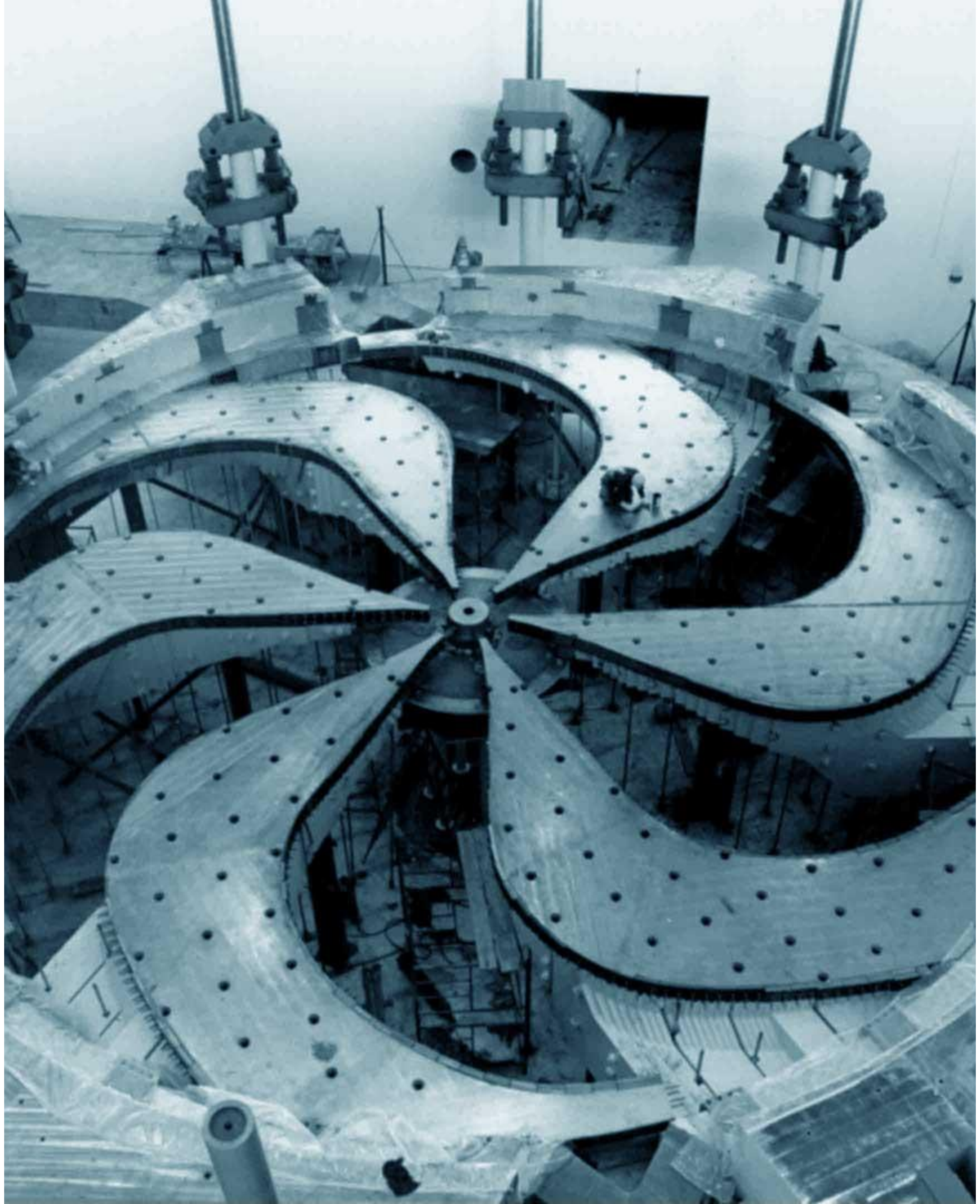
TRIUMF

Results in Scientific Computing

Lightning talks



Discovery, accelerated

B. Velghe, D. Bryman, W. Fedorko, M. Yu

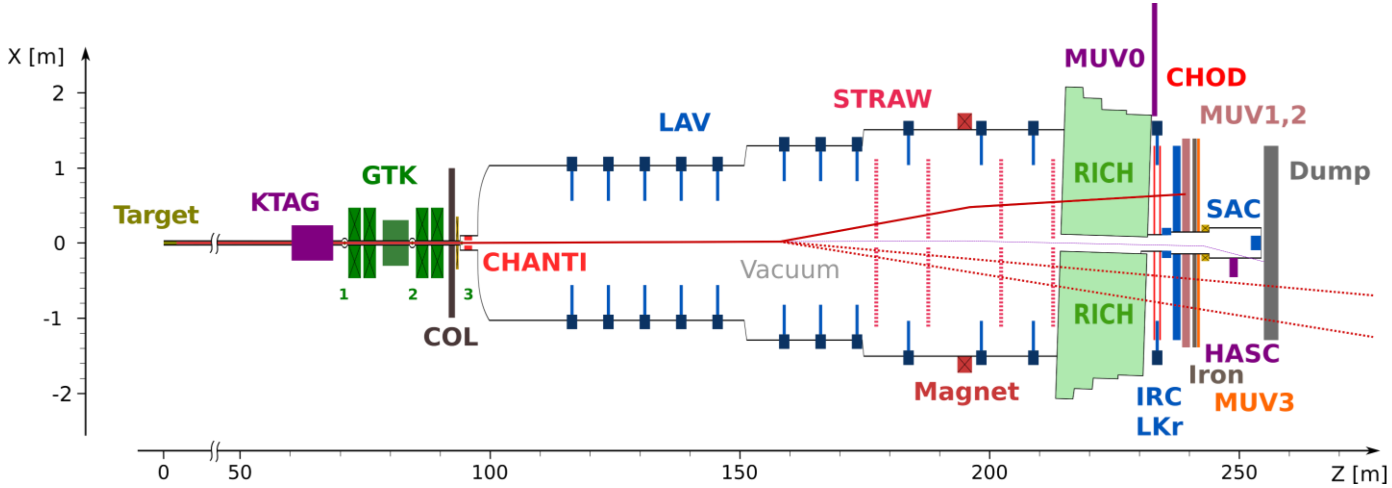
Calorimetric Particle Identification at NA62

Main goal: Study the rare **K →πνν** decay
Probe for new physics

$$\mathcal{B}_{\mathrm{exp.}} = \left(10.6^{+4.0}_{-3.4}\Big|_{\mathrm{stat.}} \pm 0.9_{\mathrm{syst.}}\right) \times 10^{-11}$$

[NA62 Collaboration, 21']

Kaon decay-in-flight: Main backgrounds are the common kaon decay modes (K →μν, K →ππ, etc.)



Multiple handles:

- Event kinematics,
- K/π timing O(100 ps),
- Track multiplicity,
- μ/ɣ vetos,
- **Particle identification**.

$$K^+ \to \mu^+\nu_\mu \ (\mathcal{B} \approx 0.64)$$
$$\downarrow \ \mathrm{mis-id}$$
$$K^+ \to \pi^+\nu\bar{\nu} \ (\mathcal{B} \approx 10^{-10})$$

Particle identification systems:

RICH, MUV3, and calorimeters (LKr, MUV1 and MUV2)
Overall Muon rejection > **10^7**

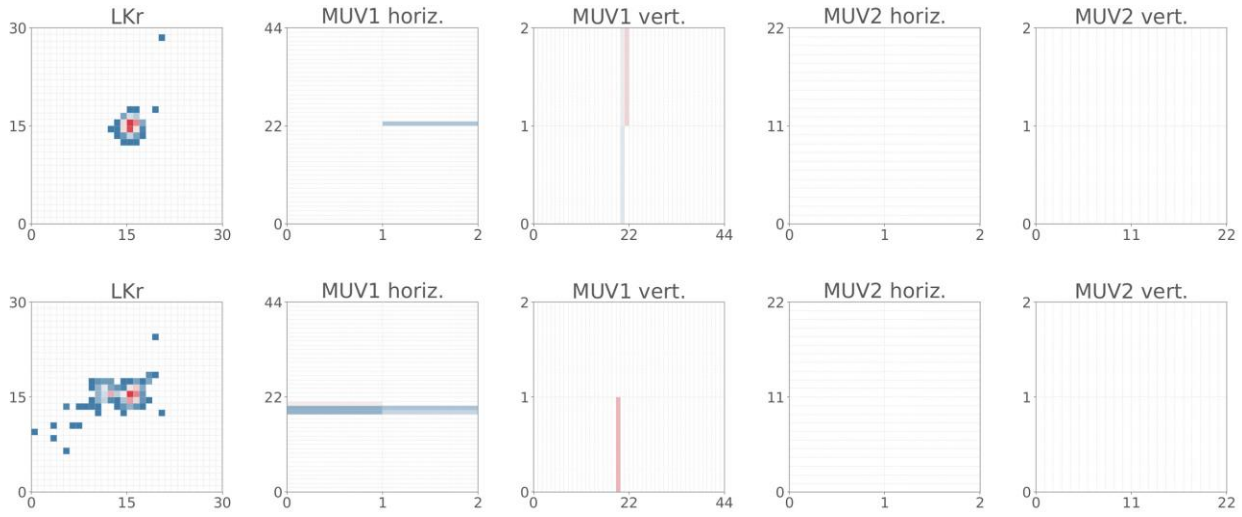
CNN-Based Approach for "CaloPID"

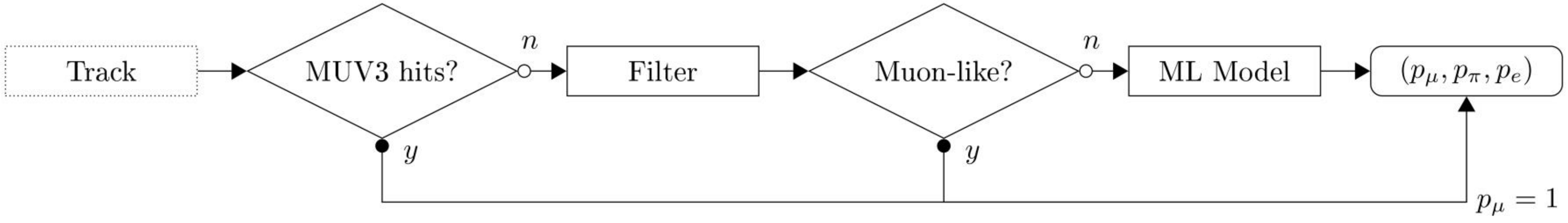
Focus on three calorimeters:

- LKr: Electromagnetic calo.
- MUV1 & MUV2: Hardronic calo

No depth information, the 3D shower is projected on a 2D plane by the readout.

