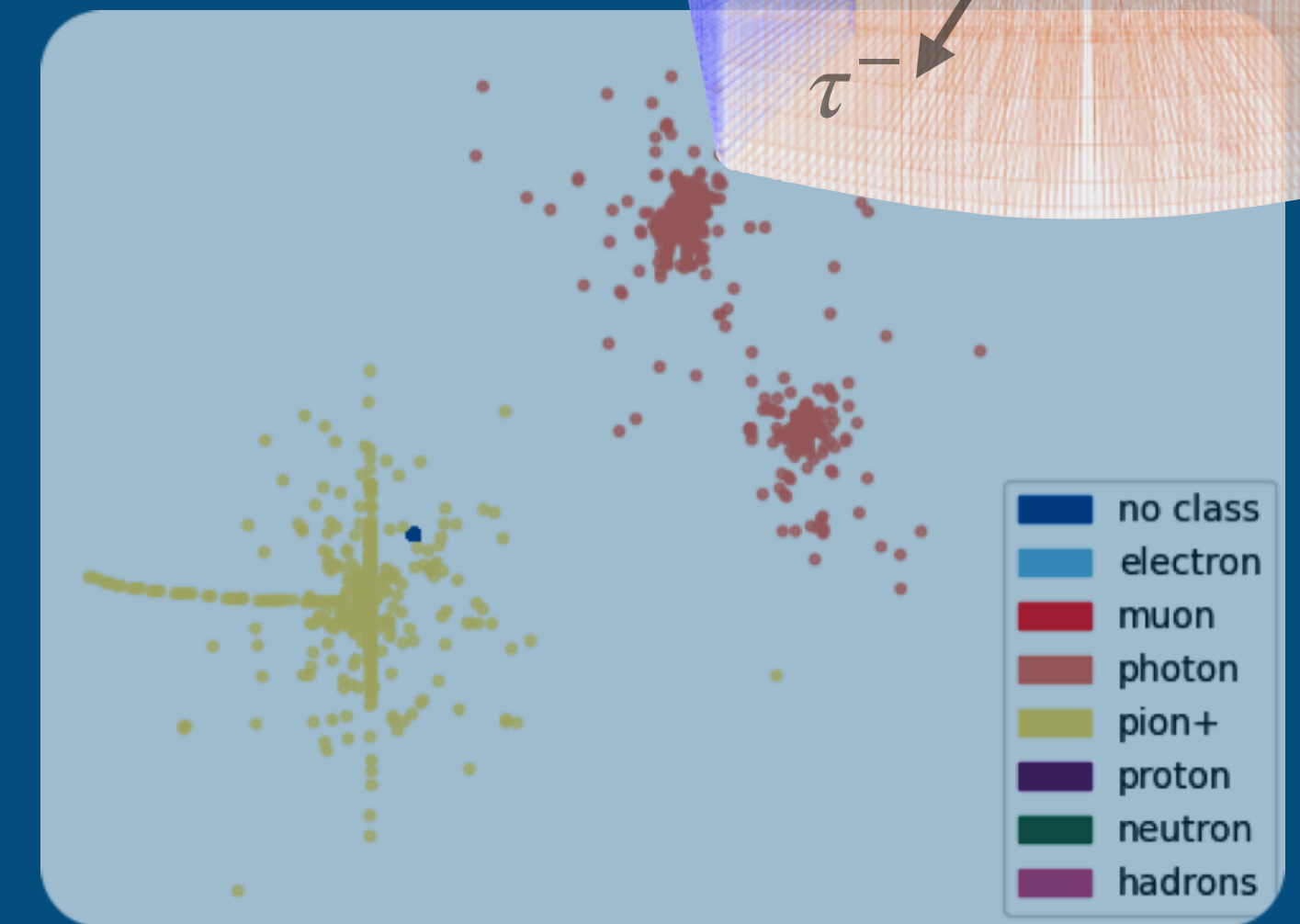
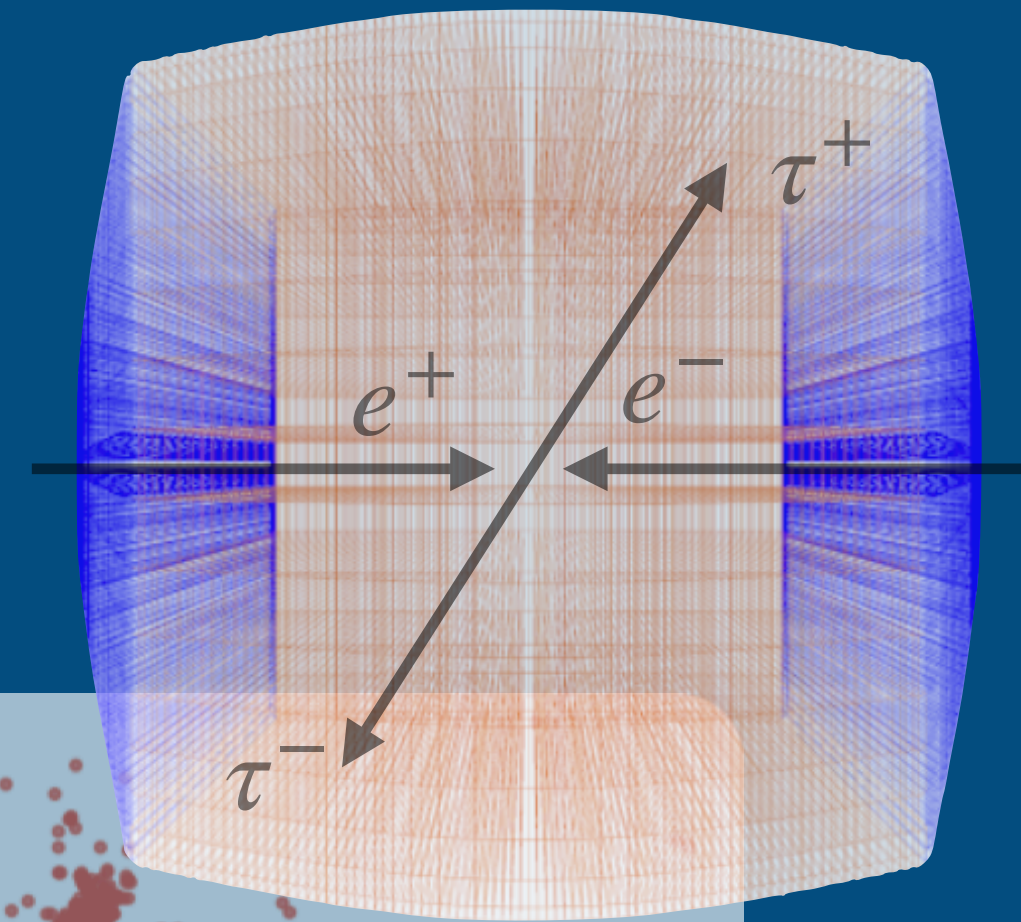


# GRAPH NEURAL NETWORK PER L'IDENTIFICAZIONE DI LEPTONI TAU IN ESPERIMENTI AI FUTURI COLLIDER $e^+e^-$

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Riunione settimanale ML\_INFNO - 3 Luglio 2023

# INTRODUCTION

- ongoing work aiming at studying and optimising the physics potential of future collider experiments (principally FCCee and CepC)
  - **case study:  $\tau$ -identification with the IDEA dual-readout calorimeter (DRC) concept**
    - leverage modern machine learning methods based on differentiable deep neural networks
    - study performance using only standalone DRC information
    - helps also in optimising the detector and design of the readout electronics
  - **tasks studied:**
    - classification of  $\tau$ -decays and separation from QCD jets based on **Dynamic Graph Neural Networks** (DGCNN)
    - development of a novel **Bayesian-DGCNN** for robust estimation of NN predictions
    - **DGCNN-based object detection** (identification of tau/jet constituents) for proto particle-flow algorithms
  - **evolutions & onngoing work:**
    - improve object detection capabilities with hybrid architectures: **GNN + encoder/decoder Transformer**
    - **model acceleration on FPGAs** for real-time use (triggers/monitor of physics streams/...)
- **plan to use the results of these studies to prepare one or more tutorials on advanced topics (Bayesian-NN, Hybrid architectures, Model Compression, ...) for ML\_INFN/AI\_INFN**

# FCC-ee & -hh

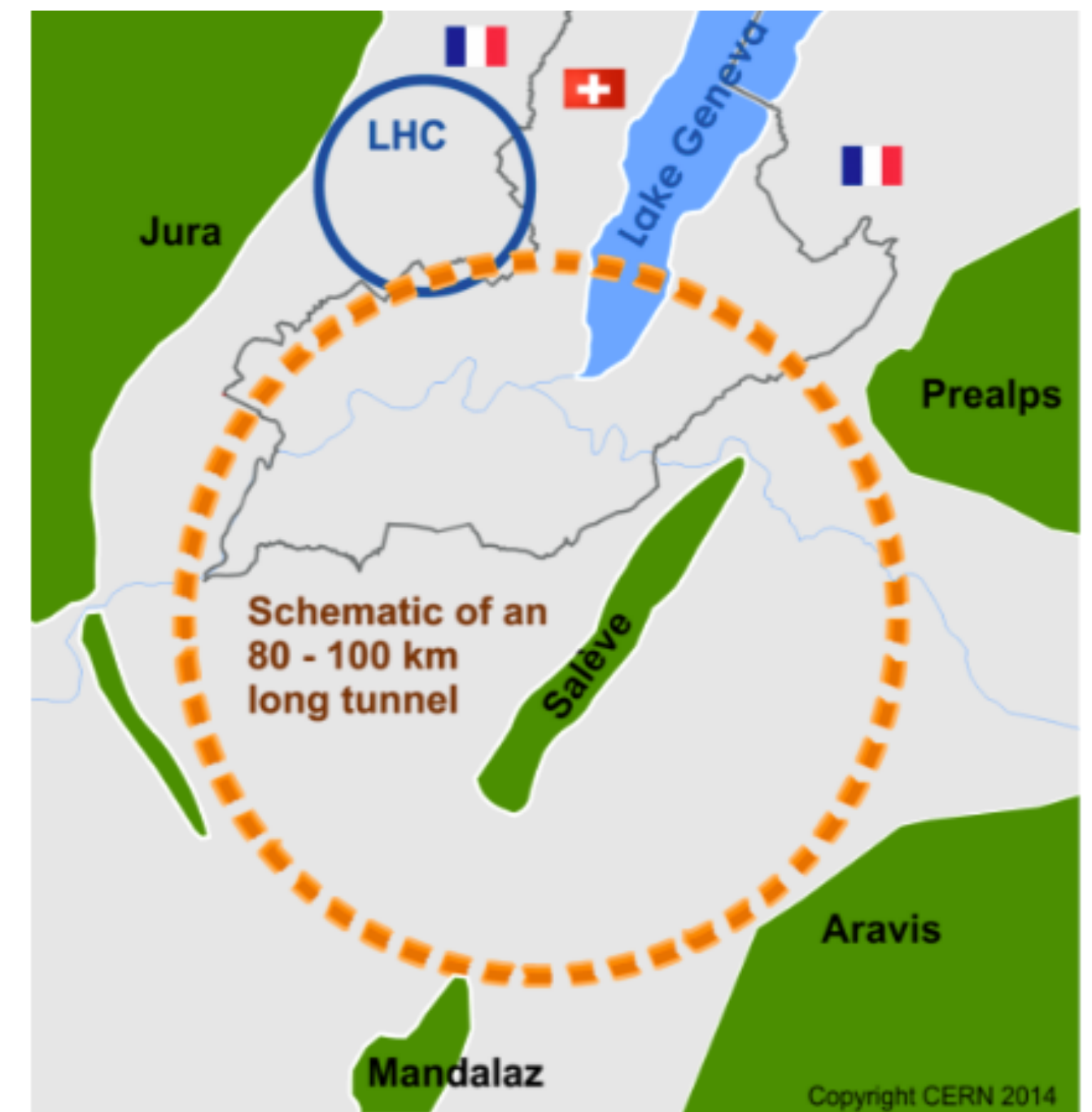
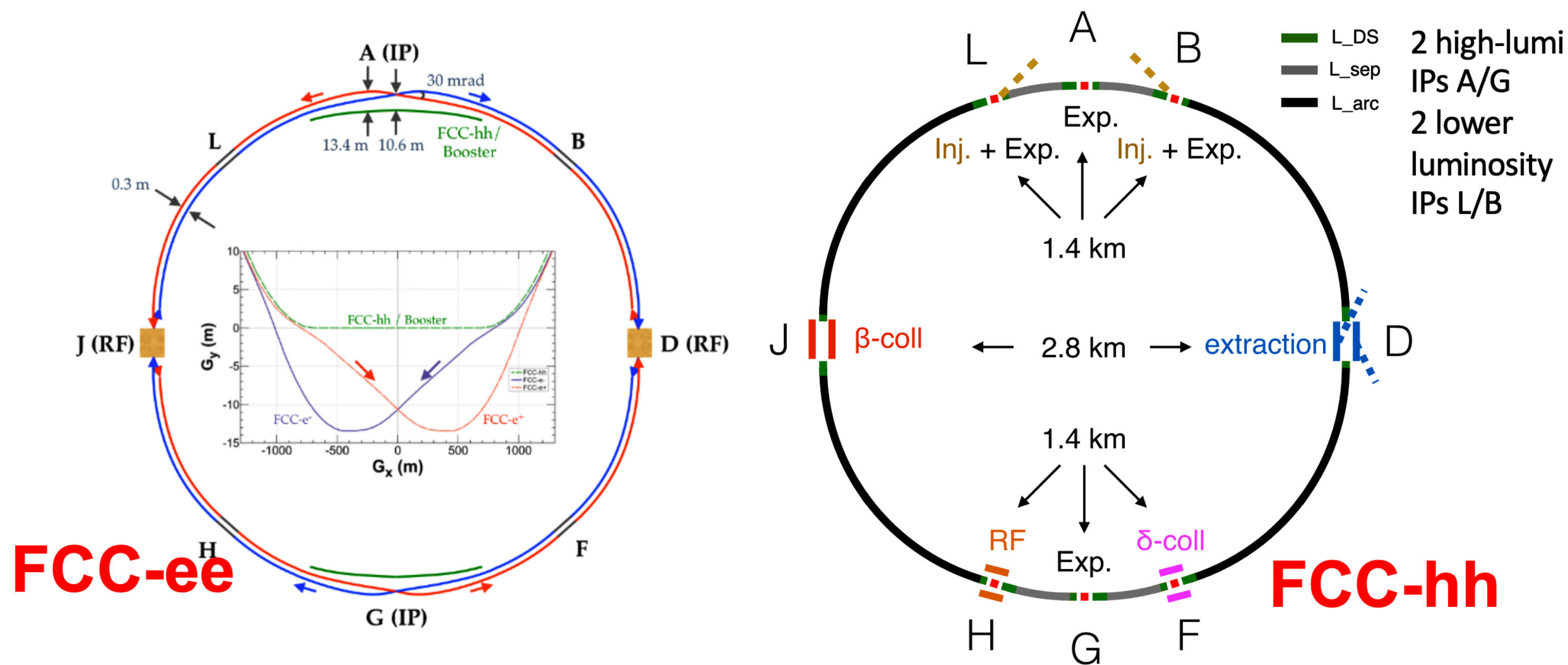
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<https://link.springer.com/article/10.1140/epjst/e2019-900087-0>

original study requested by ESPP in 2013, started in 2014 as main way to guarantee research continuity in HEP at CERN in the post HL-LHC era

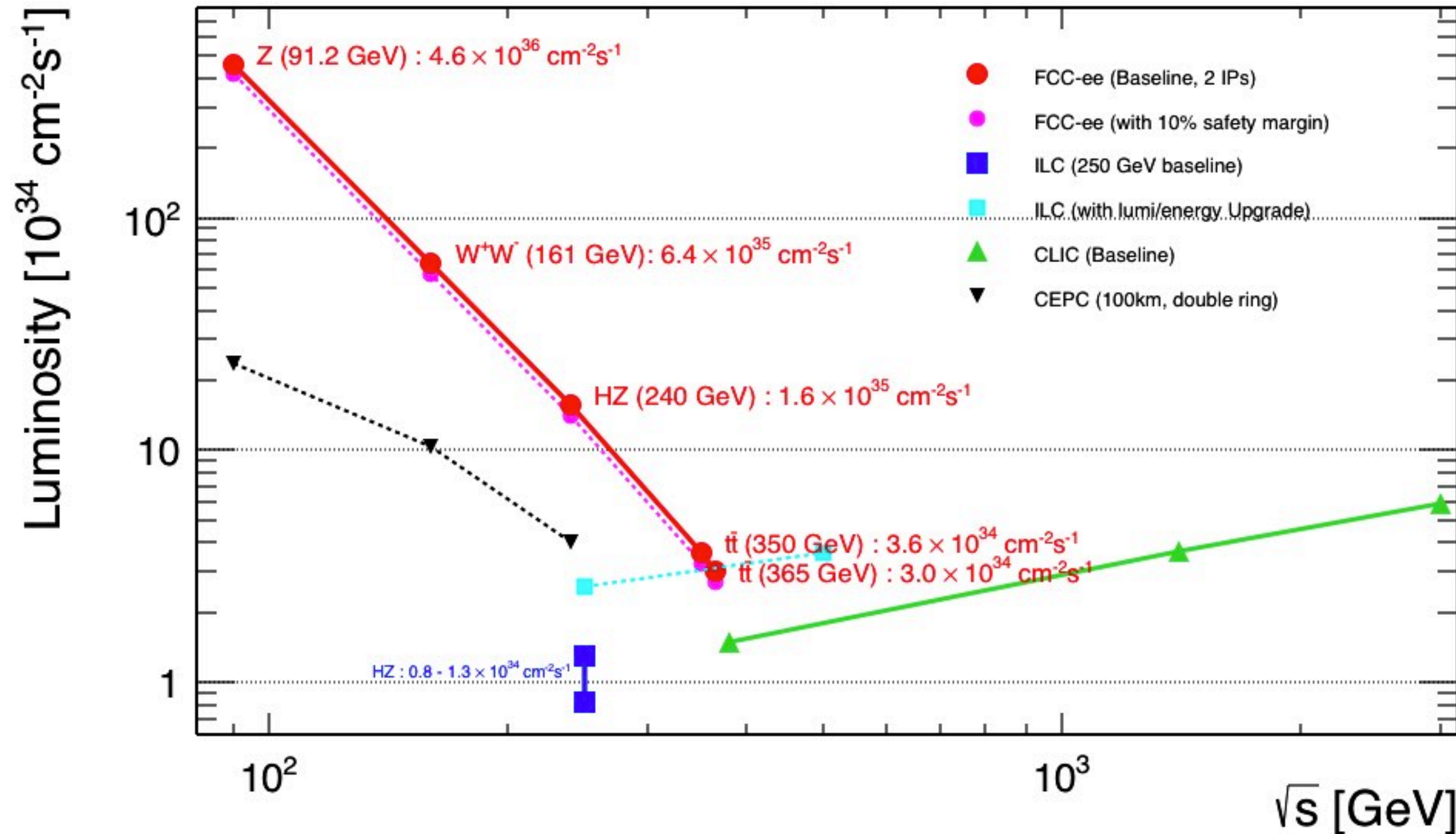
integrated project in two consecutive phases:

- stage 1: FCC-ee - ~90-400 GeV  $e^+e^-$  collider as Higgs, EW and top factory at the maximal achievable luminosity
- stage 2: FCC-hh - ~100 TeV hadron collider at the energy frontier + optional ions/eh machines

complementary physics goals & common infrastructures and civil engineering



# FCC-ee LUMINOSITY



- ◆ **100 000 Z / second**
  - **1 Z / second at LEP**
- ◆ **10 000 W / hour**
  - **20 000 W in 5 years at LEP**
- ◆ **1 500 Higgs bosons / day**
  - **10-20 times more than ILC**
- ◆ **1 500 top quarks / day**

$$\int L dt \sim 1 - 40 \text{ ab}^{-1} / \text{year}$$

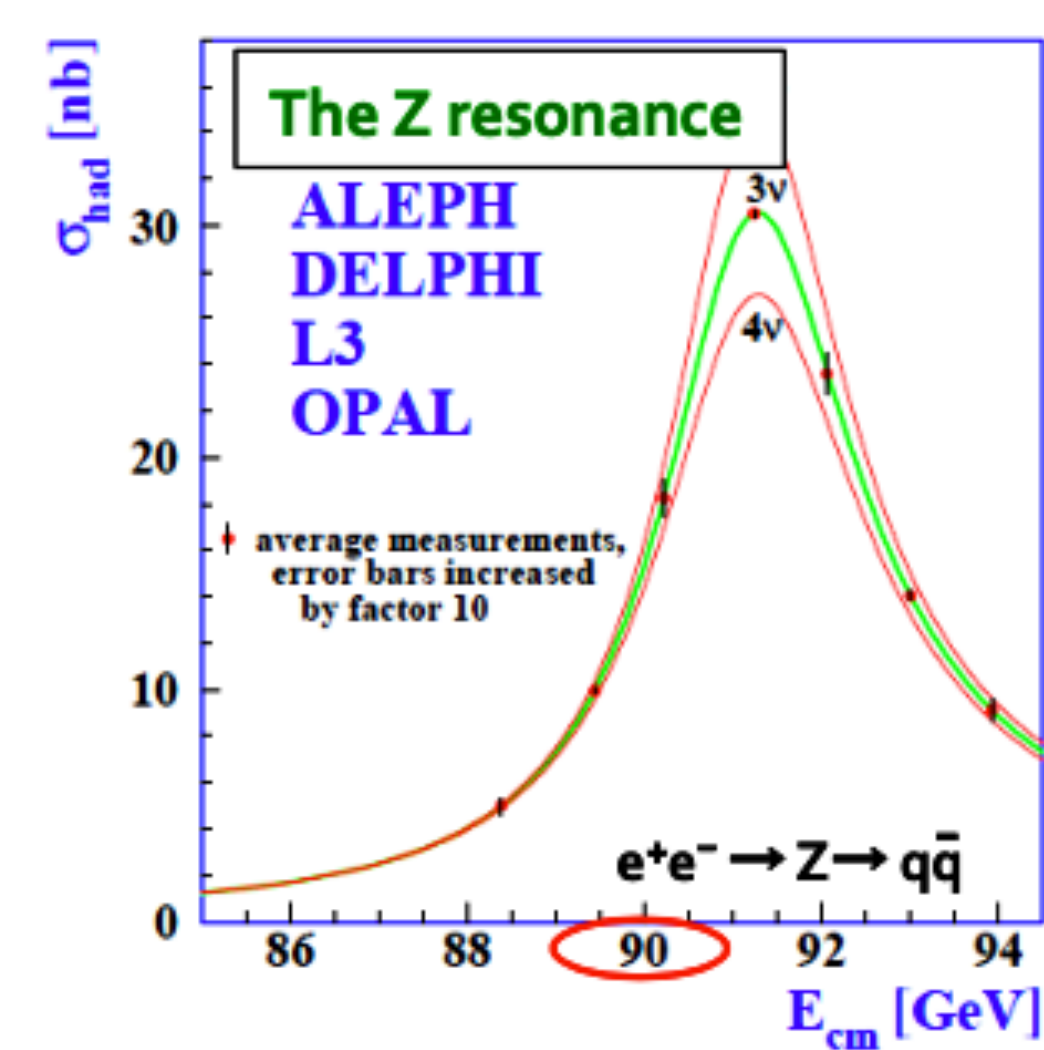
HZ    Z

luminosity  $\times 10^{3 \div 5}$  LEP thanks to the use of techniques developed for B-factories

