AI and Quantum Computing in High Energy Physics

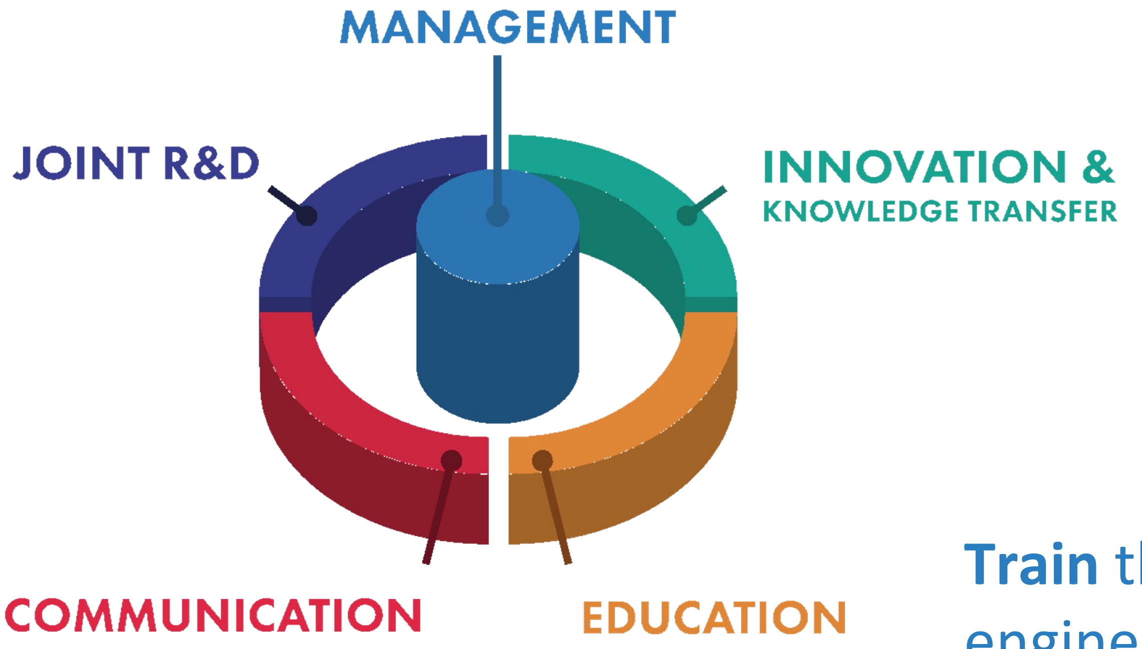
Examples from CERN openlab

Sofia Vallecorsa

CERN openlab

Collaborate and exchange ideas with other communities to generate impact.

Evaluate and test state-of-the-art technologies, **improve** them in collaboration with industry, **co-develop** new solutions.



Communicate results, demostrate impact, and reach new audiences.

Train the next generation of engineers/researchers, **promote** education and cultural exchanges.

Four Main Areas of Activity

CERN openlab

eXascale Technologies

HPC and Cloud infrastructures, frameworks, tools to support key scientific workloads and applications

Artificial Intelligence for Science

Algorithms and optimisation, interpretability, synergies between Physics and other sciences

Quantum Computing

Quantum computing in HEP and other sciences, i quantum machine learning algorithms and potential advantage. Collaborative quantum computing (simulation) platform

Multi-Science Collaborations

Expertise and knowledge sharing across sciences. Collaborations and contribute to common solutions

Artificial Intelligence in openlab

The number of ML/DL applications in HEP is increasing rapidly

>1400 publications listed on the HEPML Living Review*

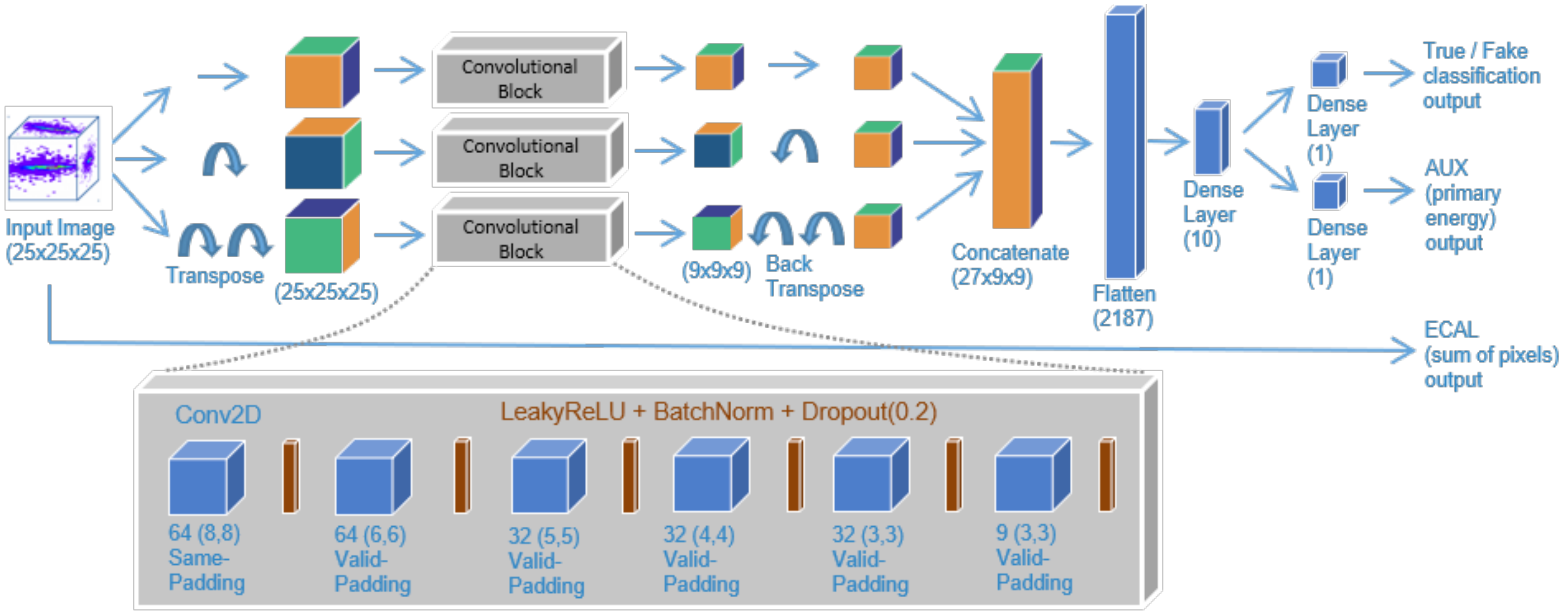
Our contributions:

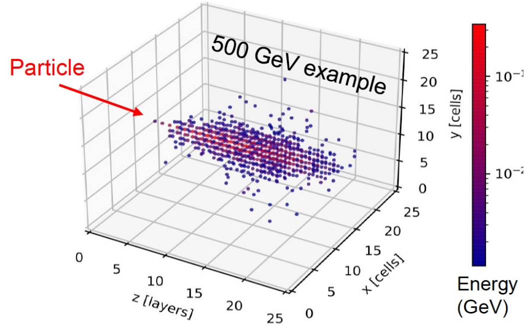
- **Generative models** for detector simulation
- **Optimised inference and training:** computing resources
- **Raw data processing** for neutrino experiments
- **Recurrent Neural Networks** for infrastructure characterization
- **Quantum Machine Learning**
- **Computer vision projects** (UNOSAT)

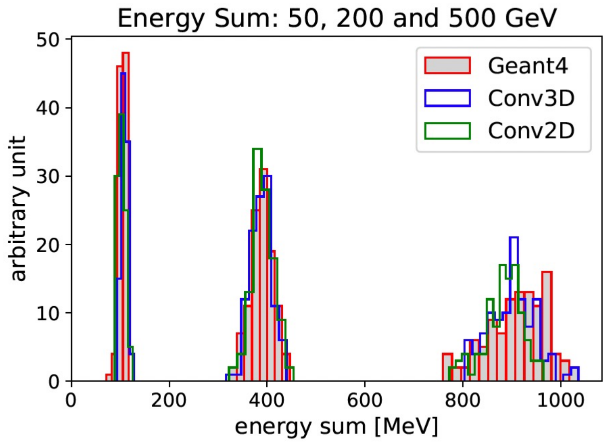
*https://github.com/iml-wg/HEPML-LivingReview

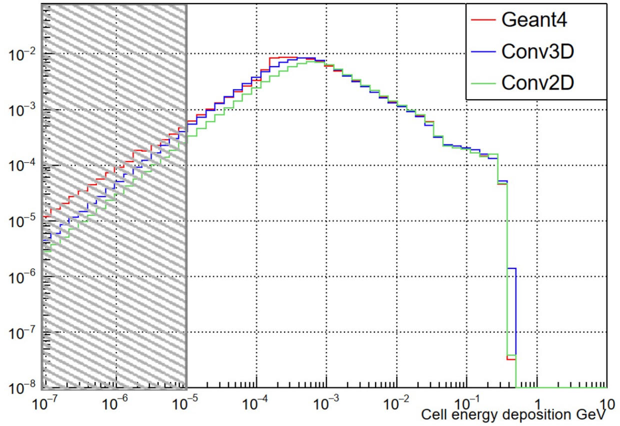
Rehm, Florian, et al. *arXiv:2105.08960* (2021).

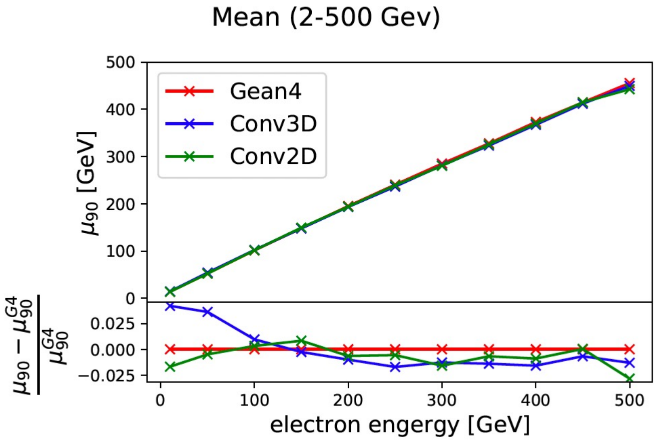
Calorimeter simulation: 3DGAN

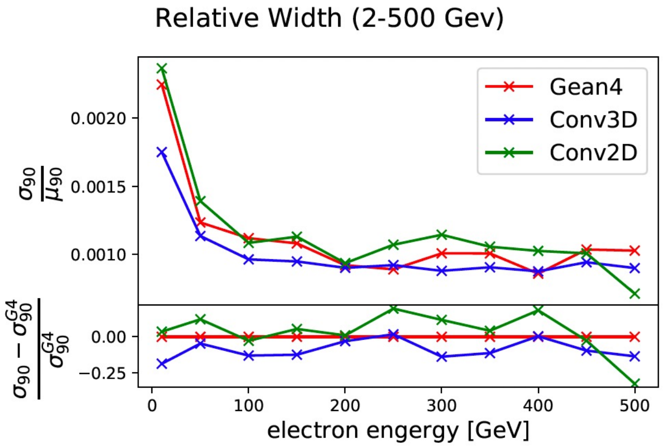












Systematics: image similarity

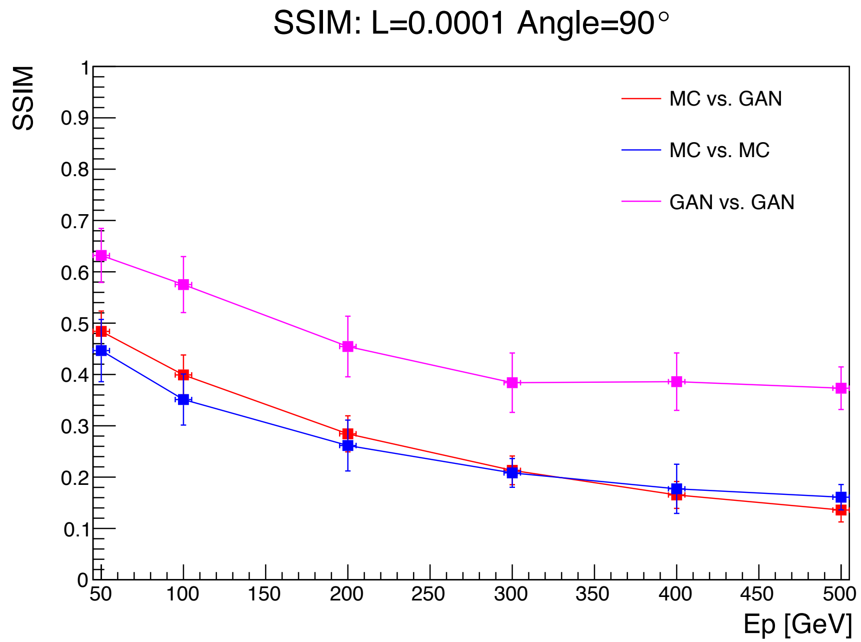
GAN can exhibit **mode-collapse** or **mode-drop**

How much **diversity** in the generated sample?

- Use the **Structural Similarity Index**

$$\mathrm{SSIM}(\boldsymbol{x},\boldsymbol{y}) = \frac{(2\mu_x\mu_y + C_1)(2\sigma_{xy} + C_2)}{(\mu_x^2 + \mu_y^2 + C_1)(\sigma_x^2 + \sigma_y^2 + C_2)}$$

where $\boldsymbol{x},\boldsymbol{y}$ are two samples to be compared



$$\mathrm{SSIM}(\boldsymbol{x},\boldsymbol{y}) = 1 \iff \boldsymbol{x} = \boldsymbol{y}$$

- Calculated on sliding windows, then averaged.
- Ours is a 3D problem: SSIM computed in ***xy* plane**, 3rd dimension is **channel**
- Adjust C1-C2 to the pixel dynamic range

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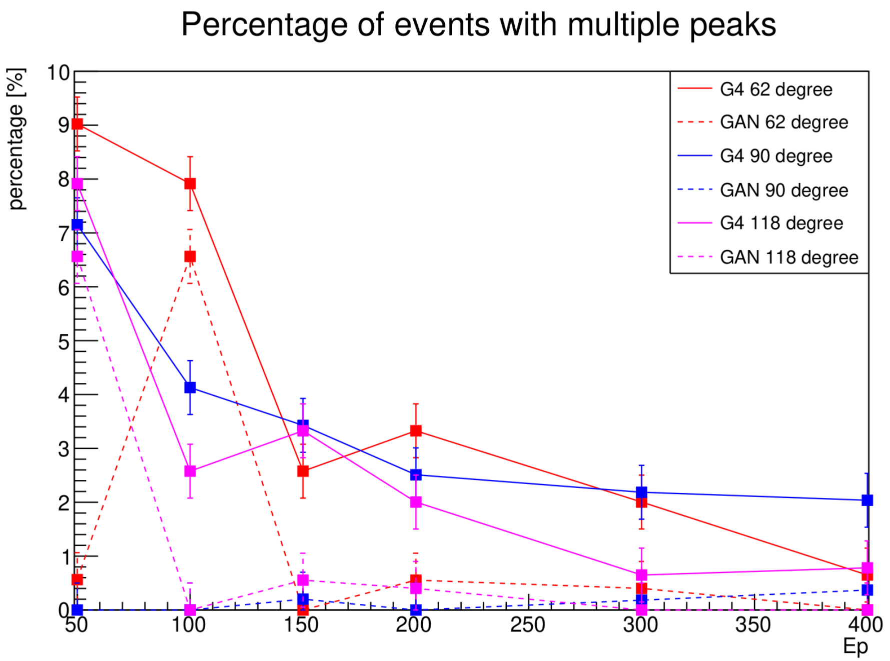
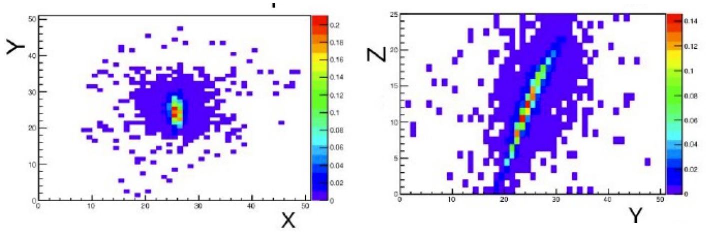
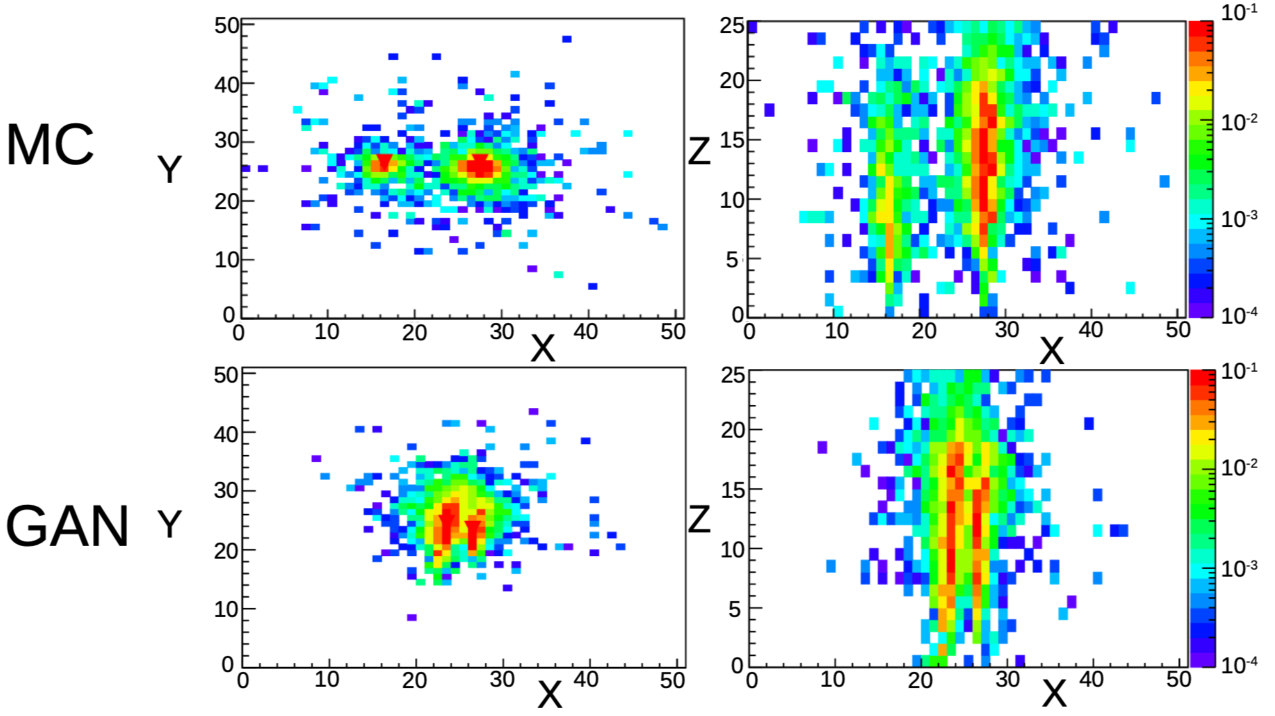
Systematics: rare events

It is important to reproduce correctly the topology and occurrence of rare events



"Standard"





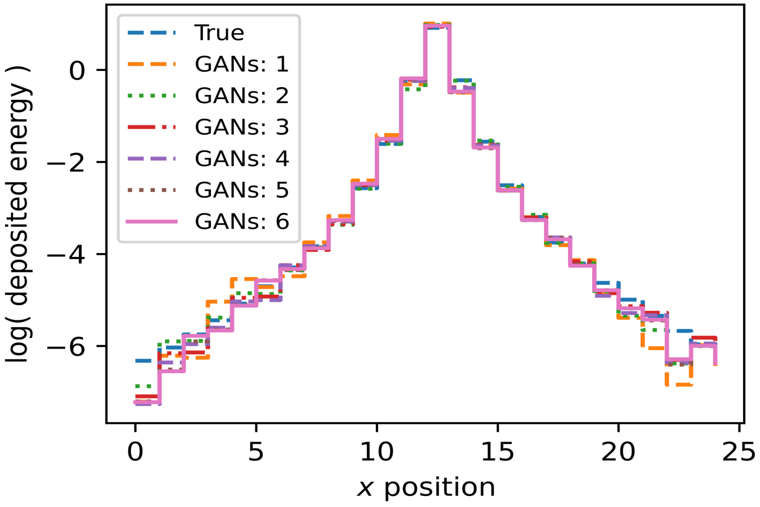
Ensemble GAN

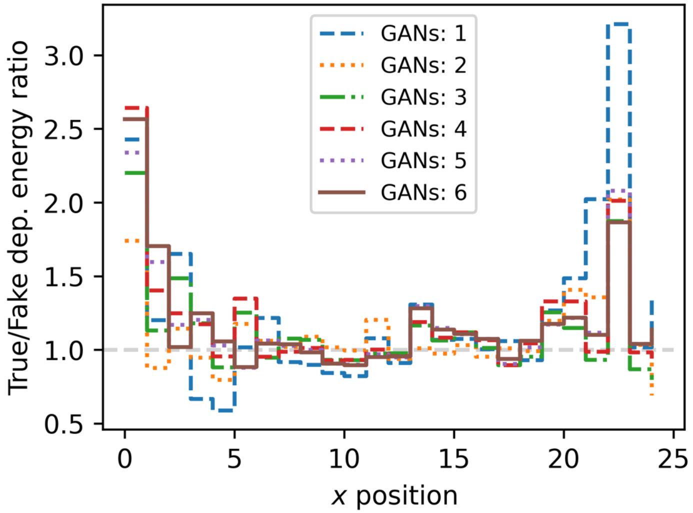
WORK in PROGRESS

Complex task can improve by **ensembling**

Building ensembles for GM is tricky

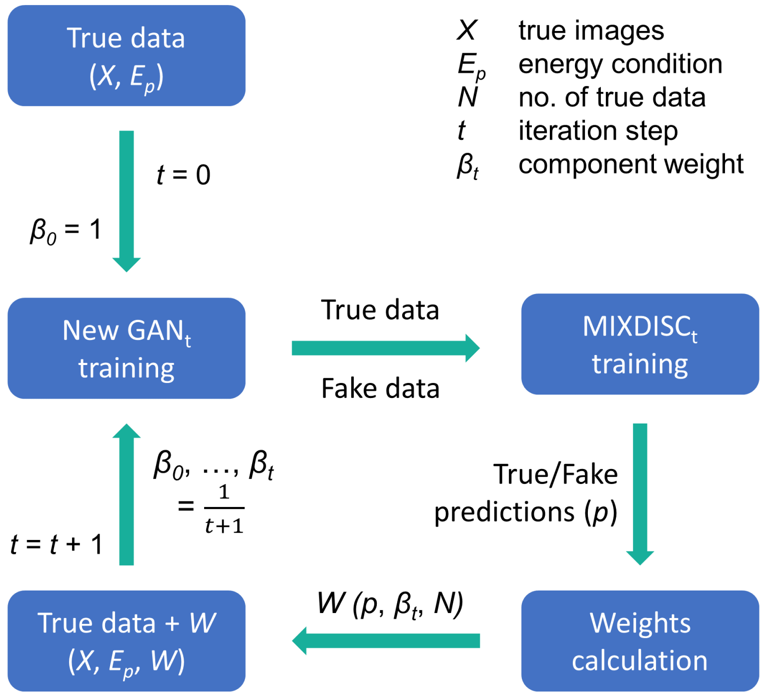
Build ensemble 3DGAN (inspired by AdaGAN model, arxiv:1701.02386)





Build a **mixture** to improve coverage by **reweighting training data**: each iteration learns a weak generator.