Direct correspondence with a 5-channel image

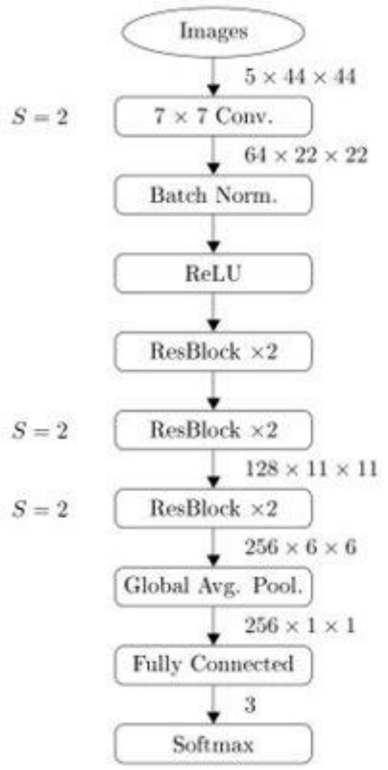


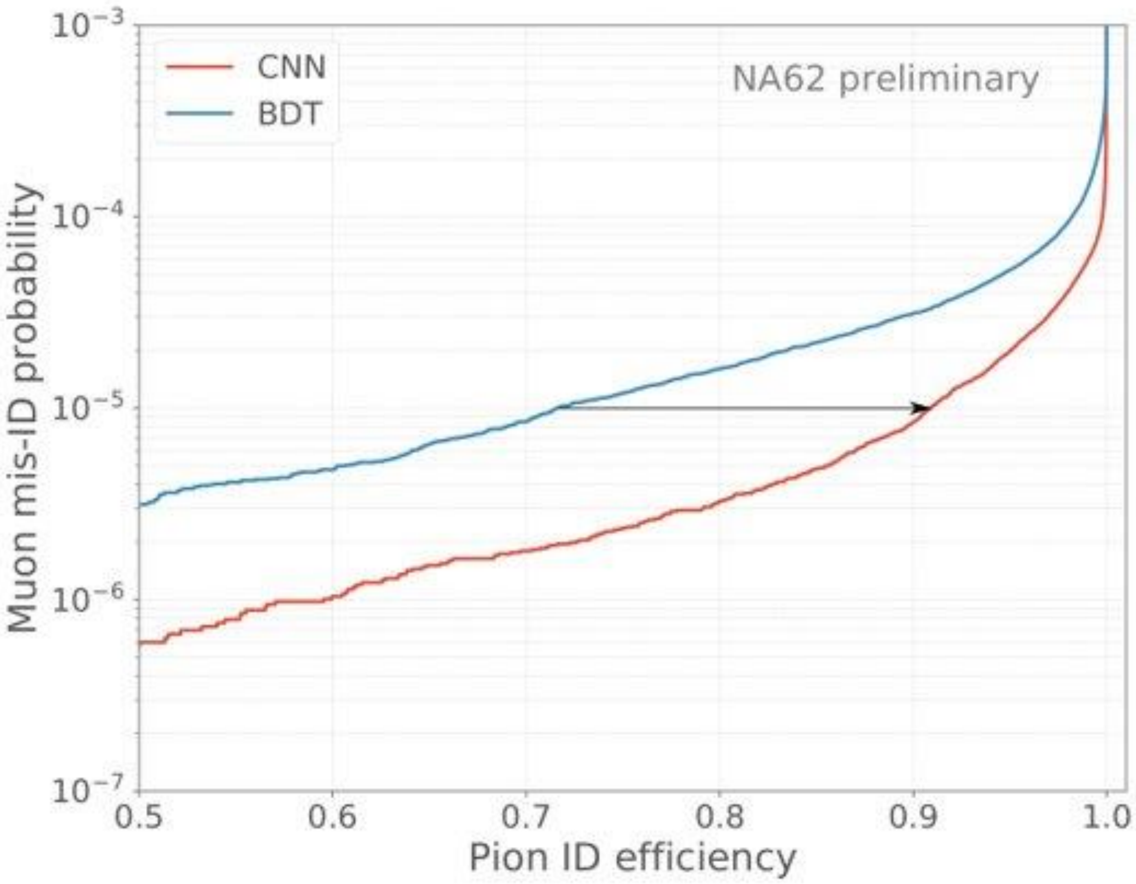


Data driven approach, training, validation and testing samples selected directly from the data. Independent test sample (*minimum bias*) used for the final evaluation.

Significant Improvement of the μ/π ID

Architecture derived from ResNet





Pion acceptance can be increased from **72 % to 92 %** over the 15 to 50 GeV/*c* (muon mis-id 10^{-5})

MACHINE LEARNING FOR PION IDENTIFICATION AND ENERGY CALIBRATION WITH ATLAS DETECTOR

ATL-PHYS-PUB-2020-018

DILIA MARÍA PORTILLO,
ALISON LISTER,MAX SWIATLOWSKI, WOJTEK FEDORKO, RUSSELL BATE

17-08-2021

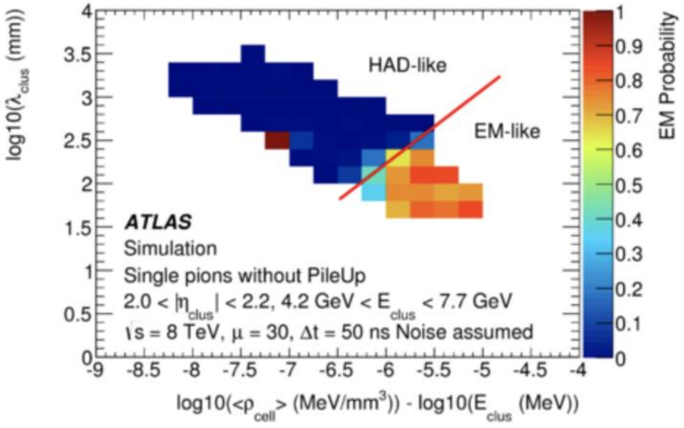
TRIUMF SCIENCE WEEK 2021

Overview

Hadronic Calibration in ATLAS

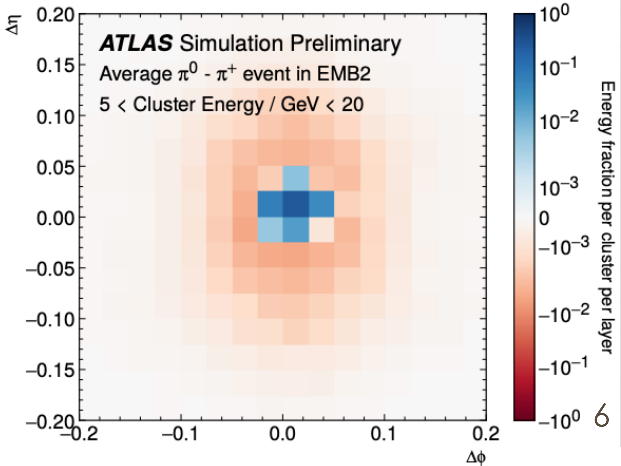
- **Hadronic showers are mostly composed of pions**
  - π^0: Captured by the **electromagnetic** calorimeter
  - $\pi^{\pm}$: Require the dense material in the **hadronic** calorimeter to be stopped

- Baseline hadronic reconstruction in ATLAS uses clusters of calorimeter cells



- Currently, clusters are calibrated in two steps:
  1. **Classified** as **electromagnetic** or **hadronic** calculating the EM probability $\mathscr{P}^{\text{EM}}_{\text{clus}}$;
  2. **Calibration** of its energy