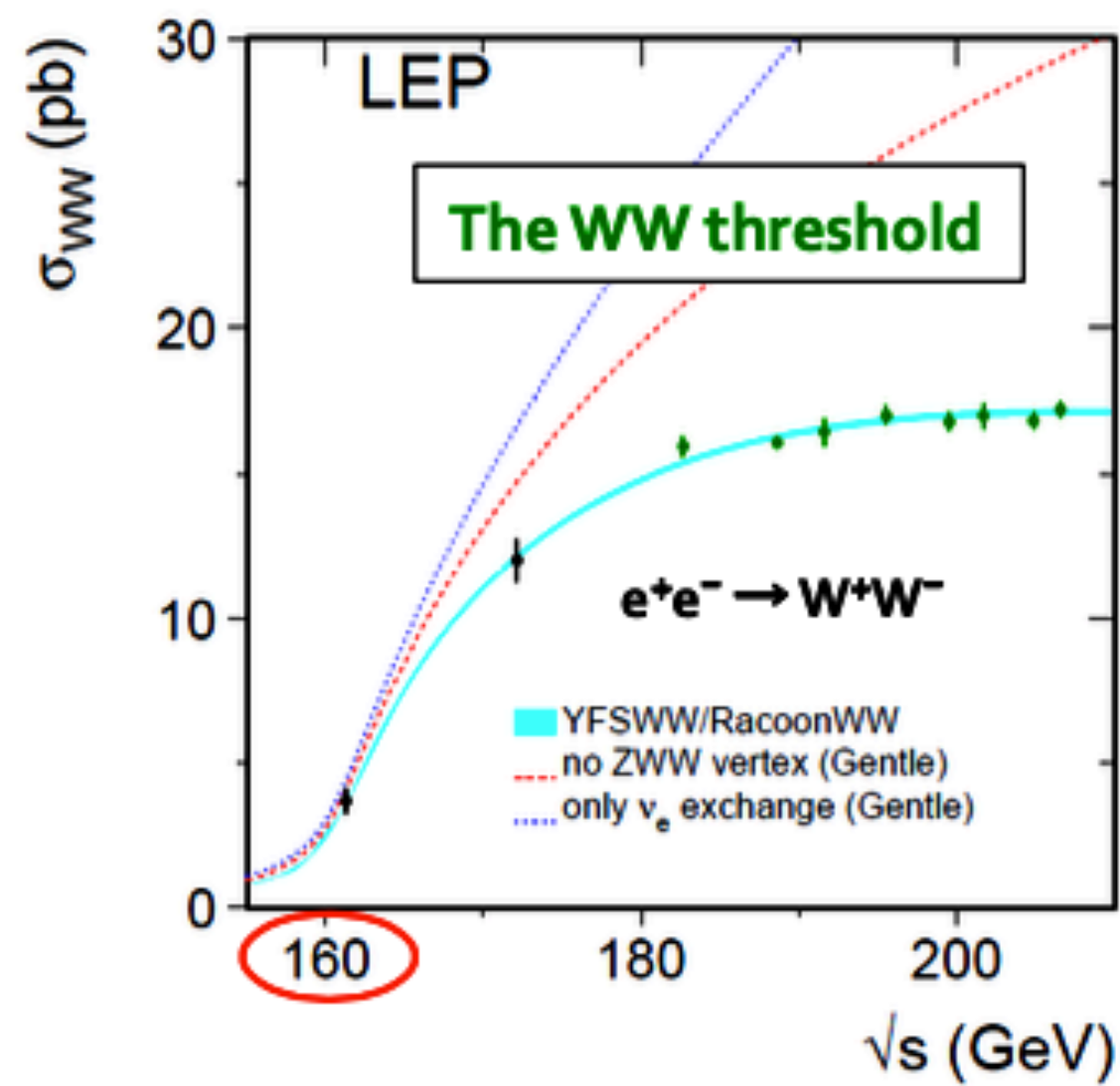
- independent rings for  $e^+$  and  $e^-$ : more bunches, higher currents w/o parasitic collisions
- crab waist and asymmetric IP, and continuous injection
- parameters optimised to keep same totale power for synchrotron radiation at all CM energies (100 MW)
  - total consumption with 50% of the klystrons active is 200 MW (compare with LHC: 210 MW and HL-LHC: 260 MW)

# FCC-ee CM ENERGY

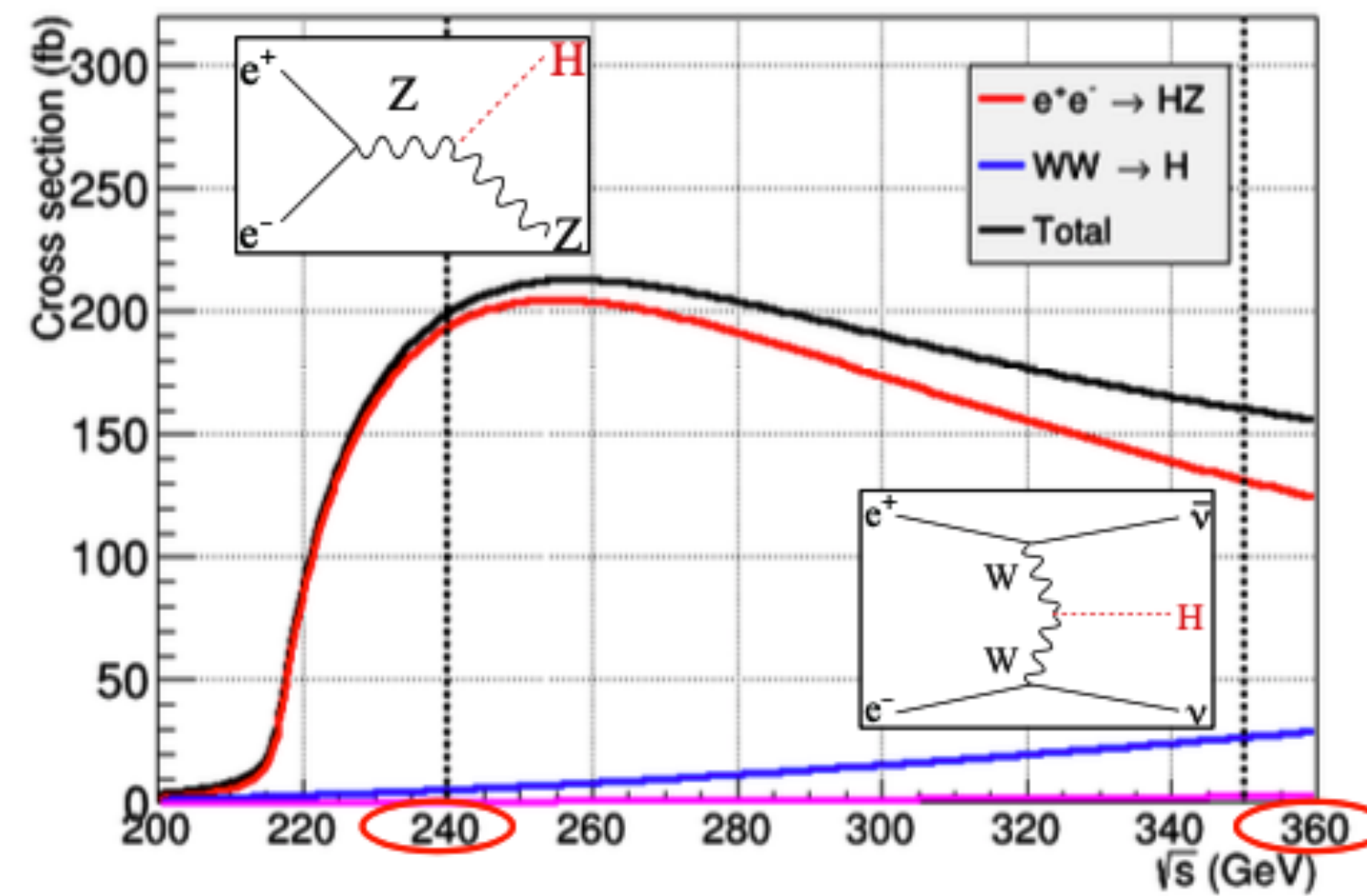
15 years physics: 4 (Z) + 2 (WW) + 3 (H) + 1 LS + 5 (tt) *not necessarily in this order* ...



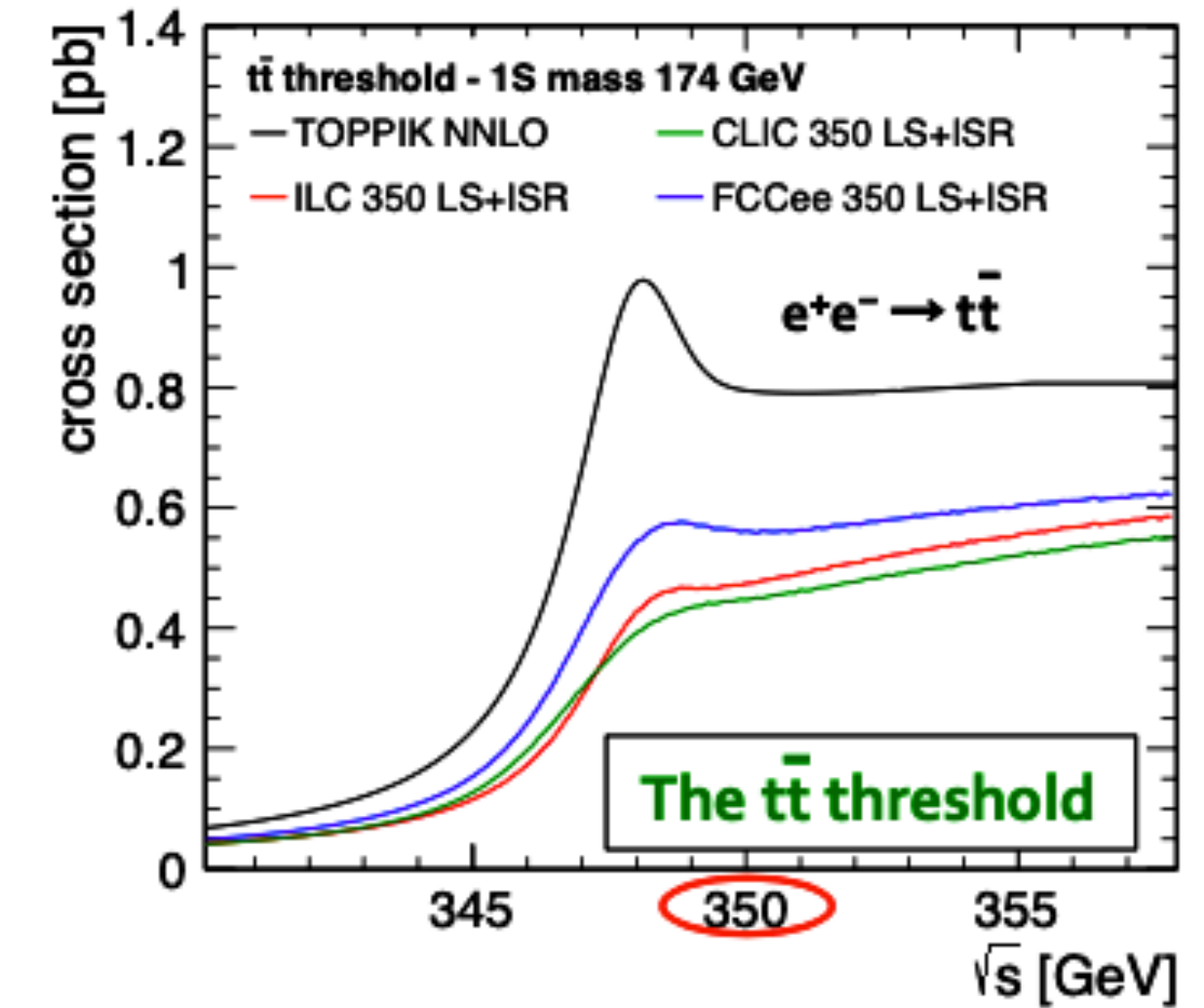
Z



WW



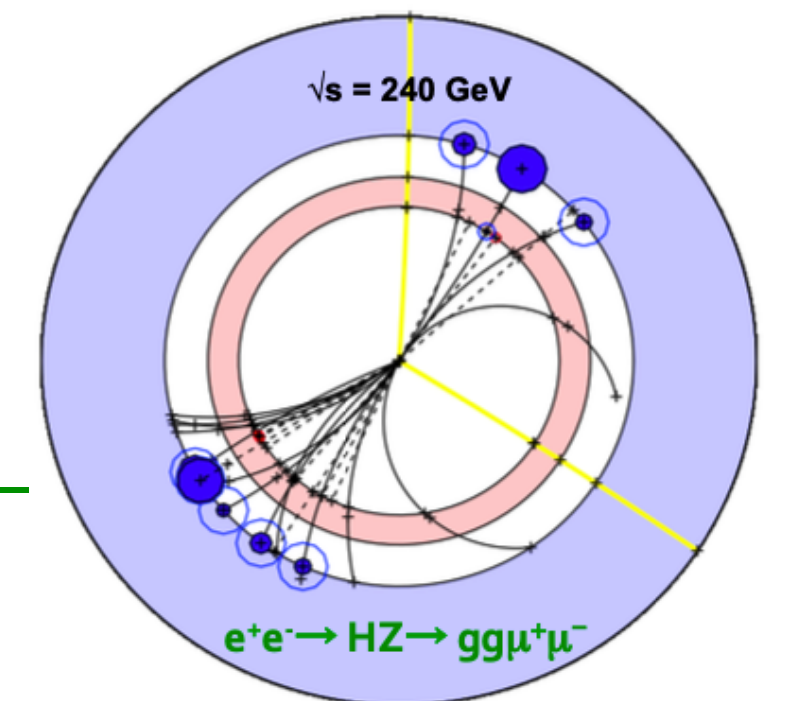
ZH e VBF-H



tt

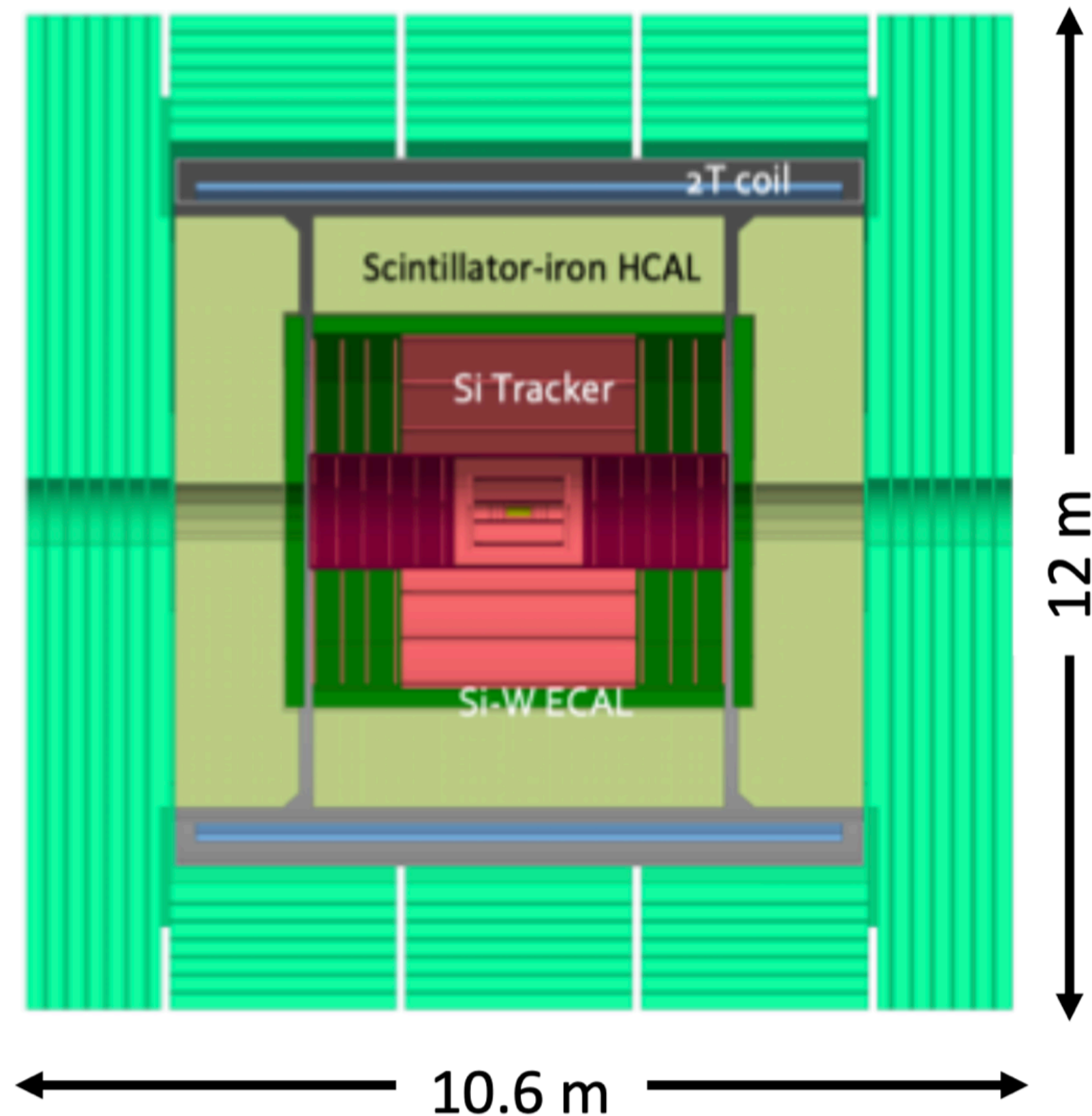
- physics at the Z pole allows study of light fermions ( $\tau$  and  $b$  - factory)
- clean environment and substantial yields open the possibility to study the properties of gluons in higgs decays:

$$e^+e^- \rightarrow HZ \rightarrow gg\mu^+\mu^-$$



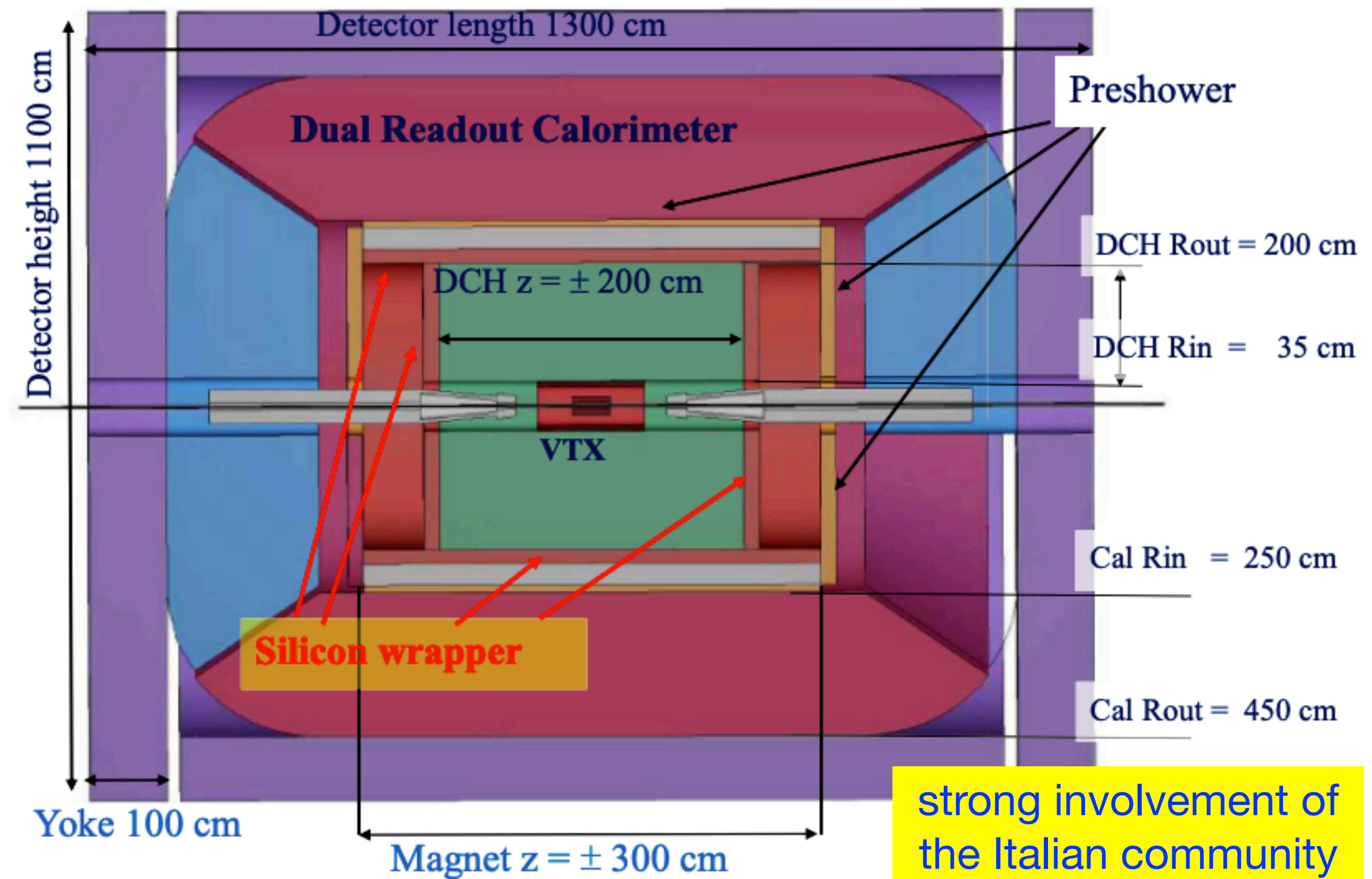
# FCC-ee CONCEPTUAL REFERENCE DETECTORS

**Clic-Like Detector:** adapted from CLIC design



- 2T B-field (CMS-style)
- Silicon ID (pixel + tracker)
- 3D imaging Silicon-tungsten ECAL
- Scintillator + FE HCAL
- MS: steel yoke instrumented with RPCs

