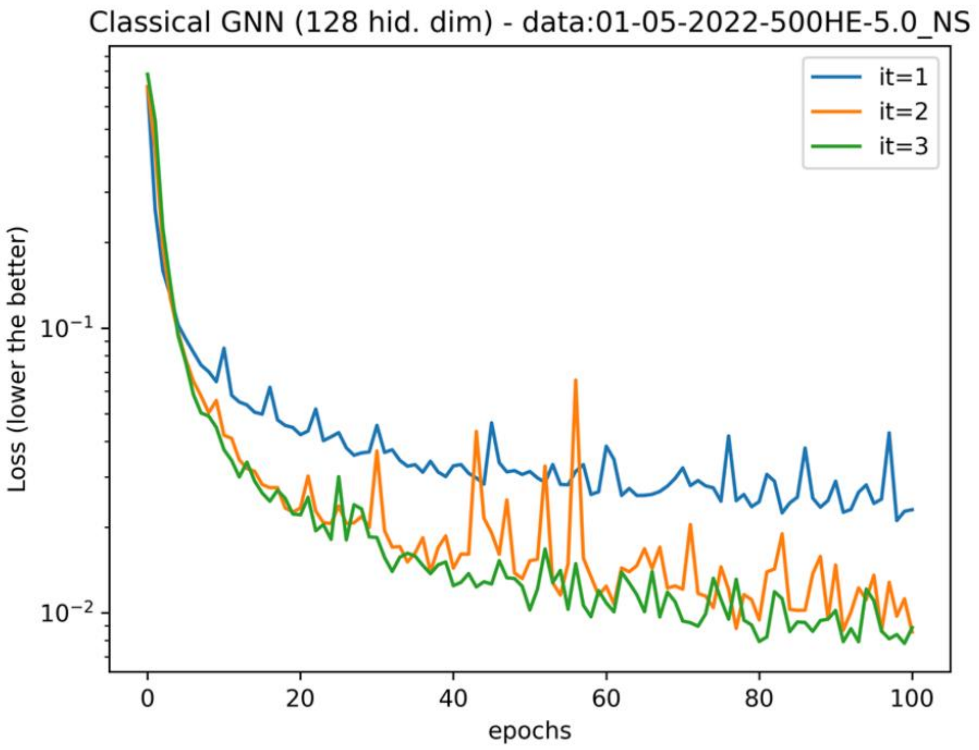
Tracking at LUXE

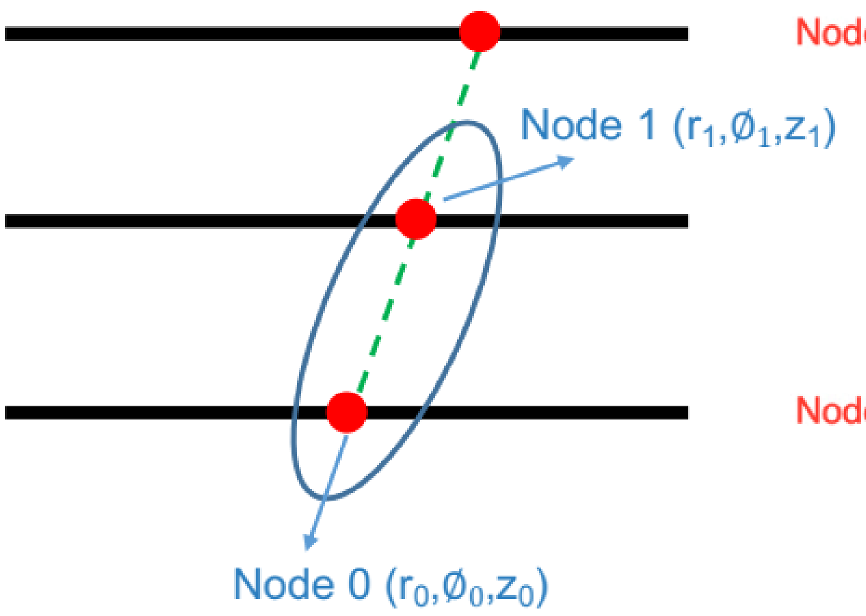


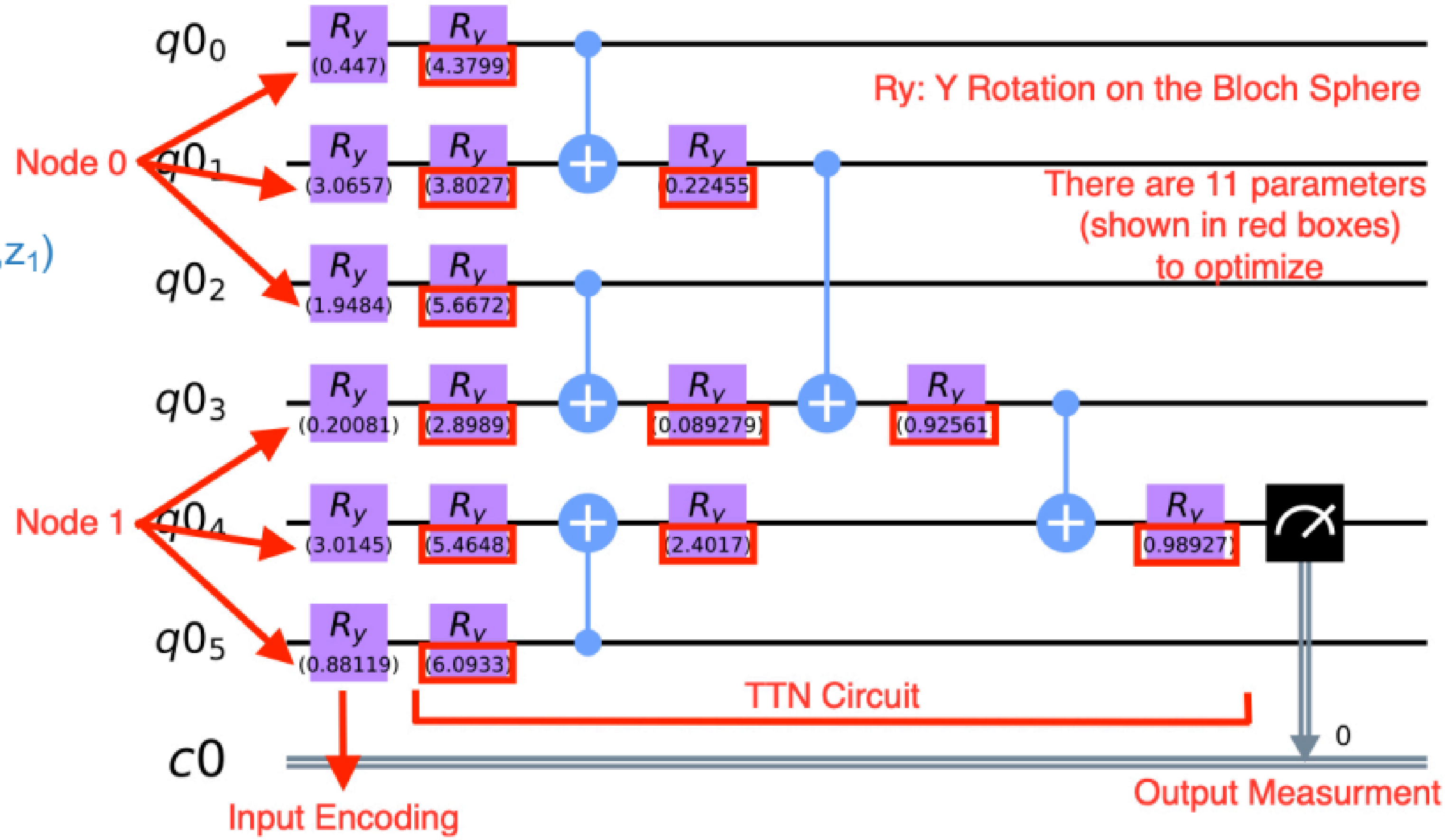