A meta-algorithm similar to **AdaBoost**



K. Jaruskova, ACAT2021

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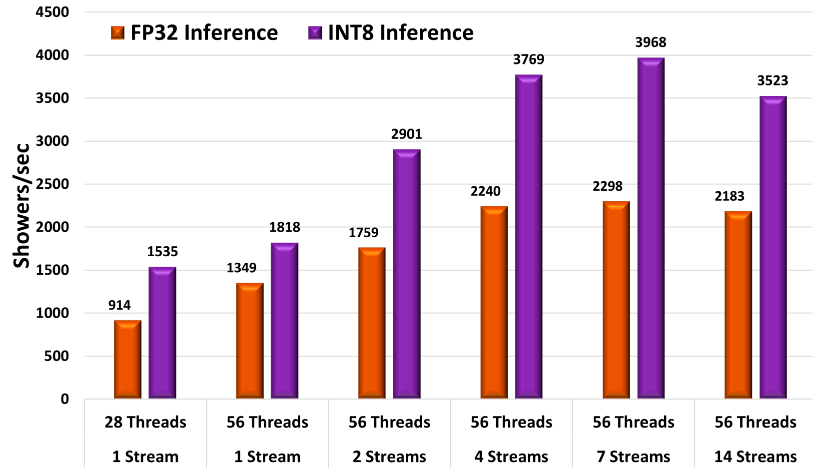
Faster then Monte Carlo?

F. Rehm, ICPRAM2021
in collaboration with Intel

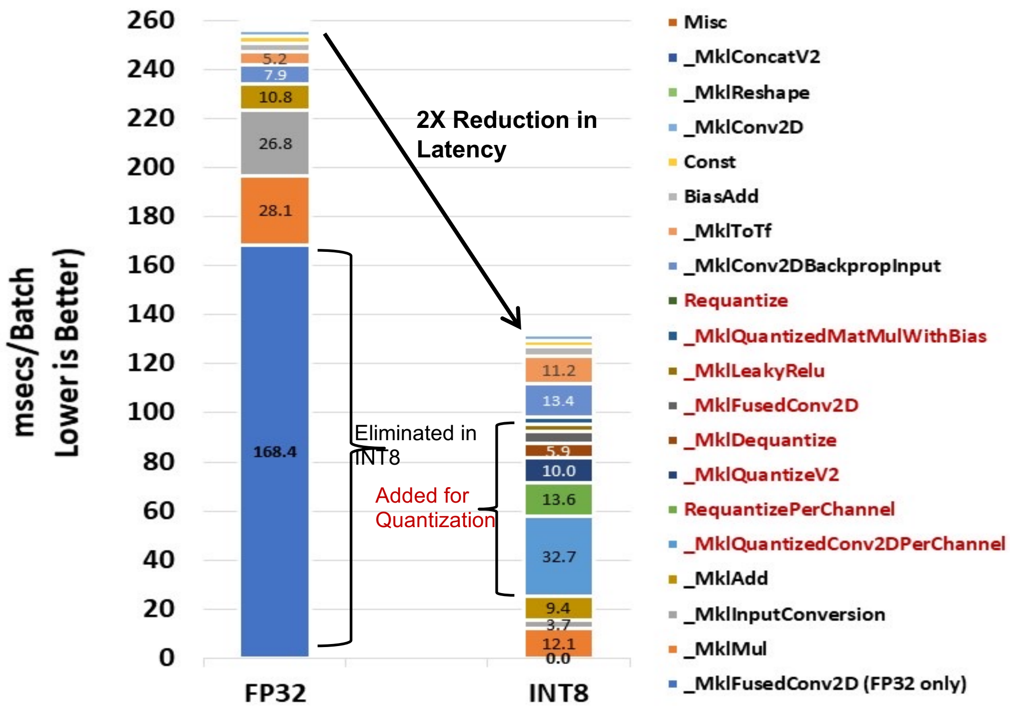


Post training quantization (INT 8) using Intel DLBoost and iLoT tool

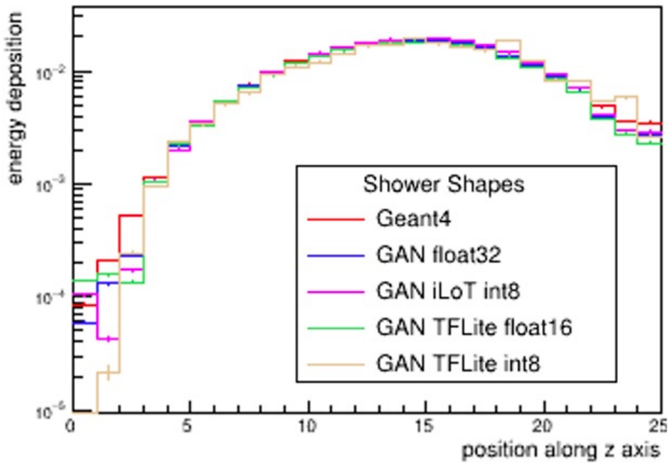
Reduced inference time but also **phsyics performance**

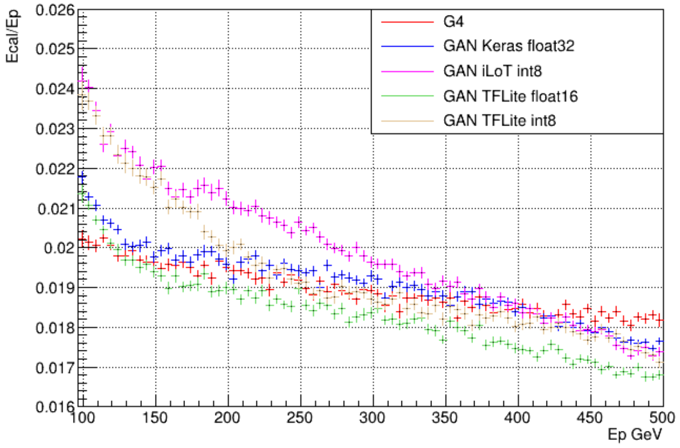
Need ad-hoc optimisation strategy

CERN 3D-GANS Inference FP32 & INT8 (DL Boost) Operation Times per Batch
on 1S Intel(R) Xeon(R) Scalable Processor 8280



FP32: 3DGAN is **38000x faster** than Monte Carlo
INT8: quantized 3DGAN is **68000x faster** than Monte Carlo

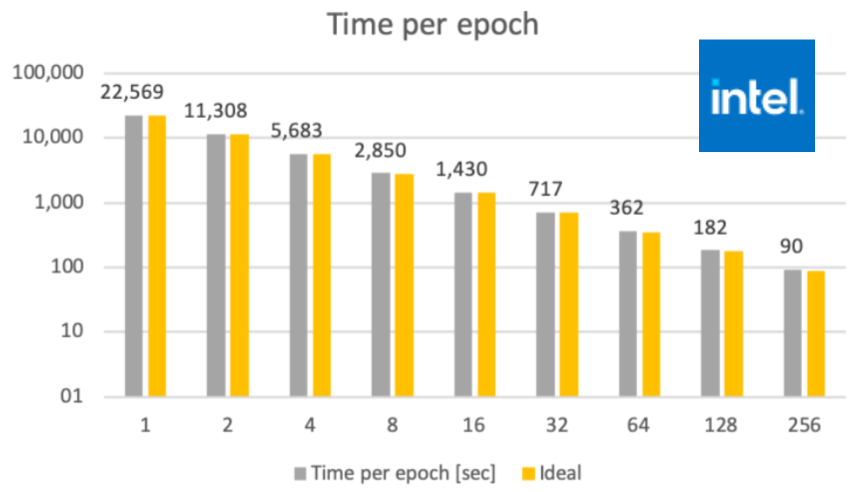


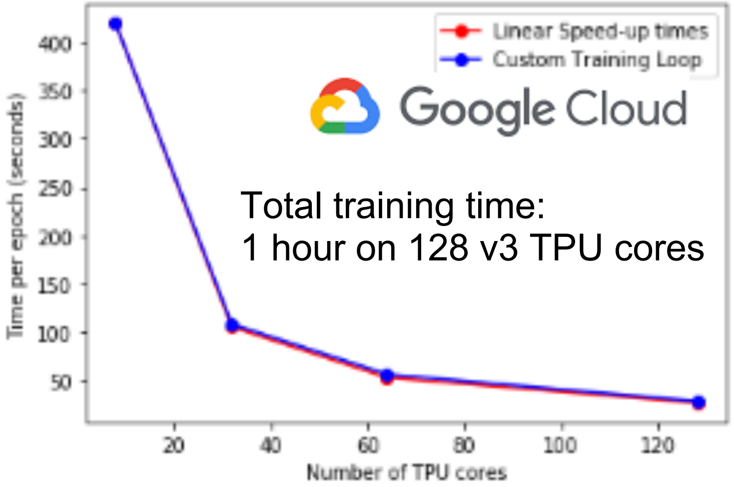


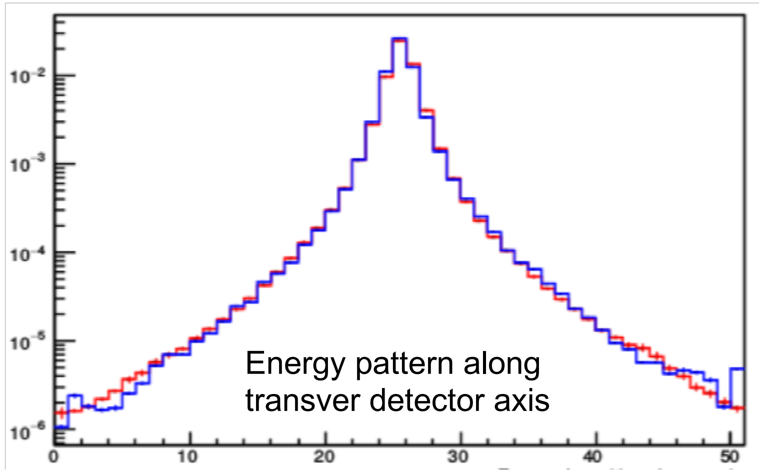
Training time

- Training 3DGAN (3M parameters) takes ~7 days on a GPU
  - **Distributed training** is essential
  - Need to keep **physics under control**
- Different data parallel approaches on different hardware on **HPC** and **Cloud**

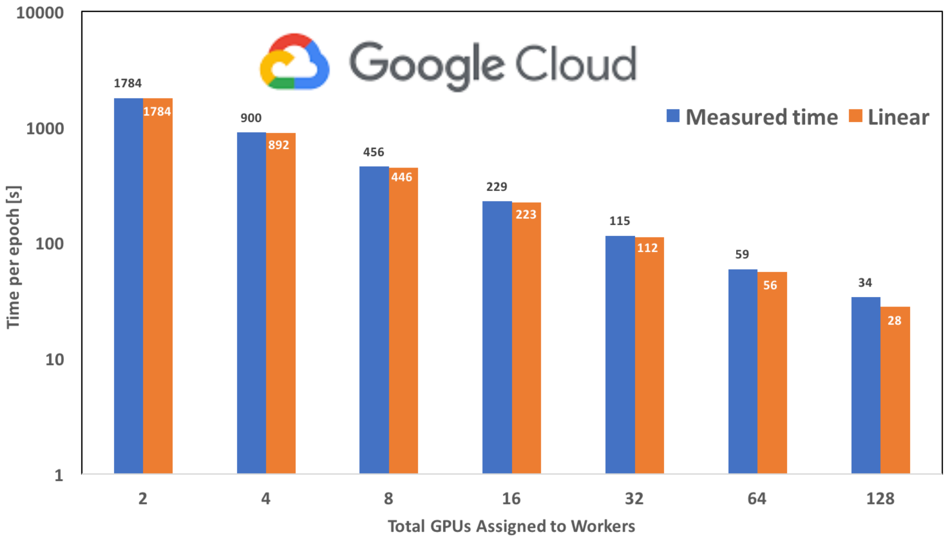
Total training time: 3 hours on 256 Intel Xeons





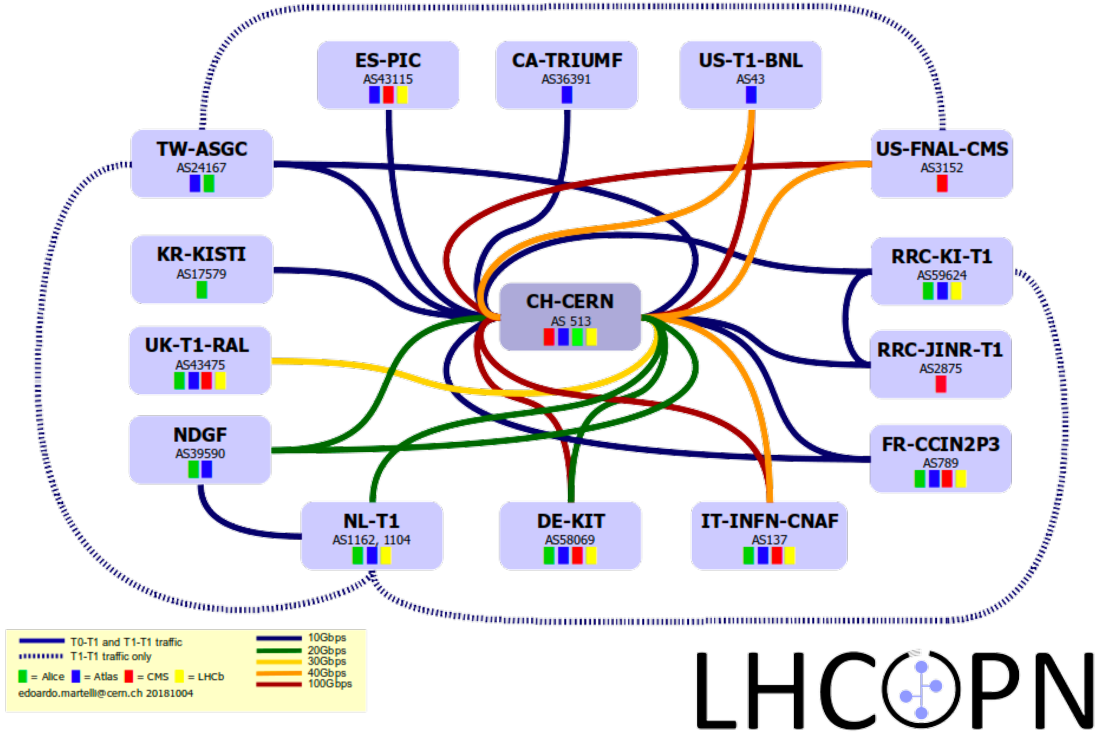


Total training time:
1 hour on 128 V100 GPUs

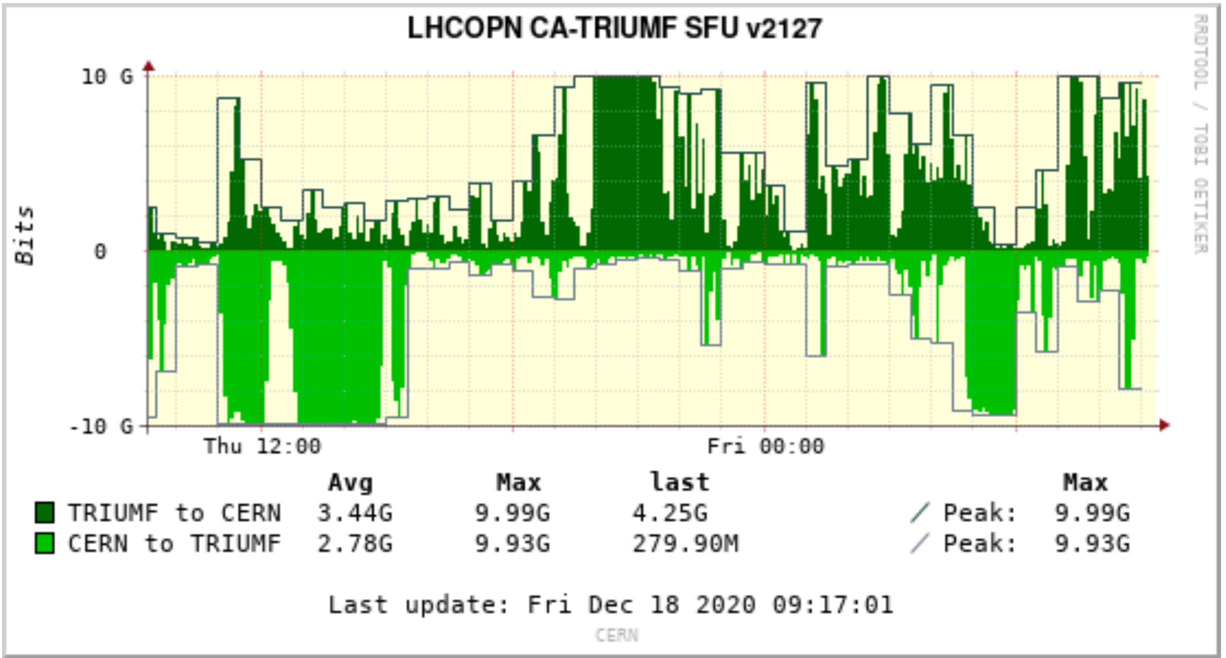


Network traffic prediction

LHCOPN (Large Hadron Collider Optical Private Network) topology



Network traffic on CERN – TRIUMF link



Predict saturation (can occur in both directions)

Optimise transfer: automatically modify network devices configuration (SDNC)

(Add extra path/link to balance traffic).