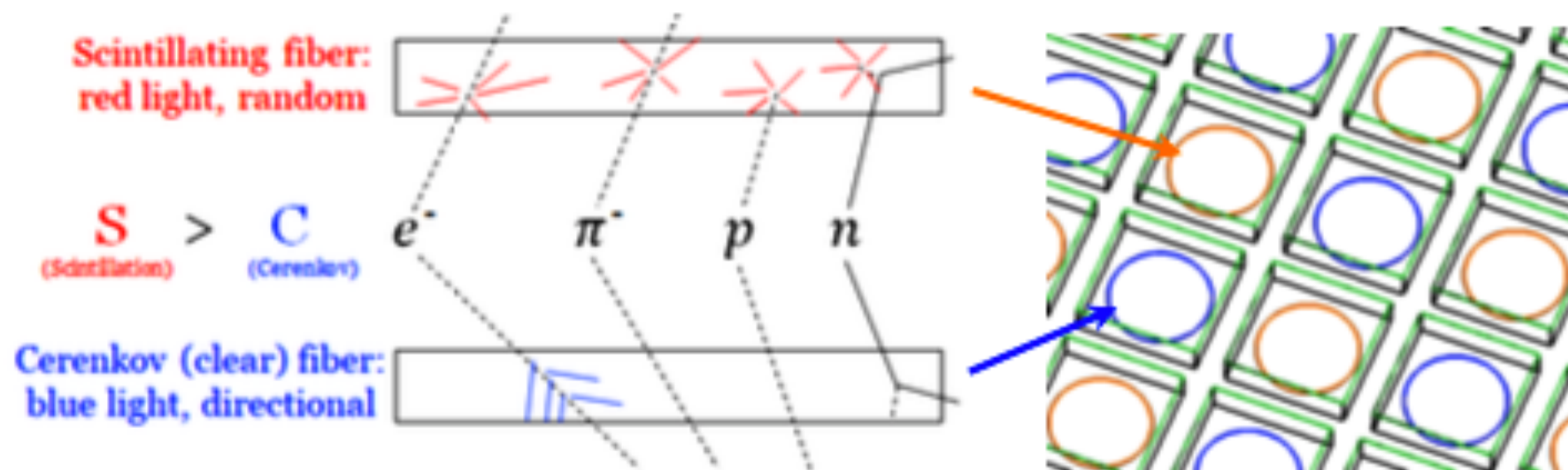
**International Detector for Electron-positron Accelerators:** specific design for FCC-ee / CepC



- 2T SC solenoid 2T ultra-thin and transparent before calorimeters
- Silicon vertex detector + short-drift, ultra-light wire chamber
- Silicon wrapper pre-shower/timing counter
- **Single Dual-readout calorimeter for EM&HAD calorimetry** + optional crystal DR EM
- MS: thin iron yoke equipped with RPCs

# DRC PRINCIPLE

correct shower energy event by event for non-compensation by measuring the EM fraction in hadronic shower by sampling with two readouts of different e/h response: Cherenkov (C) mostly sensitive to the em shower component, Scintillation (S) sensitive to all

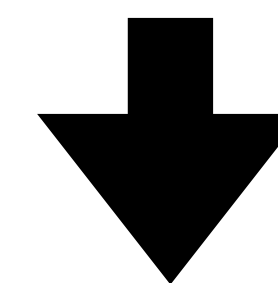


different patterns of S vs C light from different particles, combined with the fine segmentation provided by the fibres can be leveraged also for powerful particle identification ...

$\langle f_{em} \rangle$  fluctuations largely determine energy resolution for jets

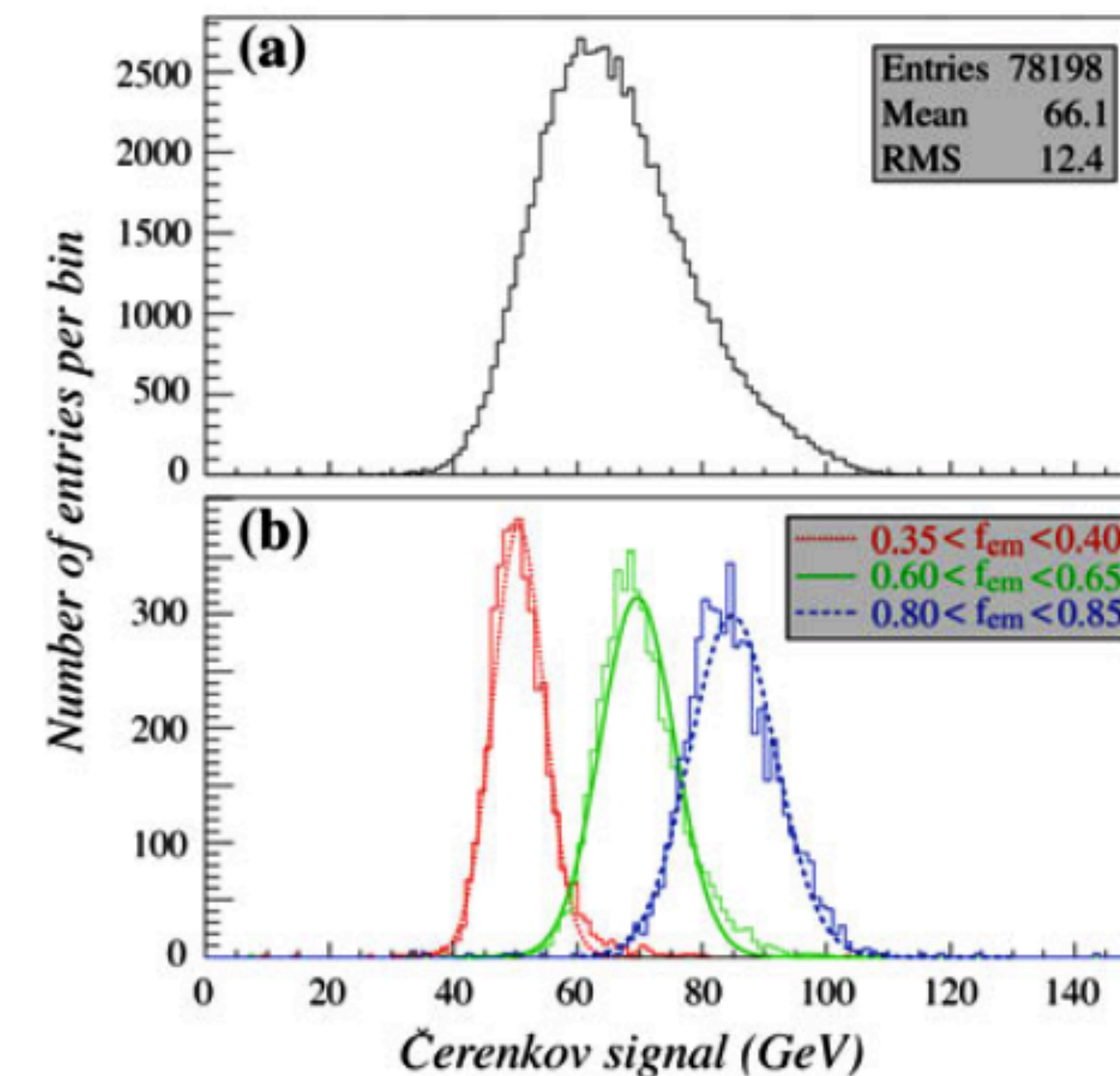
$$S = E[f_{em} + (h/e)_s(1 - f_{em})]$$

$$C = E[f_{em} + (h/e)_c(1 - f_{em})]$$

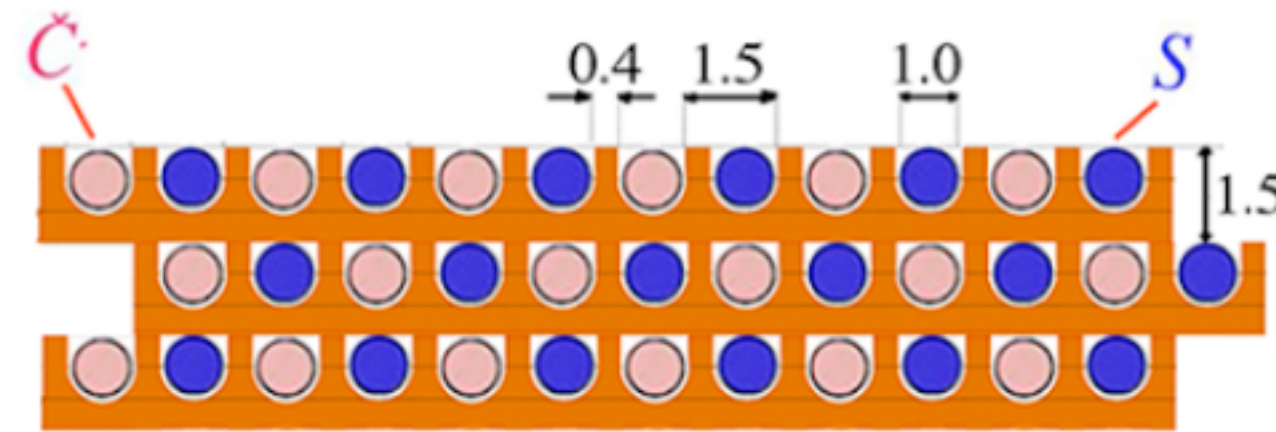
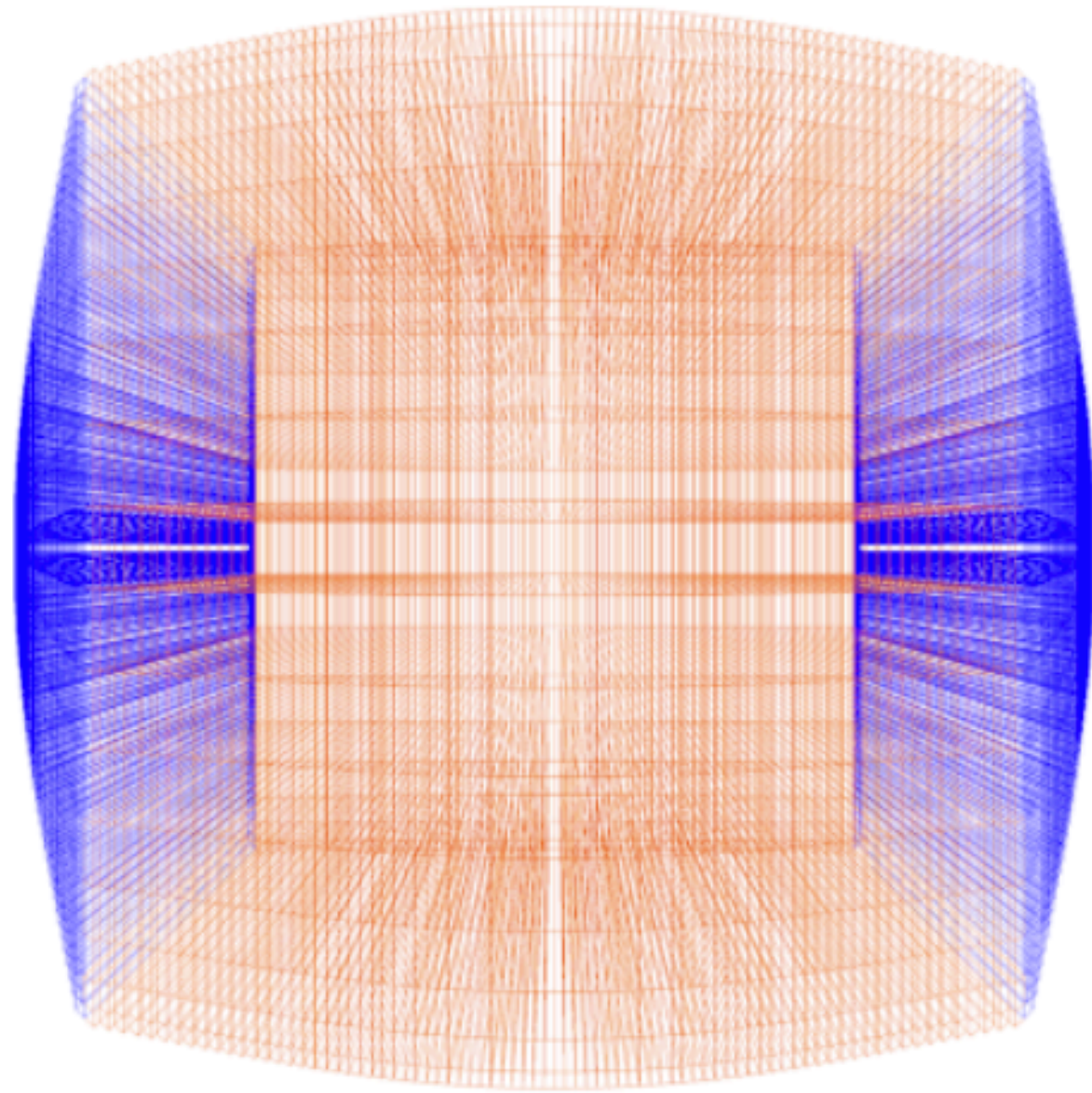


two equations in two unknowns:  $f_{em}$  and  $E$

$$E = \frac{S - \chi C}{1 - \chi} \quad \frac{1 - (h/e)_s}{1 - (h/e)_c} = \chi$$

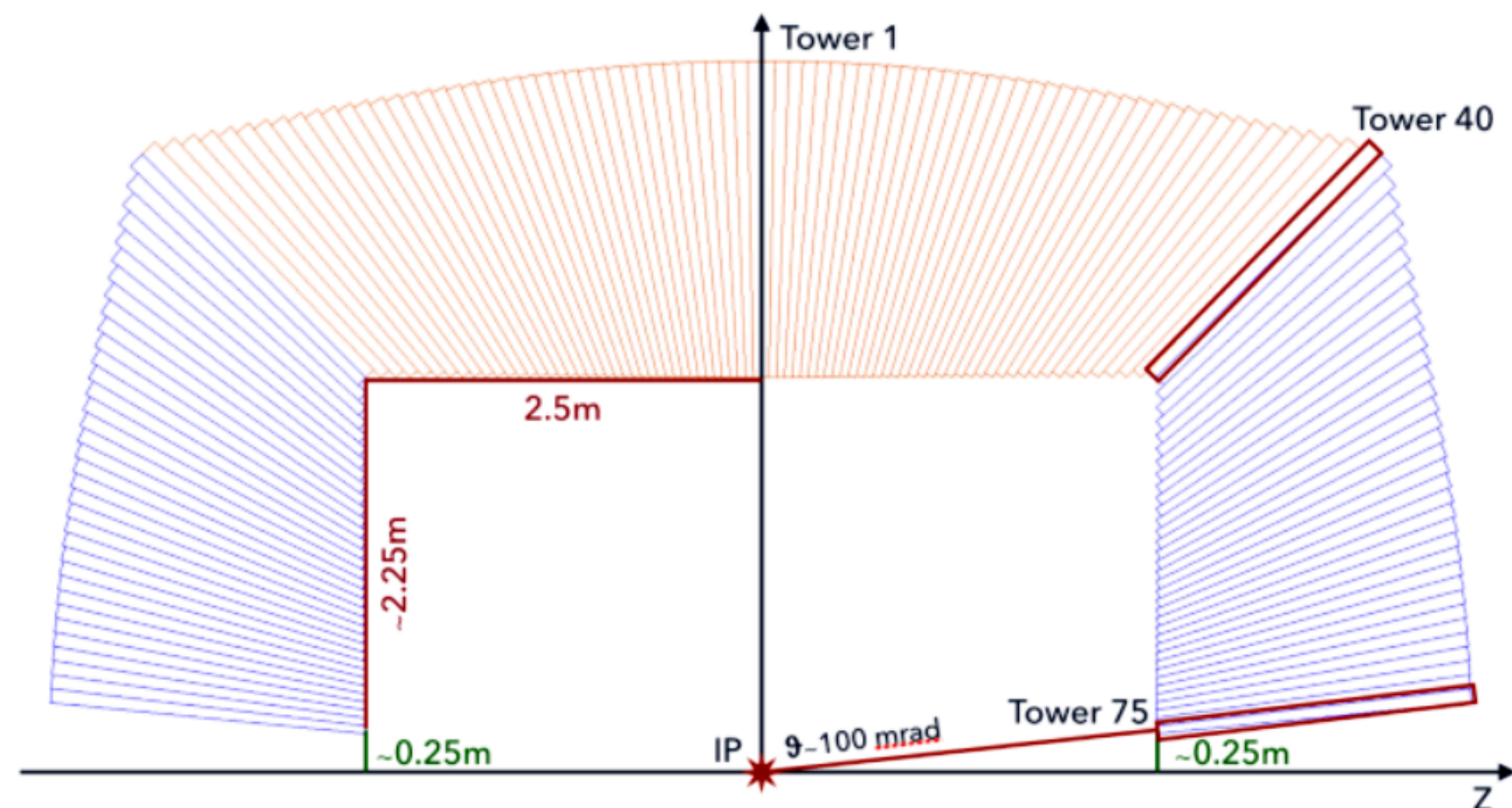


# IDEA DRC FULL SIMULATION



- full G4 simulation of the calorimeter geometry:
  - includes B field and solenoid material in front of the calorimeter
  - fiber-sampling calorimeter: Cu absorber, 1mm fibres, 1.5mm pitch
  - read out of each single fibre via SiPM
  - 130 M channels, excellent granularity and lateral shape sensitivity:

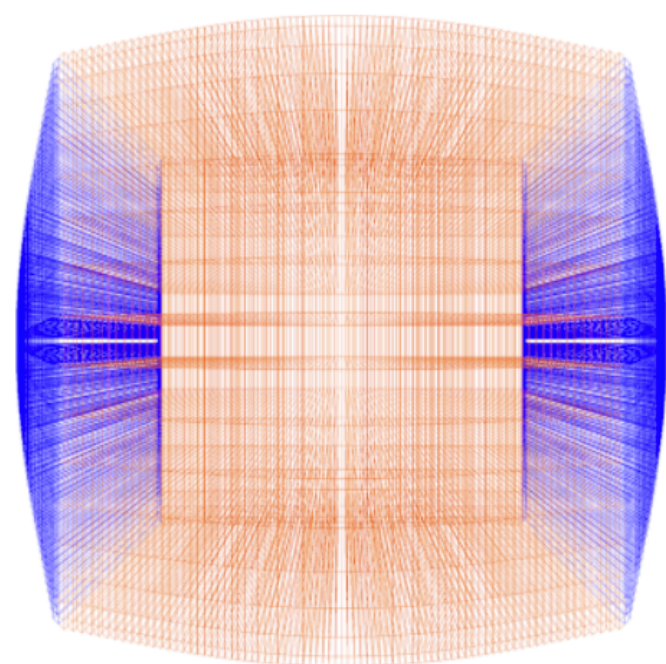
$$\Delta\theta, \Delta\phi = \sim 0.035^\circ$$



- parametrised simulation of SiPM readout and signal processing
  - dark counts, crosstalk, afterpulses, saturation, noise, ...