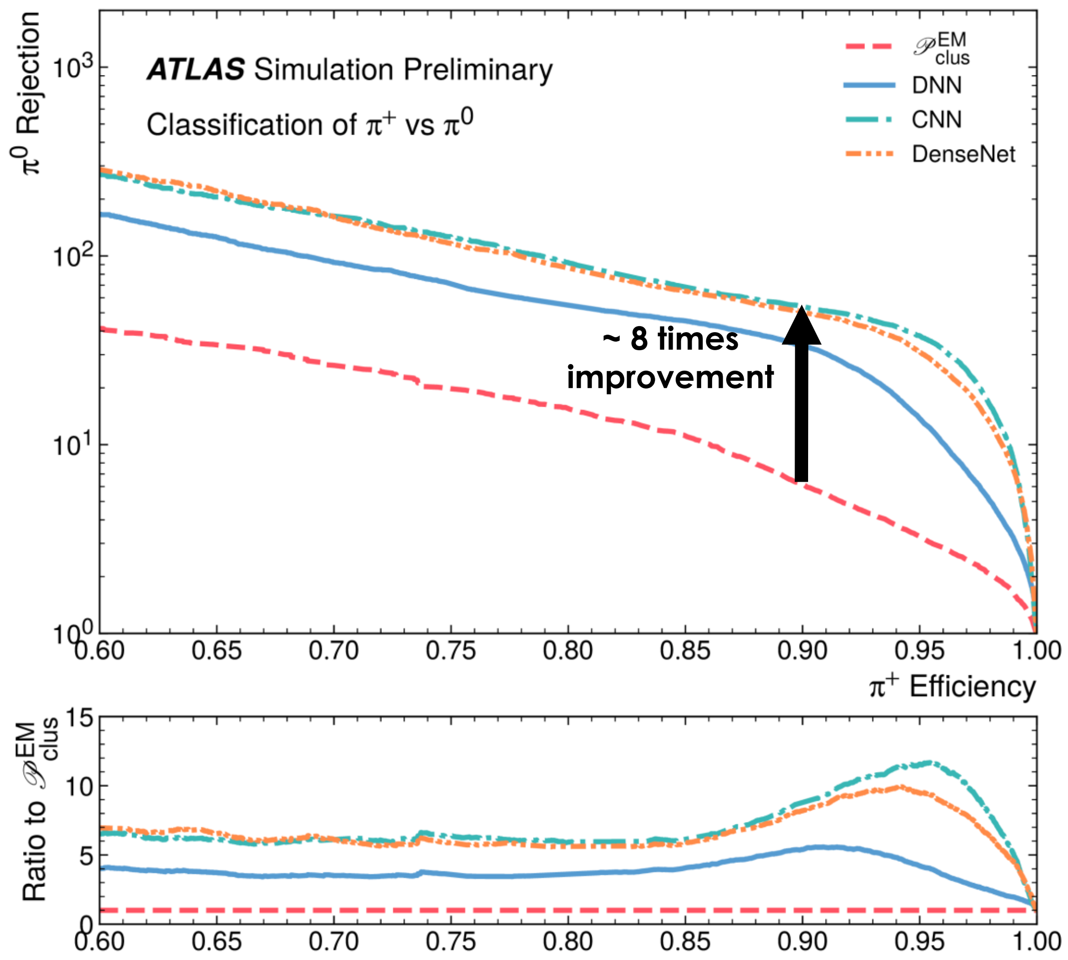
Can we use deep learning to improve these techniques?



- **Neural Networks** trained on calorimeter images can classify clusters and predict their energies
  - Studied DNNs, CNNs, and DenseNet

Cluster identification performance

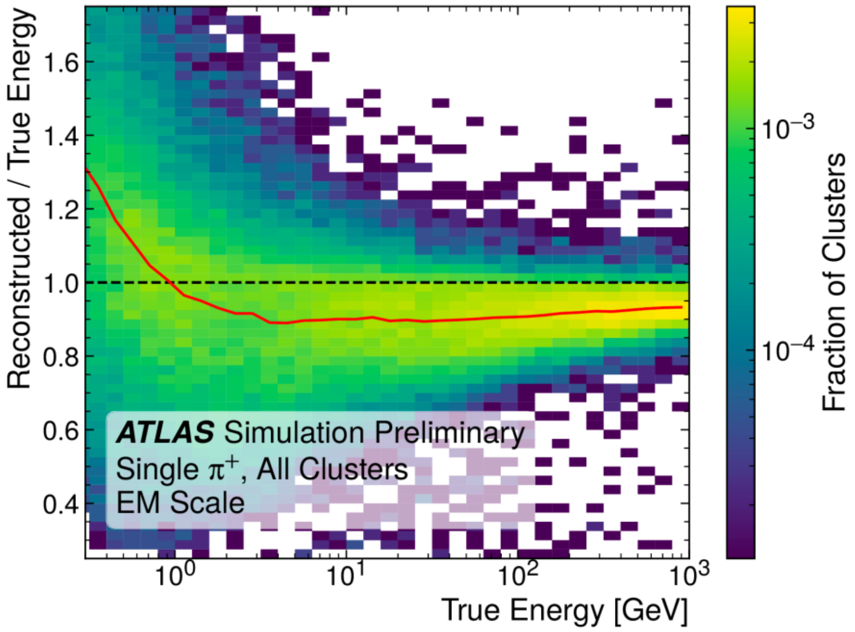
- The ML techniques all do an excellent job of distinguishing π^0 from $\pi^\pm$ showers
  - Dramatic **improvements** compared to the current classification method using $\mathscr{P}^{EM}_{clus}$



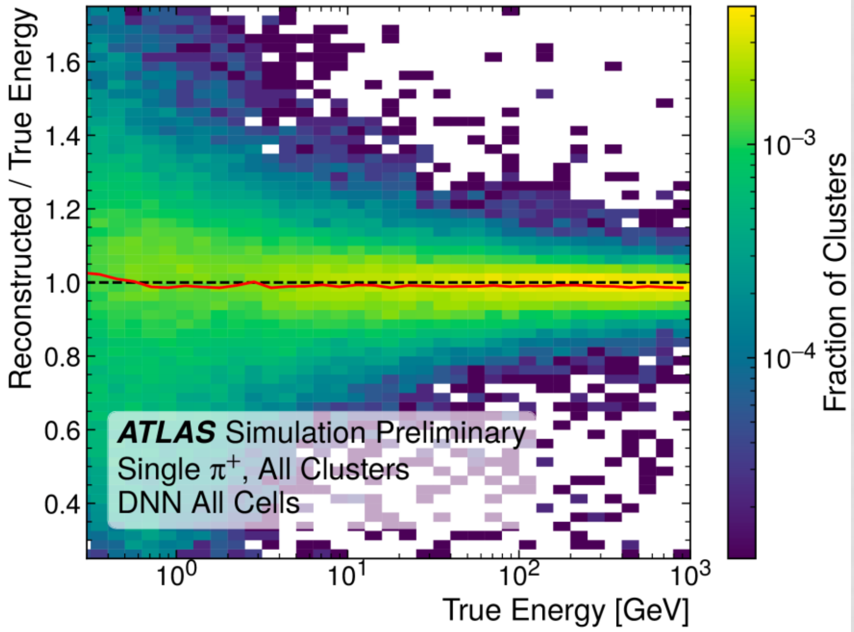
Pion Energy Calibration

- After classifying a cluster, need to calibrate its energy
- **Energy regression goal**: Correctly **predict the true energy** deposited in the cluster.
  - Quantified by measuring the cluster **energy response**: $R = \frac{E^{\text{reco}}}{E^{\text{truth}}}$ that should be ~ 1

Regression performance for charged pions



Before Calibration



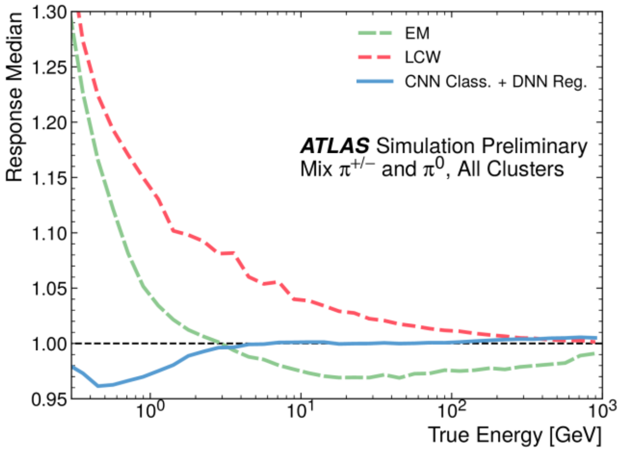
After calibration

Outlook

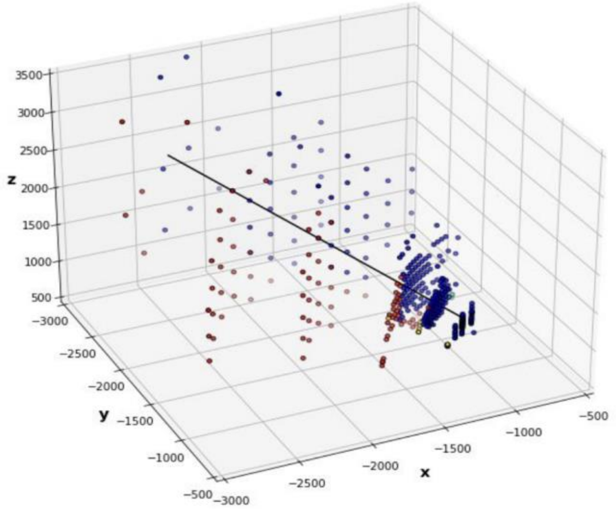
- Promising results for pion classification and energy calibration with deep-learning!

Looking forward studying more complex scenarios:

- First look at the **performance with jets**
  - π^+, π^- and π^0 mixed in a 1:1:1 ratio
  - Roughly correspond to the expected distribution in jets



- Another handy way to represent energy deposits is as a **point-cloud**
  - Points contains cell info & cluster-level info.
  - Allows for combining signals from the inner detector (tracks) and from calorimeter (clusters)



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Beamline Tuning with Reinforcement Learning