FTS

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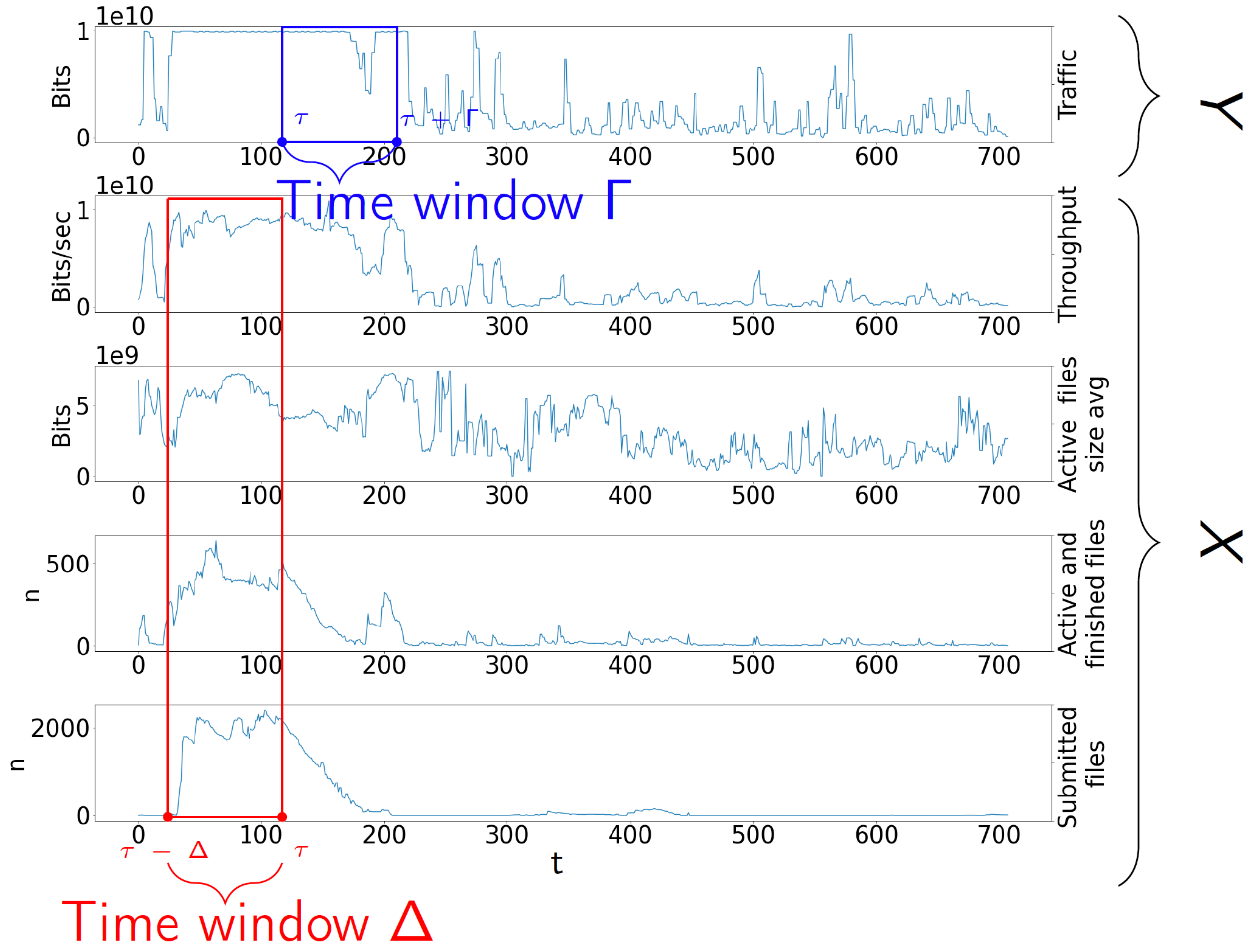
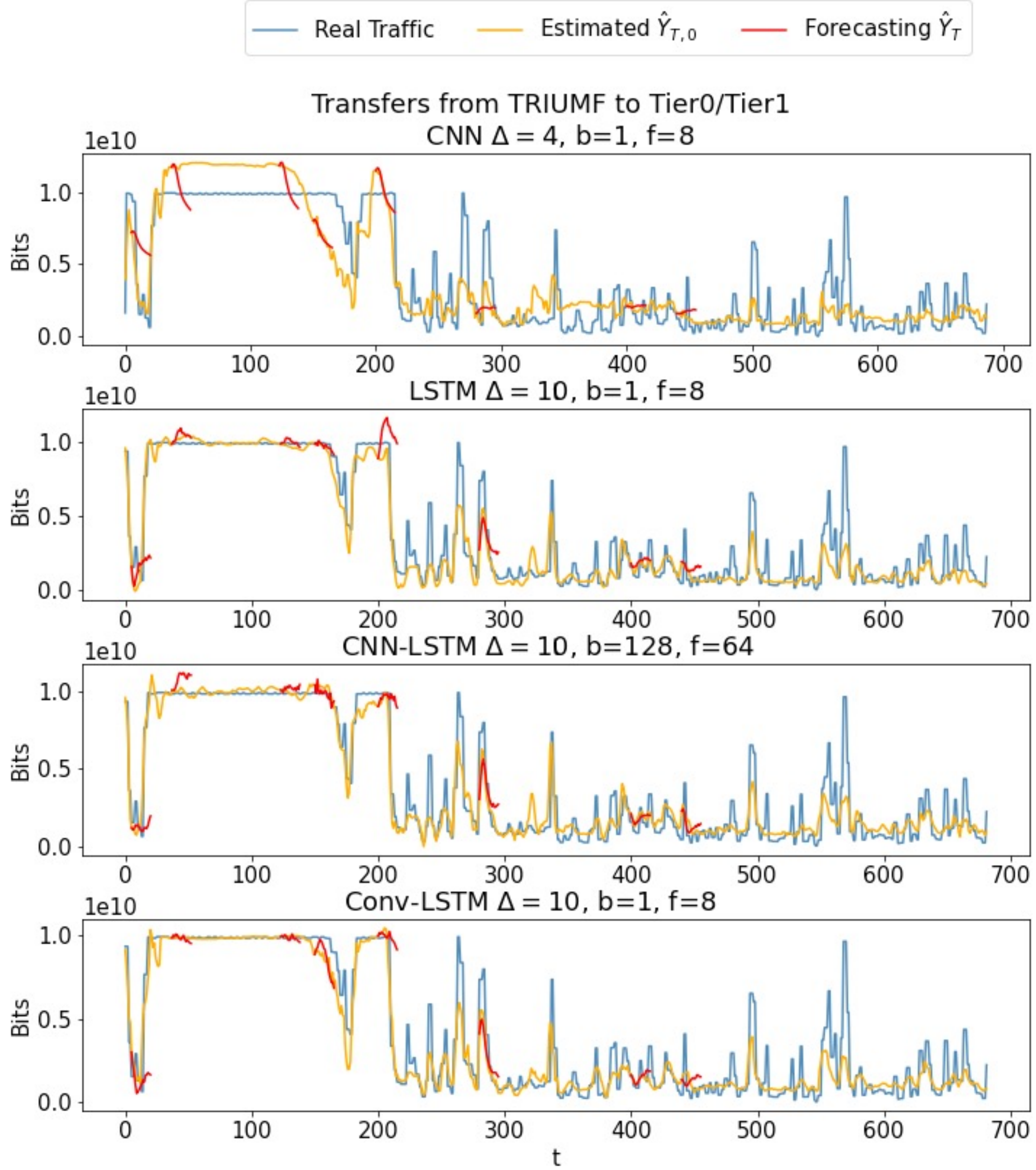
Joanna Waczynska, vCHEP2021, Grid21

arxiv: 2107.02496

Performance

Compare CNN, LSTM and hybrid architectures





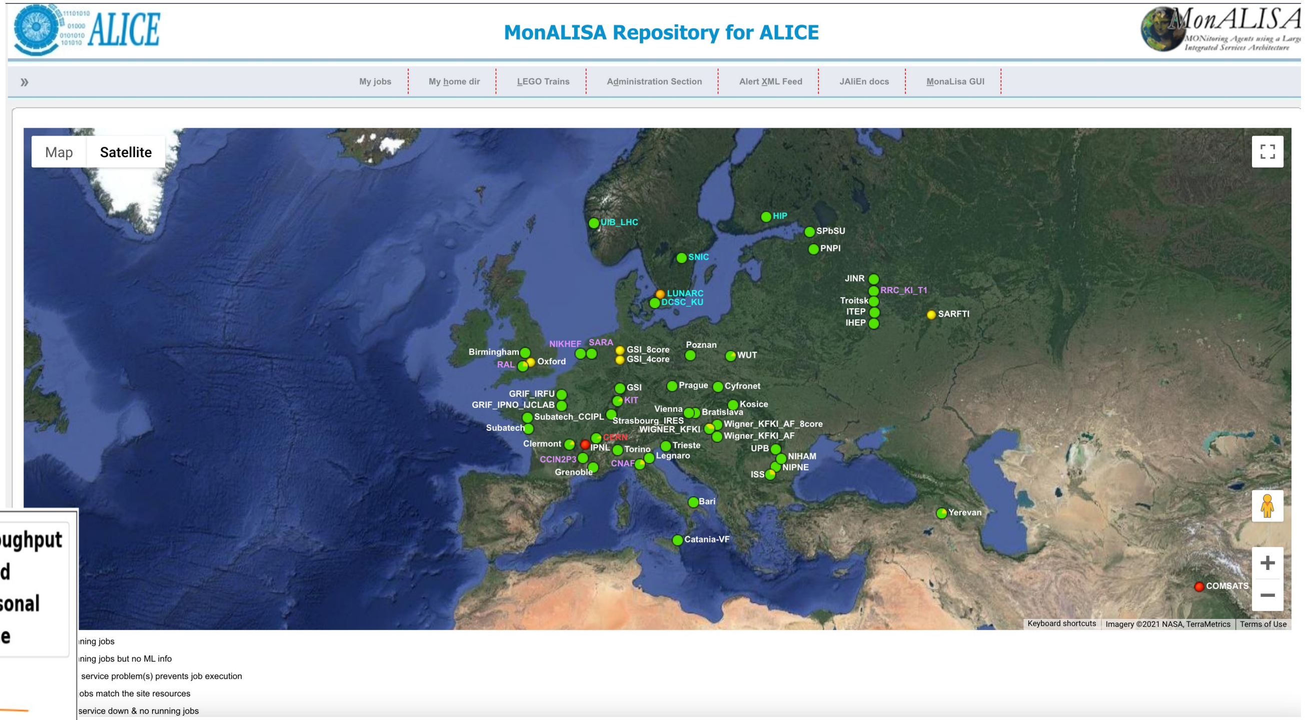
http://alimonitor.cern.ch/

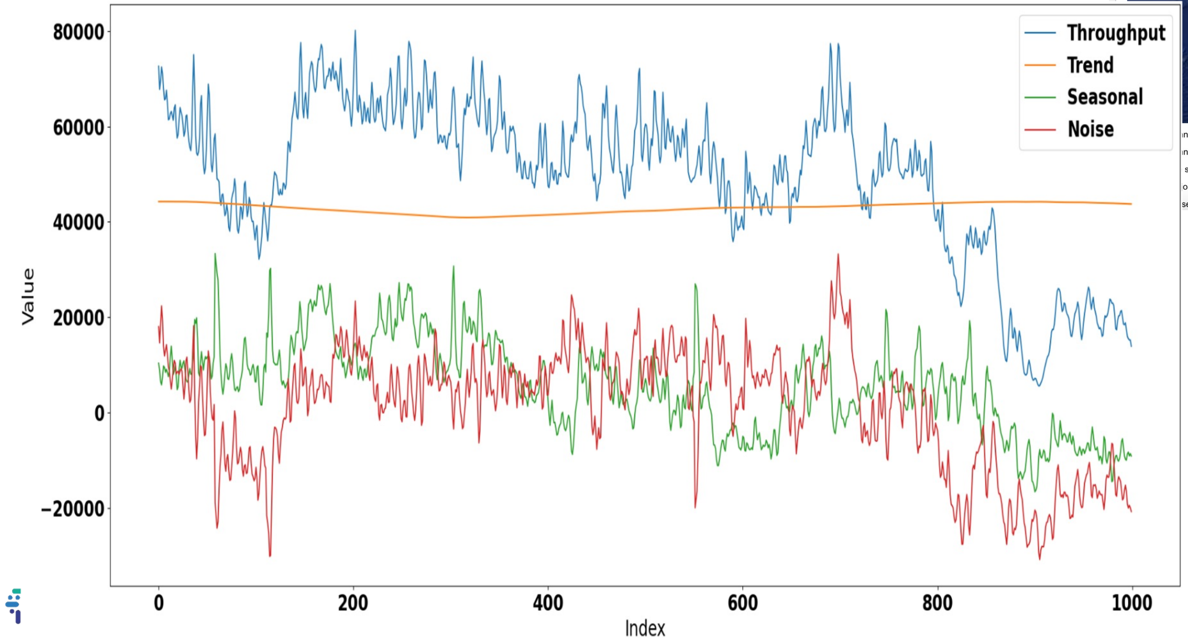
MonALISA and Alice Grid data

Legrand I., *et al.*, Computer Physics Communications 180 (2009) 2472–2498

Agent-based, dynamic service to monitor, control and **optimize distributed systems**

Analises network state and directs jobs I/O



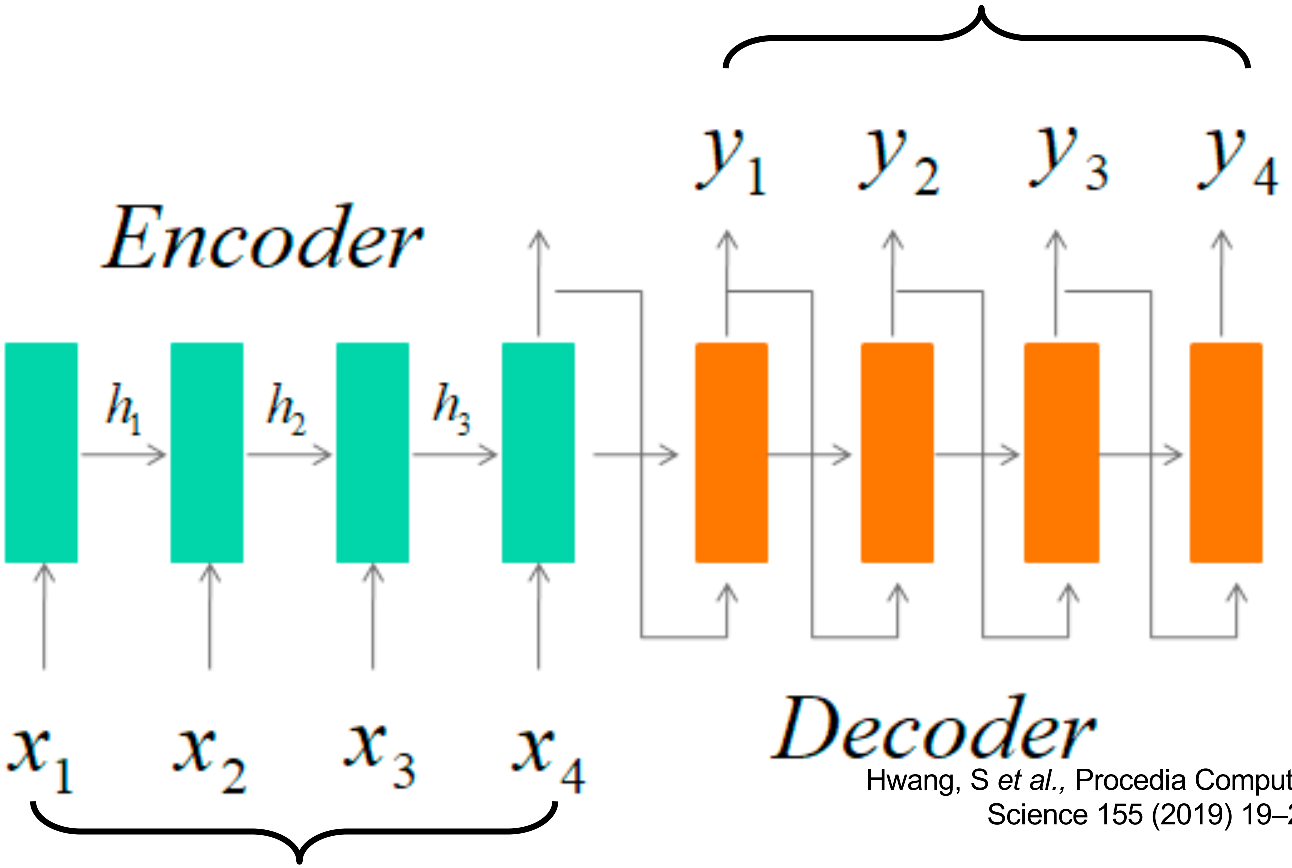


- Large fluctuations in network utilization
- Monitoring data logged every 2 minutes
- Use time stamp to associate throughput to input queries

Seq2Seq for throughput prediction

Input information: I/O queries to MonALISA

- Quantified by total Read Size:
  - $X_n = \{RS_{i,t}, \text{throughput}_t\}$
- Predict throughput
  - $Y_n = \text{throughput}_{t+n}$
- 2 hyperparameters: input & output sequence lengths



Hwang, S *et al.*, Procedia Computer Science 155 (2019) 19–26

Results

Hyper-parameters search

- Best results with **low in/out dimensions**

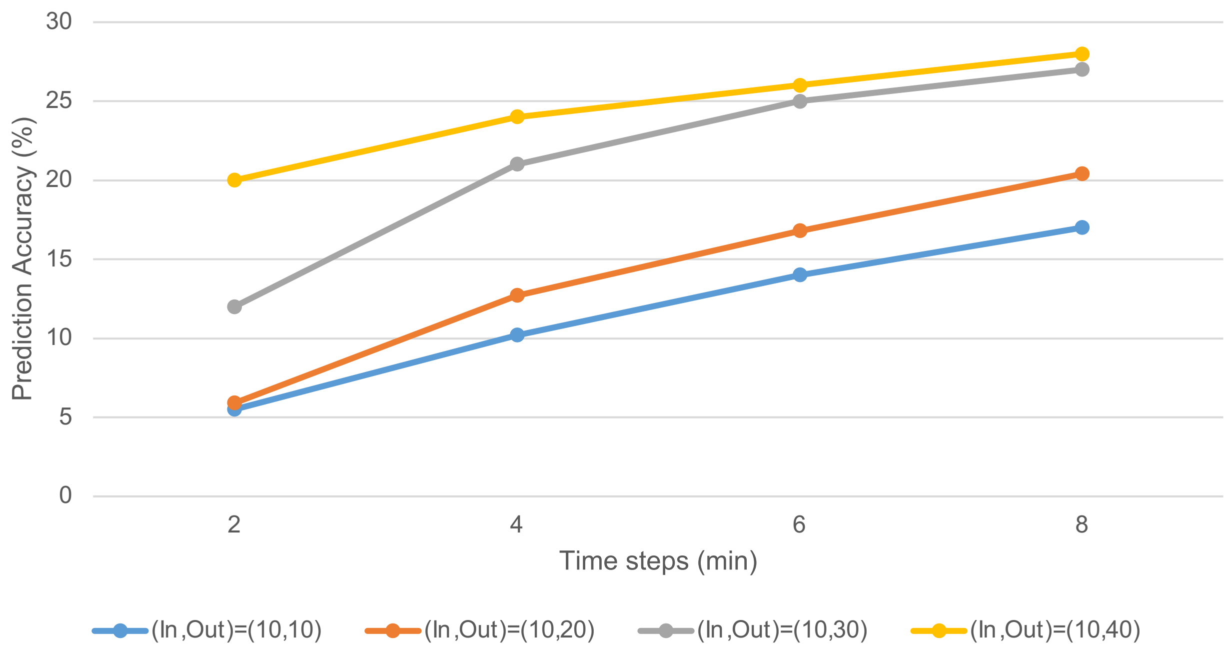
Predict next step (2min) with 5% accuracy

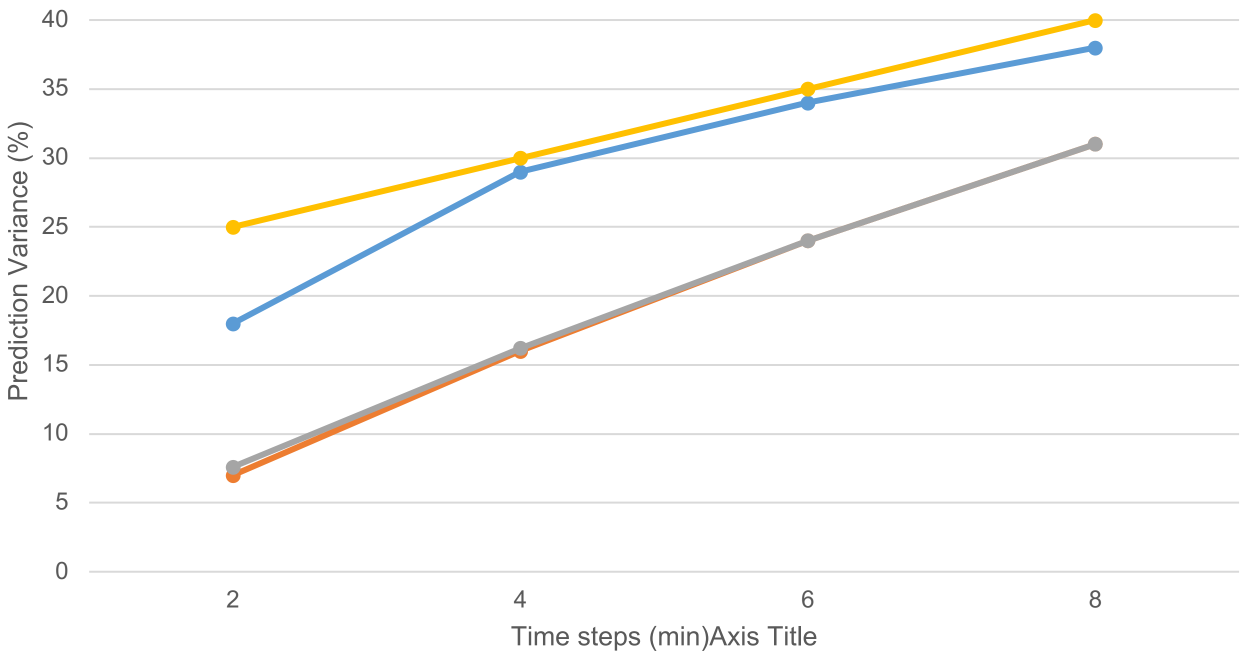
- Next step prediction is stable

Preformance **degrades when forecasting over longer time** spans

- 8 min forecast → ~15%

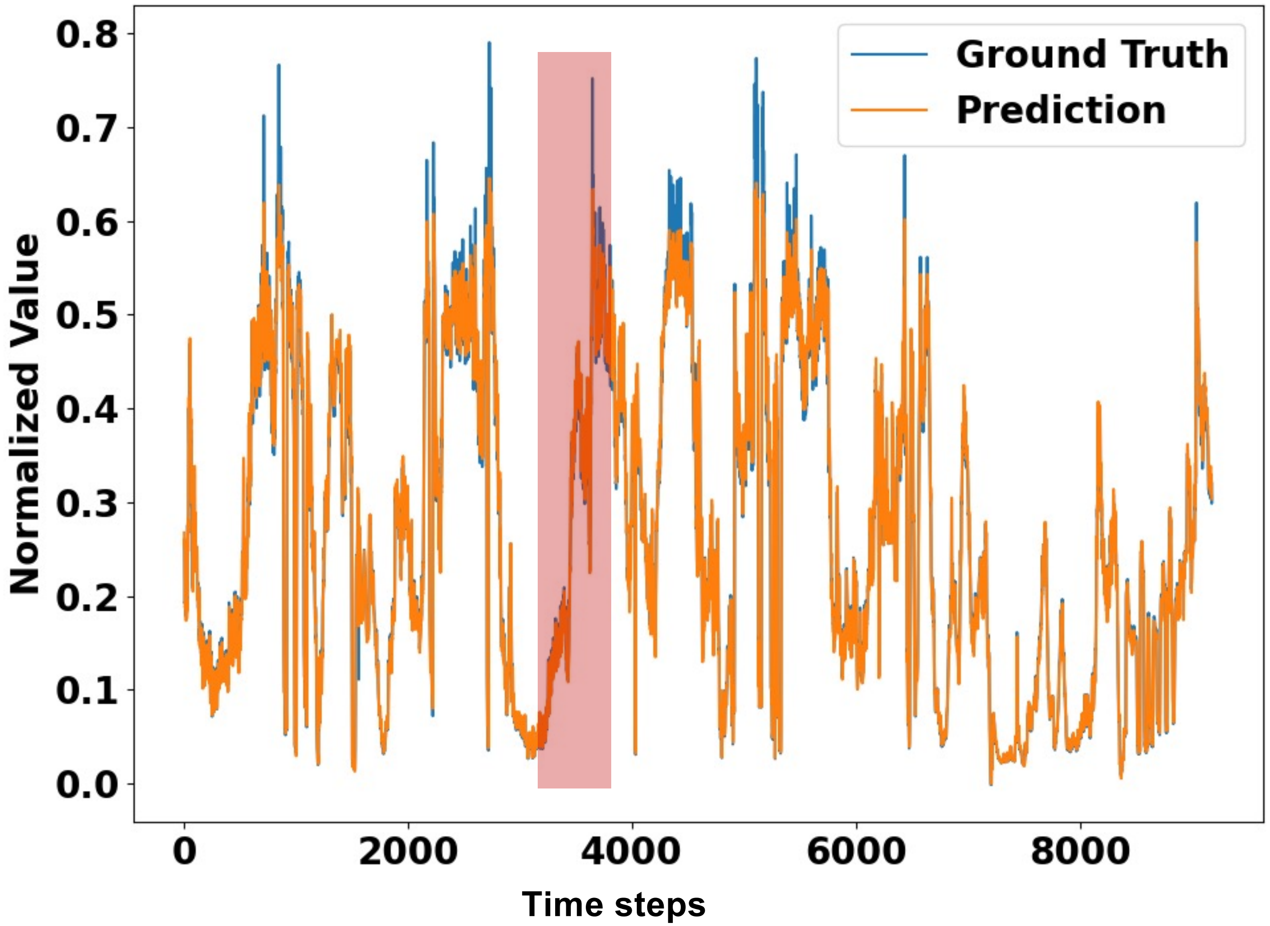
Increasing input size deteriorates the accuracy > 20%