- Ongoing tests on classical GNN w/ more training data
- Looks promising so far

From Cenk Tueysuez

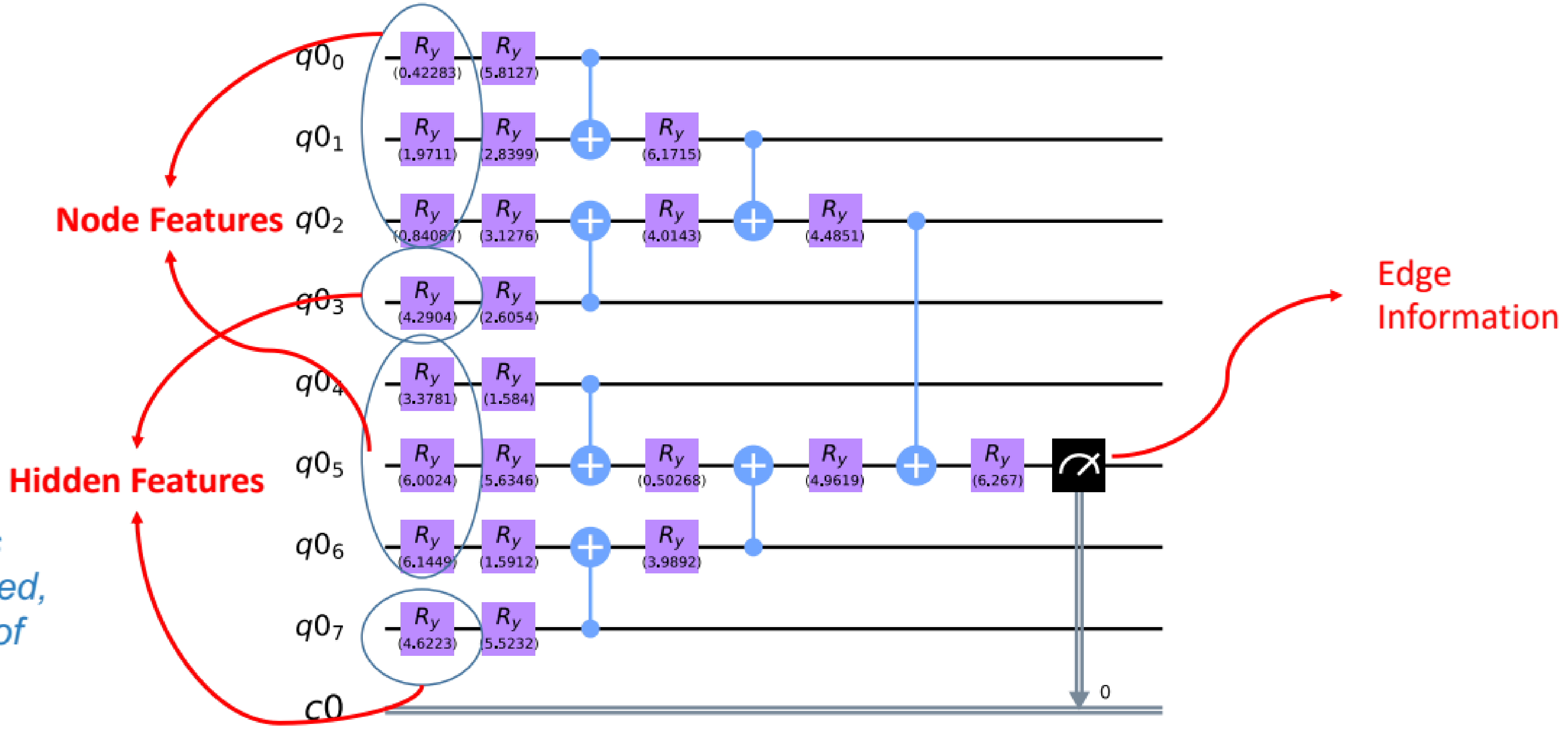
Classifier in Quantum GNN





From Cenk Tueysuez

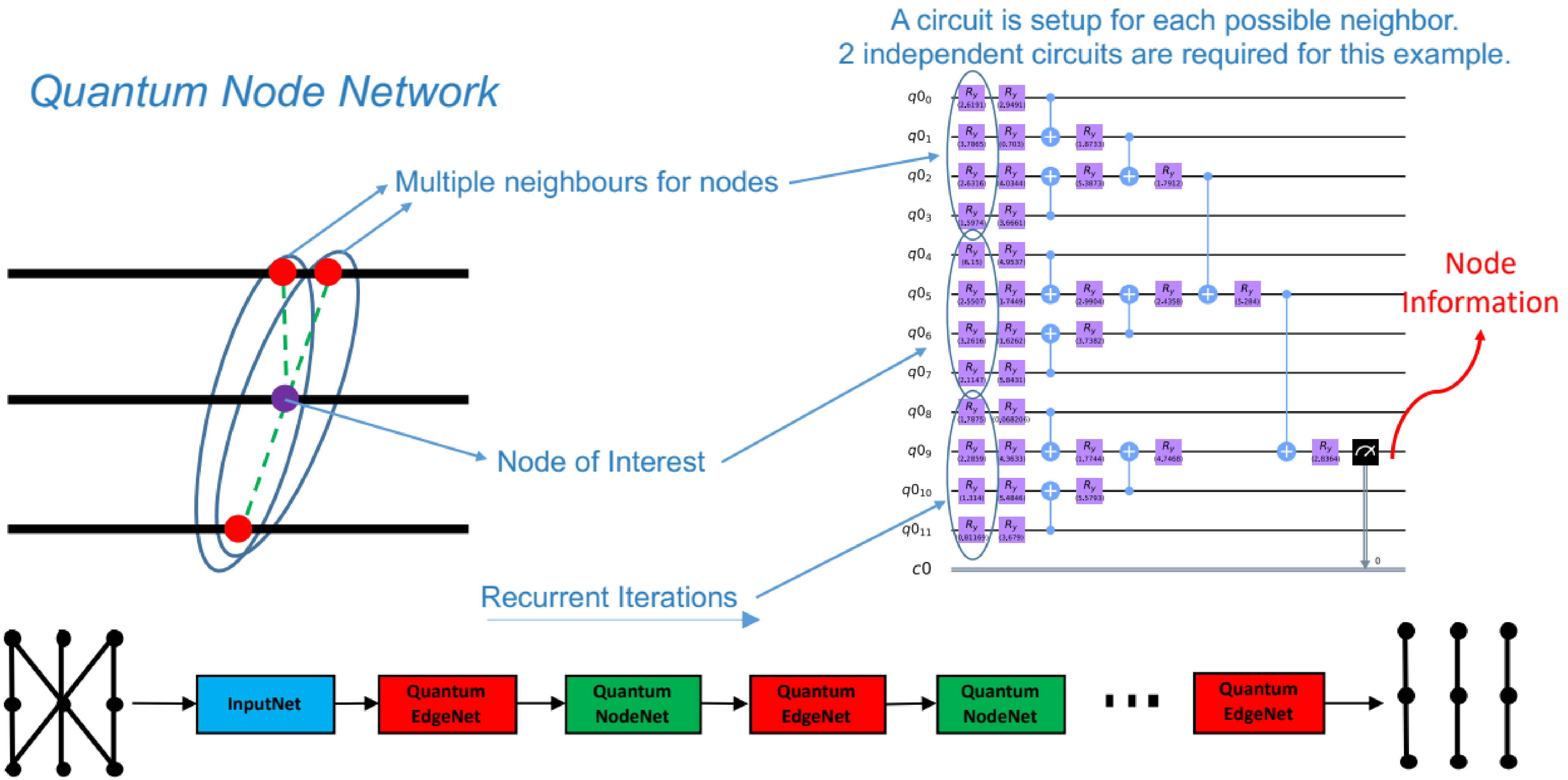
Quantum Edge Network



Number of qubits is required to be increased, to increase the size of hidden dimension.