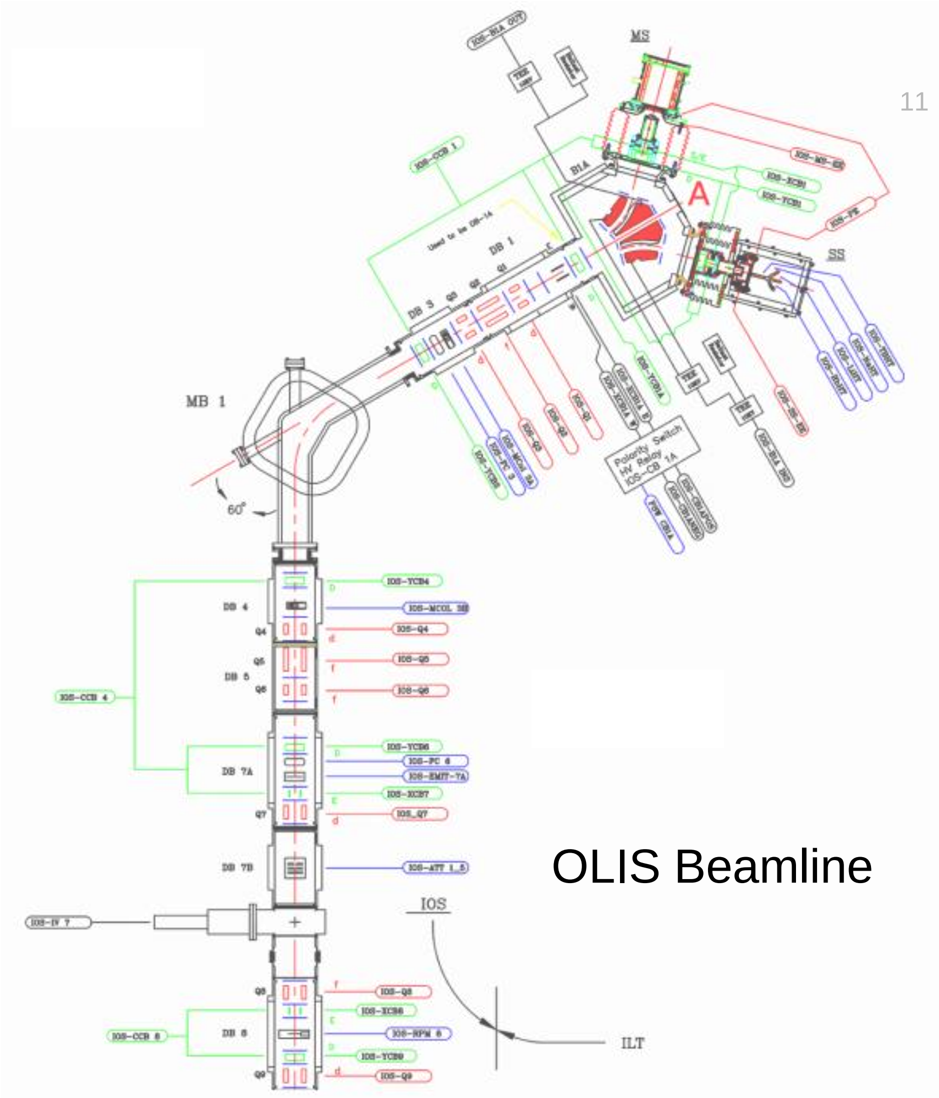
David Wang, Paul Jung, Olivier Shelbaya, Spencer Kiy, Wojtek Fedorko, Rick Baartman, Oliver Kester

2021-08-17

Discovery, accelerated

OLIS Beamline

- Starting point for AI-tuning
  - Low current
  - Non-radioactive
- Manual tuning by operators takes many hours, taking away from research beam time
- Goal for reinforcement learning agent:
  - Optimize beam transmission
  - Offset unknown misalignments
  - Improve speed and accuracy of tuning



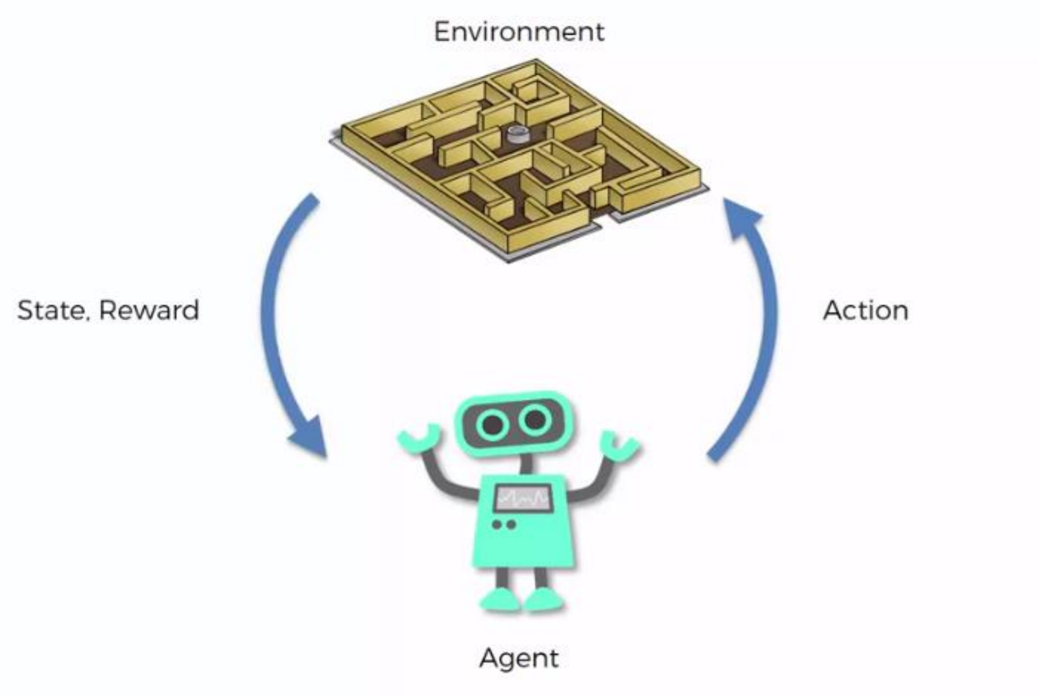
OLIS Beamline

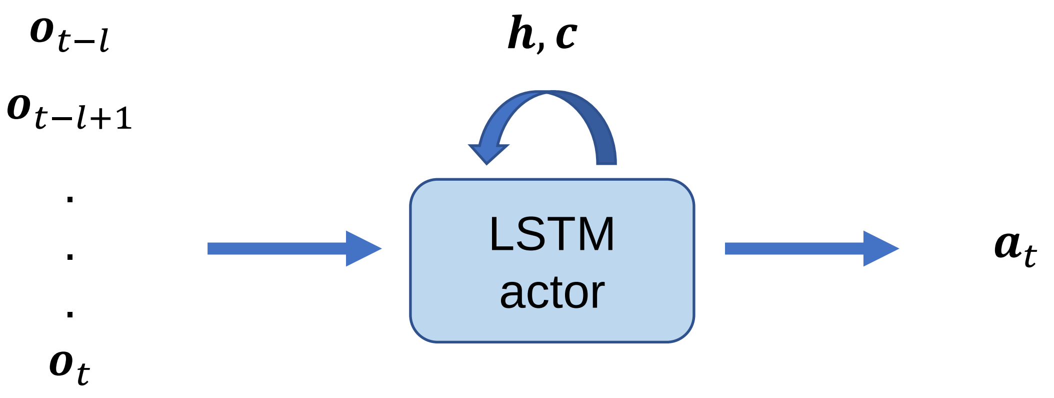
Source: Beam Physics Note TRI-BN-20-13R, Olivier Shelbaya

Source: https://towardsdatascience.com/getting-started-with-reinforcement-q-learning-77499b1766b6

Reinforcement learning

- Challenges of beamline environment:
  - Partially observed (only a few measurable spots)
  - Continuous and large action spaces
- Proposed Algorithm: Recurrent Deep Deterministic Policy Gradients (RDPG)
  - Actor-critic algorithm utilizing actor and critic networks to optimize agent learning
  - Long Short-term Memory (LSTM) networks to operate in partially observed environment

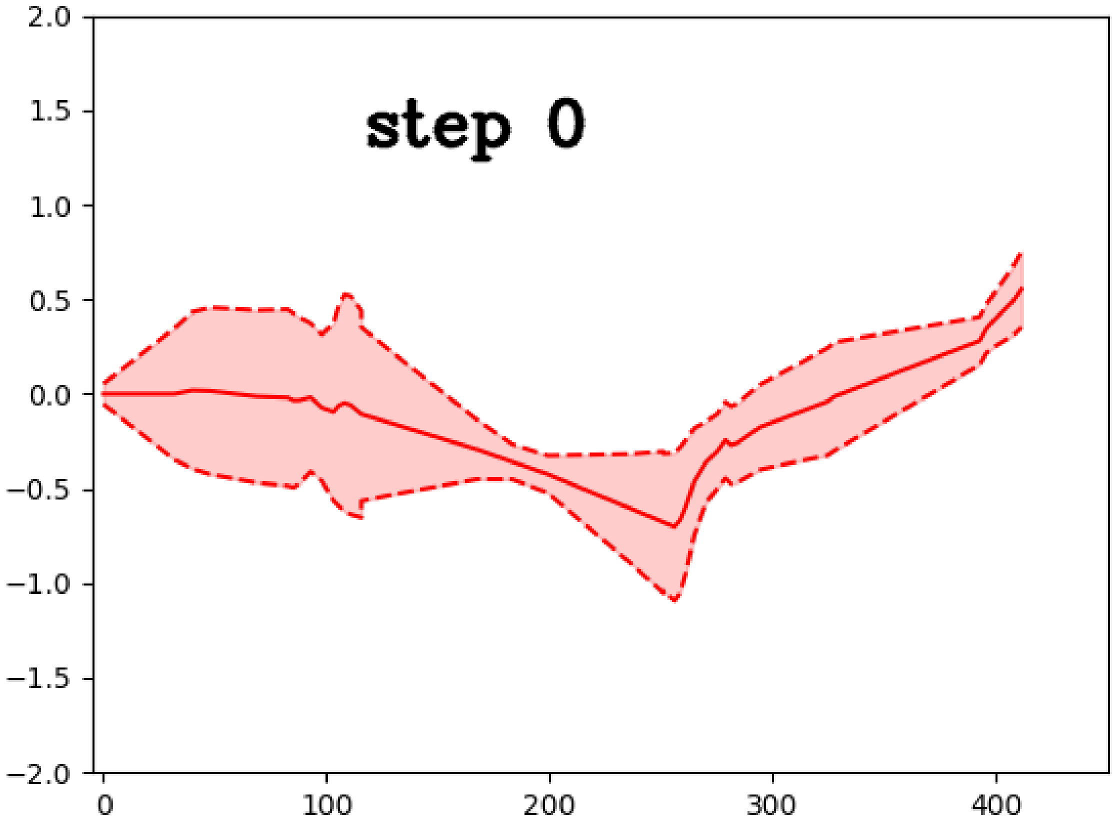




o_t : observation
for example, current measured at 2 faraday cups
a_t : predicted action
for example, angles to rotate each steerer
l : memory length of LSTM actor
h, c : hidden states of LSTM actor