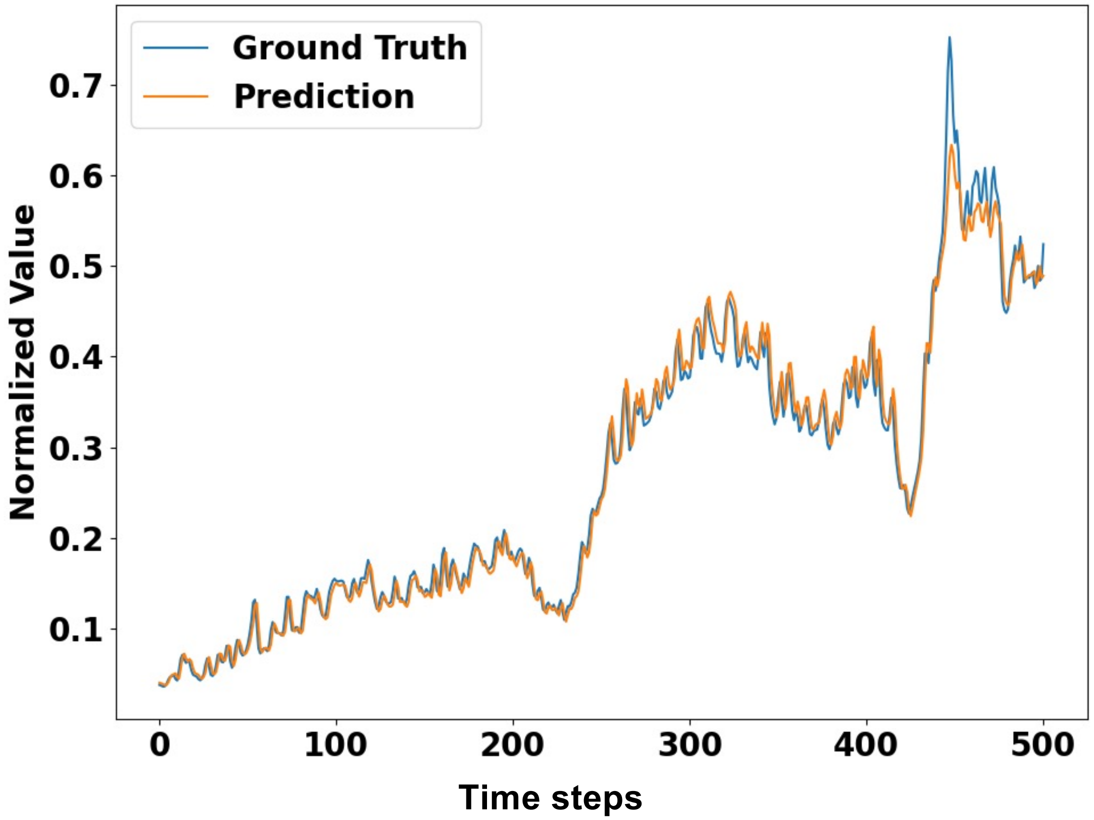




t+2min prediction

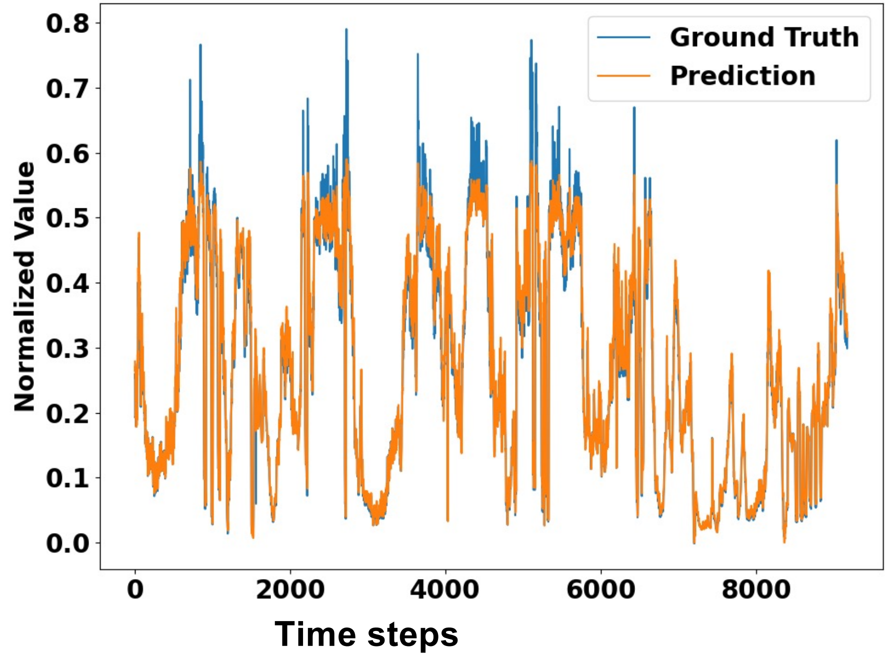
(in,out)=(10,10)



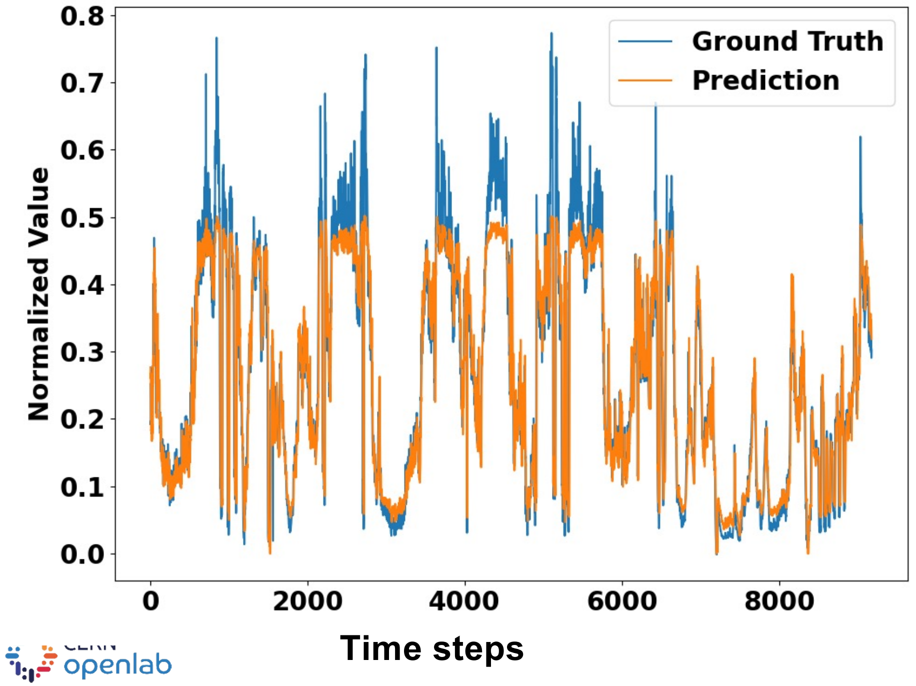


Extended forecasting

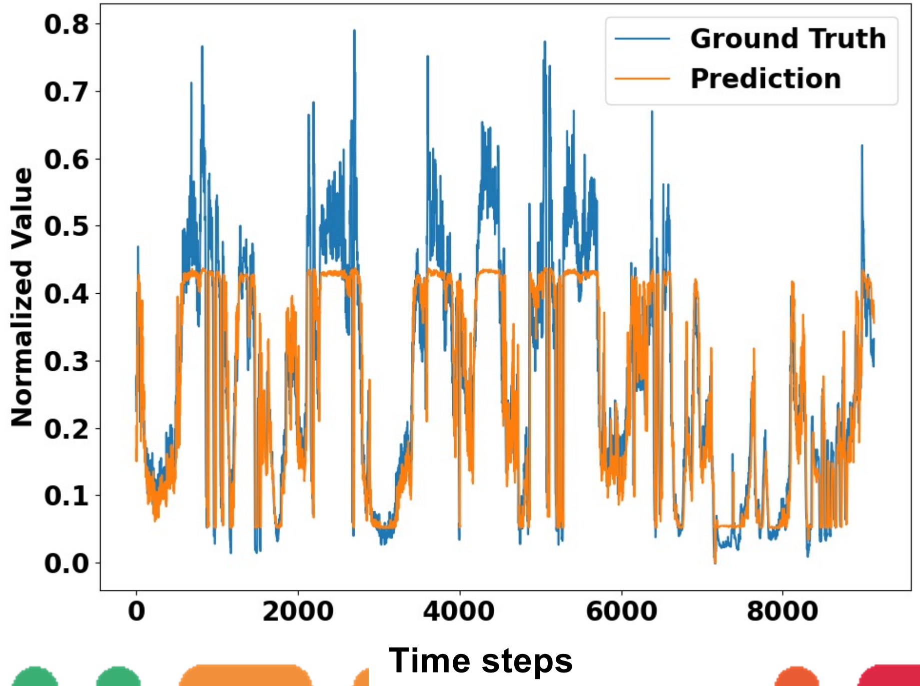
(in,out)=(10,10)
t + 4min



(in,out)=(10,10), **t + 8min**



(in,out)=(30,30), **t + 20min**



Murnane, Xiangyang, https://indico.cern.ch/event/852553/contributions/4062229/

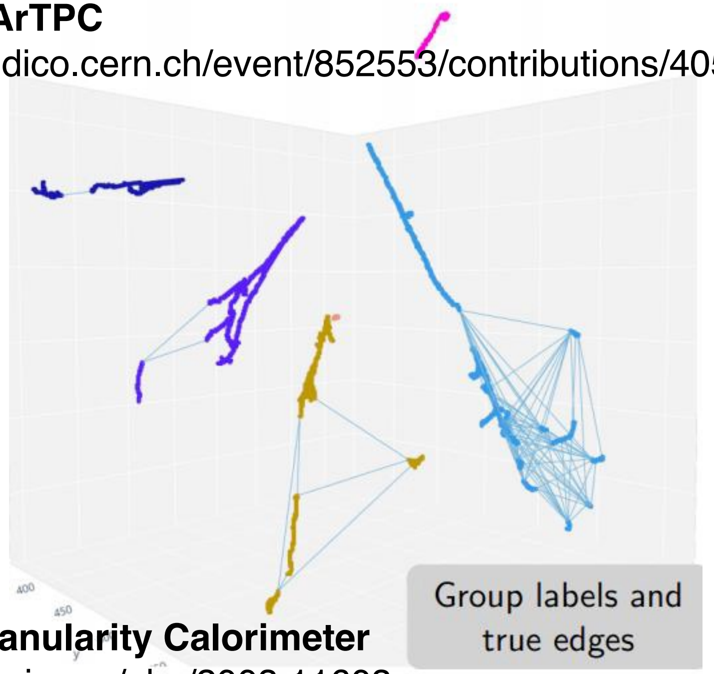
Graph Neural Networks

Next generation detectors will present challenges to **image-based methods**

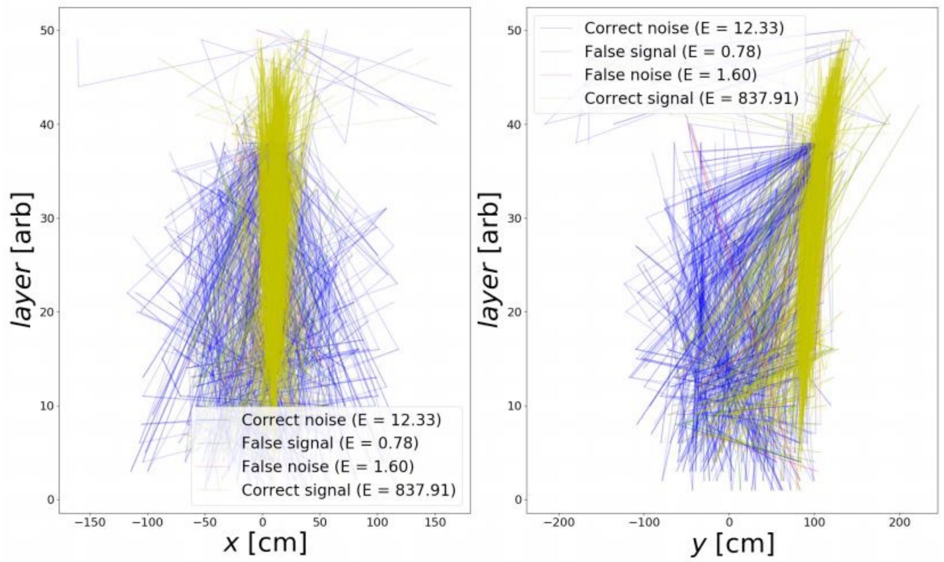
Graphs can capture inherent **sparsity** and **relational** structure

- **Approximate geometry** of the physics problem
- **Generalize** other ML techniques
- E.g. Message passing convolution generalizes CNN from flat to arbitrary geometry