# DATASETS



- Pythia8  $e^+e^- \rightarrow Z \rightarrow \tau$  and  $qq$  at Z pole
- 5000 events for each decay mode

- **Information available for each fibre:**

- geometrical quantities:  $\Delta\theta$ ,  $\Delta\phi$  wrt the tau/jet cluster center
- energetic quantities: # of photo-electrons in fibres and energy (scintillation and Cherenkov)
- SiPM information (1 SiPM per fibre): Integral and Peak of the SiPM output, Time of Arrival, Time over Threshold, Time of Peak

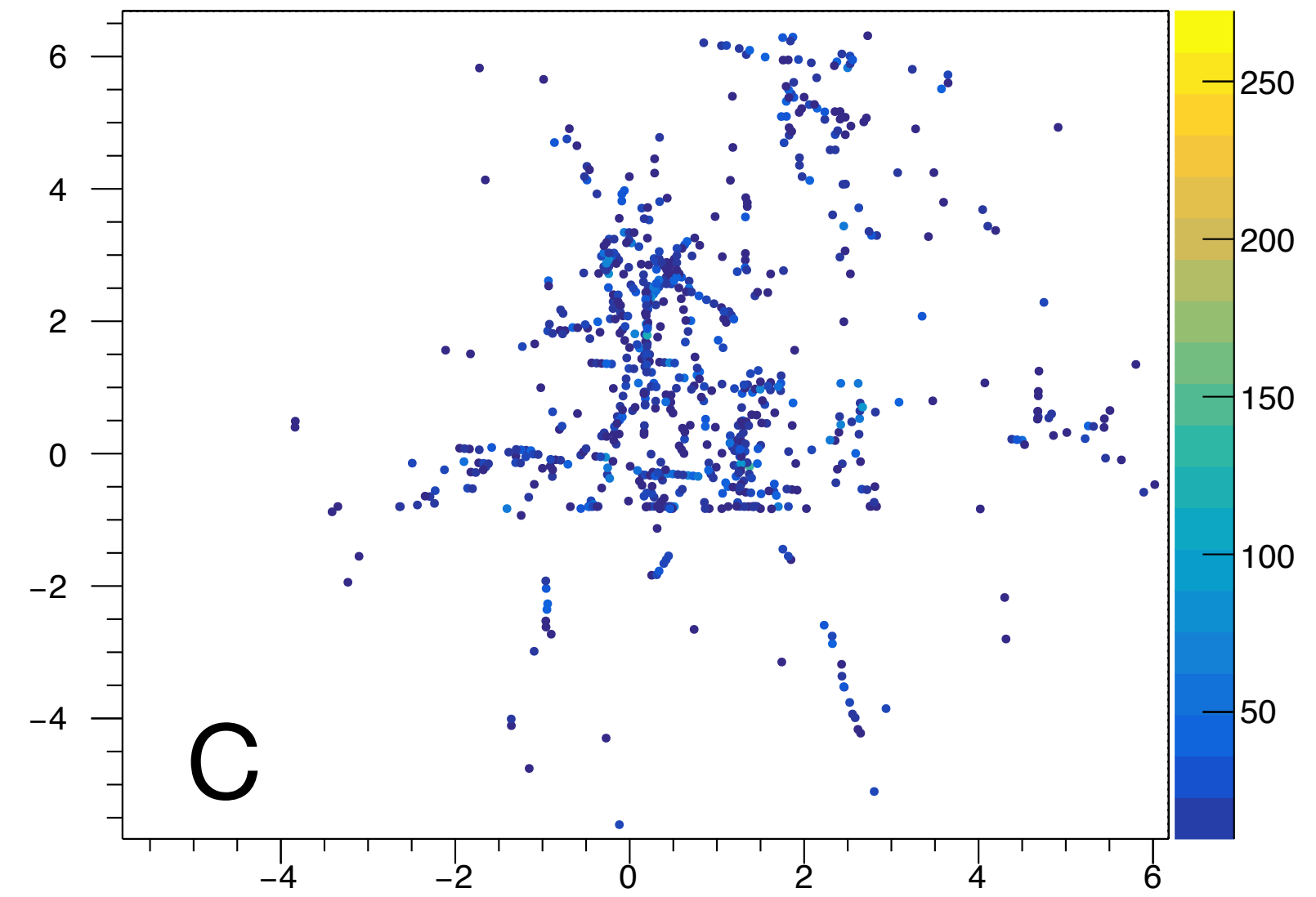
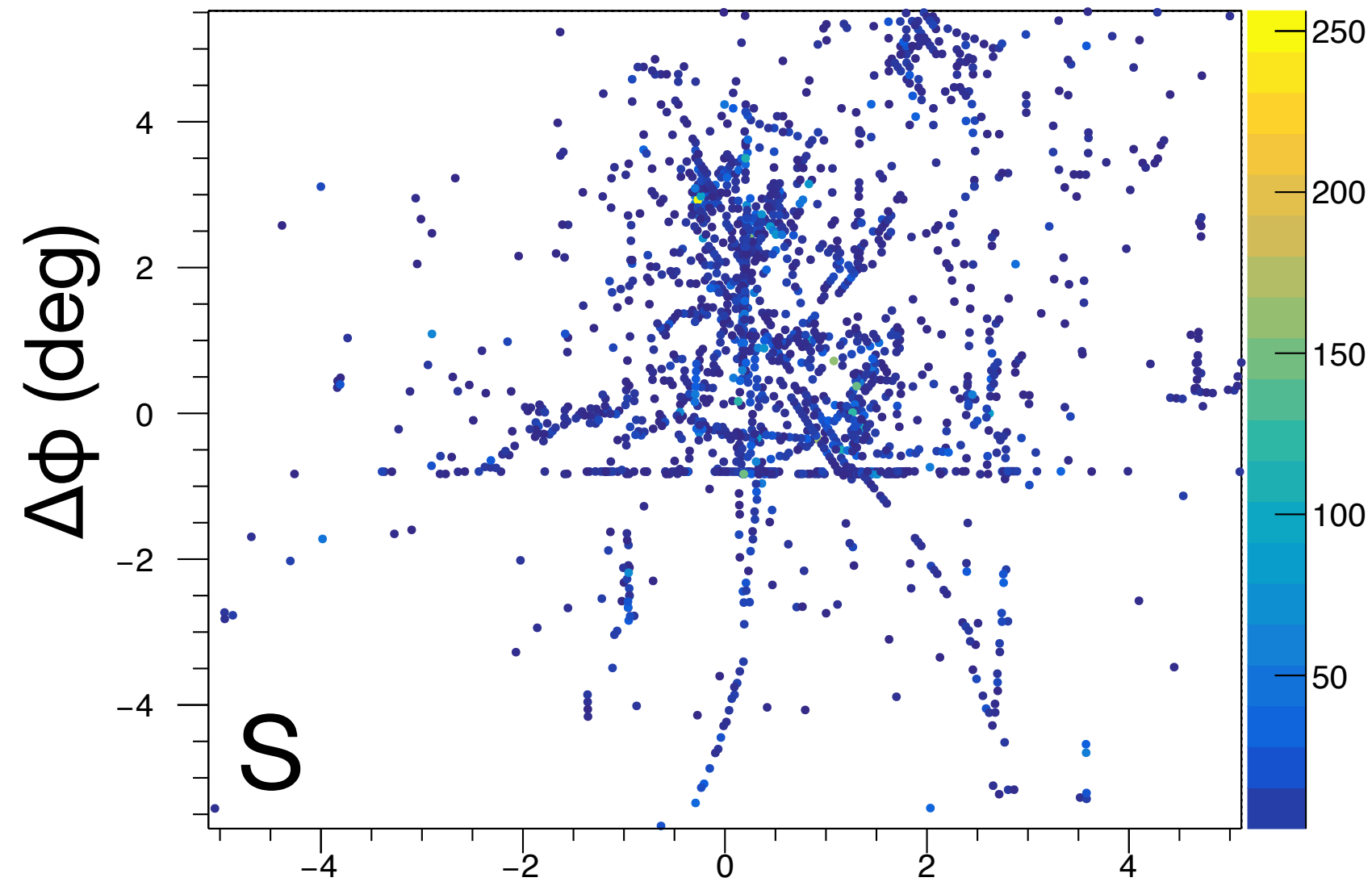
- **Ground truth labels:**

- fiber type (scintillating or cherenkov)
- decay type label

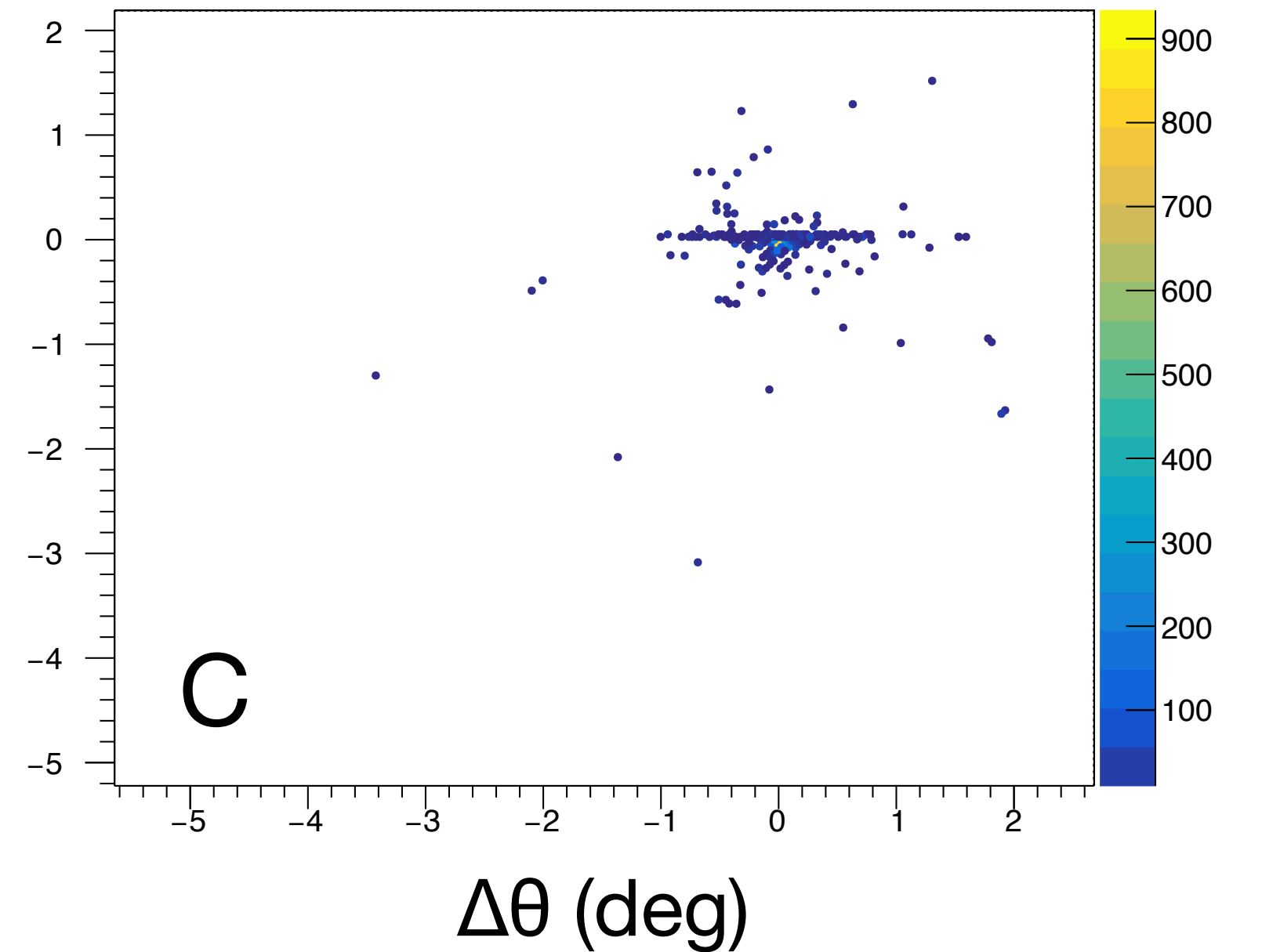
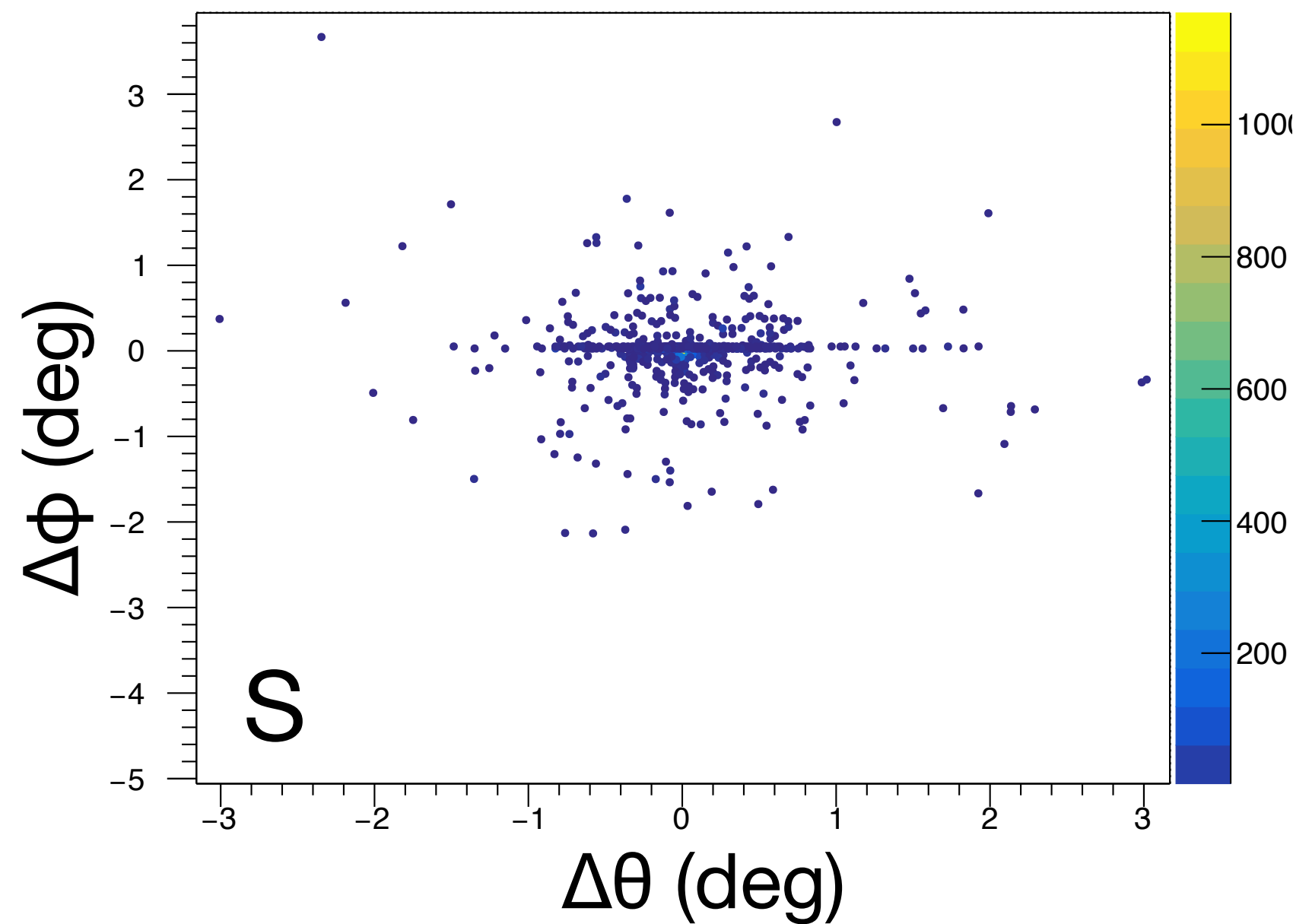
Decay	Label 8-class
$\tau^- \rightarrow e^- \nu_e \nu_\tau$	0
$\tau^- \rightarrow \pi^- \nu_\tau$	1
$\tau^- \rightarrow \pi^0 \pi^- \nu_\tau$	2
$\tau^- \rightarrow \pi^0 \pi^0 \pi^- \nu_\tau$	3
$\tau^- \rightarrow \pi^- \pi^- \pi^+ \nu_\tau$	4
$\tau^- \rightarrow \pi^0 \pi^- \pi^- \pi^+ \nu_\tau$	5
$\tau^- \rightarrow \mu^- \nu_\mu \nu_\tau$	6
$Z \rightarrow q\bar{q} \rightarrow jet\ jet$	7

# EXAMPLES OF EVENTS WITH FULL GRANULARITY

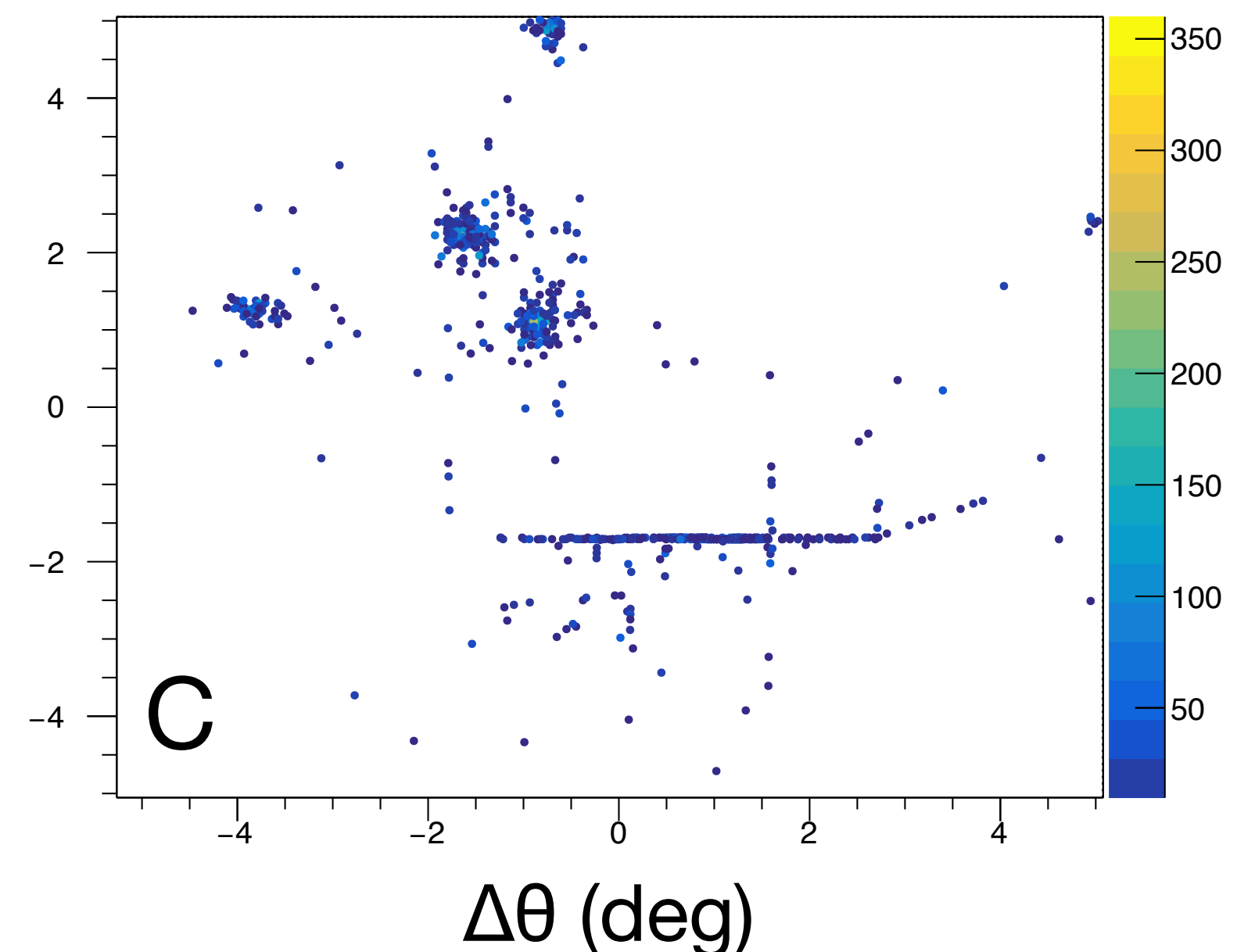
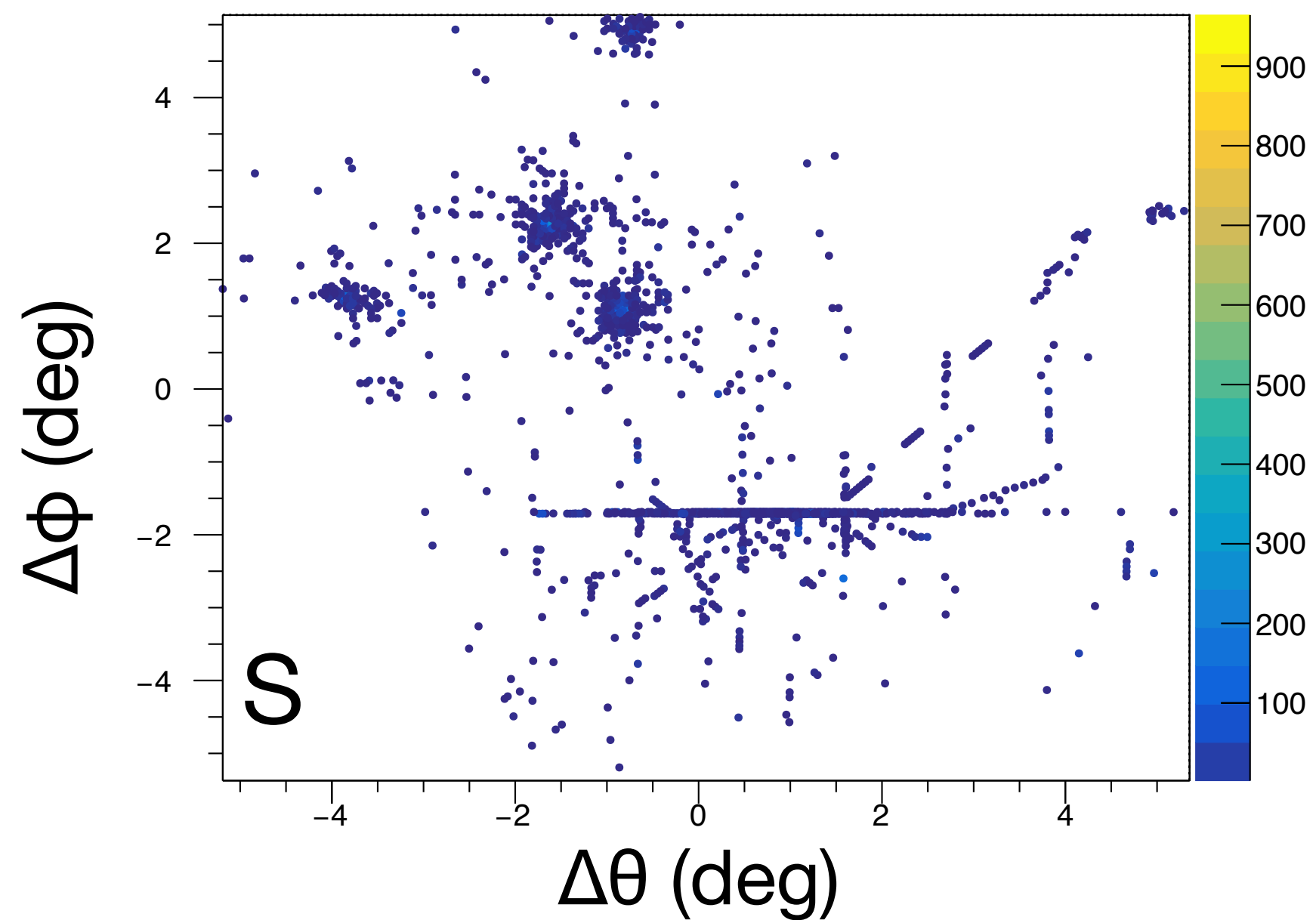
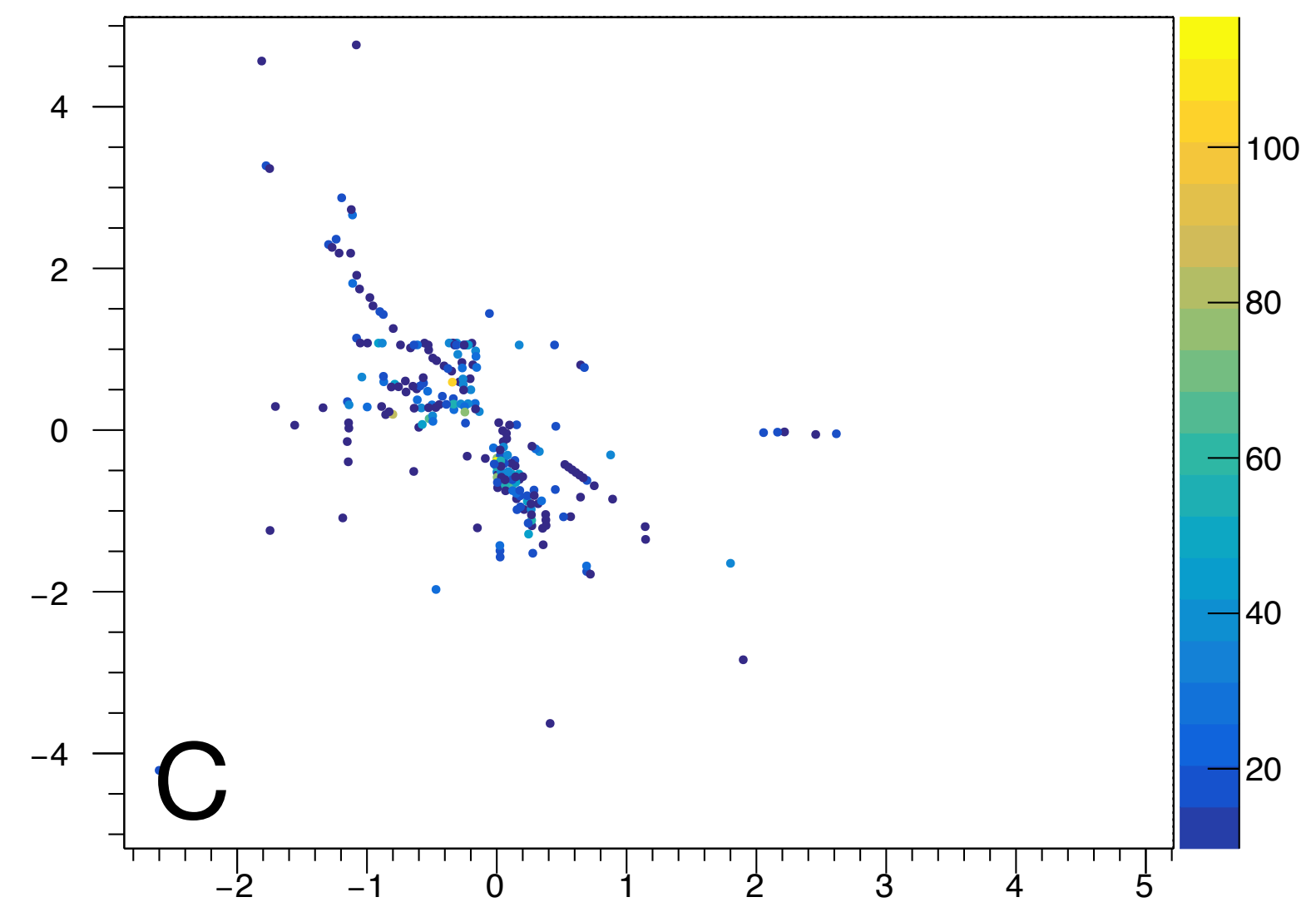
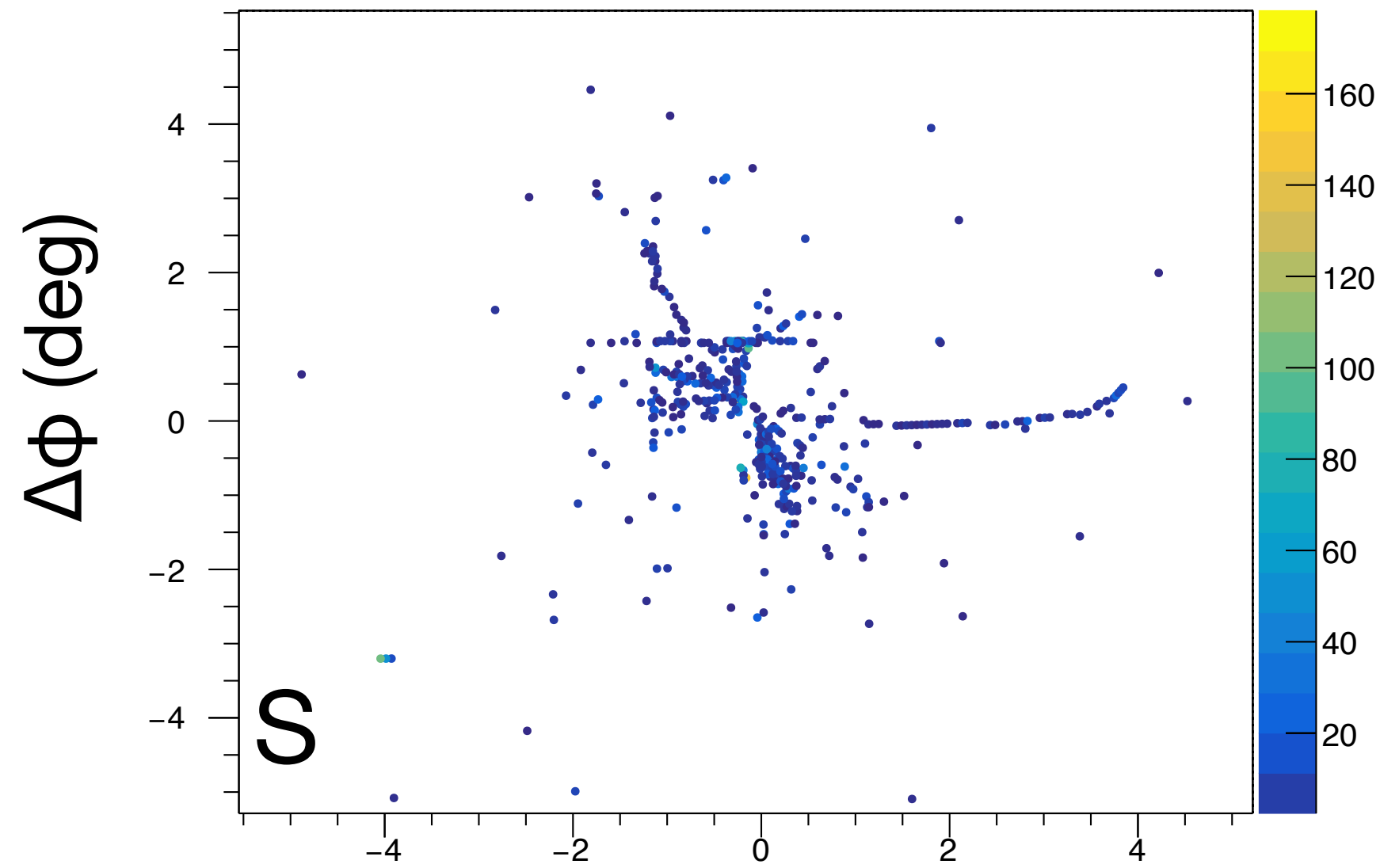
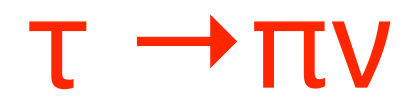
$Z \rightarrow qq$  Jets