Current Progress and Next Steps

- Beamline simulation
  - Approximate as a Gaussian particle distribution
  - Analyze in only 1 dimension
  - Use centroid (solid line) and envelope (dotted line) to determine transmission
- Current model trains well on simulation
  - Using realistic observations but artificial reward function
- Plans:
  - More realistic simulations of measurement and reward
  - Develop strategy and tools for real beamline tuning
  - Extend to ISAC and other beamlines



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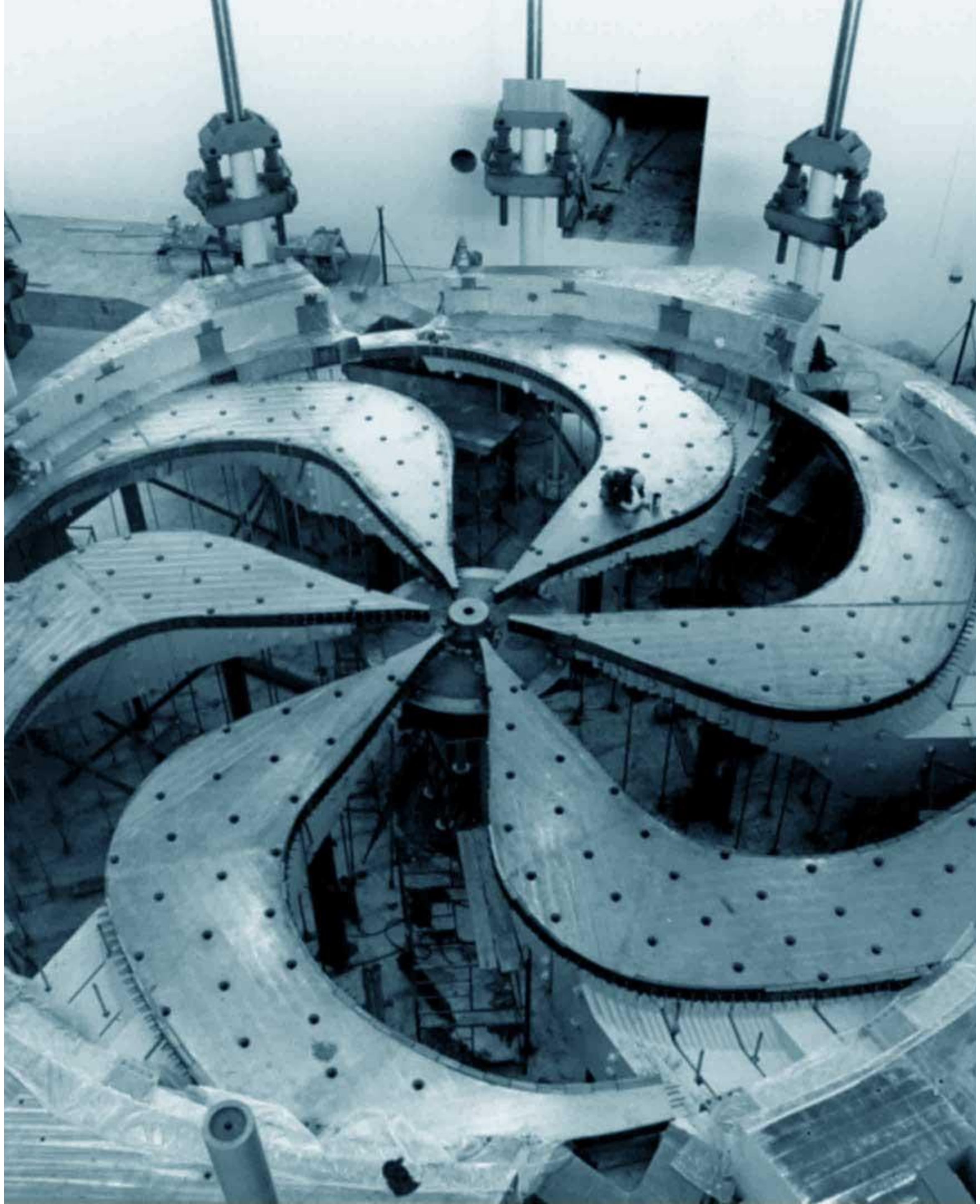
Quantum Computing for Nuclear Physics:

Improving Hamiltonian Encodings with the Gray Code

Peter Gysbers
O. Di Matteo, A. McCoy, T. Miyagi,
R. Woloshyn, P. Navrátil

Phys. Rev. A **103**, 042405 (2021)
arXiv: 2008.05012
Science Week – Aug 17, 2021



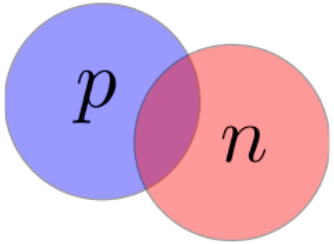
Discovery, accelerated

The Nuclear Many-Body Problem

- General goal: solve the Schrodinger equation

$$E\left|\Psi\right\rangle = H\left|\Psi\right\rangle$$

- This project: the deuteron

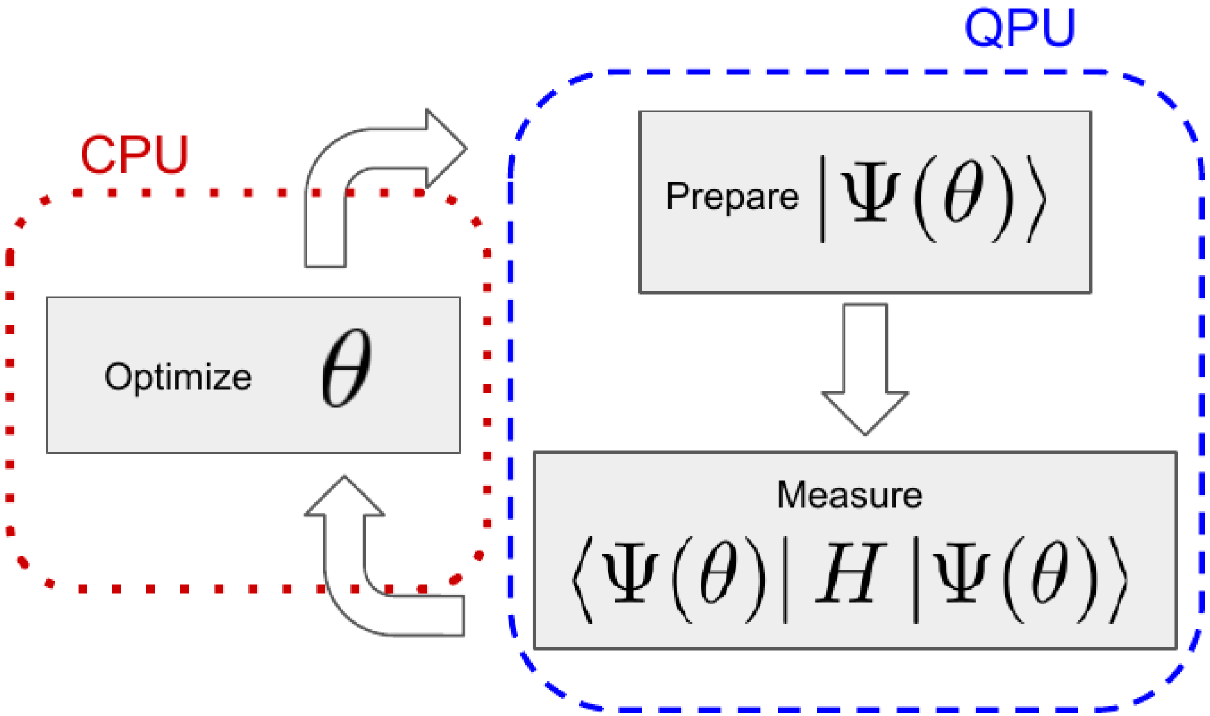


- Method: solve for coefficients of an ansatz

$$\left|\Psi(\theta)\right\rangle = \sum_{n=0}^{N-1} c_n(\theta)\left|n\right\rangle$$

Variational Quantum Eigensolver (VQE)

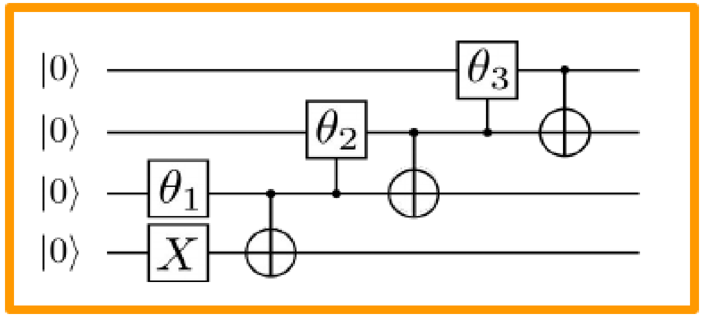
- Hybrid algorithms are most useful on current (noisy & small) devices

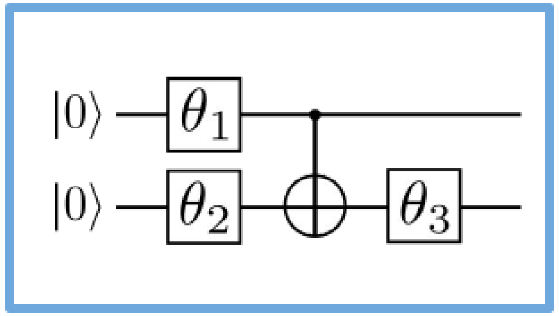


Encodings and Circuits

- Occupation (one-hot) encoding vs. Gray code encoding

Basis (N states)	Encoding	
	Occupation (N qubits)	Gray Code ($\log_2(N)$ qubits)
$\vert 0\rangle$	$\vert 1000\rangle$	$\vert 00\rangle$
$\vert 1\rangle$	$\vert 0100\rangle$	$\vert 10\rangle$
$\vert 2\rangle$	$\vert 0010\rangle$	$\vert 11\rangle$
$\vert 3\rangle$	$\vert 0001\rangle$	$\vert 01\rangle$