Dune LArTPC
https://indico.cern.ch/event/852553/contributions/4059542/

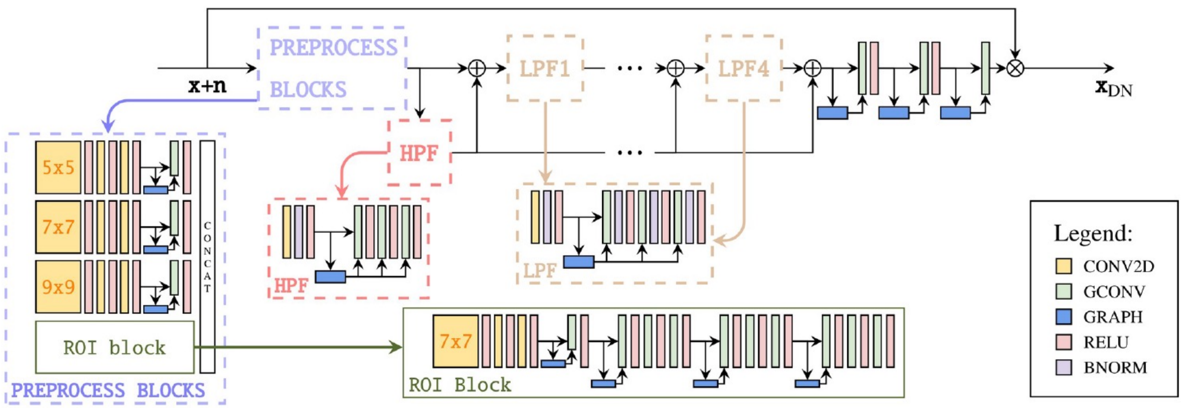


High Granularity Calorimeter
https://arxiv.org/abs/2003.11603

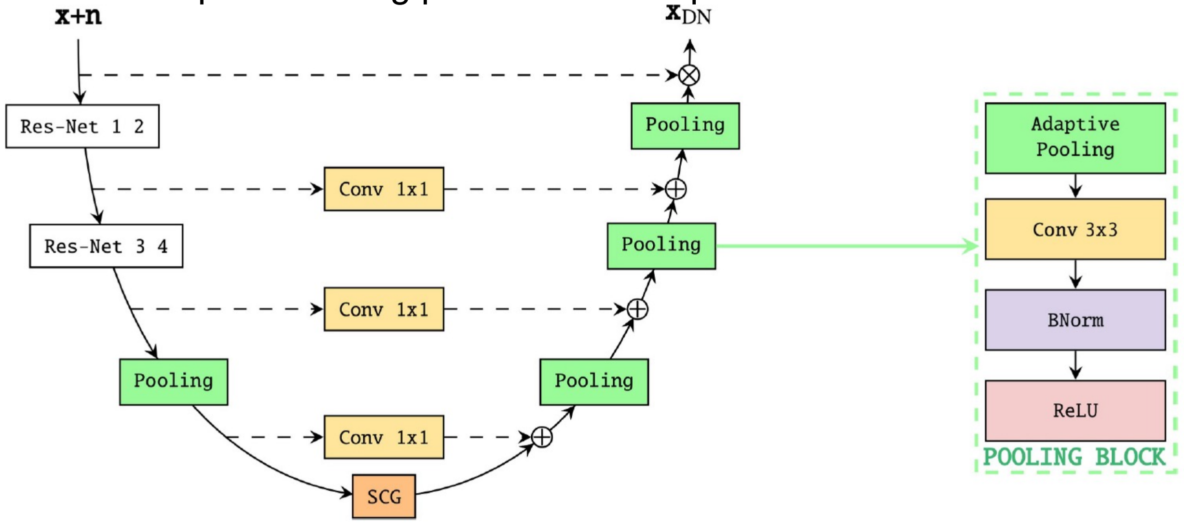


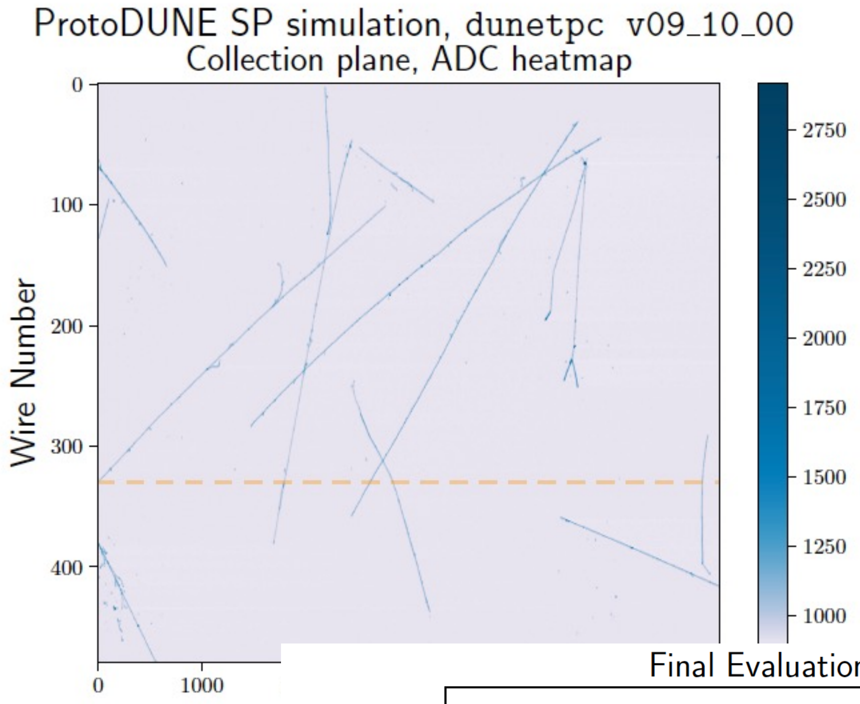
Raw data denoising with hybrid models

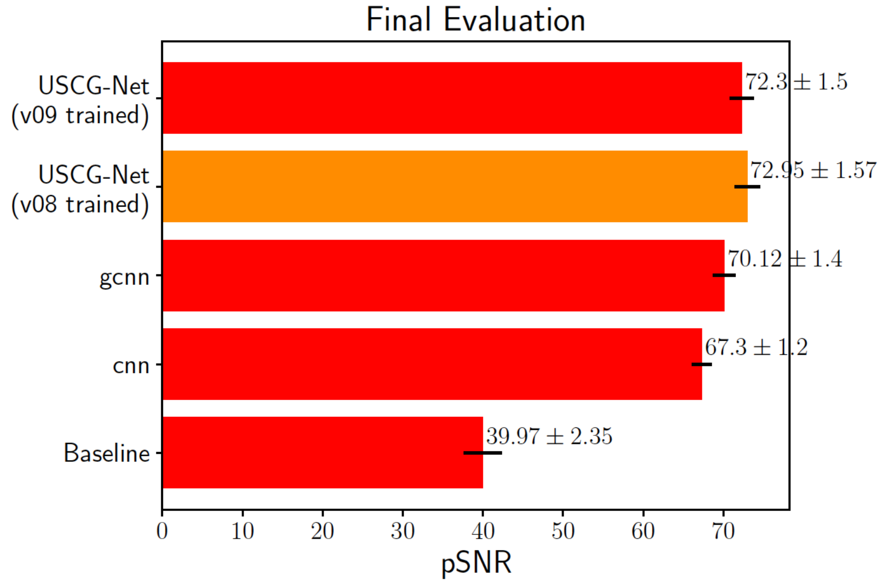
GConV: https://arxiv.org/abs/1907.08448



USCG Net https://arxiv.org/pdf/2009.01599.pdf





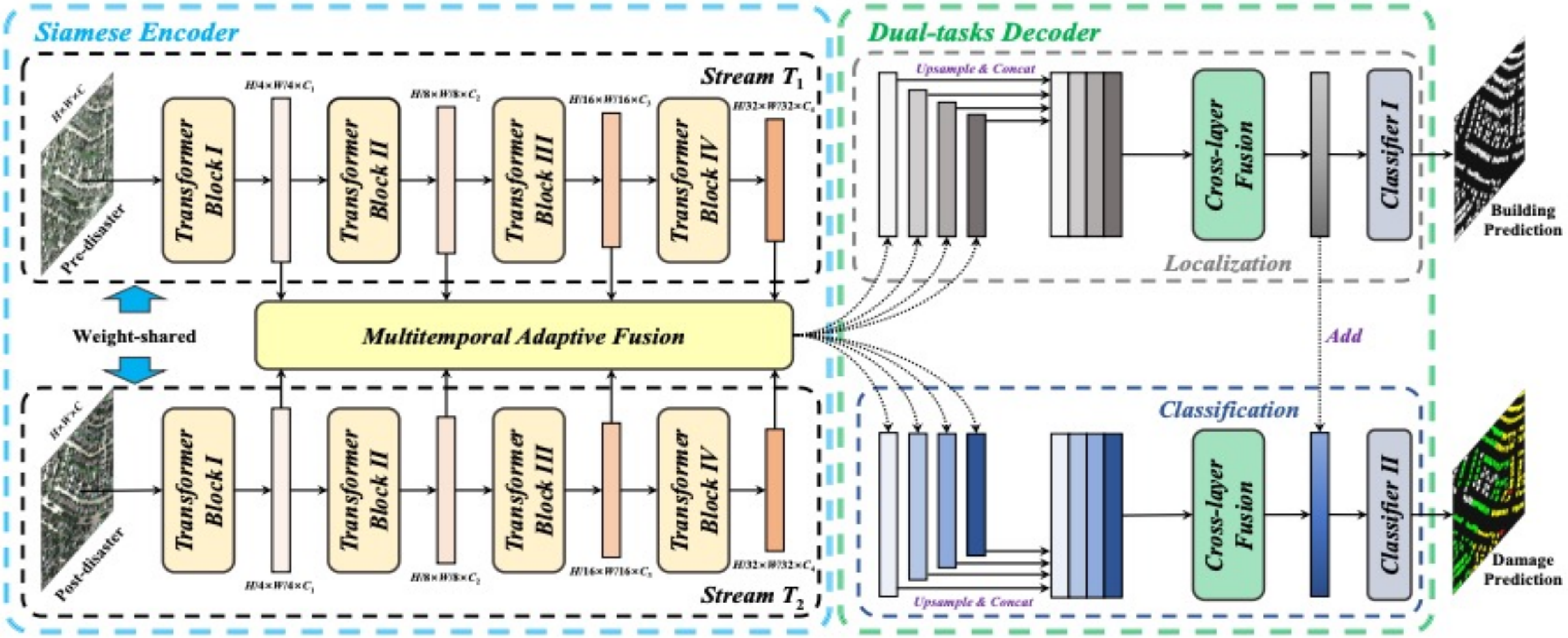


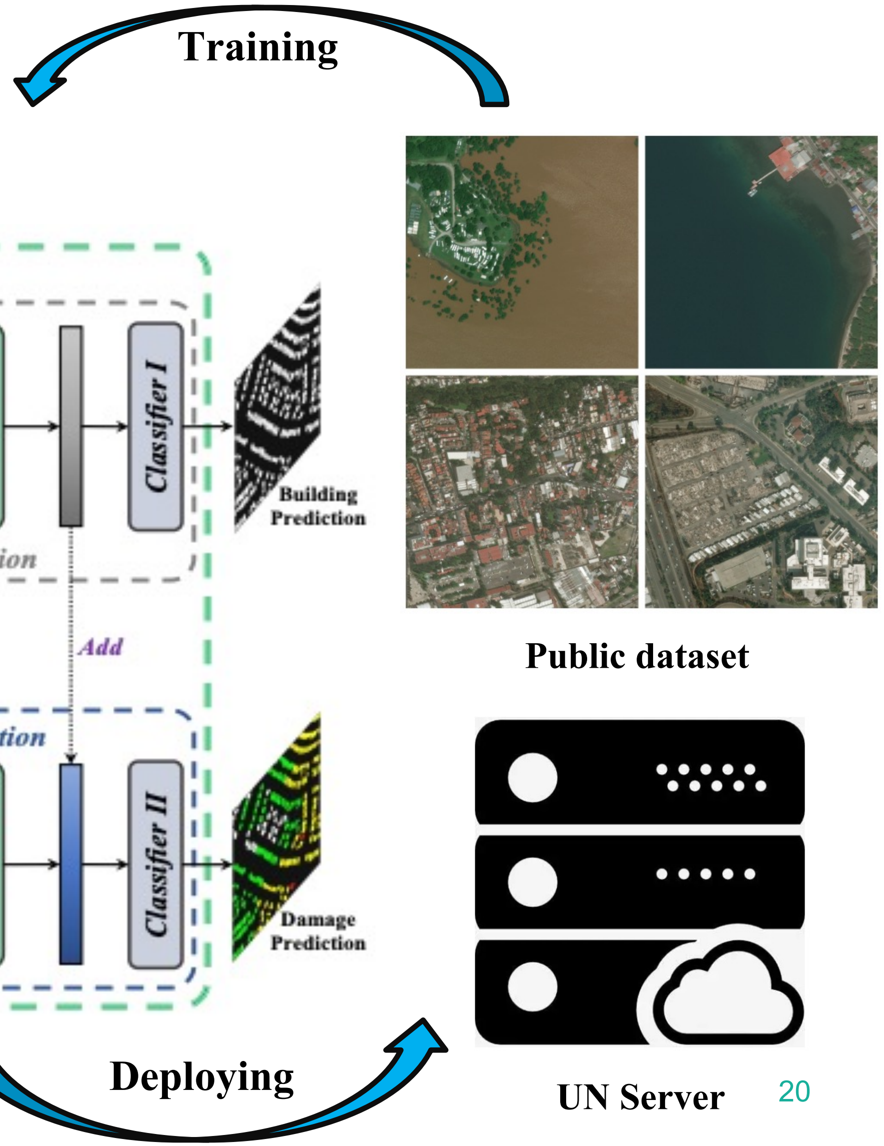
Transformers for building damage detection

arxiv:2201.10953

Inspired by the SegFormer architecture

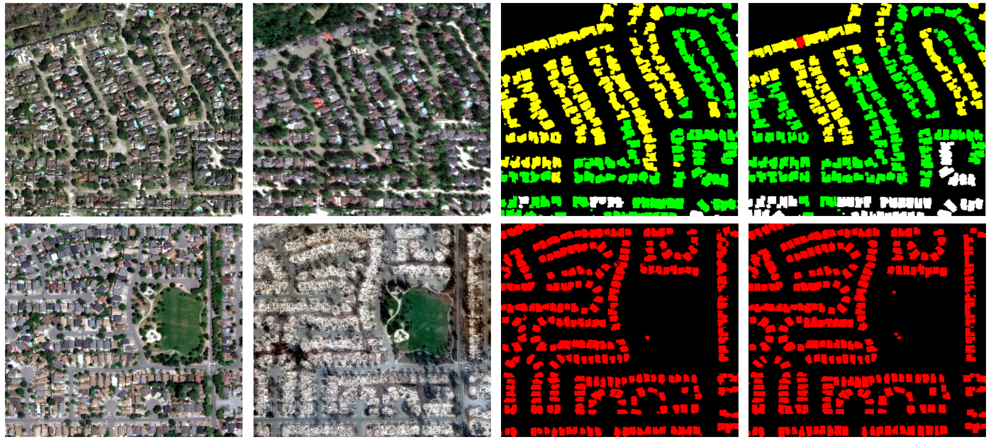
Two tasks: **localization** and per-pixel **damage classification**





Performance

xBD dataset (https://xview2.org/dataset) from **Maxar Open Data Program**



T_1 (Pre-damage) | T_2 (Post-damage) | Prediction | Reference

Method	F_1^{oa}	F_1^{loc}	F_1^{dam}	Damage F_1 per class			
				No	Minor	Major	Destroyed
xView2 Baseline	26.54	80.47	3.42	66.31	14.35	0.94	46.57
Siamese-UNet	71.68	85.92	65.58	86.74	50.02	64.43	71.68
MaskRCNN	74.10	83.60	70.02	**90.60**	49.30	72.20	**83.70**
ChangeOS	75.50	85.69	71.14	89.11	53.11	72.44	80.79
DamFormer	**77.02**	**86.86**	**72.81**	89.86	**56.78**	**72.56**	80.51

Use modified F_1 score combining localization, damage assessment scores*

Transfer learning

Pre-damage

Post-damage

Natural & Man-made damages

CERN openlab

*suggested in the "CV for Building damage assessment challenge" (https://www.xview2.org/)

Quantum Machine Learning

CERN QTI and its Roadmap

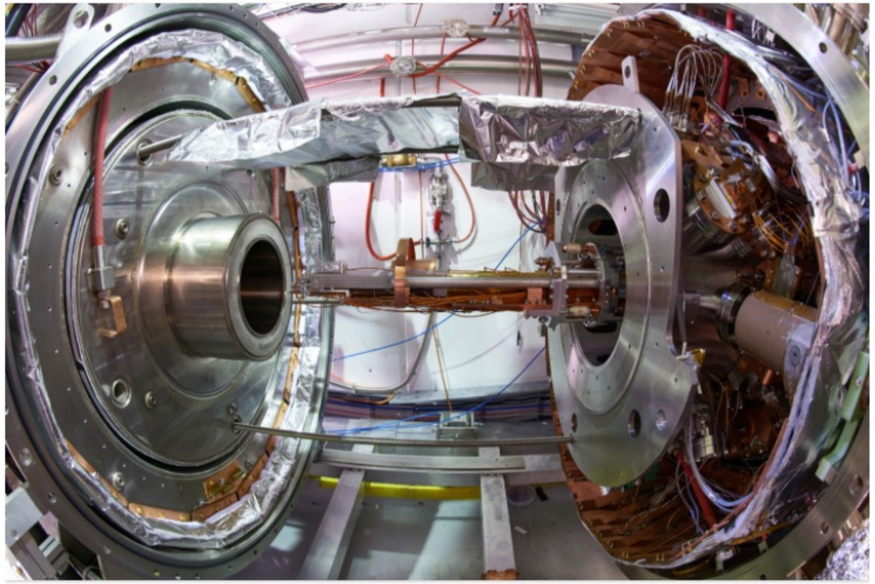
CERN established the QTI in 2020

Voir en français

CERN meets quantum technology

The CERN Quantum Technology Initiative will explore the potential of devices harnessing perplexing quantum phenomena such as entanglement to enrich and expand its challenging research programme

30 SEPTEMBER, 2020 | By Matthew Chalmers



The AEgIS 1T antimatter trap stack. CERN's AEgIS experiment is able to explore the multi-particle entangled nature of photons from positronium annihilation, and is one of several examples of existing CERN research with relevance to quantum technologies. (Image: CERN)

- Roadmap in 2021
- Publicly available in Zenodo: accessed more than 5,200 times

T1 - Scientific and Technical Development and Capacity Building

T2 - Co-development

APPLICATIONS | NEWS

CERN unveils roadmap for quantum technology

4 November 2021

QUANTUM TECHNOLOGY INITIATIVE

Credit: CERN

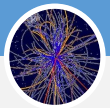
T3 - Community Building

T4 - Integration with national and international initiatives and programmes

openlab

https://doi.org/10.5281/zenodo.5553774

Scientific Objectives



- Assess **potential quantum advantage** in HEP
- Develop **common libraries, methods, tools**; benchmark as technology evolves
- Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

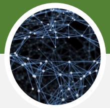
Computing & Algorithms

- Develop techniques for **quantum simulation** in collider physics, QCD, cosmology within and beyond the SM
- Co-develop quantum computing and sensing approaches by providing **theoretical foundations**

Simulation & Theory

- Develop and promote **expertise in quantum sensing**
- Develop quantum sensing approaches for **low-energy particle physics measurements**
- Assess **novel technologies and materials** for HEP applications

Sensing, Metrology & Materials



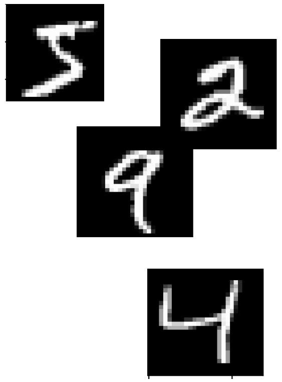
- **Co-develop CERN technologies relevant to quantum infrastructures**
- Contribute to the **deployment and validation of quantum infrastructures**
- Assess **impact of quantum communication on computing applications**

Communications & Networks

Quantum Machine Learning

- ML/DL to help discover **new quantum algorithms/improve quantum circuits**
- **Quantum Computing to accelerate ML/DL** training or inference

Quantum circuits are **differentiable** and **can be trained** minimizing a cost function that depends on the training data



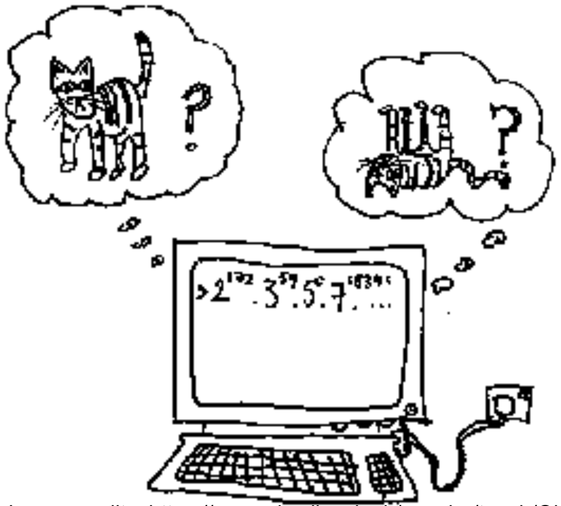


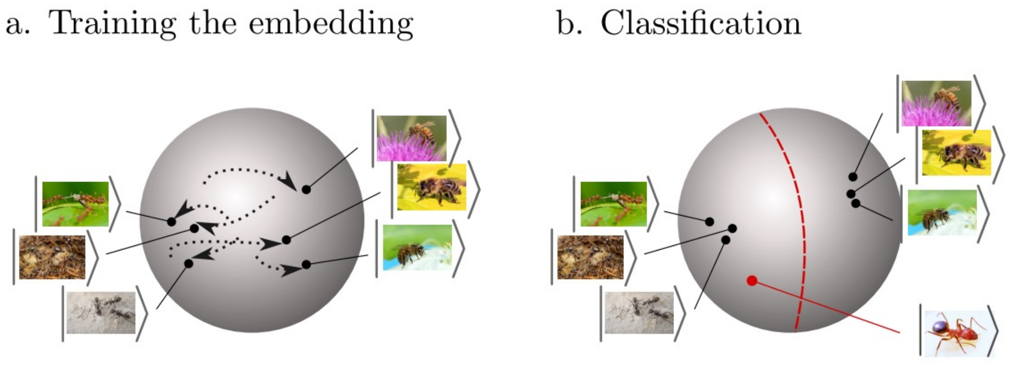
Image credits: https://www.physik.uzh.ch/~psaha/teach/Qbit/

5,2,9,4,…

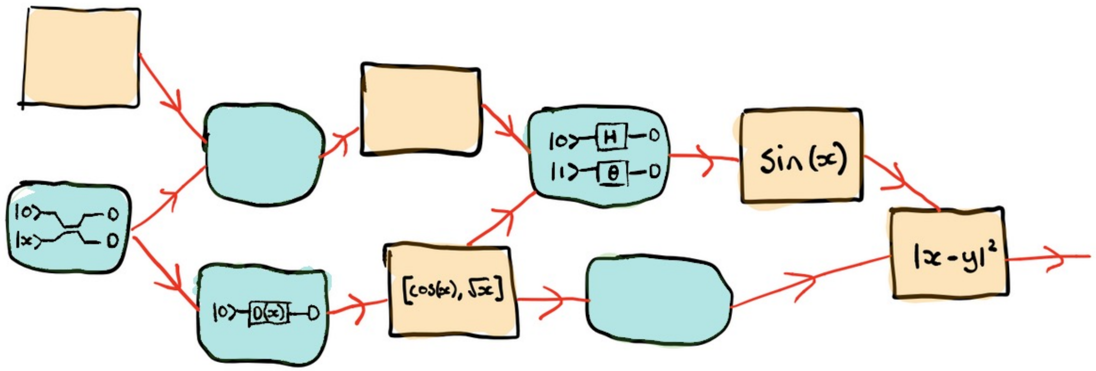
Classical ML/DL are **flexible** algorithms
but rely on **large data sets**

QML in practice…

- How to represent classical data in quantum states?
- How to introduce non-linearities in quantum circuits?
- SGD-based optimisation?
- Back-propagation and automatic differentiation



M. Schuld et al., arXiv: 2001.03622v2



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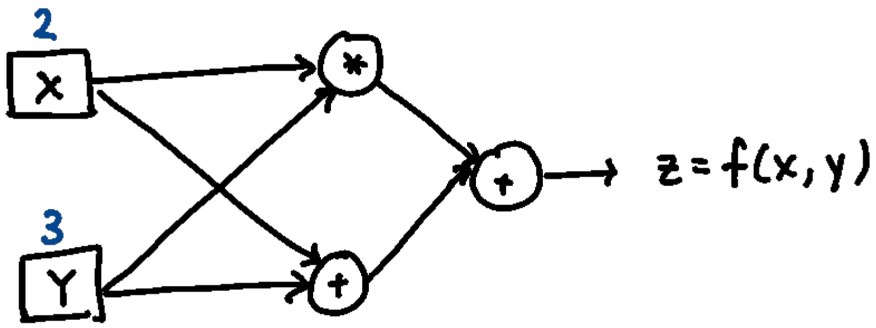


Mitarai et al. (2018)
Schuld et al. (2018)

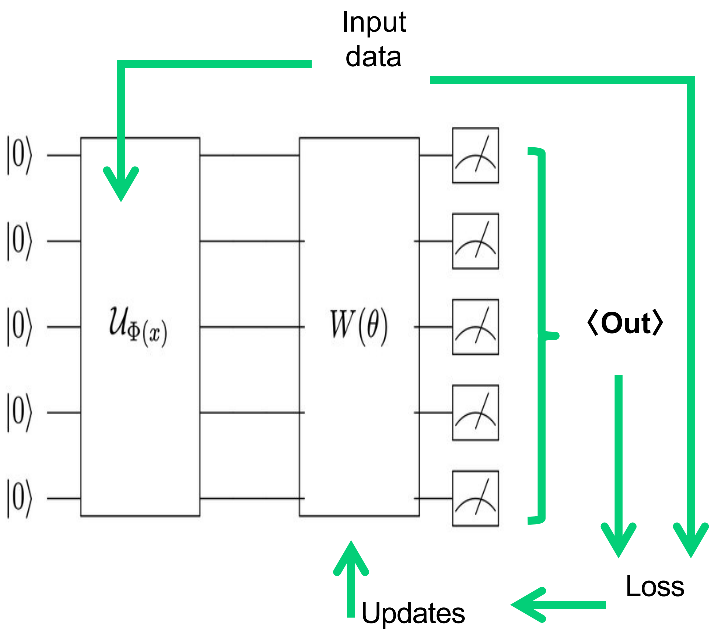
QML implementations

Variational algorithms

Parametric ansatz

Can use **gradient-free** methods or **SGD**

Data Embedding can be **learned**

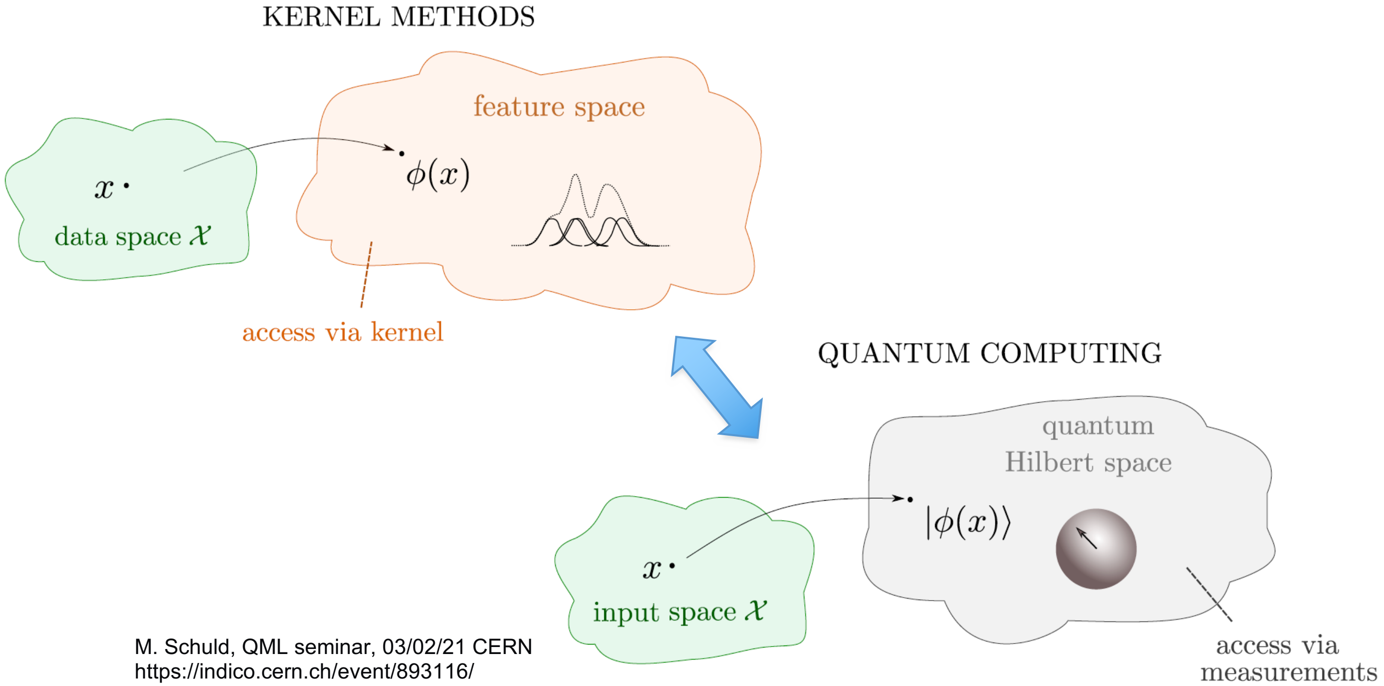


Kernel methods

Feature maps as **quantum kernels**

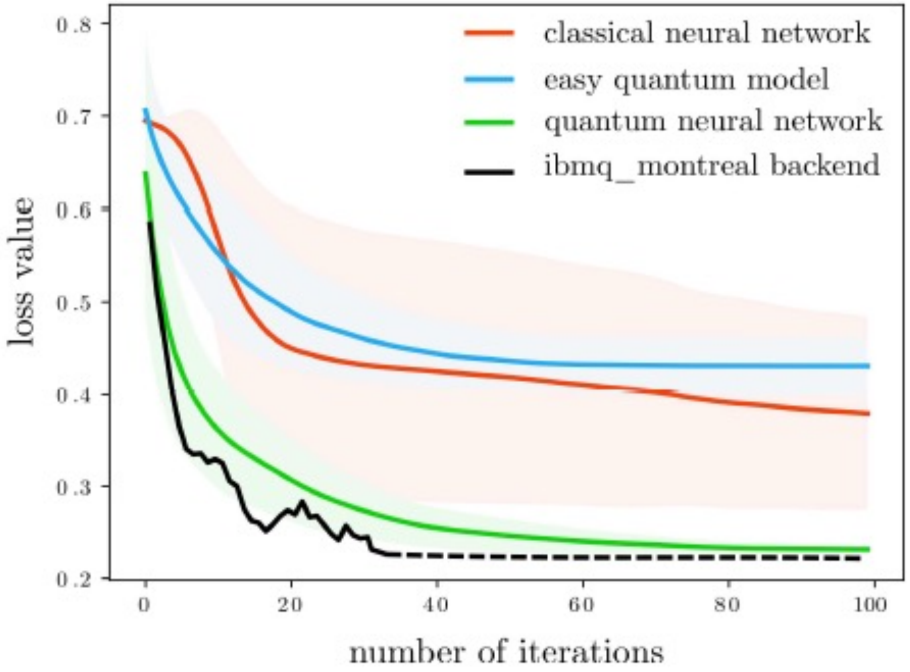
Use classical **kernel-based training**

- **Convex** losses**, global** minimum
- Compute pair-wise distances in N_{data}



M. Schuld, QML seminar, 03/02/21 CERN
https://indico.cern.ch/event/893116/

Quantum Advantage for QML?