$\tau \rightarrow e\nu\nu$



# EXAMPLES OF EVENTS WITH FULL GRANULARITY



# MAIN ISSUES IN TRAINING A DL MODEL TO IDENTIFY TAUS IN DRC

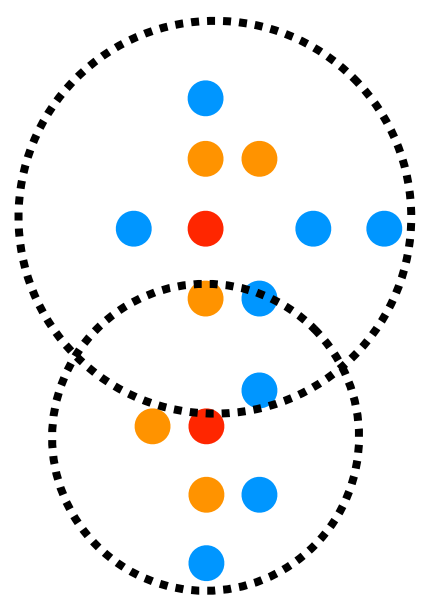
- **sparsity of data representation:** fired fibres are 5-10% of the total ← makes use of CNN architectures inefficient and hard to train
  - **solution:** use point-cloud/graph representations
- ability to **extract confidence measures on the prediction** of the ANN models ← modern modern ANNs are known to be not well calibrated (e.g. softmax outputs vs true class probabilities)
  - **solution:** calibrate the ANN output, for example by using dropout to adjust the output, or by using conformal predictions or bayesian weights to directly quantify the model uncertainty

# DATA REPRESENTATION

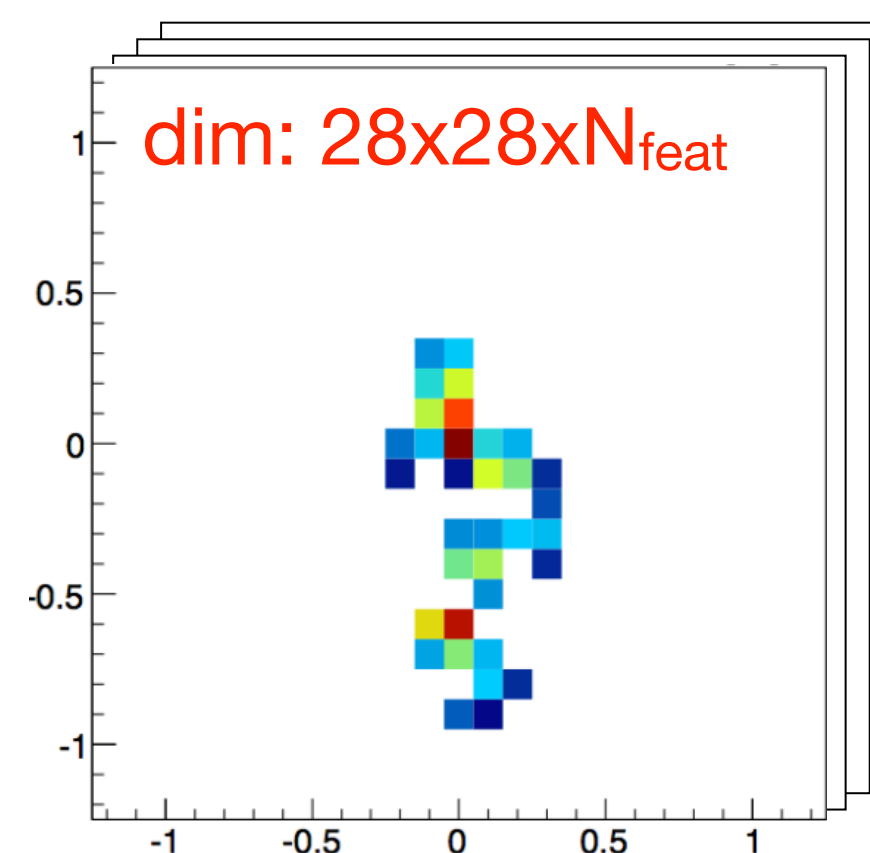
- **Image-based:** treating the energy deposition on each fiber as the pixel intensity creates an image of the event in fixed-shape mesh
  - natural representation for Convolutional Neural Networks
  - unclear how to incorporate additional information from the fibers
  - very sparse and inefficient representation: jets/tau decays have  $O(10)$  to  $O(100)$  particles  $\rightarrow$  more than 90% of the pixels are blank
- **Point cloud-based:** unordered sets of entities distributed irregularly in space, analogous to the point cloud representation of 3D shapes
  - clouds allow rich internal structures
  - straightforward to incorporate additional information of the fibers (fibre type, energy, time information, ...)
  - the architecture of the neural network has to be carefully designed to fully exploit the potential of this representation  $\rightarrow$  Graph Neural Networks (also RNN, Transformers, ...)

## Example

boosted  $W \rightarrow qq'$

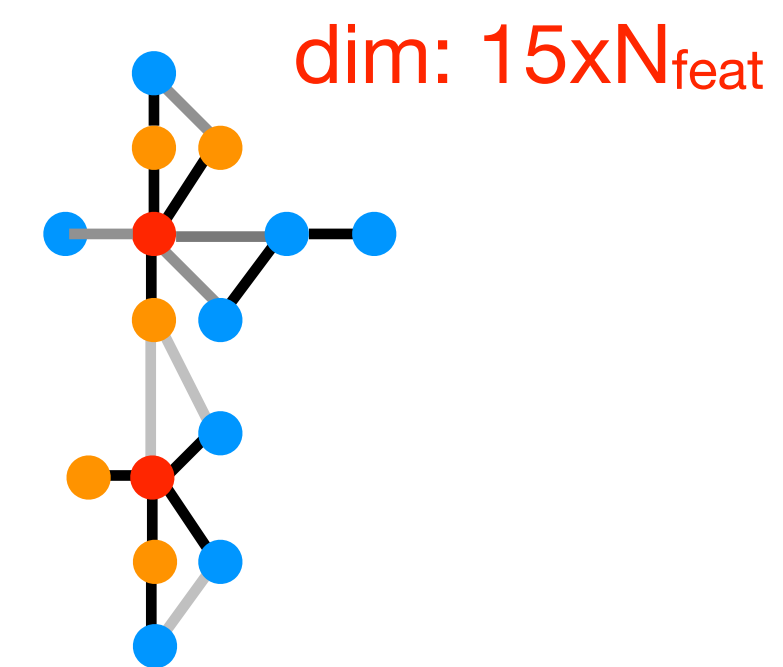


fixed-mesh image rap.

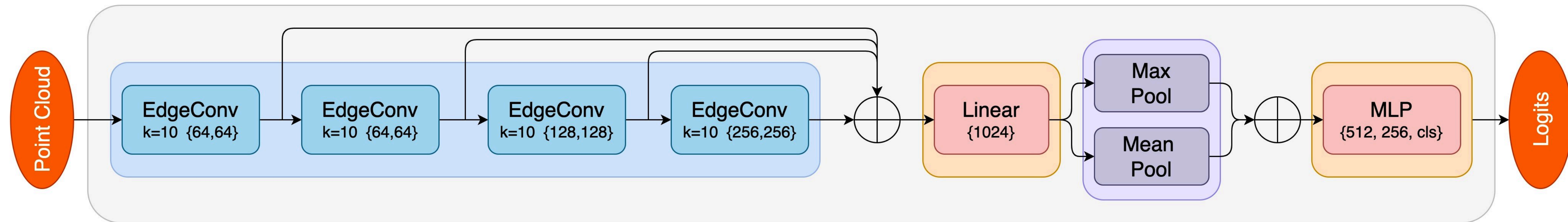


VS

graph representation



# DGCNN ARCHITECTURE



Input:

$x = \{\theta, \phi, \text{geometrical features, SiPM features, ...}\}$

local feature extractor

feature aggregator

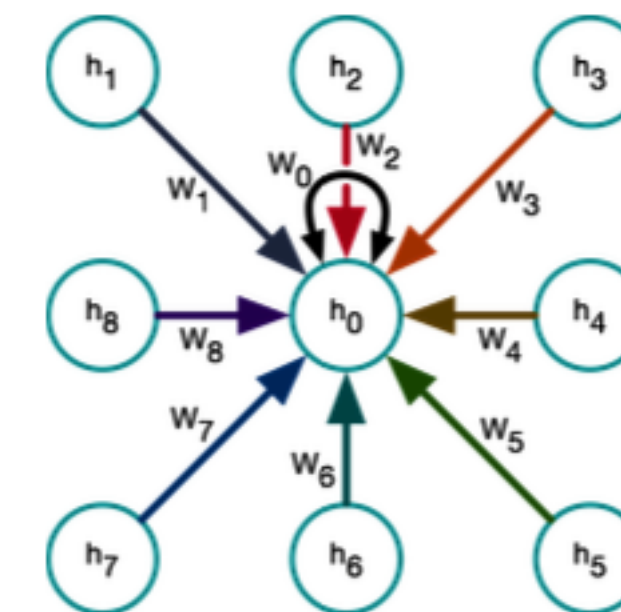
MLP global classifier

- simple and flexible architecture optimised for point cloud inputs able to learn both local (through the edge convolution) and global (through skip connections & feature aggregator) structures on the input data
- simplify inclusion of additional features and SiPM information
- # of input fibres fixed and treated as model hyper parameter, discarding those with lowest signals or adding zero valued vectors and masking in case of events with lower active fibres
- hyper-parameters chosen using a validation set

# EDGE CONVOLUTION

Regular convolution operators cannot be applied on point clouds:

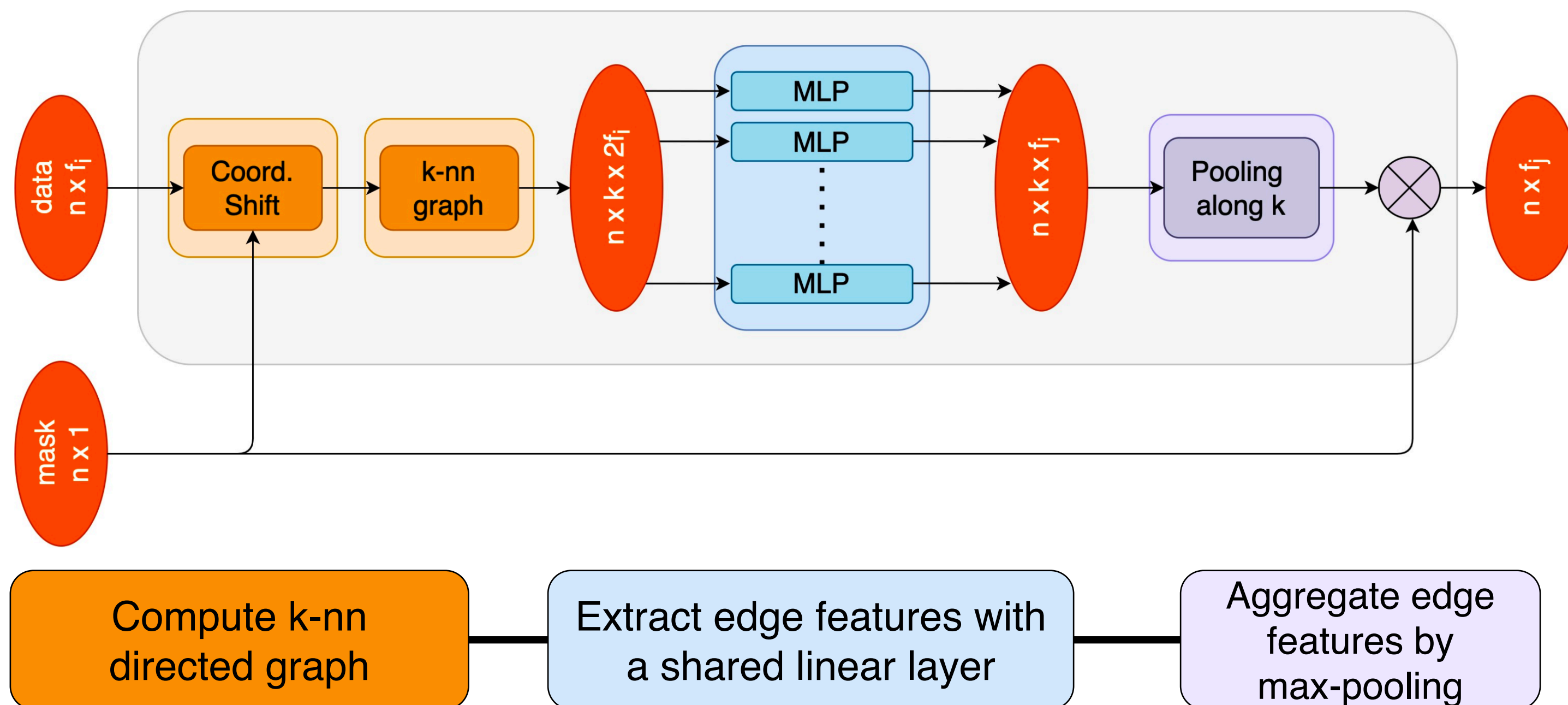
- points distribution is usually irregular (unlike uniform grids of the pixels in an image)
- they're not invariant under permutation of the points



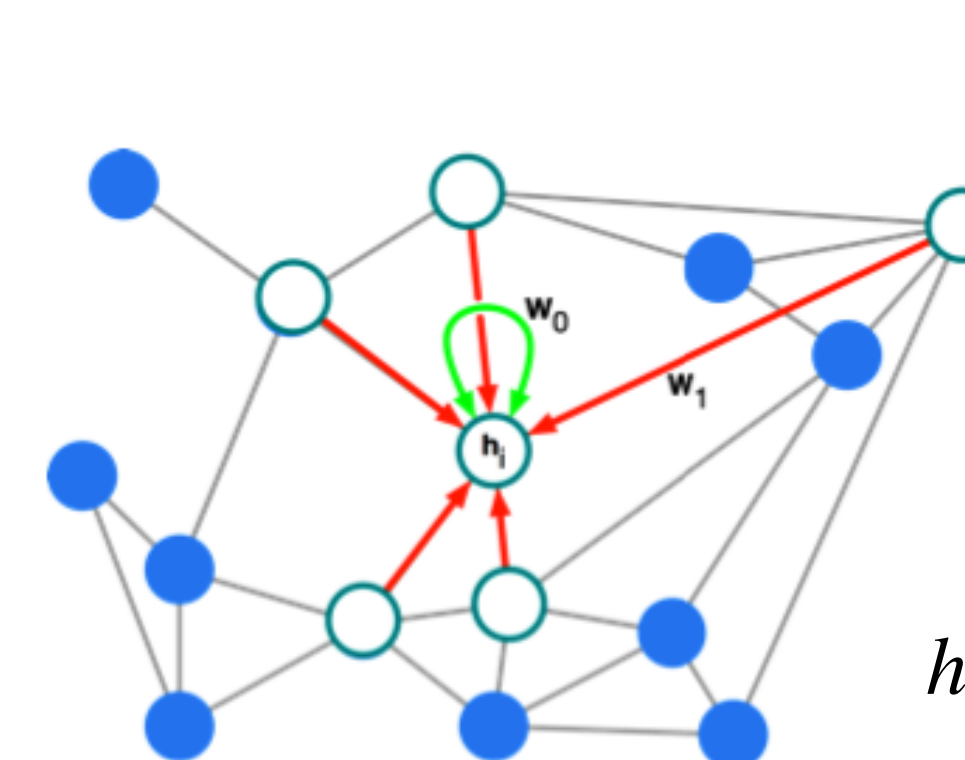
CNN-conv

$$h'_o = \sum_{i=0}^8 h_i w_i$$

Viable solution: **EDGE convolution**: point cloud represented as a graph with **Vertices** (the points themselves) and **Edges** (connections between each point to its  $k$  nearest neighbouring points): results in a **regular distribution** for each point, for which is possible to define convolution operations



ex.  $k=6$



EDGE-conv

$$\sum_{j \in N_k(h_i)} ; \max_{j \in N_k(h_i)} ; \dots$$

$$h'_i = \max_{j \in N_k(h_i)} f_w(h_i, h_j)$$

$$f_w(h_i, h_j) = \text{ReLU}(w(h_j - h_i) + w_0 h_i)$$

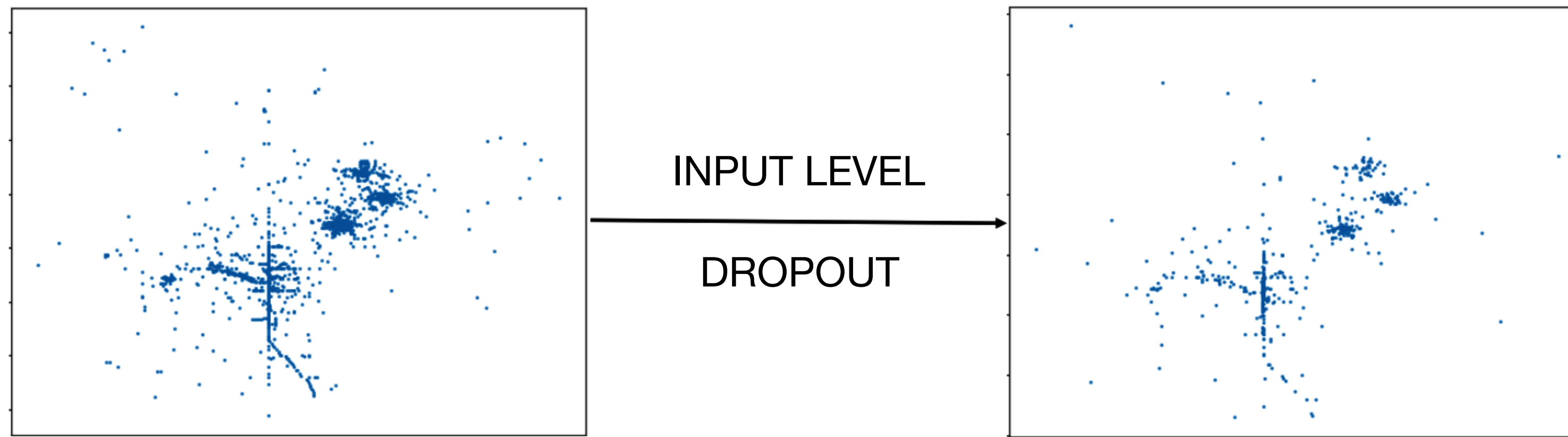
# $\tau$ DECAY IDENTIFICATION WITH DGCNN