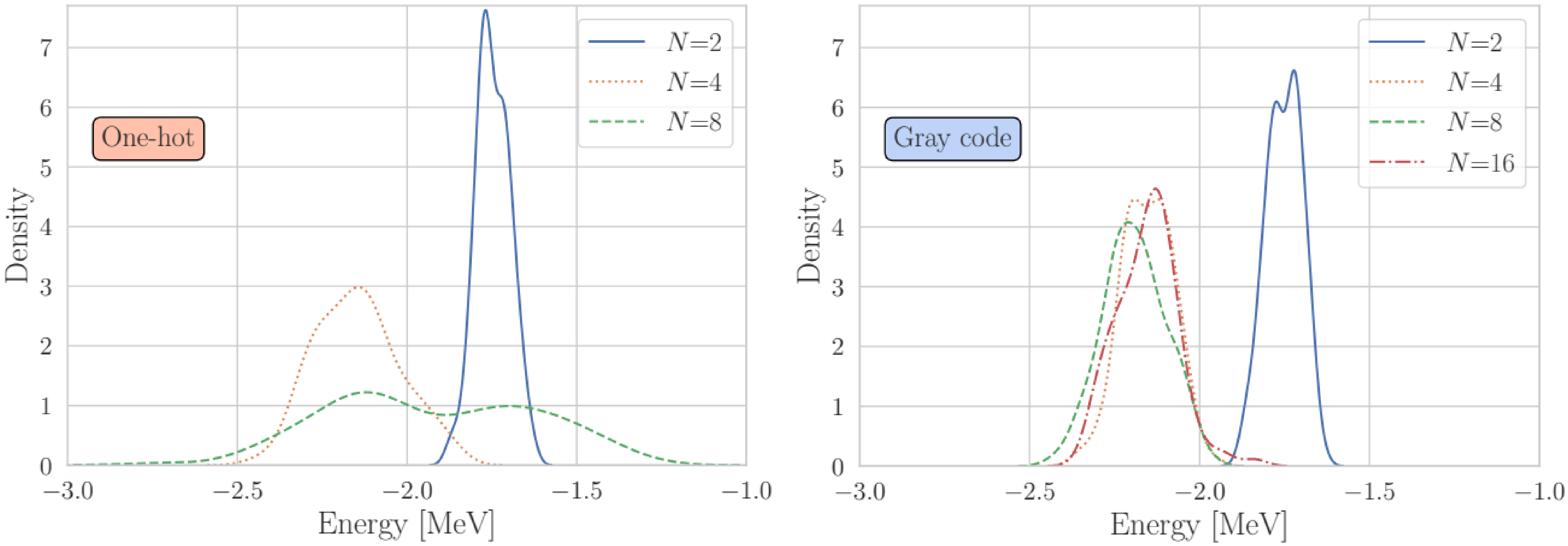




Results

- Occupation (one-hot) encoding vs. Gray code encoding

VQE trials: 100



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Thank you
Merci

www.triumf.ca

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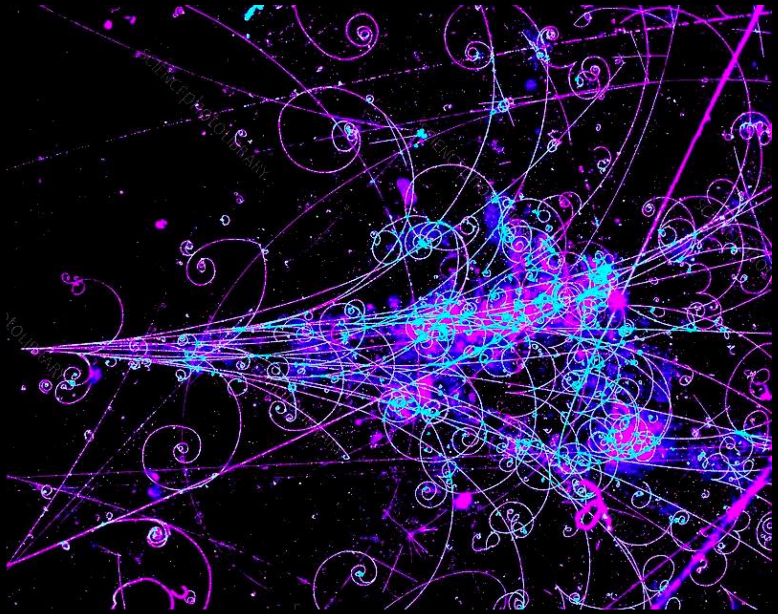
Discovery,
accelerated



Towards Calorimeter Data Generation with Quantum Variational Autoencoders

Abhishek Abhishek, Eric Drechsler, Wojtek Fedorko

TRIUMF Science Week, 16. August 2021

SFU

ATLAS EXPERIMENT

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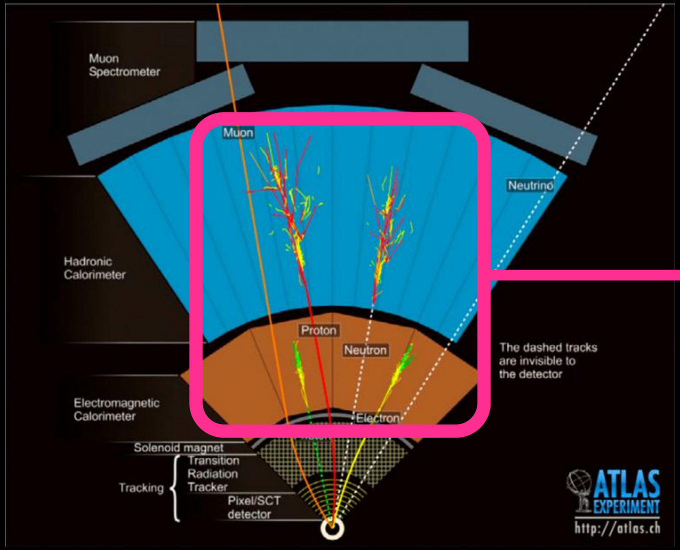
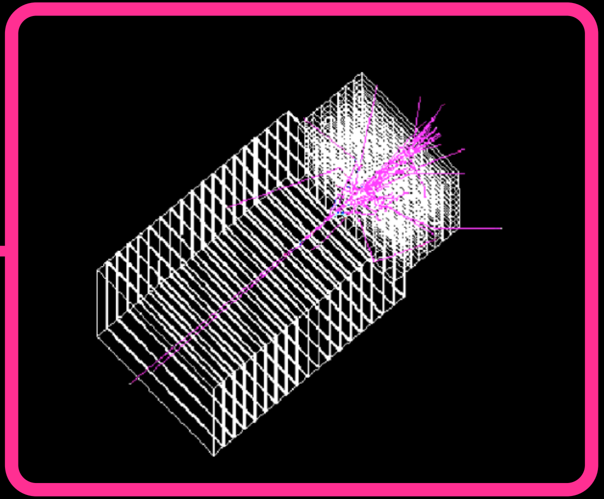
HL-LHC Computing Bottleneck: Calorimeter Shower Simulation

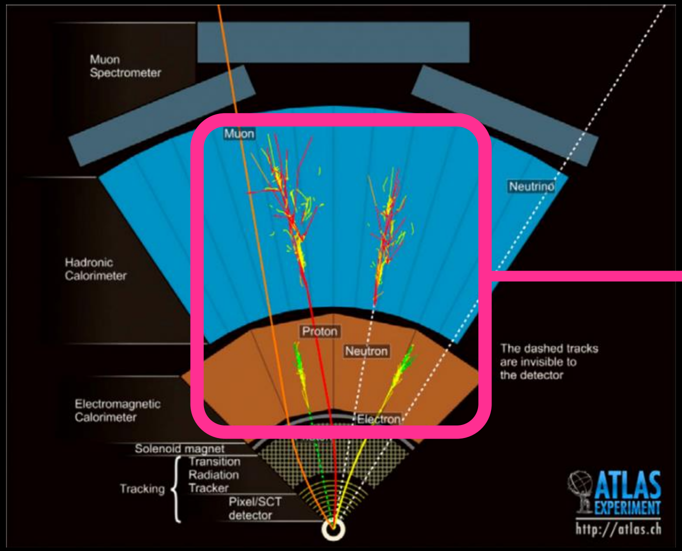


Cross-section ATLAS Detector

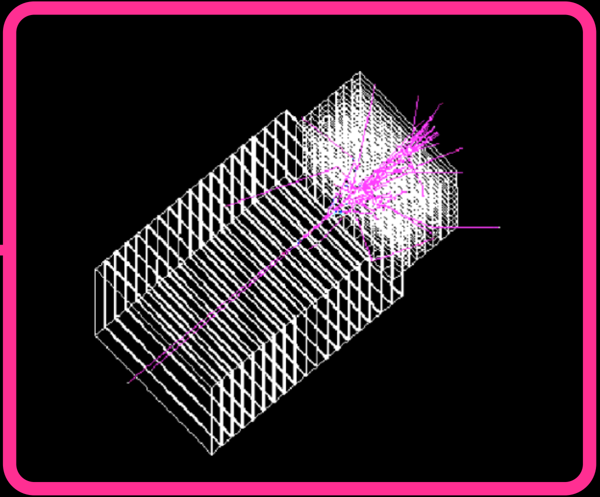


Representation of single GEANT4 simulated EM shower

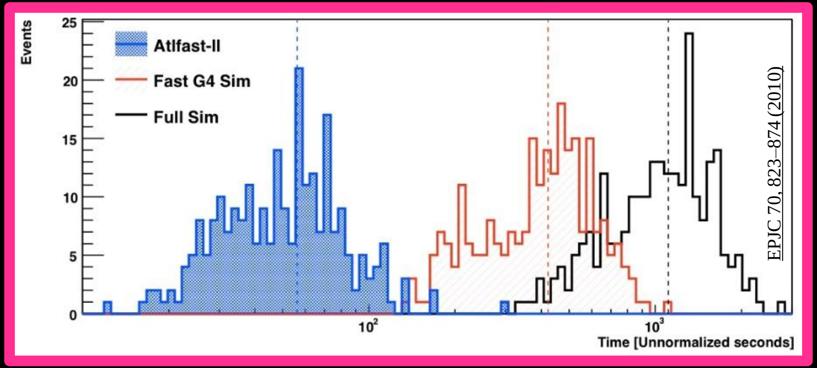
HL-LHC Computing Bottleneck: Calorimeter Shower Simulation