Advantage definition

Practical implementation vs asymptotic complexity

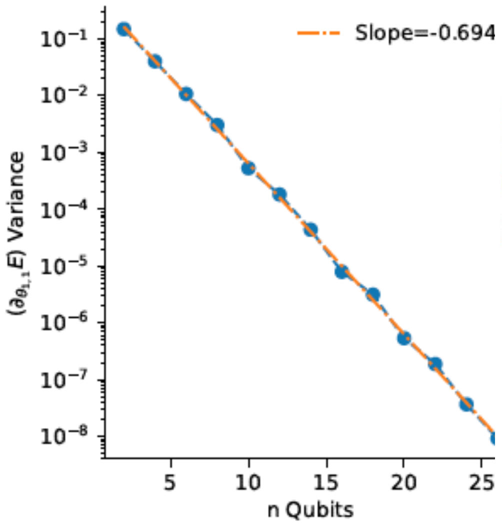
Performance metrics

A change of paradigm in the study of QML algorithms brign interesting insights in classical models as well

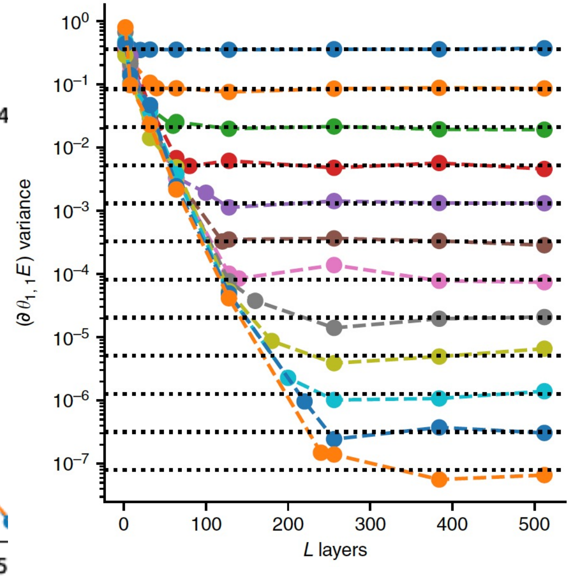
see recent work by M. Schuld and N. Killoran (arxiv:2203.01340)

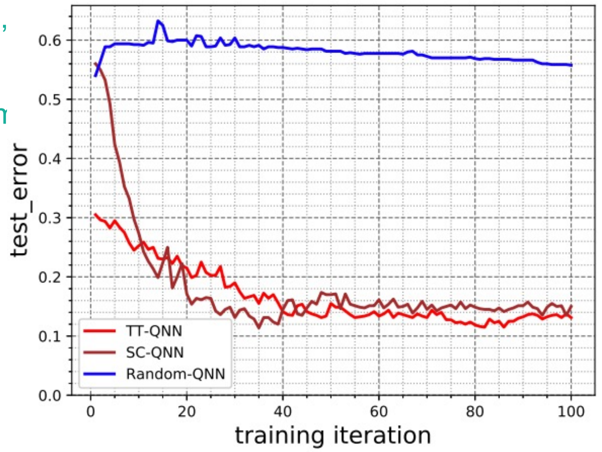
Model Convergence

- Classical gradients **vanish exponentially** with the number of layers (J. McClean *et al.*, arXiv:1803.11173)
  - Convergence still possible if gradients consistent between batches.
- Quantum gradient decay exponentially in the number of qubits
  - Random circuit initialization
  - Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
  - Ansatz choice: TTN, CNN (Zhang *et al.*, arXiv:2011.06258, *Physical Review X* 11.4 (2021): 041011.)
  - Noise induced barren plateau (Wang, S *et al.*, Nat Comm (2021))



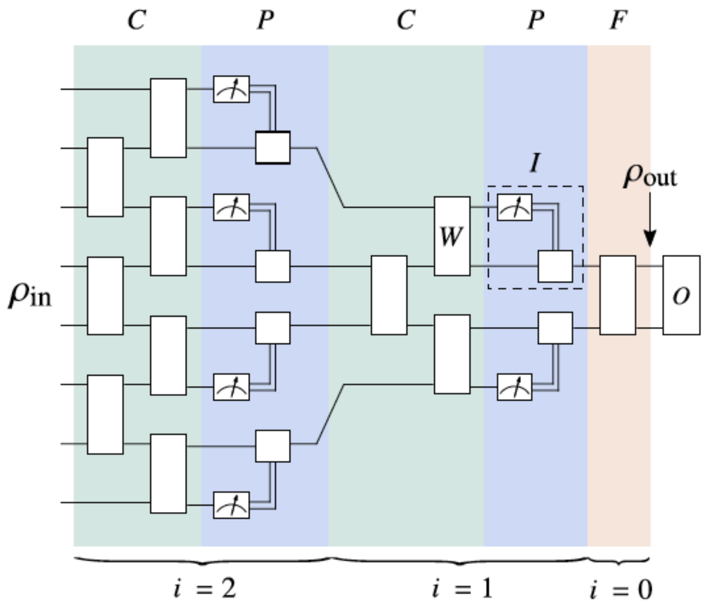
J. McClean *et al.*, arXiv:1803.11173





TTN for MNIST classification (8 qubits), Zhang *et al.*, arXiv:2011.06258

QCNN: A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011



Example QML projects

Quantum Classifiers for Higgs boson identification

arXiv:2104.07692

Quantum **Tree Tensor Networks** for particle trajectory **reconstruction**

arXiv:2007.06868, arXiv:2012.01379, arXiv:2109.12636

Hybrid **quantum-classical tracking hits embedding**

EPJ Web of Conferences (Vol. 251, p. 03065)

Quantum Generative Adversarial Networks for detector simulation

arXiv:2103.15470, arXiv:2101.11132, arXiv:2203.01007

Quantum Born Machines for event generation

ACAT2021

Quantum **Boltzmann Machines** for beam **optimization** in accelerators

BQiT 2021

Quantum algorithms for anomaly detection

Su Yeon Chang

Quantum generation of energy profiles

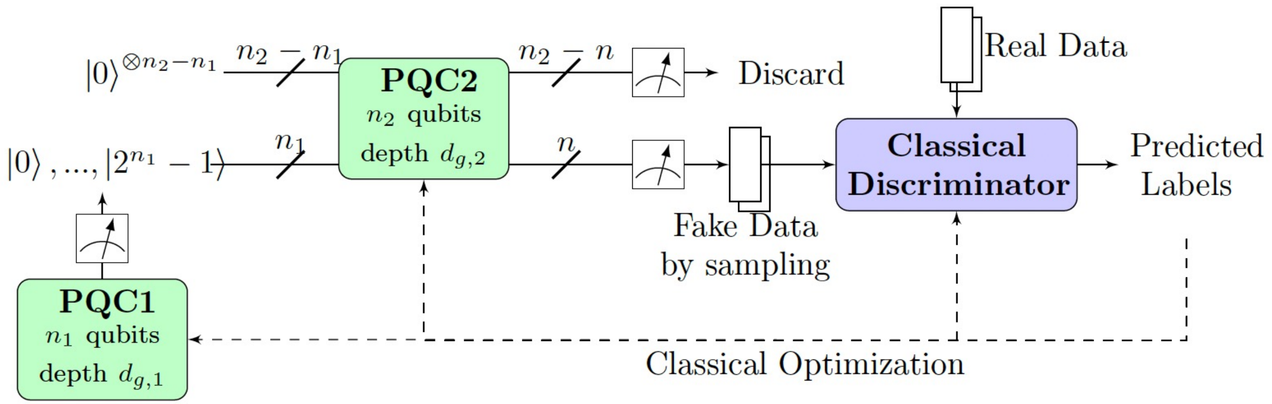
Simplify simulation problem

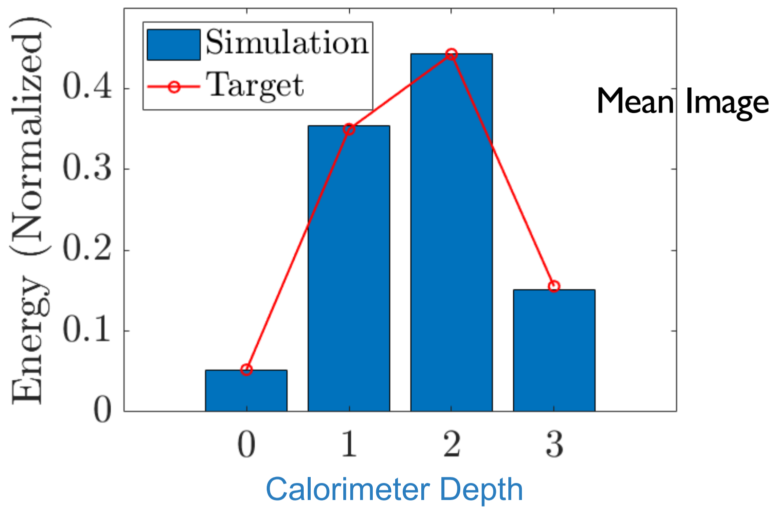
1D & 2D energy profiles from detector

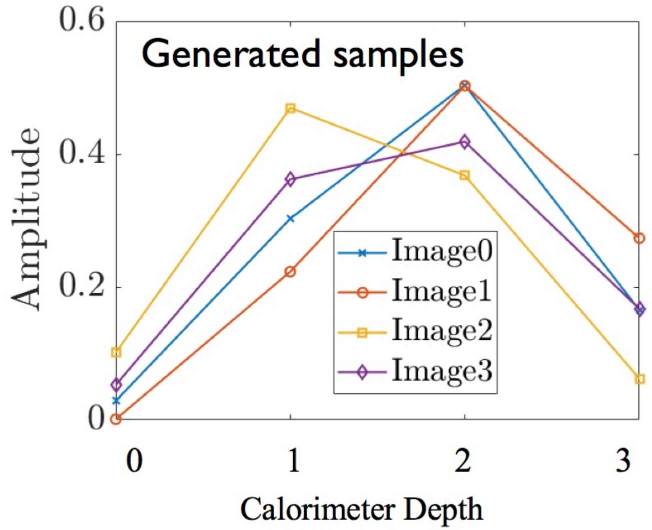
Two-steps quantum generator to sample images

PQC1 – Reproduce distribution over images

PQC2 – Reproduce amplitudes over pixels on one image







Benchmarks on hardware

- Train models using **noisy simulator** and test the inference of the model on the **superconducting** (IBMQ) and **trapped-ion** (IONQ) **quantum hardware**
  - For IBMQ machines, choose the qubits with the lowest CNOT gate error

Device	Readout error CX error	$D_{KL}/D_{KL,ind}$ $(\times 10^{-2})$
ibmq_jakarta	0.028 $1.367 \cdot 10^{-2}$	0.14 ± 0.14 6.49 ± 0.54
ibm_lagos	0.01 $5.582 \cdot 10^{-3}$	0.26 ± 0.11 6.92 ± 0.71
ibmq_casablanca	0.026 $4.58 \cdot 10^{-2}$	4.03 ± 1.08 6.58 ± 0.81
IONQ	NULL $1.59 \cdot 10^{-2}$	1.24 ± 0.74 10.1 ± 5.6

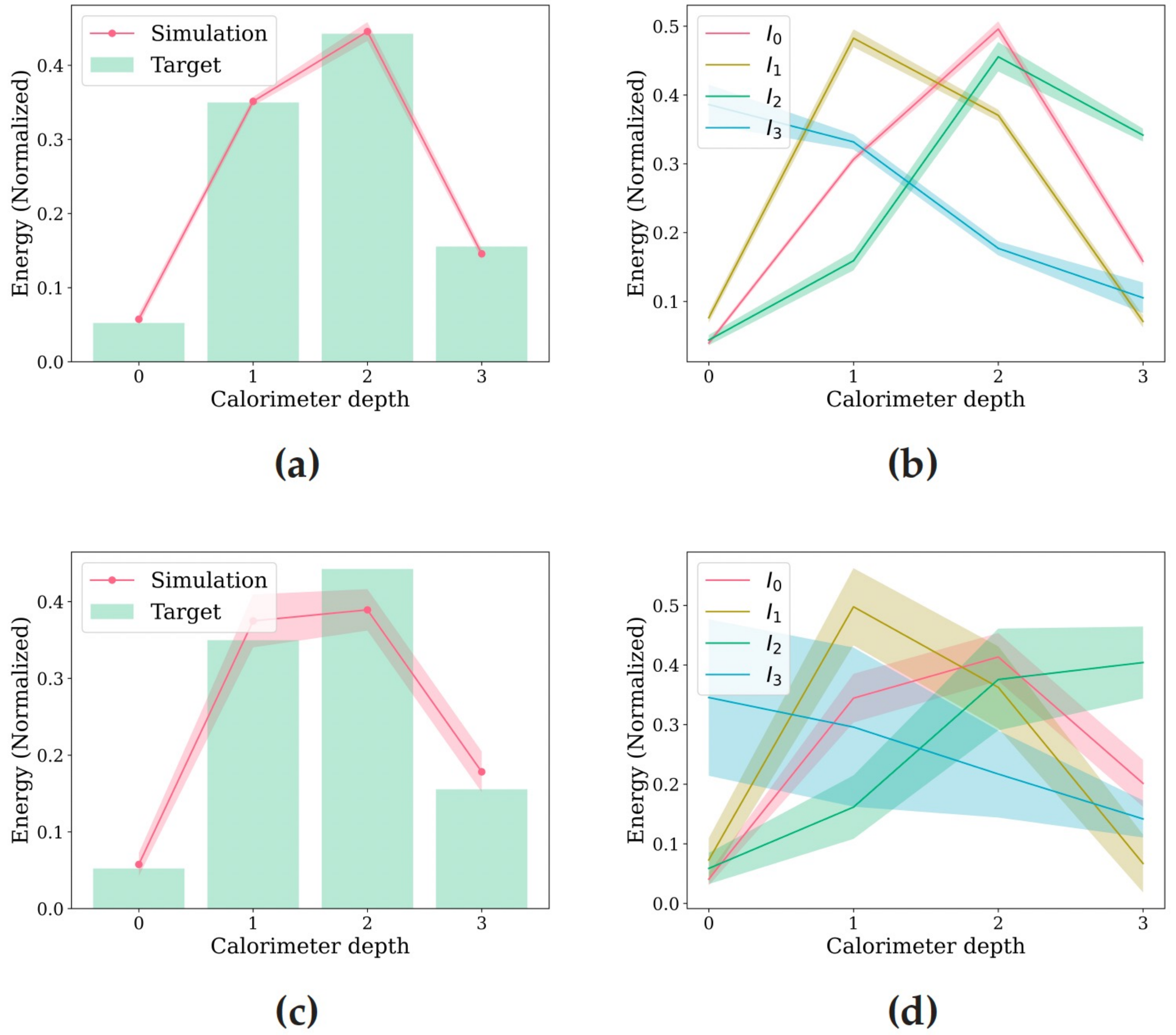


Figure 4: Mean (a,c) and individual images (b,d) obtained by inference test on ibmq_jakarta (a,b) and IONQ (c,d).

STUDY ON IMPACTS OF QUANTUM NOISES ON QGAN TRAINING

S.Y. CHANG[1,2], F. REHM[1,3], S. KÜHN[4], S. VALLECORSA[1], K. JANSEN[5], L. FUNCKE[6], T. HARTUNG[4,7], M. GROSSI[1], K. BORRAS[3,5], D. KRUECKER[5]
[1]CERN, Openlab, [2]EPFL, [3] RWTH Aachen University [4] The Cyprus Institute, [5] Deutsches Elektronen-Synchrotron DESY, [6]MIT, [7]University of Bath

INTRODUCTION

- **Artificial noises** are often injected in machine learning for a more robust, more stable and faster converging model.
- Current and near future quantum devices still have **considerable levels of noise**.
- Possibility to replace the artificial noise in classical ML with the intrinsic noise in quantum ML (QML).

OBJECTIVES

- Investigate the **impact of different errors** in the training of quantum Generative Adversarial Networks (qGAN) [1] for a simplified High-Energy Physics (HEP) use case.
- Provide a broad exploratory study to unfold the hidden impact of noise in QML.

ACAT2021 (arxiv:2203.01007)
Collaboration with DESY, RWTH AACHEN UNIVERSITY
(see K. Borras' talk on wednesday)

getting state $|k\rangle$ = normalized energy at pixel k.

- Input dataset = scalars following the real energy distribution

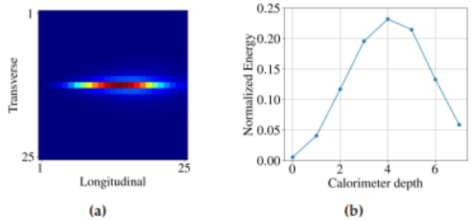


Figure 2: (a) Original calorimeter output generated by *Geant4*. (b) Reduced energy distribution used for our qGAN training.

REFERENCES

[1] Christa Zoufal, Aurélien Lucchi, and Stefan Woerner. Quantum generative adversarial networks for learning and loading random distributions. *npj Quantum Information*, 5(1):103, Nov 2019.

QUANTUM GAN

- **Hybrid model** with a n-qubit quantum generator and a classical discriminator [1]

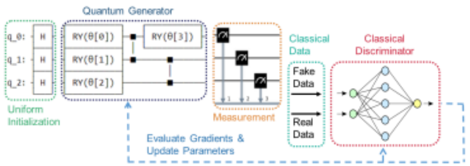


Figure 3: Schematic Diagram of qGAN.

- Relative entropy (or *Kullback-Leibler (KL) divergence*) $D_{KL}(p\|q) = \sum_j p(j) \log \frac{p(j)}{q(j)}$ as accuracy metrics.

ERPARAMETER SCAN

perform a scan on different **subsets of hyperpa-eters**: decay rate γ, generator lr_g, and discrimi-r learning rate lr_d.

the qGAN training using a noise model **with lout error** in form of bit flips occurring indepen-tly for each qubit with a flip probability p.

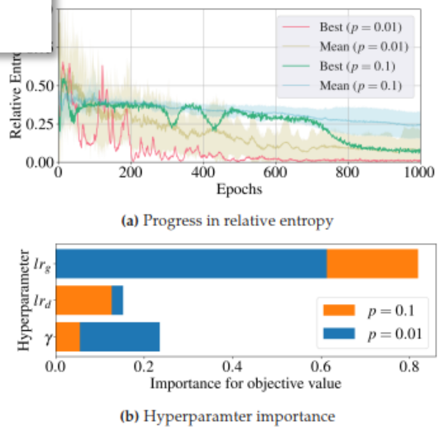


Figure 5: Results of the scan on different hyperparameters for the readout error $p = 0.01$ and 0.1

- Higher relative entropy for higher noise level, even with the optimal hyperparameters.
- Impact of generator learning rate becomes higher as the flip probability increases.

INSTABILITY OF QGAN TRAINING

- Repeat the qGAN training with the *qiskit* noise model with readout error only using the same hyperparameters and **investigate its statistical error**.

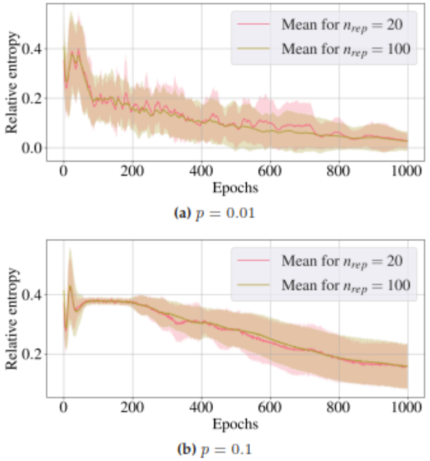


Figure 4: Progress in relative entropy averaged over n_{rep} = 20 and 100 runs for $p = 0.01$ and 0.1.

Flip probability p	$n_{rep} = 20$	$n_{rep} = 100$
0.01	0.026 ± 0.028	0.028 ± 0.040
0.05	0.029 ± 0.022	0.027 ± 0.020
0.1	0.153 ± 0.097	0.159 ± 0.077

Table 1: Relative entropy at the end of the training

- The model is stable on the "ensemble" of simulations, but unstable for the individual runs.
→ Fixed standard deviation despite increase in the number of simulations.

DISCUSSION

- The **instability of the qGAN model** cannot be resolved even with large number of simulations.
→ Further study going on to find the origin of the instability.
- Small levels of quantum noise help to improve the performance of the model, while error mitigation is required for large noise.
- Effect of error mitigation in the full noise model and the real quantum hardware needs to be further studied.

ERROR MITIGATION

- We compare the training results with and without **error mitigation method** implemented by *qiskit*.

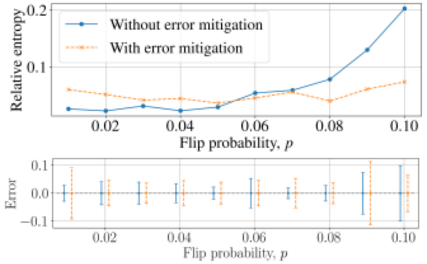


Figure 6: Mean (above) and standard deviation (below) of the final relative entropy, averaged over 20 simulations, with and without error mitigation w.r.t. the readout error.