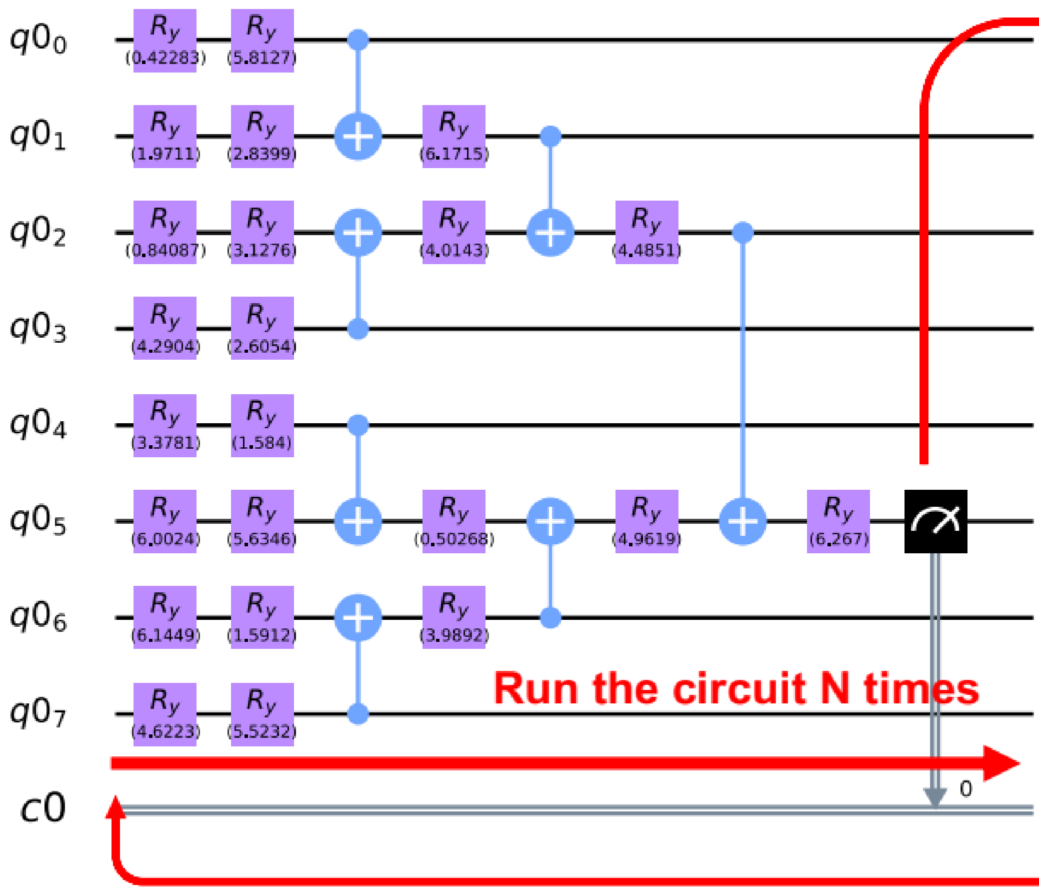
Quantum Node Network

From Cenk Tueysuez



From Cenk Tueysuez

Training in Quantum GNN



Averaging the measurement outcomes gives a probability of being an edge.

Calculate an error from the ground truth data.

Calculate the gradients of the parameters using parameter shift rule.

Update the parameters:

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \nabla_{\theta} \mathcal{J}(\theta)$$

Repeat!