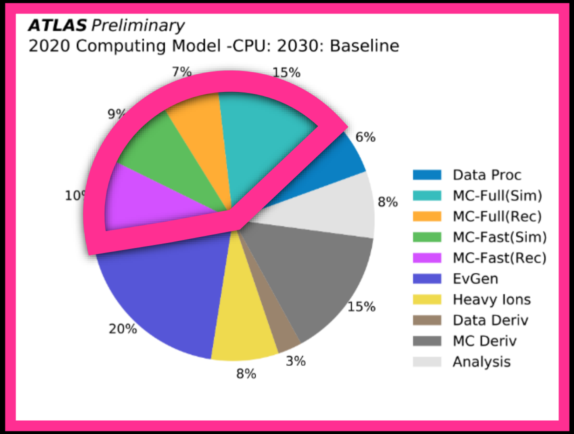
Cross-section ATLAS Detector



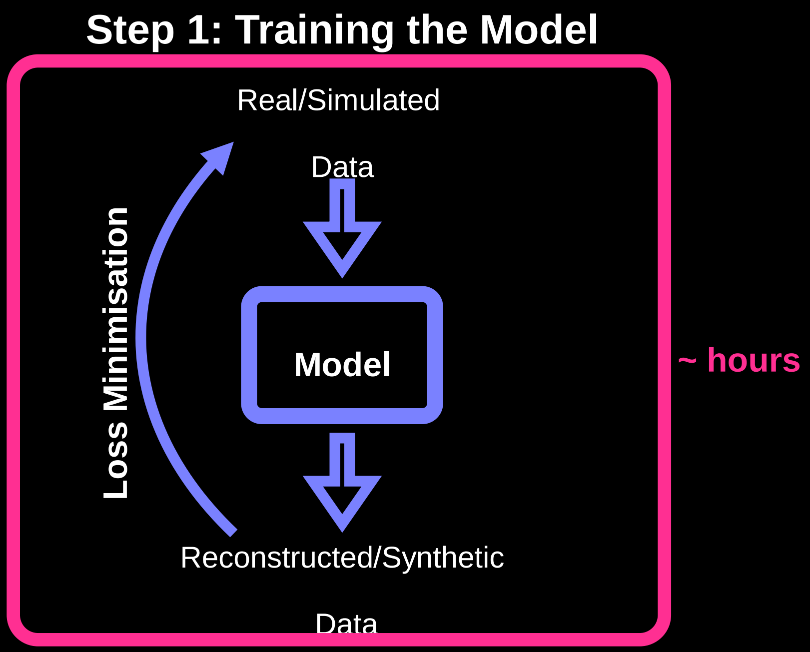
Representation of single GEANT4 simulated EM shower

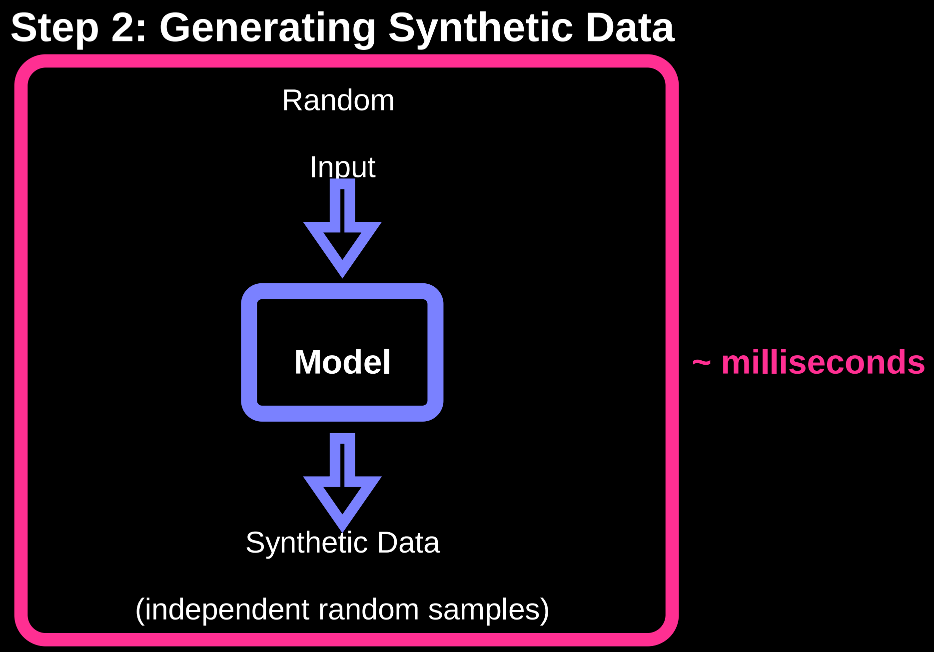


CPU time for simulating 250 ttbar events



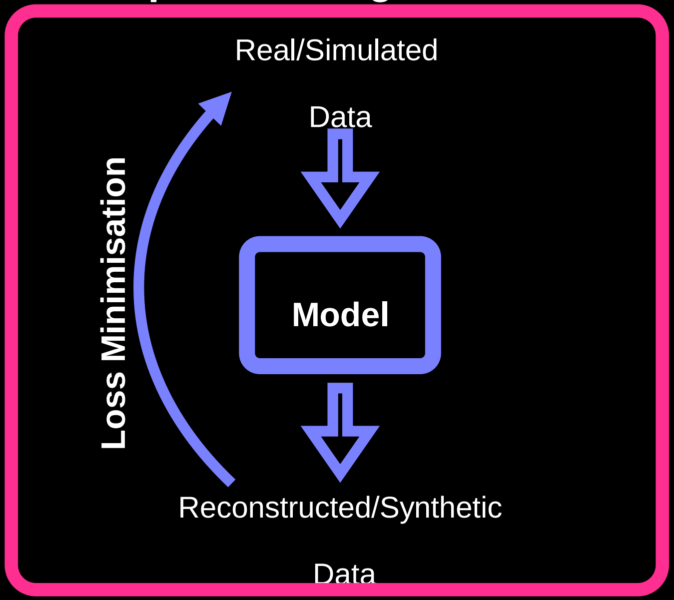
Generative Models for Synthetic Shower Generation





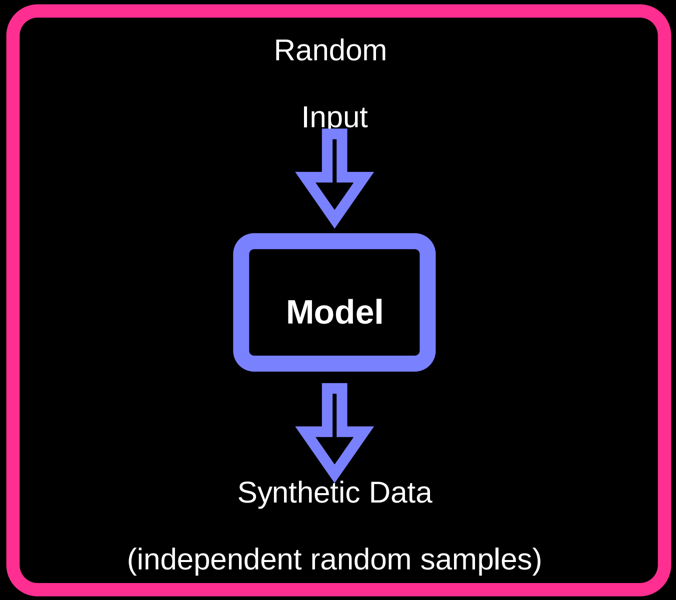
Generative Models for Synthetic Shower Generation

Step 1: Training the Model



~ hours

Step 2: Generating Synthetic Data

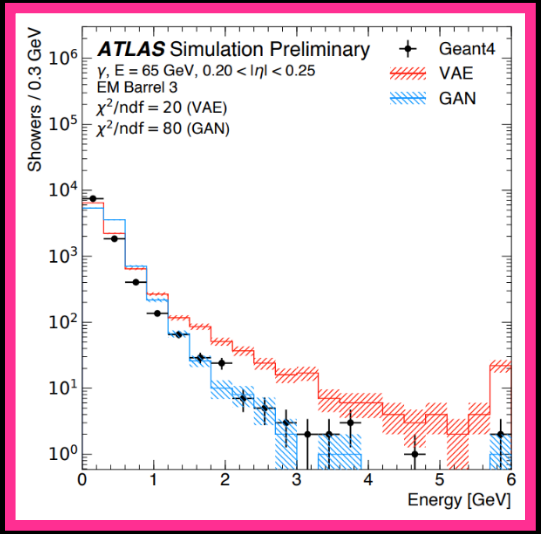


~ milliseconds

Example: Variational Autoencoder trained with modified loss

$$\mathcal{L}(x,x';\theta,\phi) = w_{\text{reco}}\mathbb{E}_{\zeta\sim q_\phi(\zeta|x)}[\log p_\theta(x|\zeta)] - w_{\text{KL}} D_{\text{KL}}[q_\phi(\zeta|x)||p_\theta(\zeta)] - w_{E_{tot}}\Big|\sum_i x_i - \sum_i x'_i\Big| - \sum_l w_l\Big|\frac{1}{E_{tot}}\sum_j^{N_l} x_j - \frac{1}{E'_{tot}}\sum_j^{N_l} x'_j\Big|$$