- Low readout error ($p < 0.06$) helps the qGAN training, while error mitigation plays an important role for high readout error.
- Large standard deviation in the relative entropy which cannot be overcome with error mitigation.

INCLUDING CNOT ERROR

- We run the training with a custom noise model consisting of 2.5% readout noise per qubit and 1.5% two qubit gate level noise (called CNOT error).
- We found new optimized hyperparameters to reduce the number of epochs to only 300 while reaching a good accuracy.

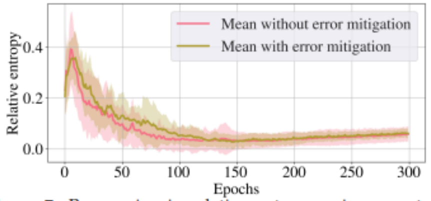


Figure 7: Progression in relative entropy using a custom noise model with and without error mitigation.

- For the chosen noise levels one cannot see any improvement when including error mitigation.

ONGOING RESEARCH

- Train the qGAN on real quantum hardware.
- Apply other error mitigation methods and compare the resulting outcomes.

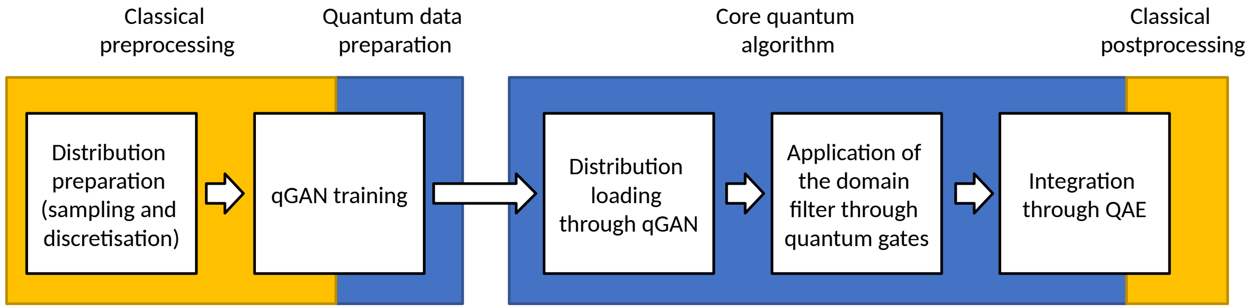
qGAN as a data loader

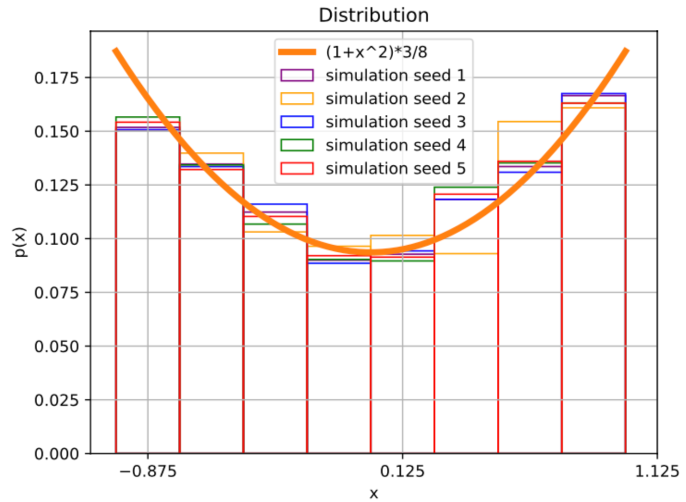
Use **Quantum Amplitude Estimation** to accelerate **Monte Carlo Integration**

Data encoding into quantum states affects the quality of the integration

Test different approaches including **QGAN**

M. Grossi, arxiv:2201.01547





Loading of $1 + x^2$ distribution:

- 10k events
- 3 qubits
- best entanglement is the circular

FR-PHENO-2022-01

arXiv:2201.01547v1 [hep-ph] 5 Jan 2022

Quantum integration of elementary particle processes

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Abstract

We apply quantum integration to elementary particle-physics processes. In particular, we look at scattering processes such as $e^+e^- \to q\bar{q}$ and $e^+e^- \to q\bar{q}'W$. The corresponding probability distributions can be first appropriately loaded on a quantum computer using either quantum Generative Adversarial Networks or an exact method. The distributions are then integrated using the method of Quantum Amplitude Estimation which shows a quadratic speed-up with respect to classical techniques. In simulations of noiseless quantum computers, we obtain per-cent accurate results for one- and two-dimensional integration with up to six qubits. This work paves the way towards taking advantage of quantum algorithms for the integration of high-energy processes.

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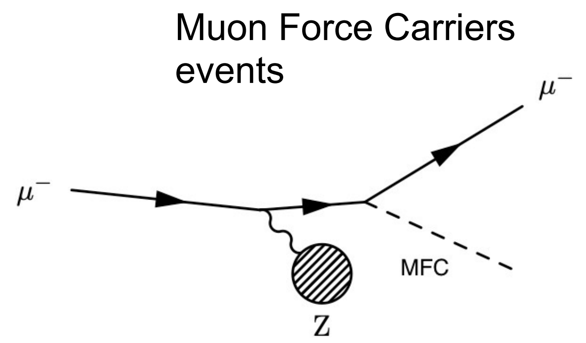
A purely quantum model

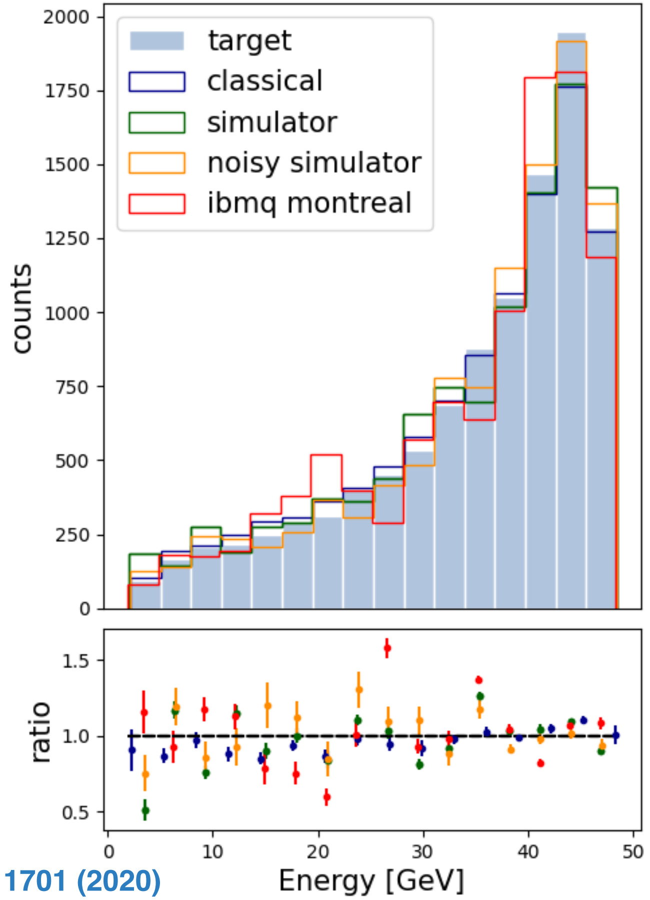
Quntum Circuit Born Machine



- Sample from a variational wavefunction $|\psi(\theta)\rangle$ with probability given by the **Born rule**: $p_\theta(x) = |\langle x|\psi(\theta)\rangle|^2$
- Only able to generate **discrete** PDFs (continuous in the limit #qubits $\to \infty$)
- **Typically trained** using **Maximum Mean Discrepancy**:

MMD(P,Q) = $\mathbb{E}_{\substack{X\sim P \\ Y\sim P}}[K(X,Y)] + \mathbb{E}_{\substack{X\sim Q \\ Y\sim Q}}[K(X,Y)] - 2\mathbb{E}_{\substack{X\sim P \\ Y\sim Q}}[K(X,Y)]$

with K a gaussian kernel



Do not have classical equivalent!

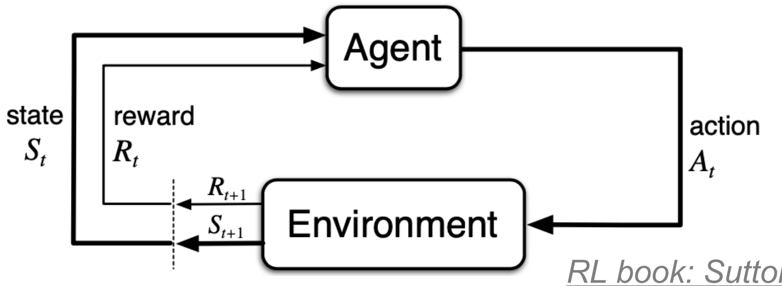
Galon, I, Kajamovitz, E et al. "Searching for muonic forces with the ATLAS detector". In: Phys. Rev. D 101, 011701 (2020)

M. Shenk, V. Kain
BQiT 2021
2021 CERN openlab Tech Workshop

Quantum Reinforcement Learning

Return is estimated by **value function *Q(s, a)***

- **Use greedy policy** *(maximize Q(s,a))*
- **Q-learning** – learn Q(s, a) using **function approximator**
  - **DQN: Deep Q-learning** *(feed-forward neural network)*
  - **QBM-RL** *(Quantum Boltzmann Machine)*

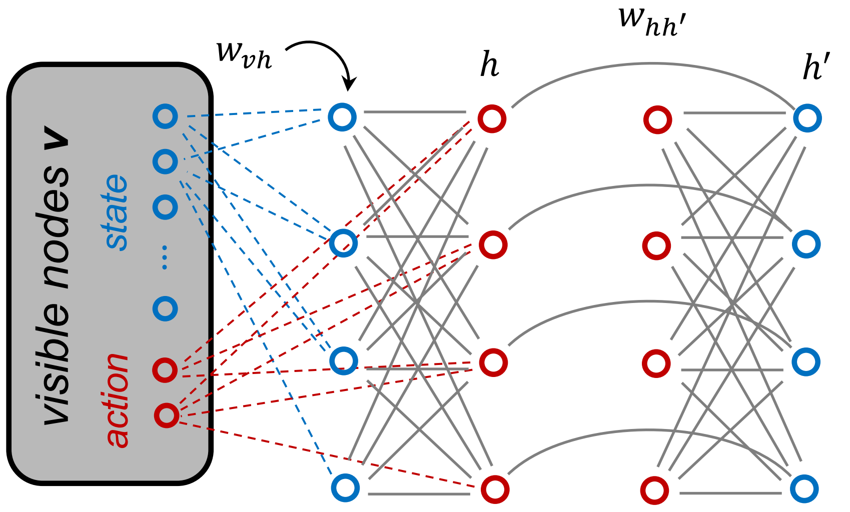


RL book: Sutton & Barto

Free Energy RL: clamped QBM

- **Network of coupled, stochastic, binary units** (spin up / down)
- $\hat{Q}(s, a) \approx$ **negative free energy** of classical spin configurations c
- **Sampling** c using **(simulated) quantum annealing**
- **Clamped:** visible nodes not part of QBM; accounted for as biases
- **Using 16 qubits of D-Wave Chimera graph**
- **Discrete, binary-encoded** state and action spaces

Clamped QBM

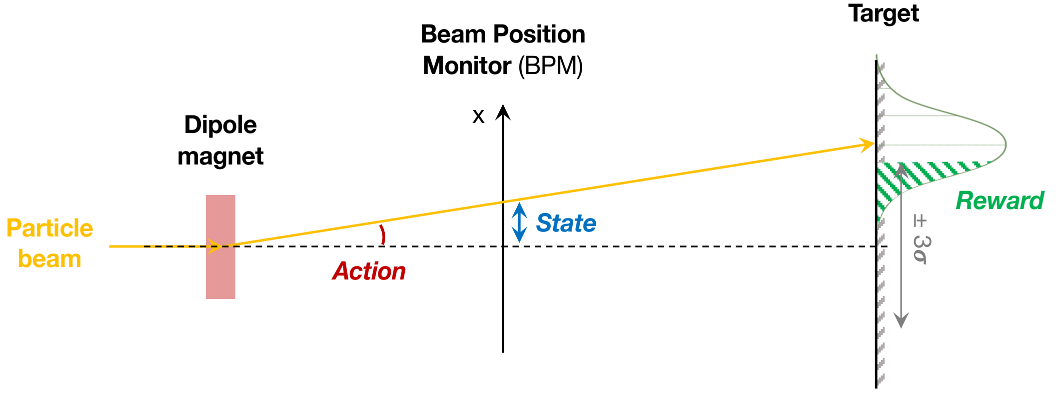


$$\hat{Q}(s, a) \approx -F(\boldsymbol{v}) = -\langle H_{\boldsymbol{v}}^{\mathrm{eff}} \rangle - \frac{1}{\beta} \sum_{c} \mathbb{P}(c|\boldsymbol{v}) \log \mathbb{P}(c|\boldsymbol{v})$$

CERN openlab

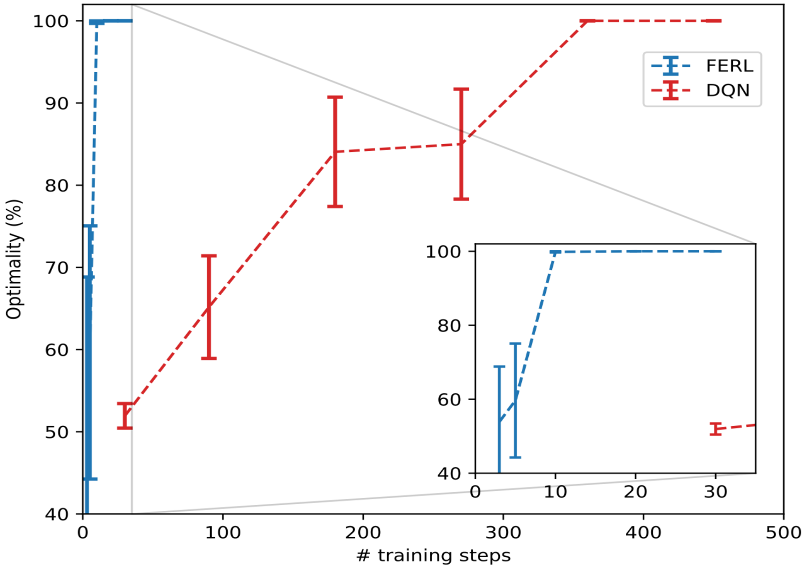
Beam optimisation in linear accelerator

- **Action: deflection** angle
- **State: BPM** position
- **Reward: integrated beam intensity on target**
- **Optimality**: what fraction of possible states does agent take the right decision

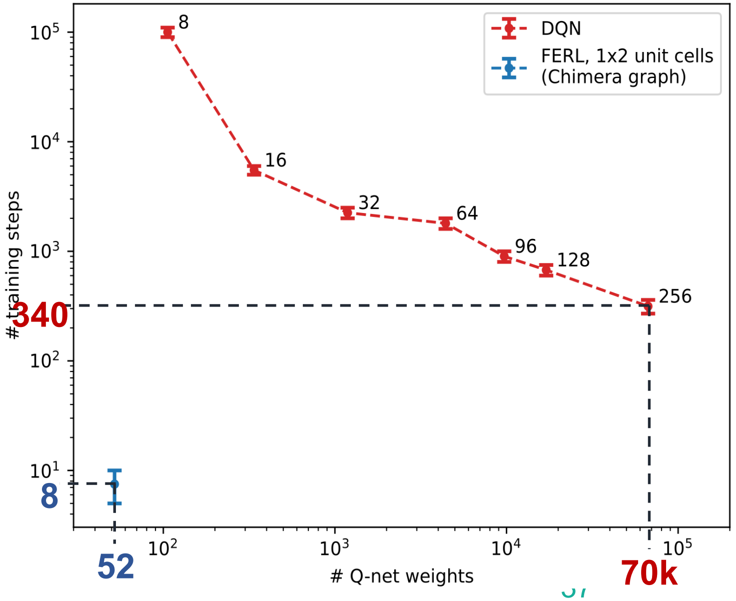


- **Training efficiency:** FERL **massively** outperforms classical Q-learning *(8±2 vs. 320±40 steps)*
- **Descriptive power:** QBM can reach high performance with **much fewer weights** than DQN *(52 vs. ~70k)*

Training efficiency



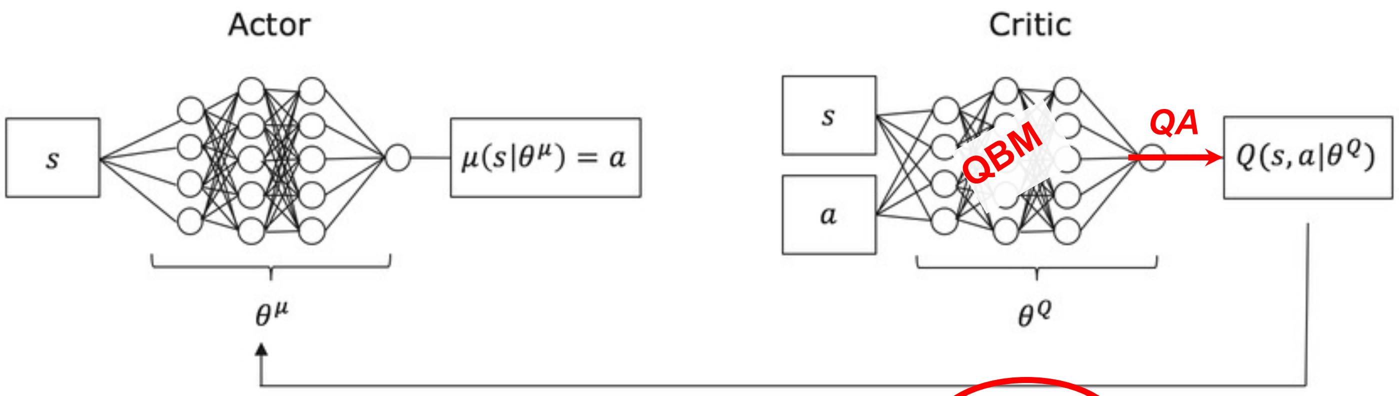
Training efficiency vs. # Q-net / QBM weights



Hybrid actor-critic

- **FERL for continous state-action spaces to tackle real-world problems:** inspired by classical actor-critic methods

- **Why use FERL in combination with classical policy network?**
  - **QBM has ideal structure** to replace classical critic
  - Can we benefit from **high training efficiency of QBM** (?!)
    Intuitively: if critic learns faster, should be beneficial for actor training



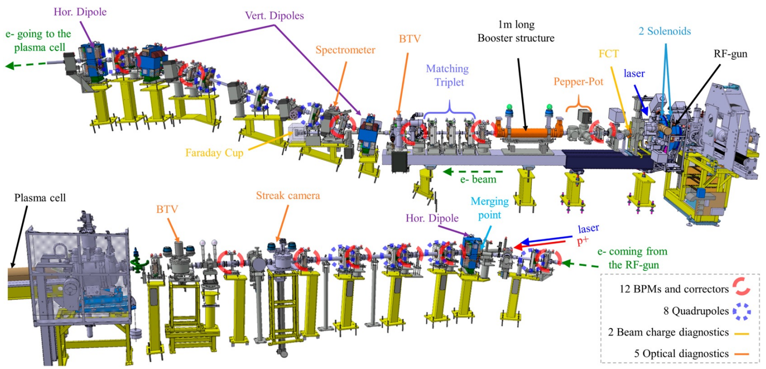
Policy Gradient: $\nabla_{\theta^\mu}\mu = \mathbb{E}_\mu[\nabla_{\theta^\mu} Q(s,\mu(s|\theta^\mu)|\theta^Q)] = \mathbb{E}_\mu[\nabla_a Q(s,a|\theta^Q) \cdot \nabla_{\theta^\mu}\mu(s|\theta^\mu)]$

Main challenge

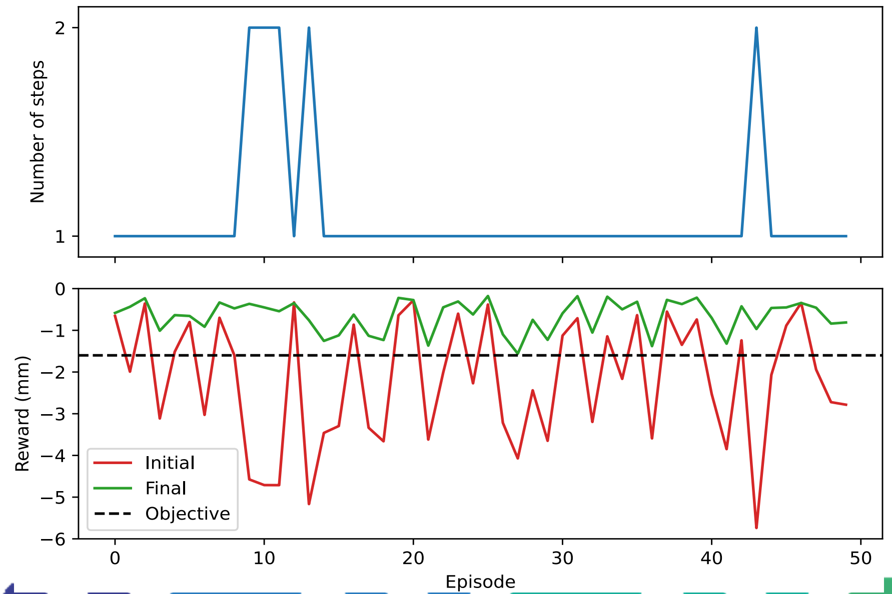
- Calculating derivative of critic wrt. action $\nabla_a Q(s,a|\theta^Q)$
- Numerical (finite difference) or semi-analytical derivative options

Q-learning on 10D AWAKE beam line

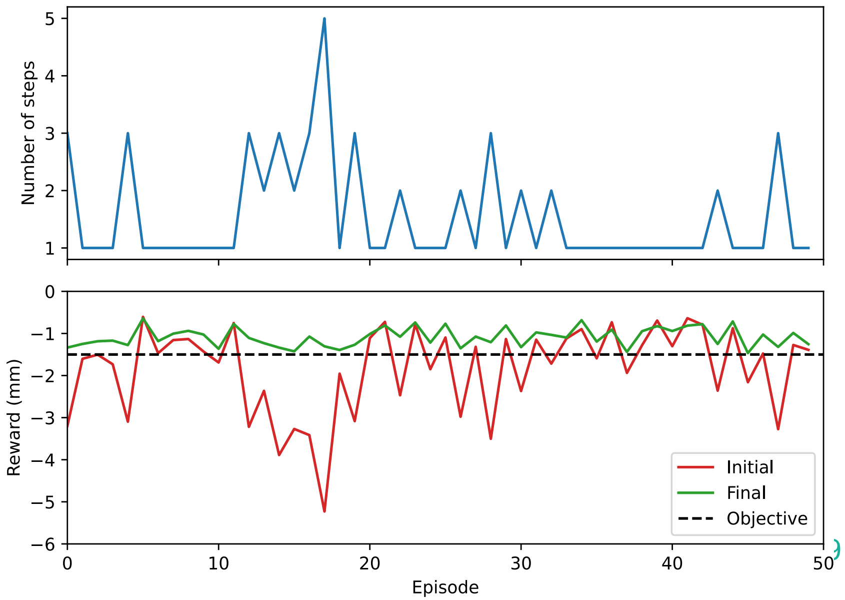
- **Trained and tested quantum actor-critic agent** on *simulated* 10D AWAKE beam line
- **Deployment on *real* beam line => agent works successfully ☺ !**
  Even with 1 broken beam position monitor (BPM) …
- **Will redo with optimized agent and fixed BPM**



Evaluation on simulated beam line



Evaluation on real beam line



Thanks!