- **Classification task:**
  - 8-classes: 7 tau decays + QCD jets
  - training/validation/test sets: 22k/6k/7k events (balanced among classes)
- **Data-preprocessing:**
  - simple geometrical clustering, no specific selection or fiducial volume applied
  - saved fibres signal around each cluster ( $\sqrt{\Delta\theta^2 + \Delta\phi^2} < 1$ )
- **DGCNN inputs:**
  - jet/tau representation: 2D point-cloud of fibres coordinates
  - fiber type (S, C), #photo-electrons, SiPM's: Integral and Peak of the SiPM output, ToT, ToA, ToP (in different combinations)



# DATA AUGMENTATION VIA DROPOUT

- overfitting and memorisation for the DGNN model controlled using two different implementations of the dropout regularisation:
  - (traditional) in the network: some of the parameters of the last MLP block are randomly zeroed during the training phase
  - (as data augmentation/perturbation regularisation) at input level: some of the fired fibers are switched off before to be exposed to the network
- much better generalisation obtained leveraging both methods
- dropout levels optimised on validation set



# IDEAL PERFORMANCE ON TEST SET

8-class classification task w/ DGCNN

input features: **coordinates**, **type** of fibre (S/C), and **#of photo-electrons** in each fibre

small confusion only  
within topologically  
similar decays

$\tau \rightarrow e\nu\nu$	98.53	0.45	0.65	0.03	0.00	0.00	0.34	0.00
$\tau \rightarrow \mu\nu\nu$	3.20	91.35	2.21	0.25	1.71	0.19	0.94	0.14
$\tau \rightarrow \pi\pi^0\nu$	1.34	3.49	86.87	4.97	1.12	1.67	0.11	0.44
$\tau \rightarrow \pi\pi^0\pi^0\nu$	0.46	0.25	12.09	83.19	0.14	3.24	0.00	0.63
$\tau \rightarrow \pi\pi\pi\nu$	0.11	3.14	1.24	0.16	87.39	6.79	0.00	1.16
$\tau \rightarrow \pi\pi\pi\pi^0\nu$	0.16	0.30	1.82	1.57	6.42	87.04	0.03	2.66
$\tau \rightarrow \mu\nu\nu$	1.24	0.25	0.06	0.00	0.03	0.00	98.42	0.00
$Z \rightarrow qq$ jets	0.13	0.21	0.21	0.59	1.87	2.29	0.03	94.67
	$\tau \rightarrow e\nu\nu$	$\tau \rightarrow \mu\nu\nu$	$\tau \rightarrow \pi\pi^0\nu$	$\tau \rightarrow \pi\pi^0\pi^0\nu$	$\tau \rightarrow \pi\pi\pi\nu$	$\tau \rightarrow \pi\pi\pi\pi^0\nu$	$\tau \rightarrow \mu\nu\nu$	$Z \rightarrow qq$ jets

average accuracy:  
**90.8%**

small confusion only  
within topologically  
similar decays

stat. uncertainty on  
accuracies  $\sim 3\div 5\%$

Predicted BR

# PERFORMANCE ONLY USING GEOMETRICAL OR GEOM. + FIBER TYPE INFORMATION

input features: **coordinates only**

Truth BR	$\tau \rightarrow e\nu\nu$	$\tau \rightarrow \pi\nu$	$\tau \rightarrow \pi\pi^0\nu$	$\tau \rightarrow \pi\pi^0\pi^0\nu$	$\tau \rightarrow \pi\pi\pi\nu$	$\tau \rightarrow \pi\pi\pi\pi^0\nu$	$\tau \rightarrow \mu\nu\nu$	$Z \rightarrow qq \text{ jets}$
$\tau \rightarrow e\nu\nu$	90.36	4.07	2.21	0.03	0.00	0.00	3.34	0.00
$\tau \rightarrow \pi\nu$	2.57	86.24	5.39	0.25	3.59	0.17	1.57	0.22
$\tau \rightarrow \pi\pi^0\nu$	2.10	18.92	72.67	2.76	1.97	1.01	0.27	0.30
$\tau \rightarrow \pi\pi^0\pi^0\nu$	0.74	3.54	58.43	33.04	0.84	2.81	0.05	0.54
$\tau \rightarrow \pi\pi\pi\nu$	0.11	9.88	6.22	0.46	75.32	6.49	0.00	1.52
$\tau \rightarrow \pi\pi\pi\pi^0\nu$	0.11	1.49	9.30	2.90	38.28	43.75	0.05	4.12
$\tau \rightarrow \mu\nu\nu$	2.50	0.70	0.17	0.00	0.03	0.00	96.60	0.00
$Z \rightarrow qq \text{ jets}$	0.08	0.33	0.63	0.94	2.92	3.09	0.08	91.92
	$\tau \rightarrow e\nu\nu$	$\tau \rightarrow \pi\nu$	$\tau \rightarrow \pi\pi^0\nu$	$\tau \rightarrow \pi\pi^0\pi^0\nu$	$\tau \rightarrow \pi\pi\pi\nu$	$\tau \rightarrow \pi\pi\pi\pi^0\nu$	$\tau \rightarrow \mu\nu\nu$	$Z \rightarrow qq \text{ jets}$
	Predicted BR							

average accuracy: **73.7%**

**coordinates + type of fibre (S/C)**

Truth BR	$\tau \rightarrow e\nu\nu$	$\tau \rightarrow \pi\nu$	$\tau \rightarrow \pi\pi^0\nu$	$\tau \rightarrow \pi\pi^0\pi^0\nu$	$\tau \rightarrow \pi\pi\pi\nu$	$\tau \rightarrow \pi\pi\pi\pi^0\nu$	$\tau \rightarrow \mu\nu\nu$	$Z \rightarrow qq \text{ jets}$
$\tau \rightarrow e\nu\nu$	96.95	0.79	0.62	0.03	0.00	0.00	1.58	0.03
$\tau \rightarrow \pi\nu$	3.09	89.03	3.48	0.41	2.02	0.39	1.44	0.14
$\tau \rightarrow \pi\pi^0\nu$	1.77	4.83	80.45	9.25	1.61	1.67	0.16	0.25
$\tau \rightarrow \pi\pi^0\pi^0\nu$	0.30	0.38	10.43	84.55	0.16	3.87	0.05	0.25
$\tau \rightarrow \pi\pi\pi\nu$	0.16	3.52	1.38	0.35	84.82	8.79	0.03	0.95
$\tau \rightarrow \pi\pi\pi\pi^0\nu$	0.11	0.24	1.98	2.60	10.19	82.60	0.08	2.20
$\tau \rightarrow \mu\nu\nu$	2.53	0.48	0.11	0.00	0.03	0.00	96.82	0.03
$Z \rightarrow qq \text{ jets}$	0.08	0.25	0.19	1.05	2.54	4.08	0.06	91.75
	$\tau \rightarrow e\nu\nu$	$\tau \rightarrow \pi\nu$	$\tau \rightarrow \pi\pi^0\nu$	$\tau \rightarrow \pi\pi^0\pi^0\nu$	$\tau \rightarrow \pi\pi\pi\nu$	$\tau \rightarrow \pi\pi\pi\pi^0\nu$	$\tau \rightarrow \mu\nu\nu$	$Z \rightarrow qq \text{ jets}$
	Predicted BR							

average accuracy: **88.3%**

**double-readout geometry alone allows excellent tau identification**

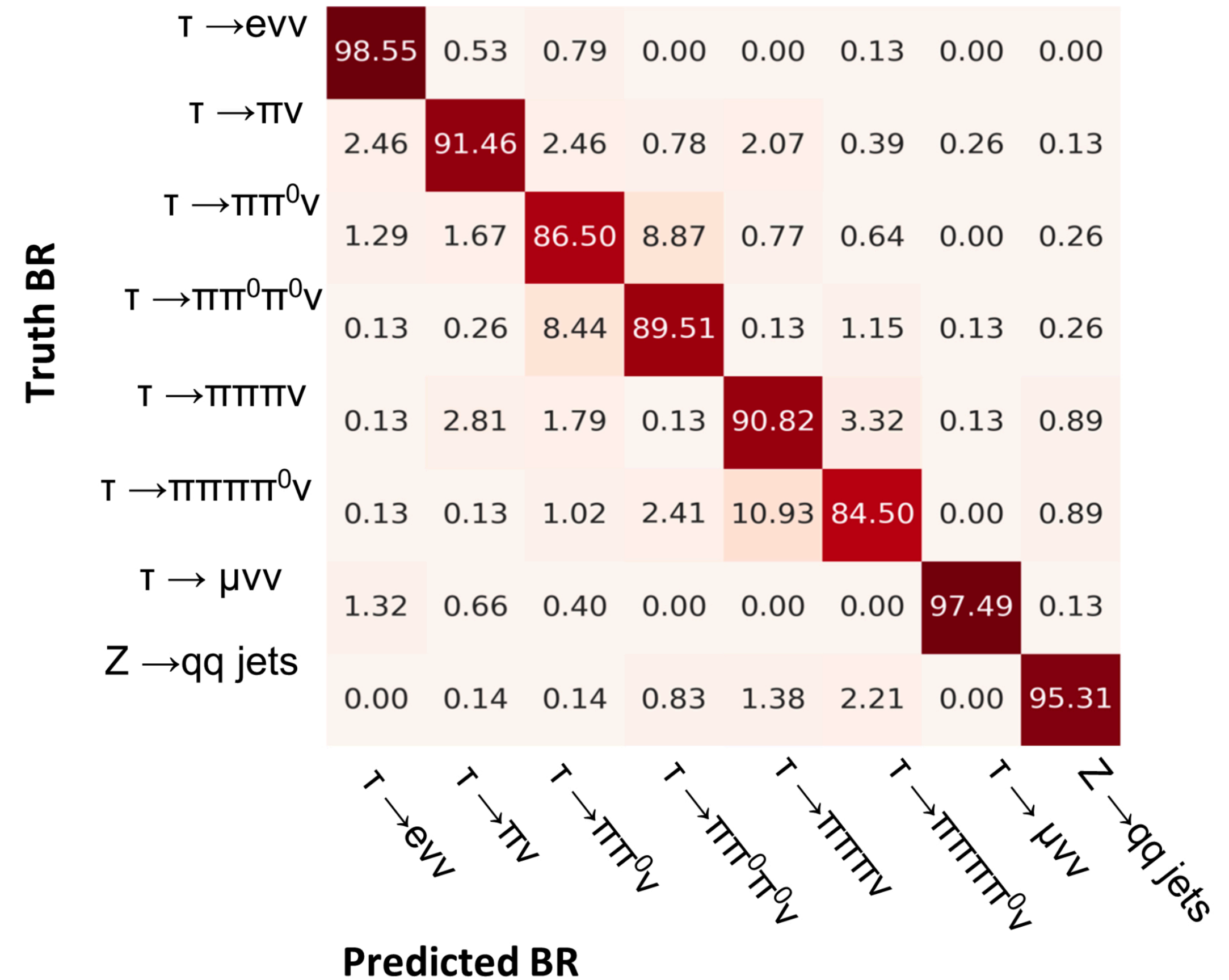
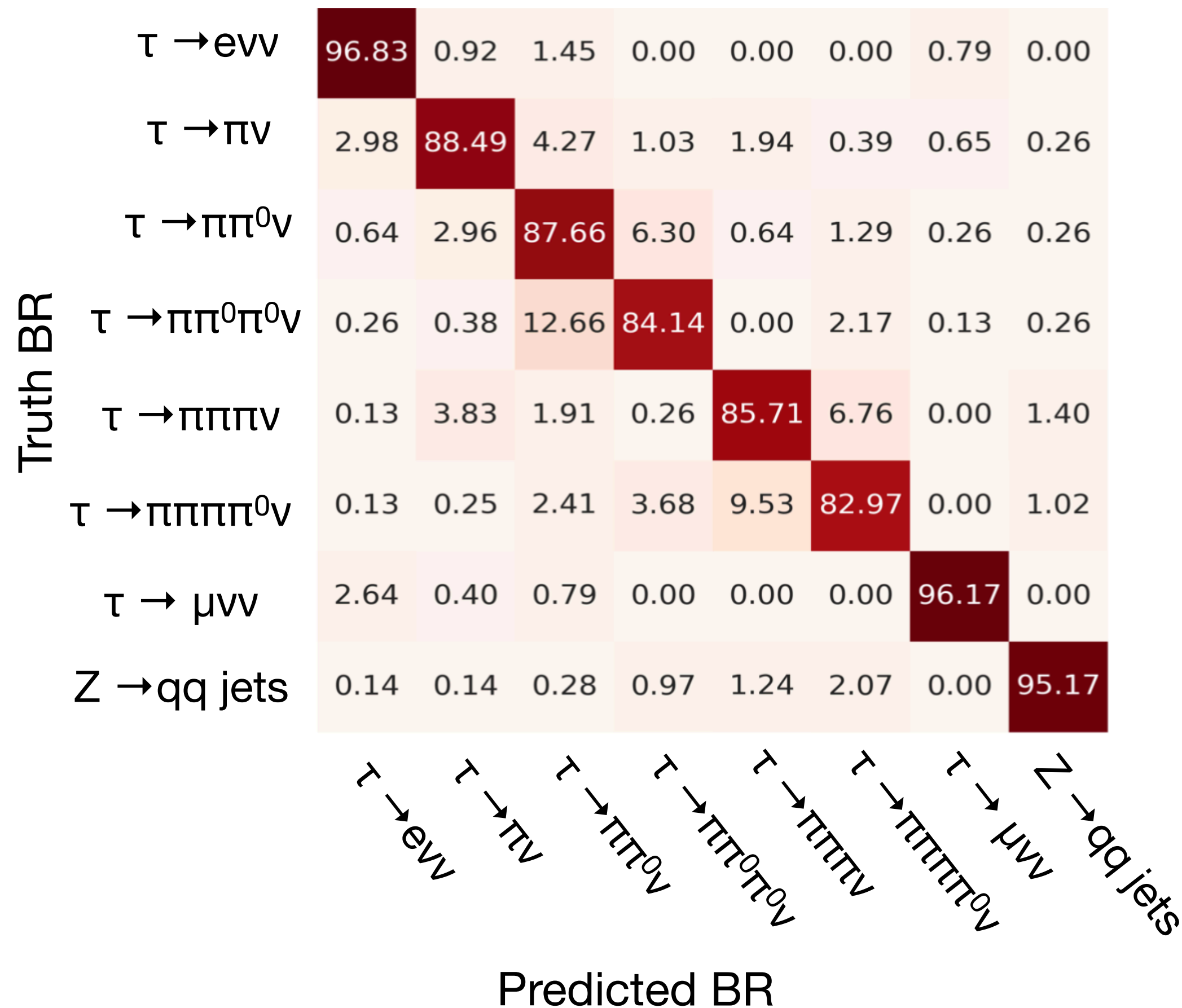
# PERFORMANCE USING REALISTIC SiPM READOUT INFORMATION