Total Energy — Energy per layer



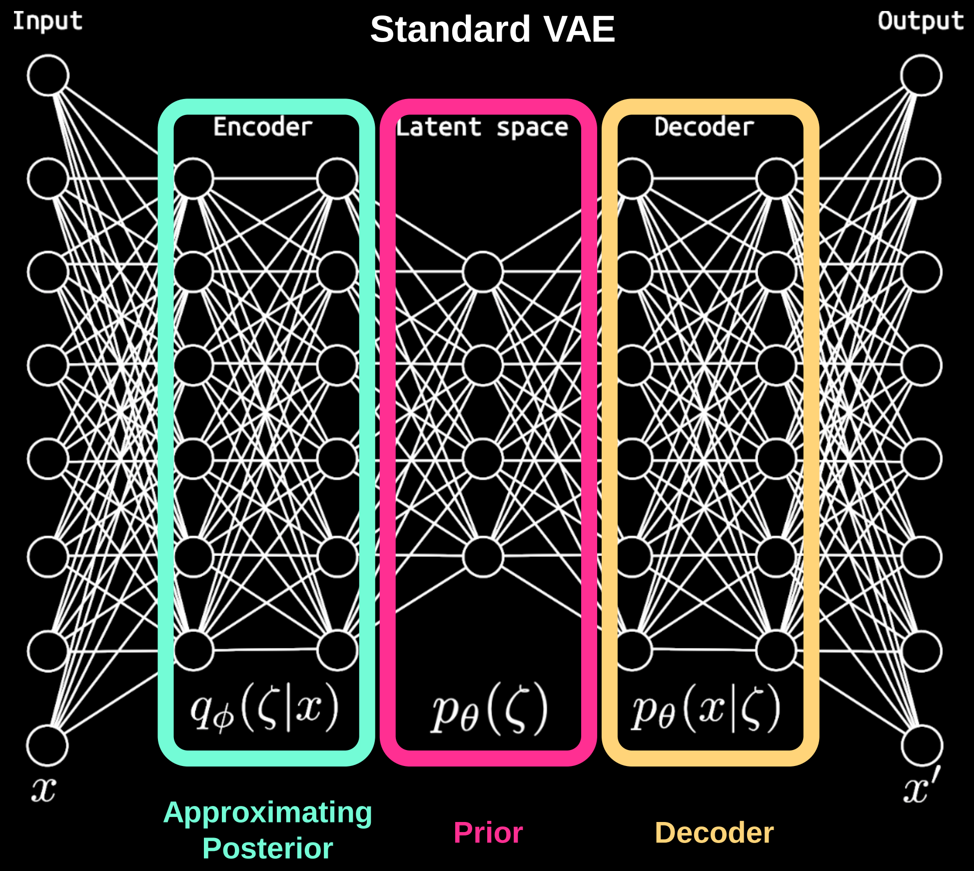
ATL-SOFT-PUB-2018-001

A. Abhishek, Eric Drechsler, Wojtek Fedorko, *Calorimeter Shower Generation with QVAE*, 16. August 2021

Discrete Variational Autoencoders

arxiv:1609.02200

Standard VAE



Discrete VAE

Flat Approximating Posterior

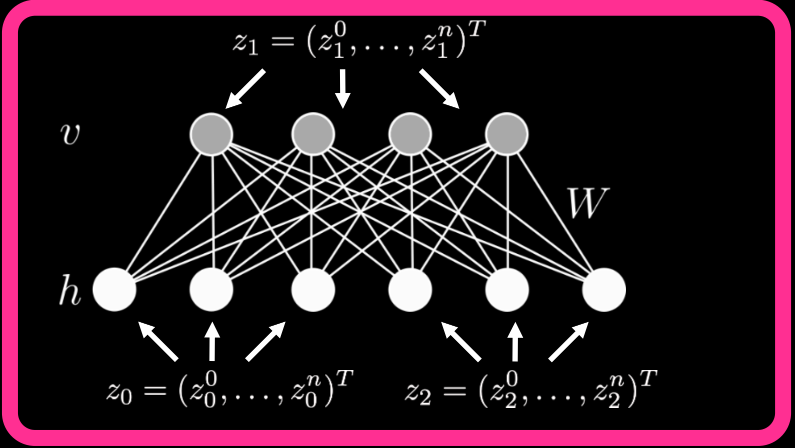
$$q_\phi(\zeta|x)$$

$$\Downarrow$$

$$q_\phi(\zeta_l|x, \{\zeta_m\}_{m<l})$$

Hierarchical Approximating Posterior

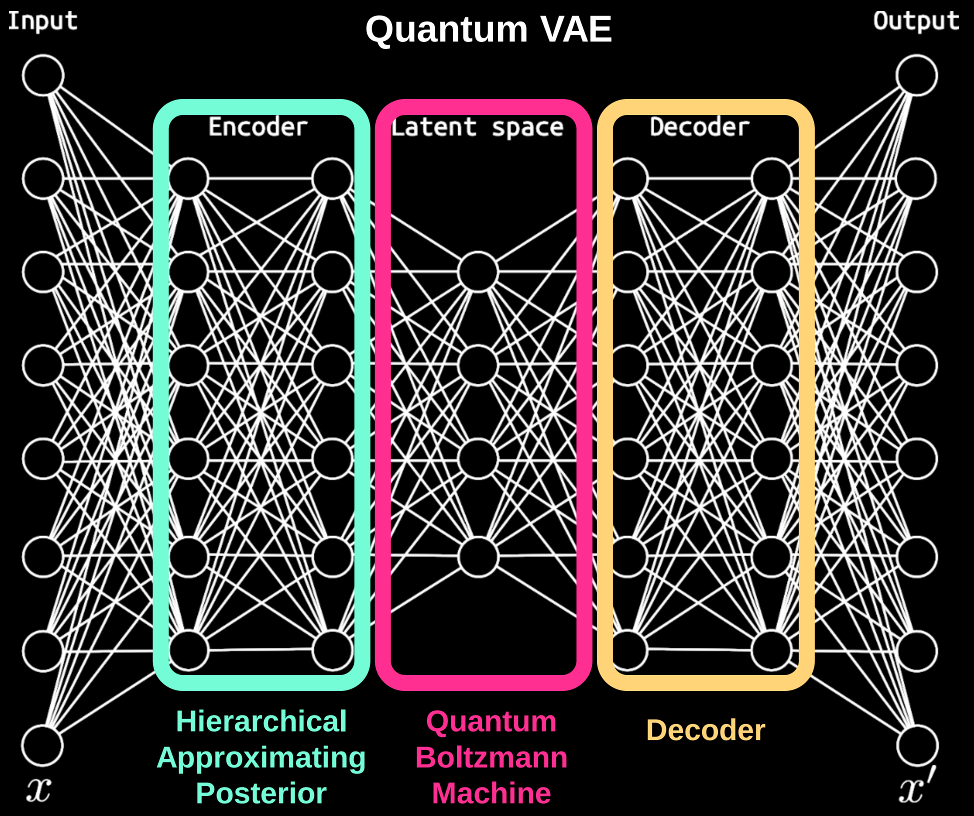
Prior: Restricted Boltzmann Machine



Discrete Latent Space: $p_\theta(\zeta) \Rightarrow p_\theta(z_0, \dots, z_l)$

Quantum Variational Autoencoders

arxiv:1802.05779

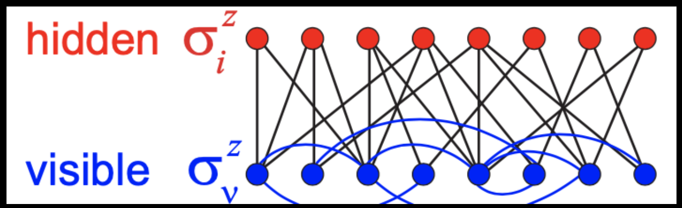


$q_\phi(\zeta_l|x, \{\zeta_m\}_{m<l})$

$$p_\theta(z) = \frac{1}{Z_\theta}\mathrm{Tr}[\Lambda_z e^{-\mathcal{H}_\theta}]$$

Prior: Quantum Boltzmann Machine

qbits on DWave QPU



Restricted BM

State Probability $$p_\theta(v,h) = \frac{1}{Z_\theta}\exp[-E_\theta(v,h)]$$

State Energy $$E_\theta(v,h) = -\sum_{i=0}^{D}\sum_{j=0}^{M} W_{ij}v_ih_j - \sum_{j=0}^{D} b_iv_i - \sum_{j=0}^{M} a_jh_j$$

Quantum BM

State Probability $$p_\theta(z) = \frac{1}{Z_\theta}\mathrm{Tr}[\Lambda_z e^{-\mathcal{H}_\theta}]$$

State Energy $$\mathcal{H}_\theta = \sum_l \sigma_l^x\Gamma_l + \sum_l \sigma_l^z h_l + \sum_{l<m} W_{lm}\sigma_l^z\sigma_m^z$$

A. Abhishek, Eric Drechsler, Wojtek Fedorko, *Calorimeter Shower Generation with QVAE*, 16. August 2021

Science, Community, Training, Collaboration

- Undergraduate coop programs
- Master of Data Science (UBC), UBC EngPhys, BCIT Capstone projects
- MITACS GRA, GRI
- Data Science Study Group w/ GAPS
  - Courses/ certificates
  - Paper reading
- Summer Schools, TRIUMF Summer Institute 2020/2021: Cornerstone Models of Quantum Computing