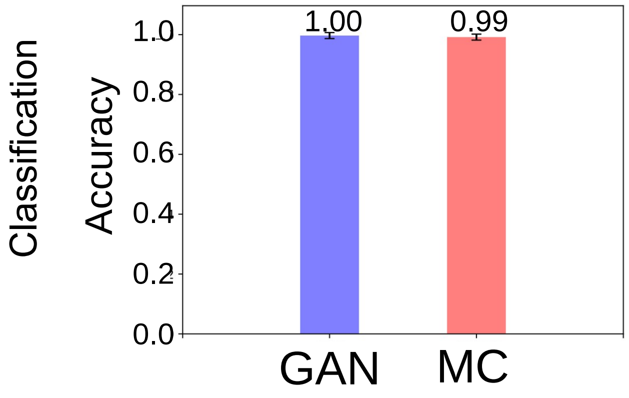
Sofia.Vallecorsa@cern.ch

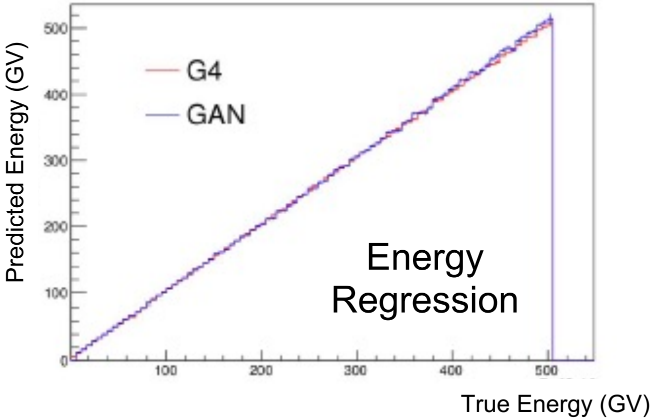
https://openlab.cern/
https://home.cern/

Physics validation

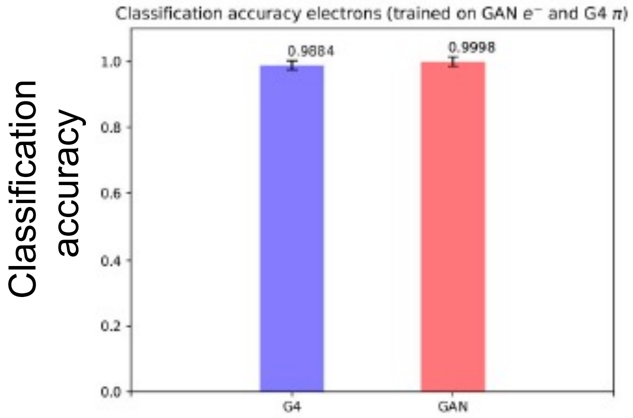
Triforce* DNN has been developed to distinguish different kind of particles and measure their energy

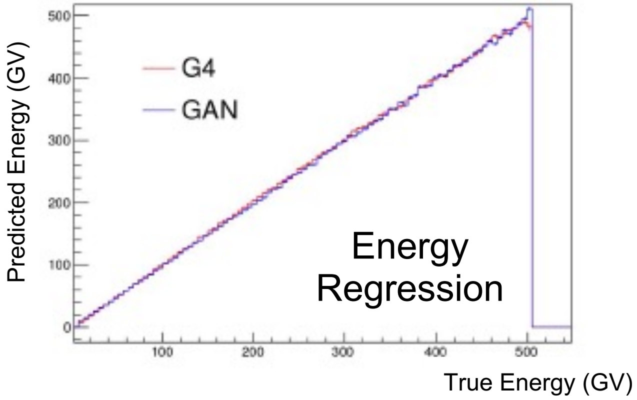
Trained on G4





Trained on GAN



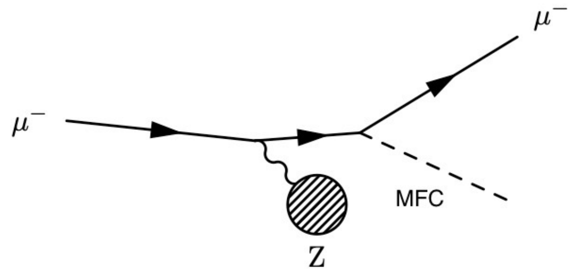


*D. Belayneh et al.,"Calorimetry with deep learning: Particle simulation and reconstruction for collider physics," 2019, https://inspirehep.net/literature/1770936

Quantum Circuit Born Machine for event generation

Muon Force Carriers predicted by several theoretical models:

- Could be detected by muon fixed-target experiments (FASER) or muon interactions in calorimeters (ATLAS).

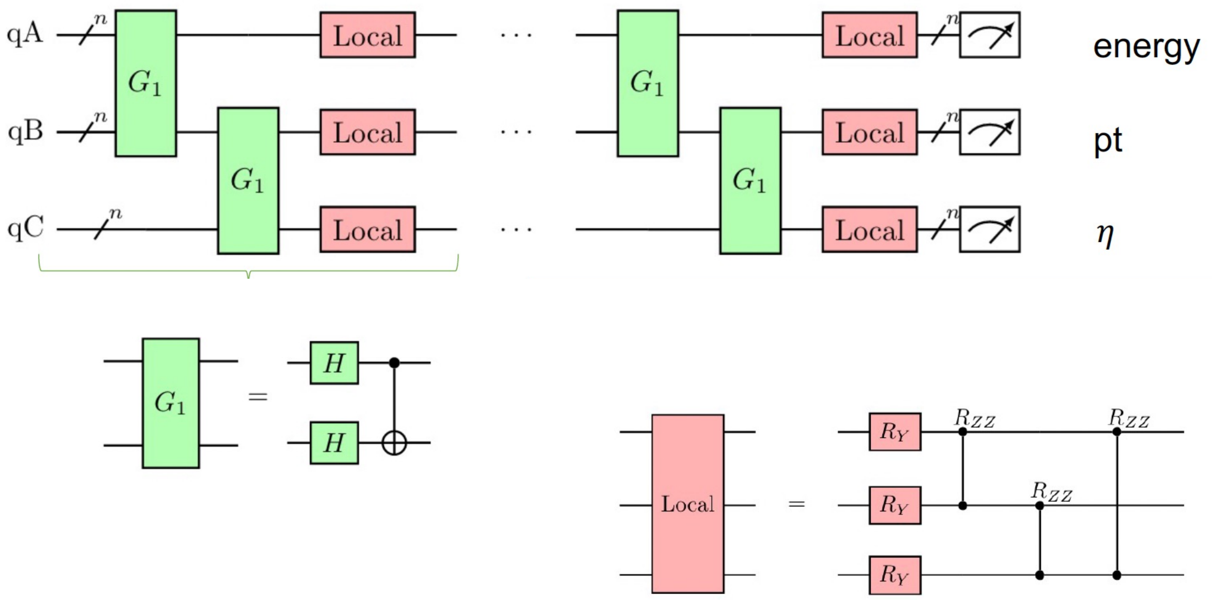


Generate **E, $\mathbf{p_t}$, η** of outgoing muon and MFC

Sample from variational wavefunction $|\psi(\theta)\rangle$ with $p_\theta(x)$ =$|\langle x|\psi(\theta)\rangle|$” given by the Born rule

Generate **discrete PDFs** (continuous in the limit #qubits $\rightarrow\infty$)

Maximum Mean Discrepancy loss function and gaussian kernel with $\sigma\in[0.1,1,10,100]$



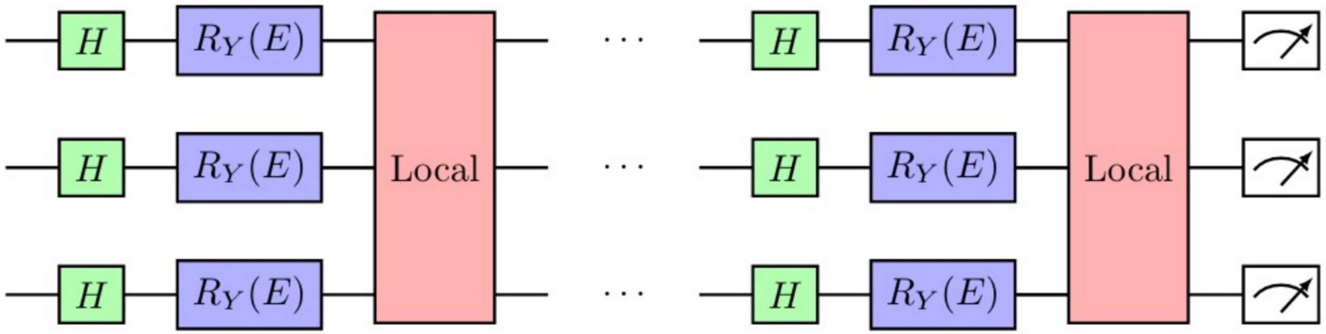
$$MMD(P,Q) = \mathbb{E}_{\substack{X\sim P\\ Y\sim P}}[K(X,Y)] + \mathbb{E}_{\substack{X\sim Q\\ Y\sim Q}}[K(X,Y)] - 2\mathbb{E}_{\substack{X\sim P\\ Y\sim Q}}[K(X,Y)]$$

Galon, I, Kajamovitz, E et al. "Searching for muonic forces with the ATLAS detector". In: Phys. Rev. D 101, 011701 (2020)

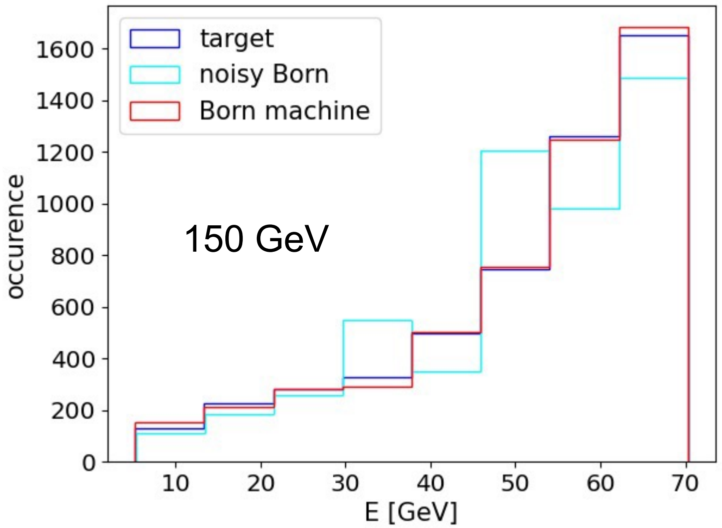
Conditional Born Machine

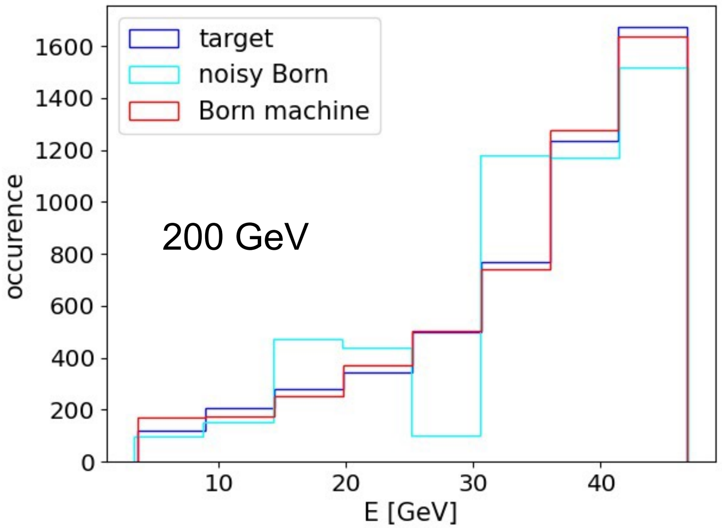
Encode $E_{\mu,i}$ condition using parametrized rotations

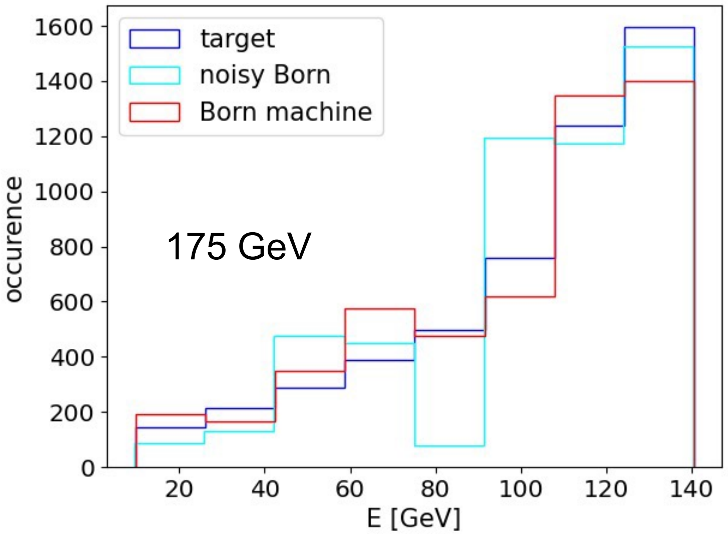
Interpolation: train on 150 and 200 GeV muons and predict 175 GeV signal



Data re-uploading makes the quantum circuit more expressive as function of the data
Noise model according to IBM Q Casablanca

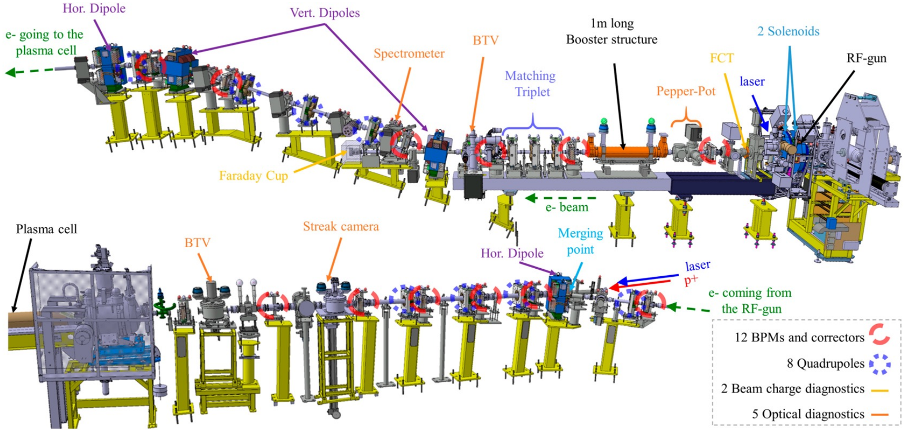




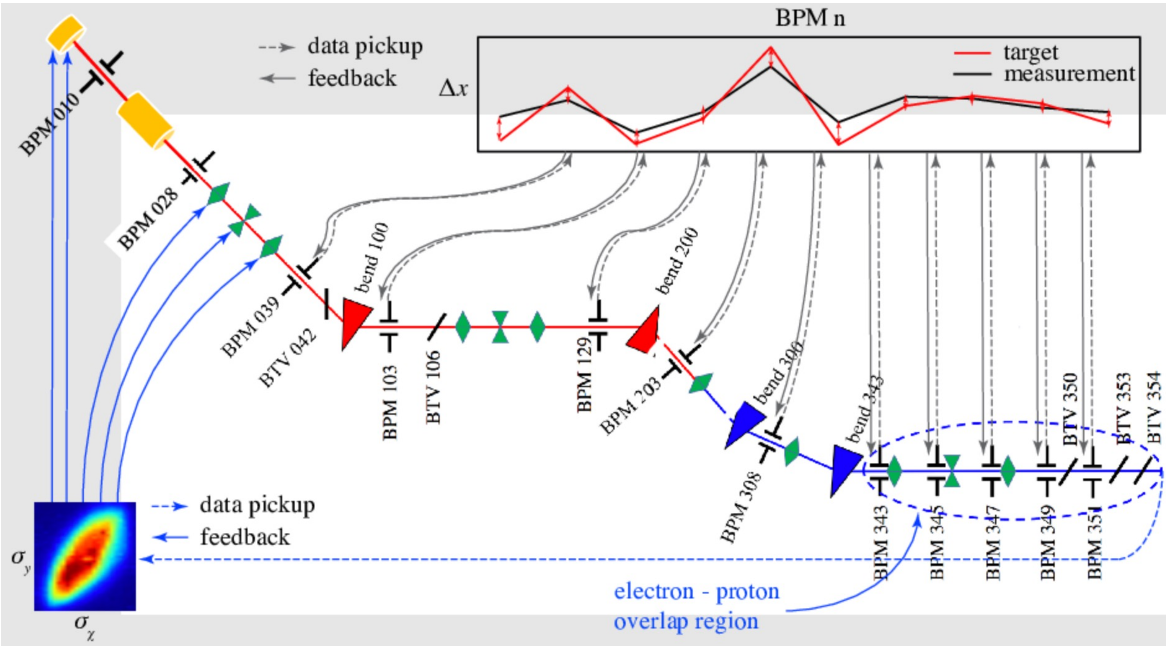


Use case II: Q-learning on 10D AWAKE beam line

Environment



- **AWAKE electron beam line** https://gitlab.cern.ch/be-op-ml-optimization/envs/awake
- **OpenAI gym template**
- **Action:** deflection angles at 10 correctors *(continous)*
- **State:** beam positions at 10 BPMs *(continuous)*
- **Reward:** negative rms from 10 BPMs



Credits: A. Scheinker

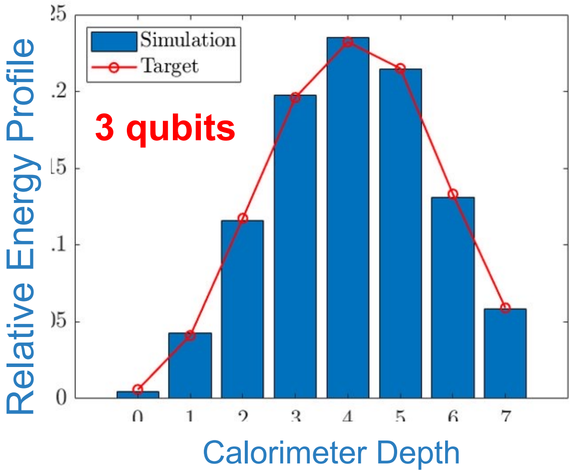
Quantum generation of energy profiles

IBM qGAN can load probability distributions in quantum states

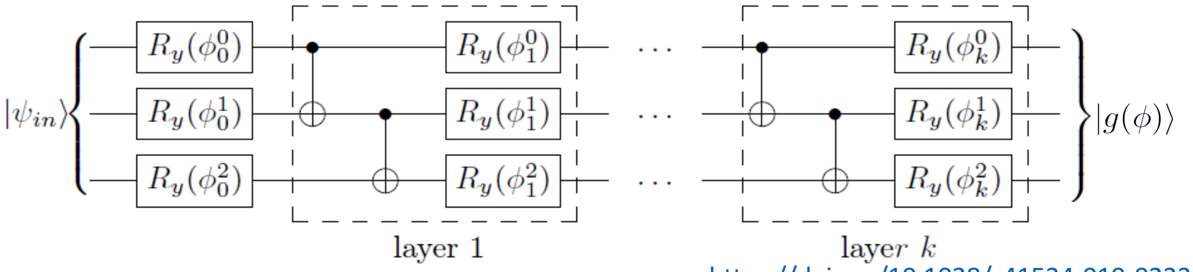
Simplify simulation problem

1D & 2D energy profiles from detector

Train a **hybrid classical-quantum** GAN to generate **average image**

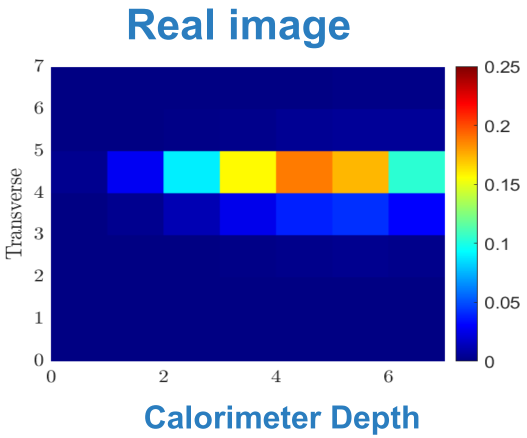


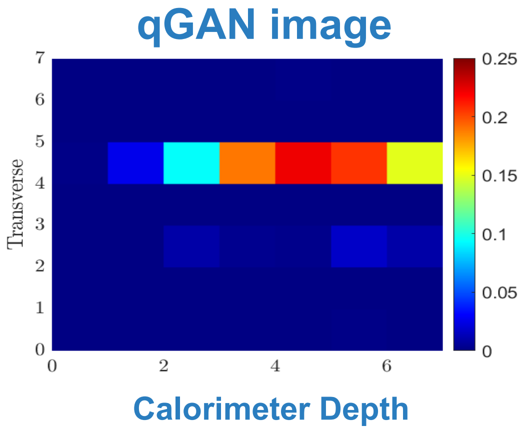
Quantum Generator: 3 R_y layers



https://doi.org/10.1038/s41534-019-0223-2

6 qubits





Need a way to **sample single images**