using only **geometry** and **Integral/Peak** of the signal

average accuracy:  
**88.8%**

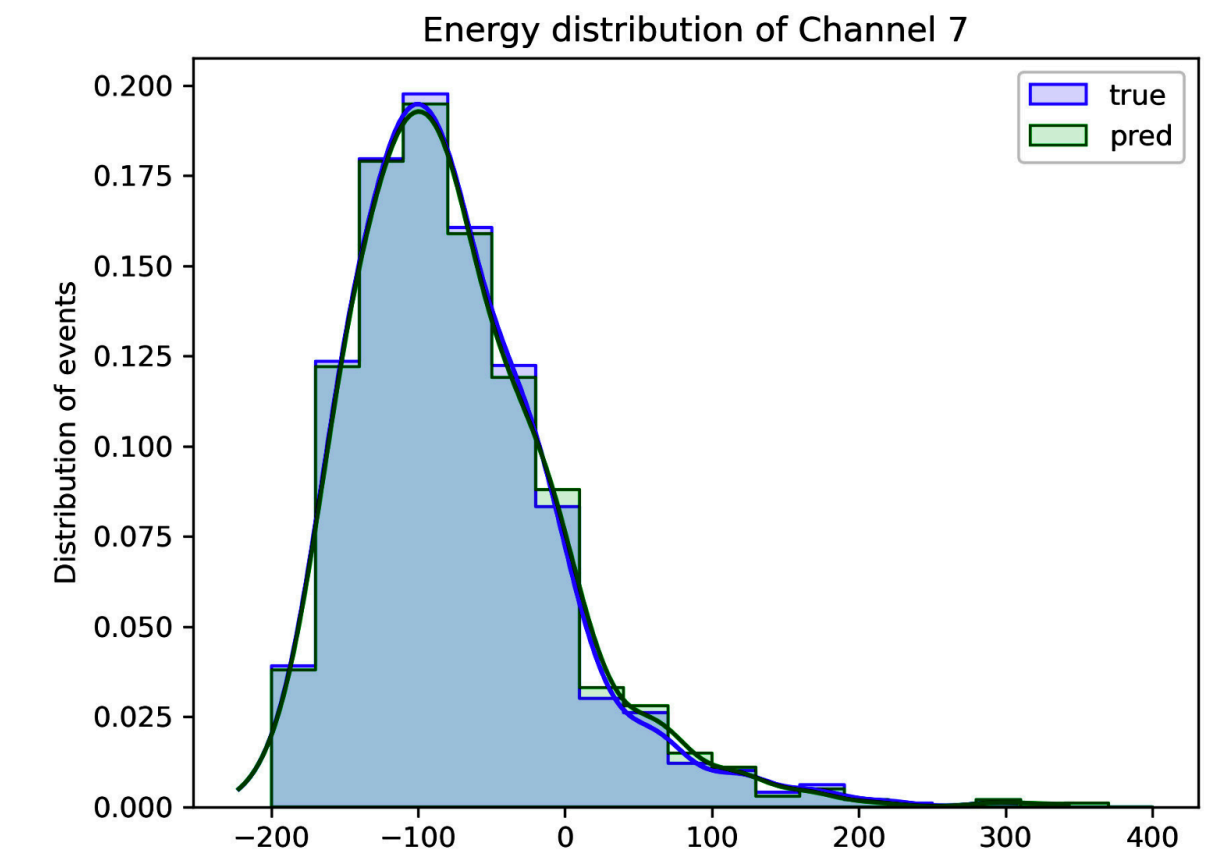
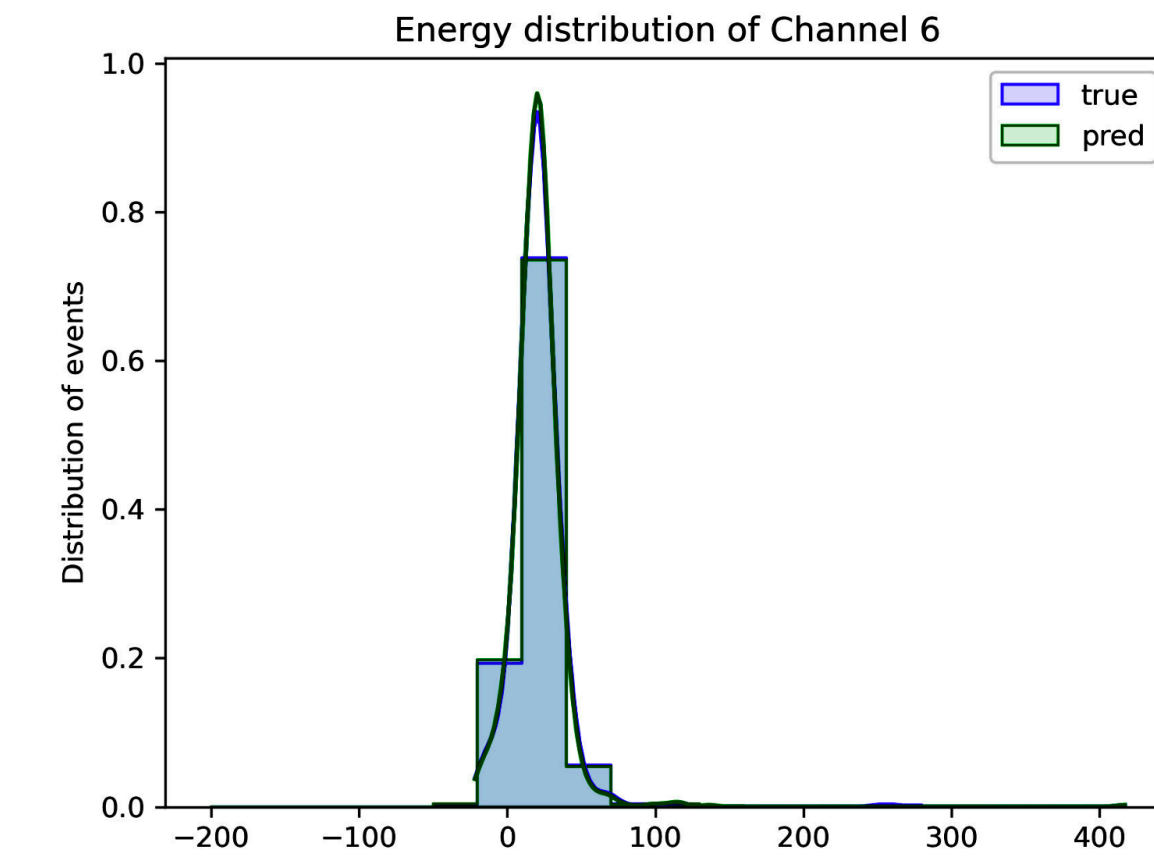
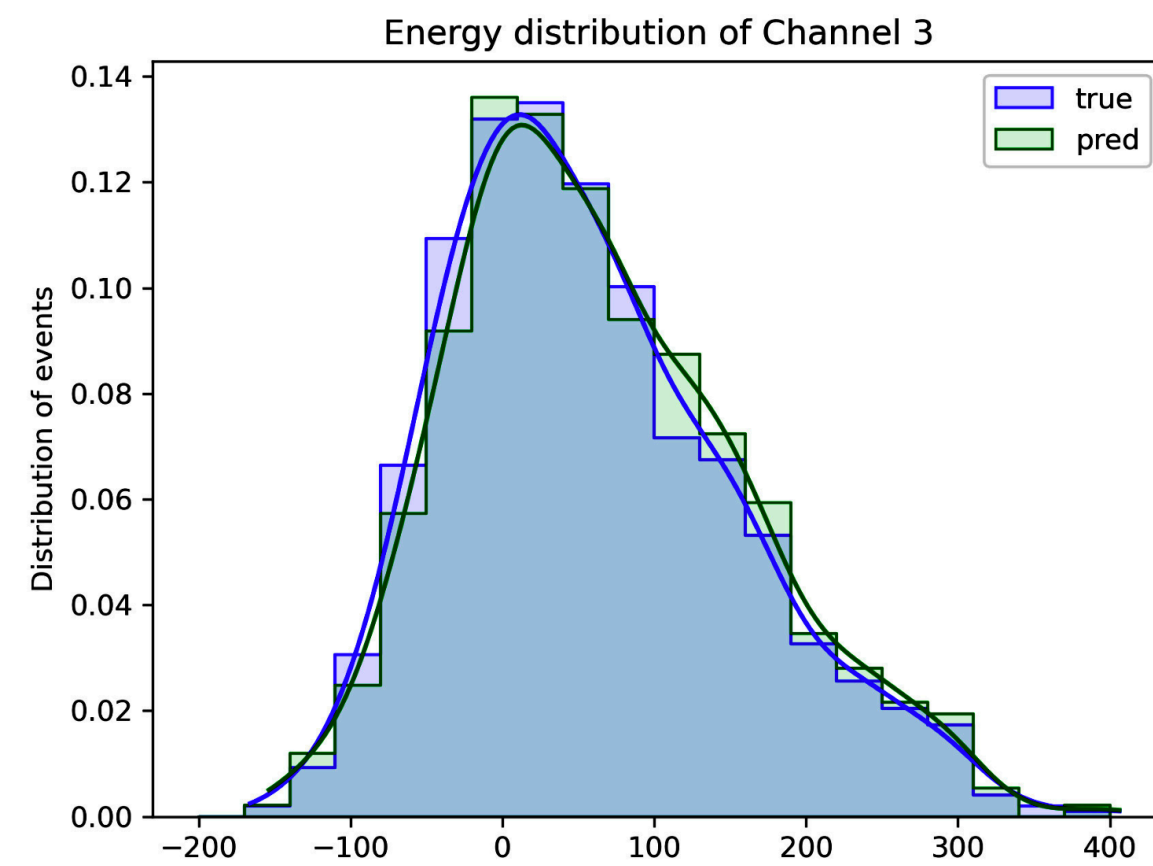
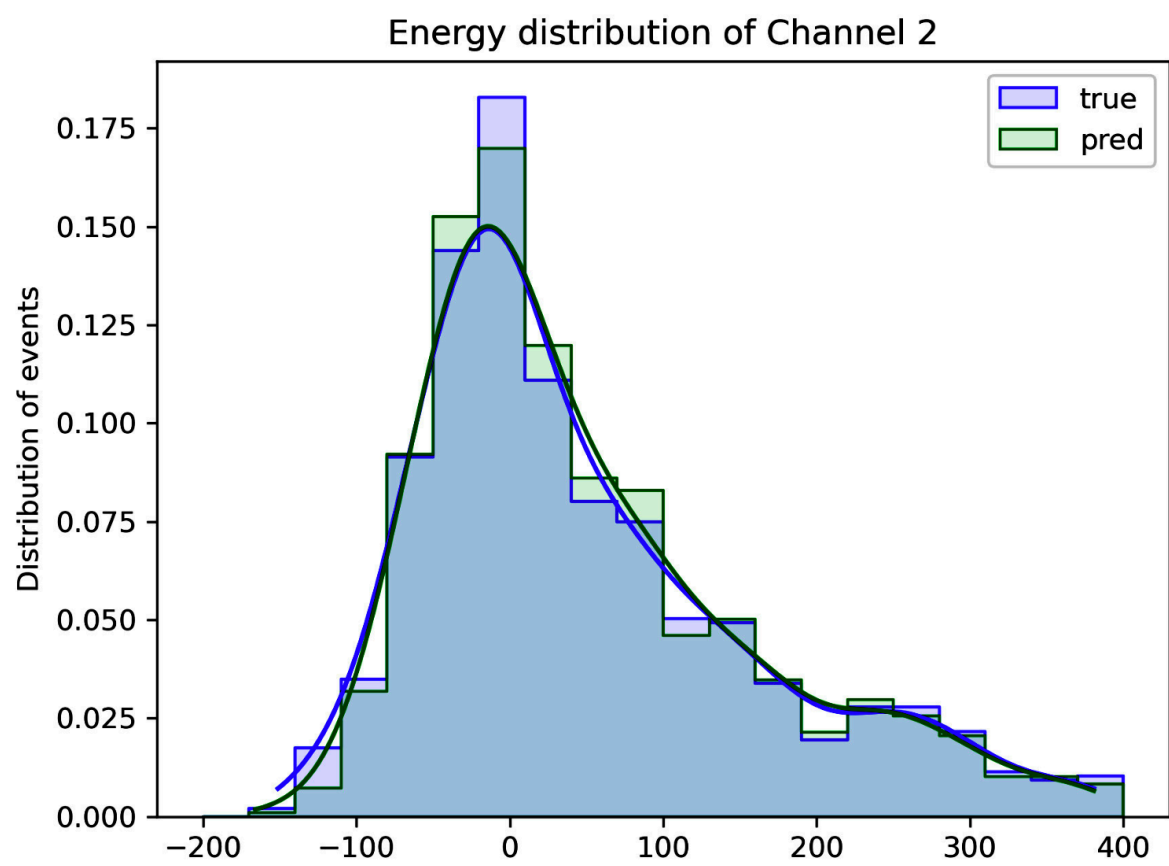
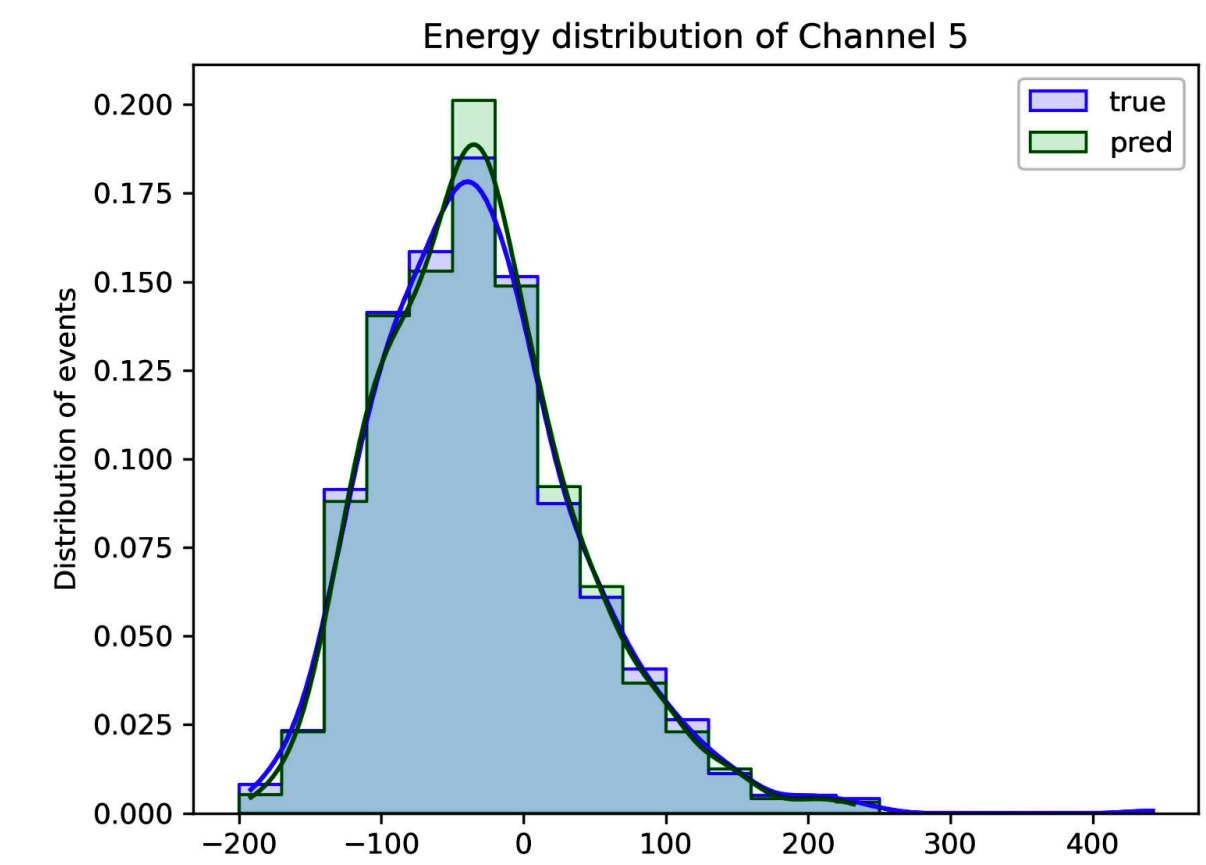
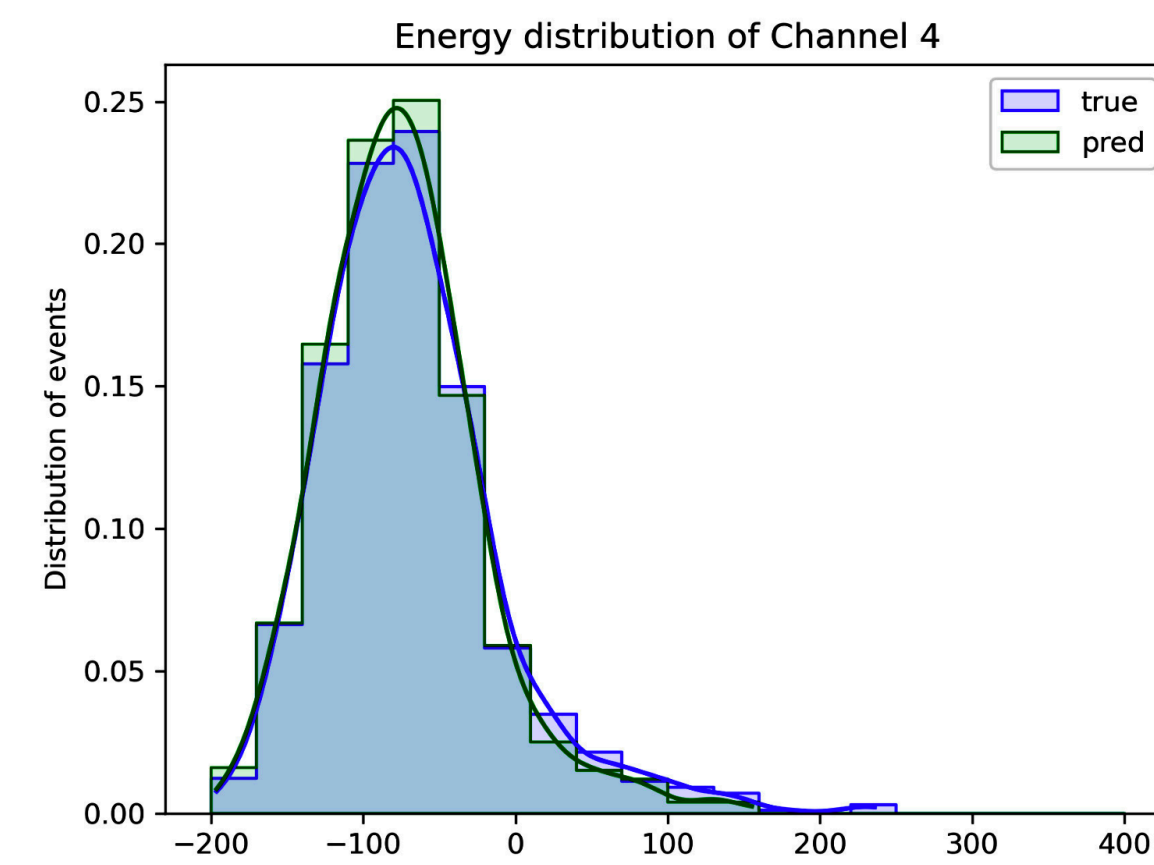
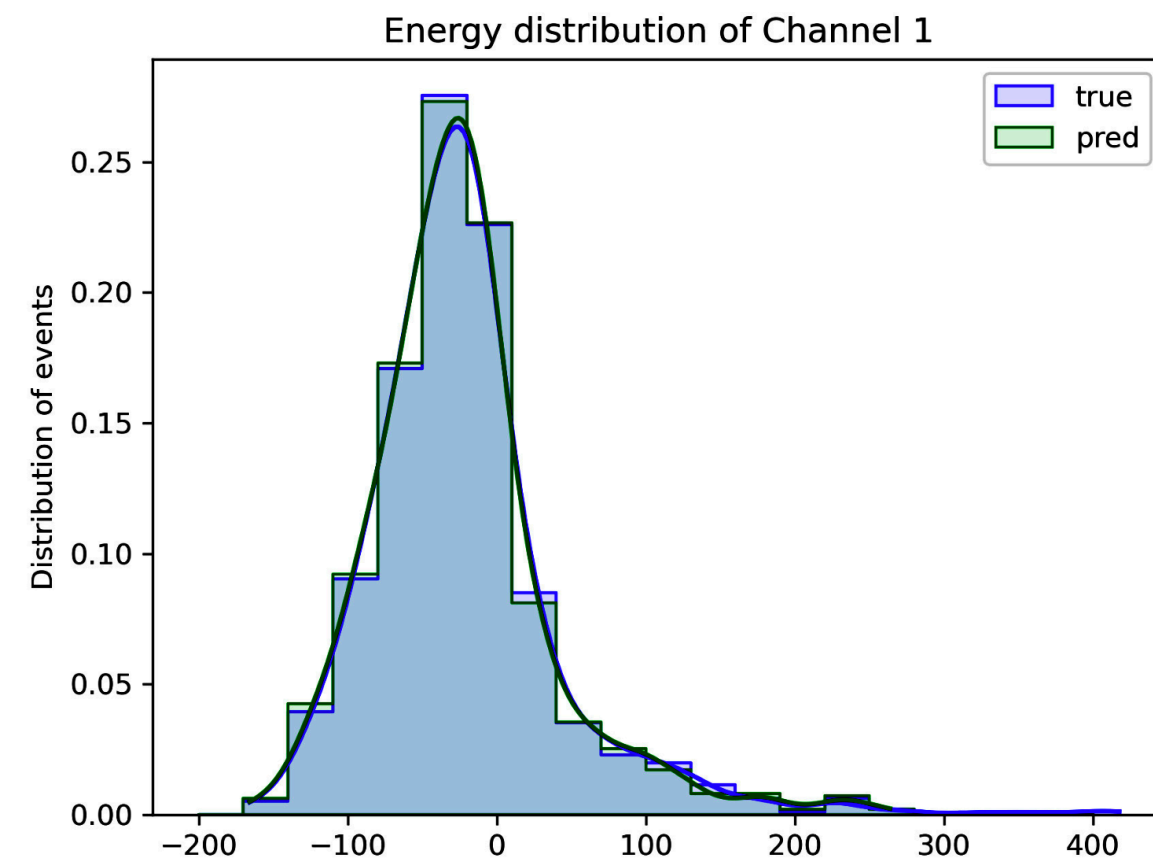
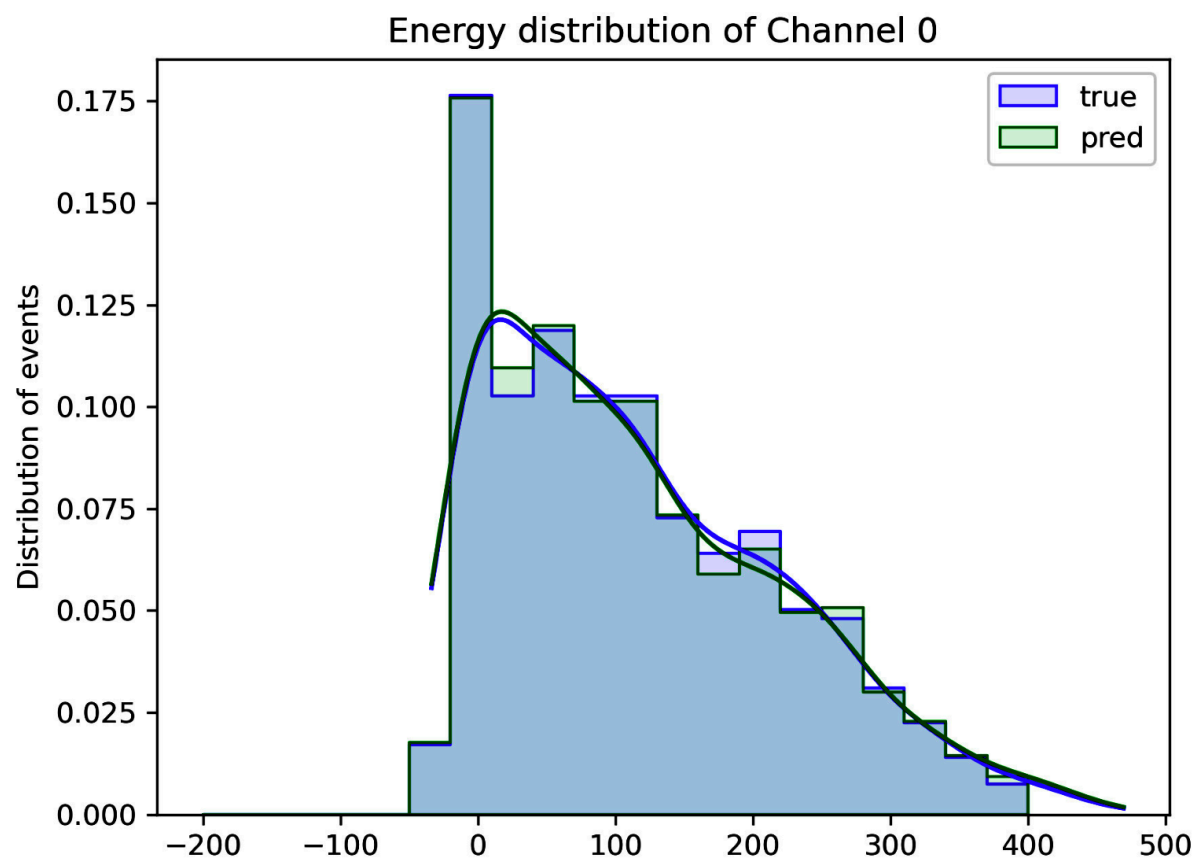
adding also SiPM **timing information**

average accuracy:  
**91.4%**



comparable identification performance w/r the ideal case

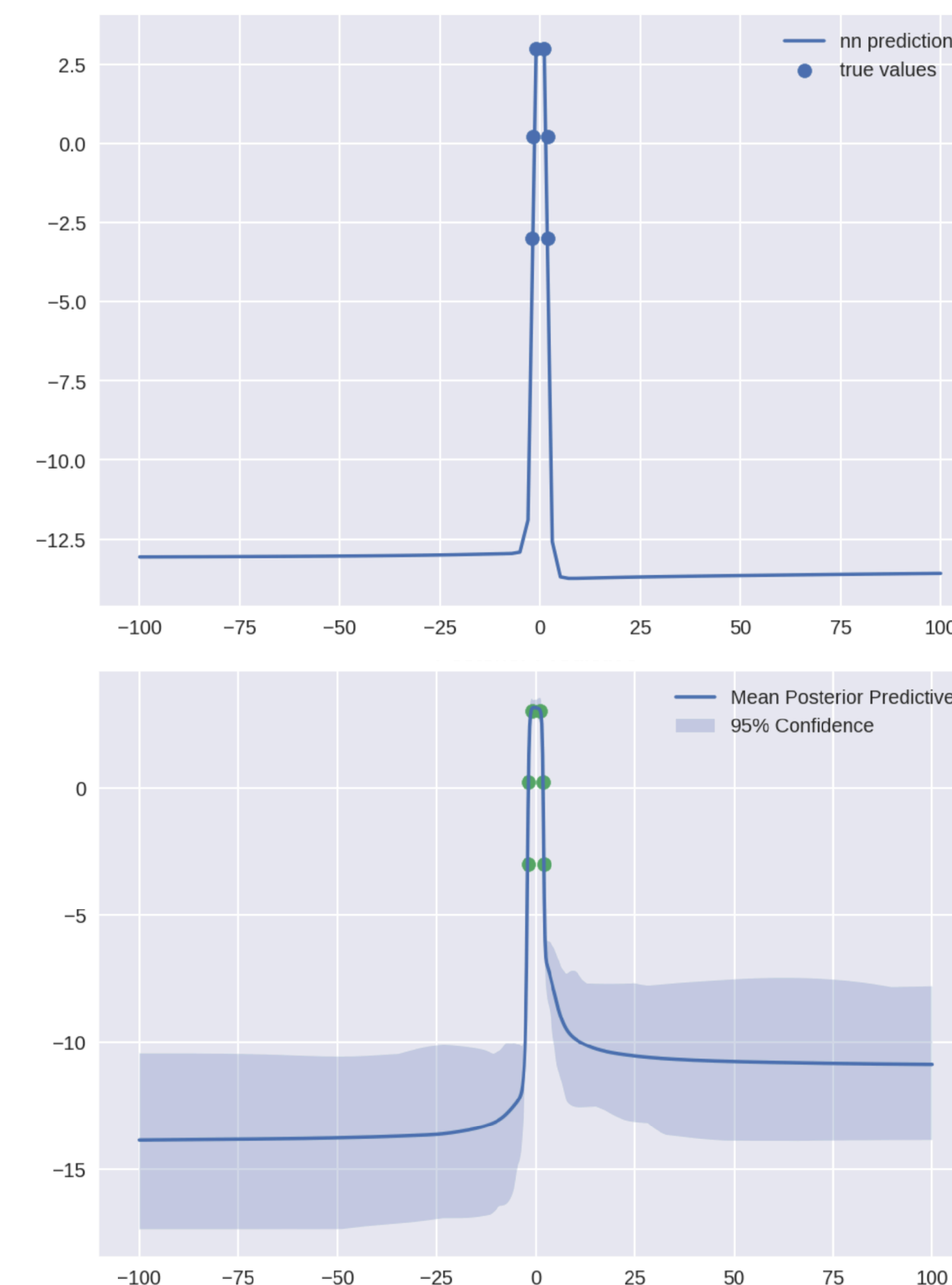
# CHECK OF POSSIBLE BIAS ON ENERGY



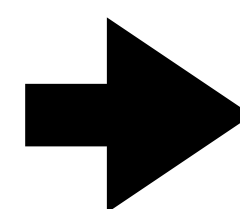
**no bias** observed over distribution of total energy per event

# UNCERTAINTY IN THE CLASSIFICATION: BAYESIAN-DGCNN

- Neural networks based on point values for weights may suffer of overconfidence when analysing new data especially for predictions in regions with few or w/o examples in the training set
- Bayesian neural networks mitigate the problem by introducing probability distributions over the weights and **predicting distributions instead of point values**
  - a Bayesian-NN learns a variational approximation of the true posterior distribution  $P(w|D)$ , and predict an estimate of the expected value  $E_{P(w|D)}[P(y|x,w)] \rightarrow$  since the weights are random variables, each predictions is a random variable too
  - allows to measure uncertainty, identify outliers in the input, regularise the whole model
- Designed and implemented in pytorch a full Bayesian version of a DGCNN (leveraging the *Bayes by Backprop* algorithm (<https://arxiv.org/abs/1505.05424>):



$$p(y|x, D) = \int p(x|y, w)p(w|D)dw$$



$$p(w|D) \approx q_{\theta}(w|D)$$

bayesian inference

generally intractable via MC integration

replace it with a variational (eg optimisation) problem

approximate p with a more tractable parametric distribution q (eg. gaussian) w/ learnable parameters (eg a NN)

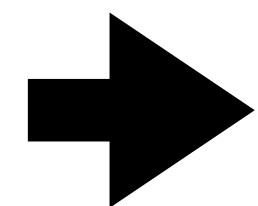
# BAYES BY BACKPROP

find optimal  $\theta^*$  by minimising the Kullback-Leibler divergence between  $p$  and  $q$

$$\theta^* = \arg \min_{\theta} \text{KL}[q_{\theta}(w | D) || p(w | D)]$$

$$\text{KL}[q_{\theta}(w | D) || p(w | D)] = \int q_{\theta}(w | D) \log \frac{q_{\theta}(w | D)}{p(w | D)} dw$$

we have another integral here, but now  $q$  is more tractable and we can approximate it via MC sampling

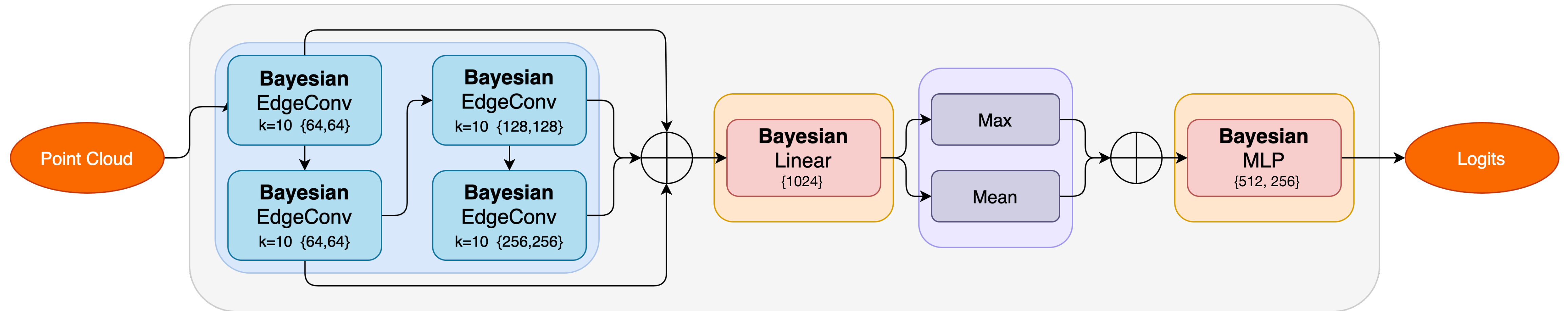


$$\theta^* \approx \arg \min_{\theta} \sum_{i=1}^n \log q_{\theta}(w^{(i)} | D) - \log p(w^{(i)}) - \log p(D | w^{(i)})$$

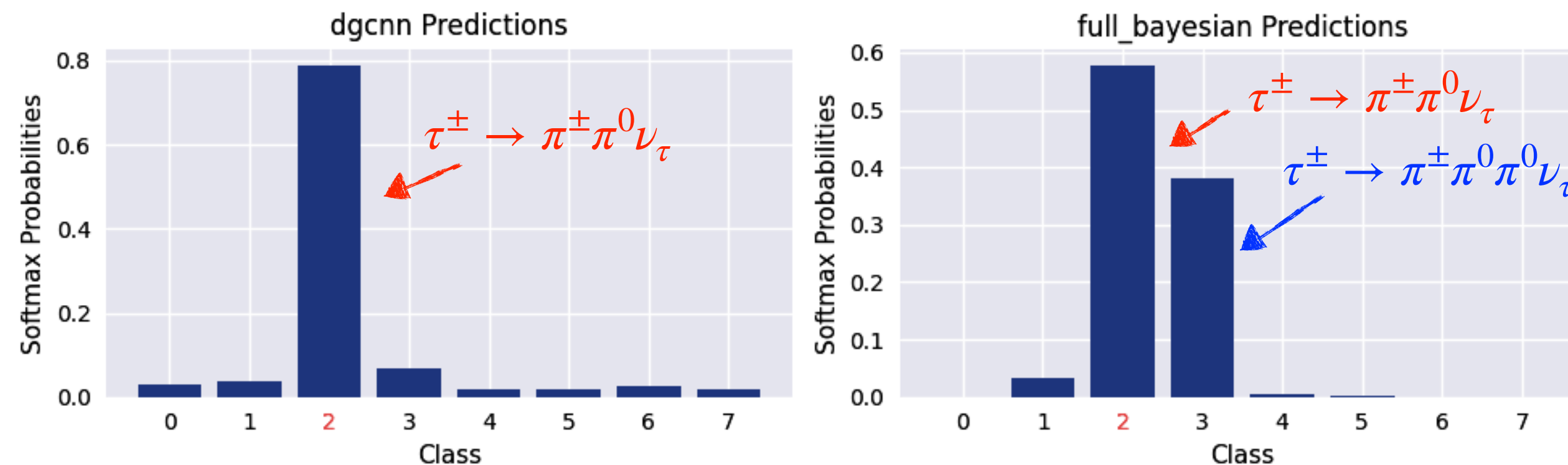
with  $w^{(i)}$  samples sampled from  $q_{\theta}(w | D)$

in practice as  $q_{\theta}$  is an ANN, the Kingma local reparameterization trick is used to make the whole expression differentiable

# BAYESIAN-DGCNN

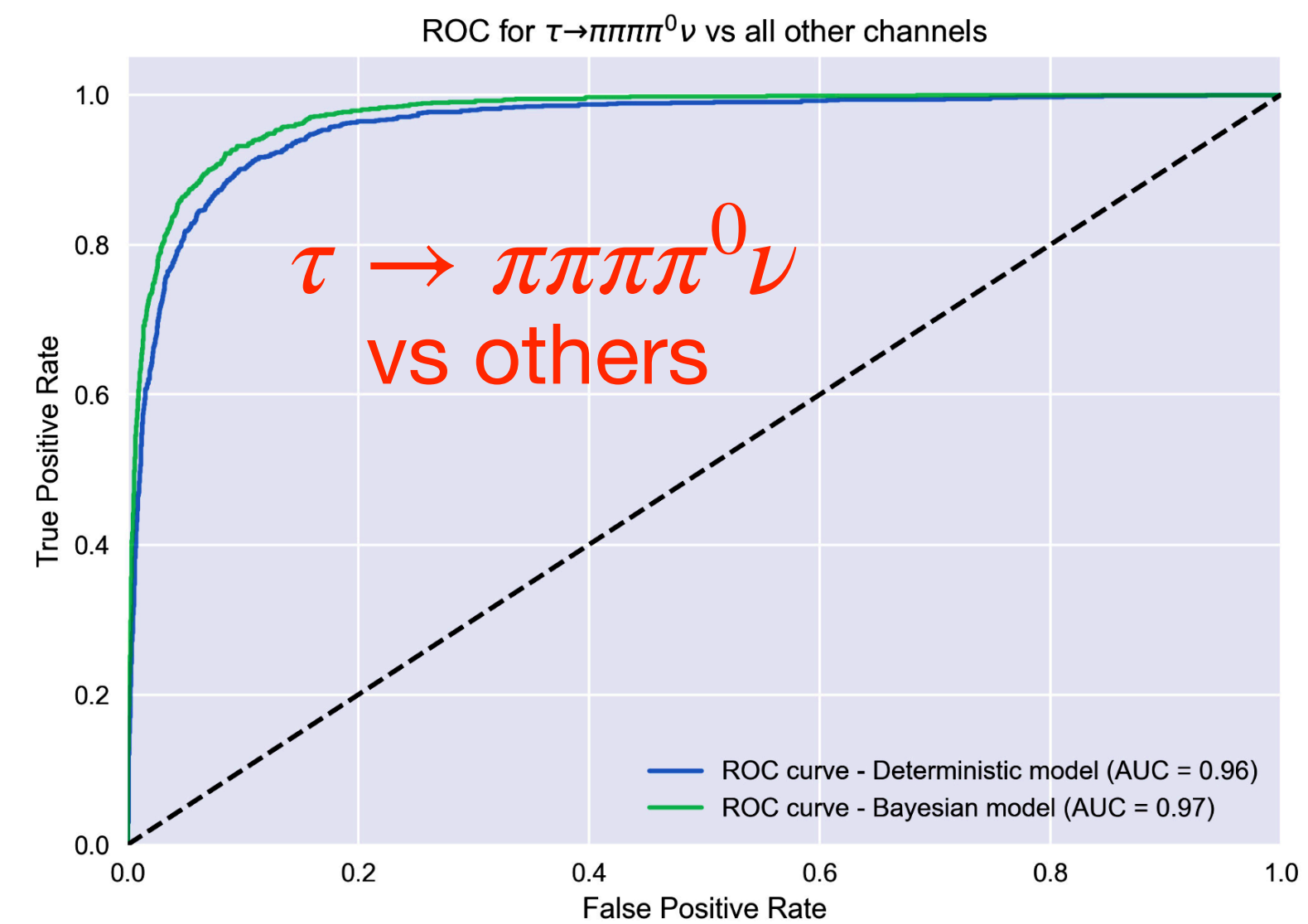
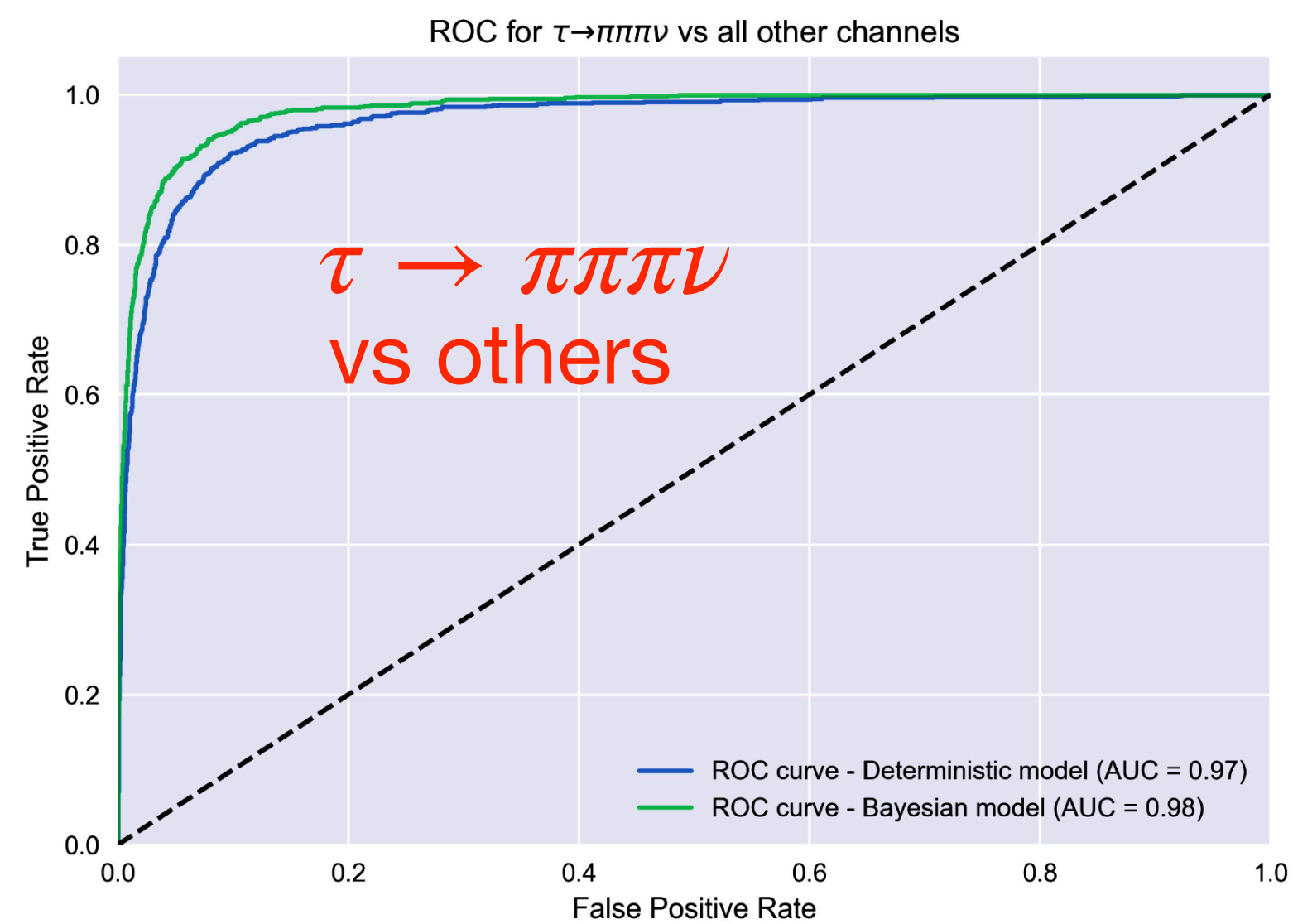
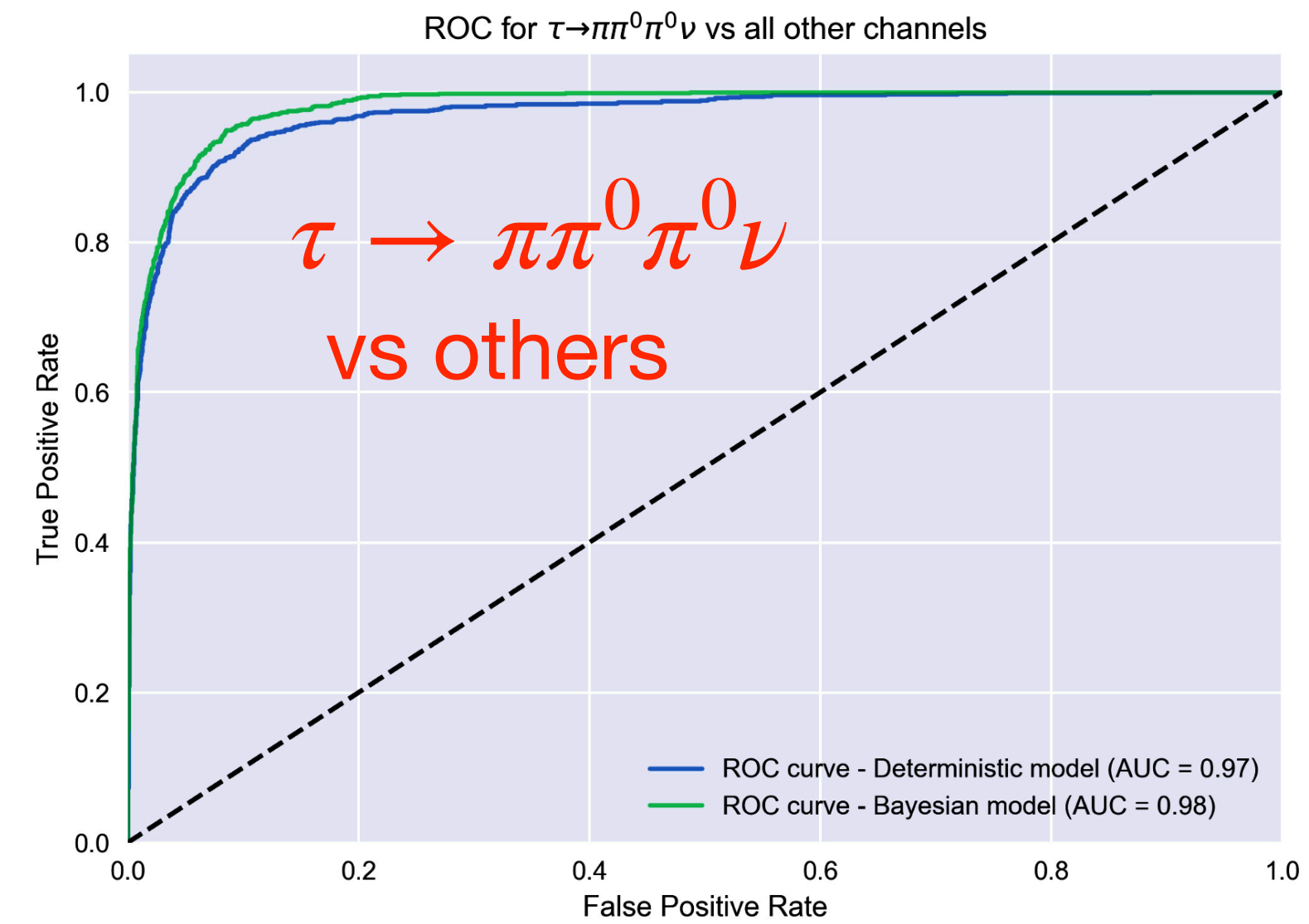
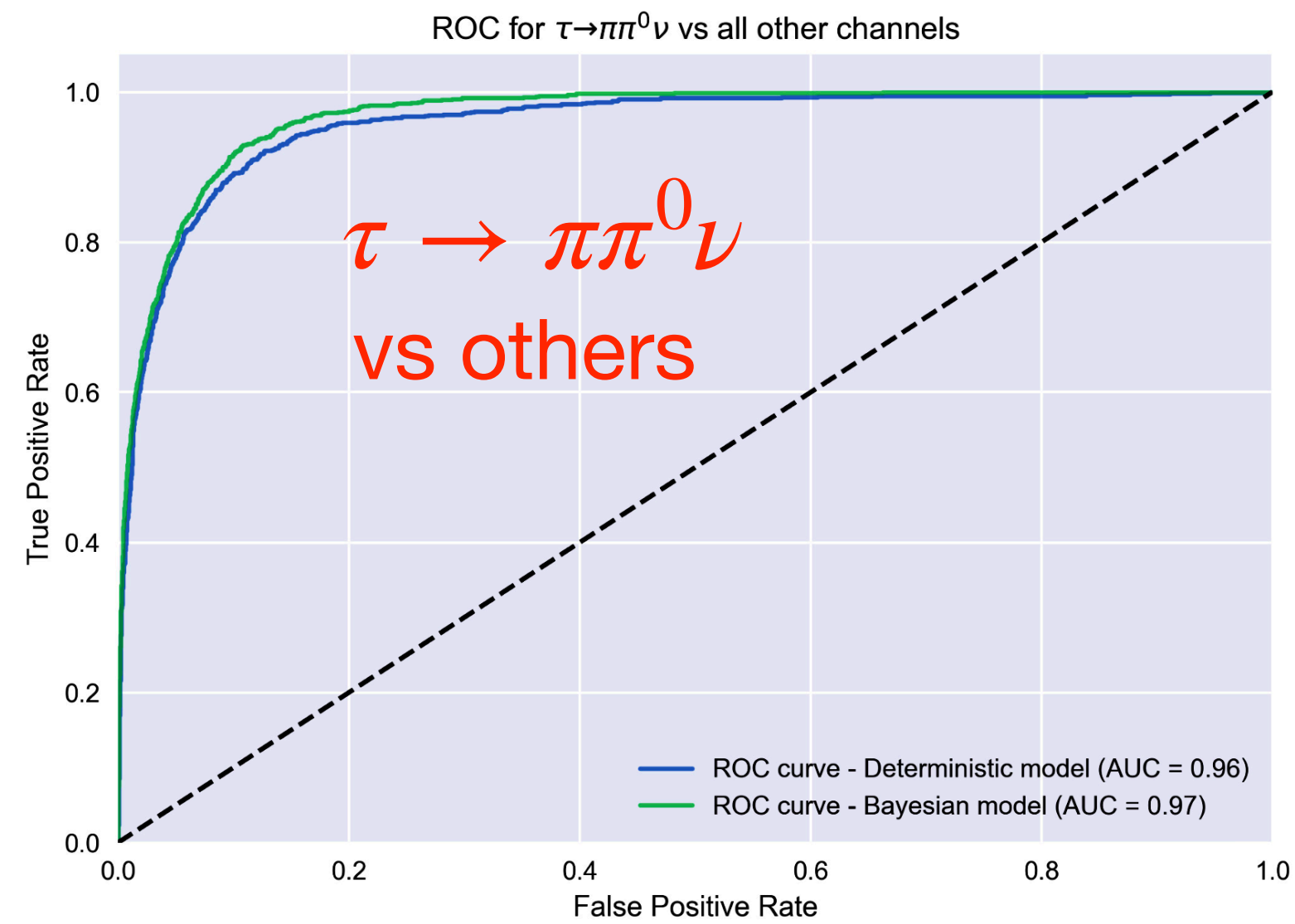


- all bayesian layers (EdgeConv, MLP, etc.), w/ gaussian priors (uncorrelated between layers and neurons)
- better classification performance wrt the point DGCNN
- class probabilities better aligned with physics expectations



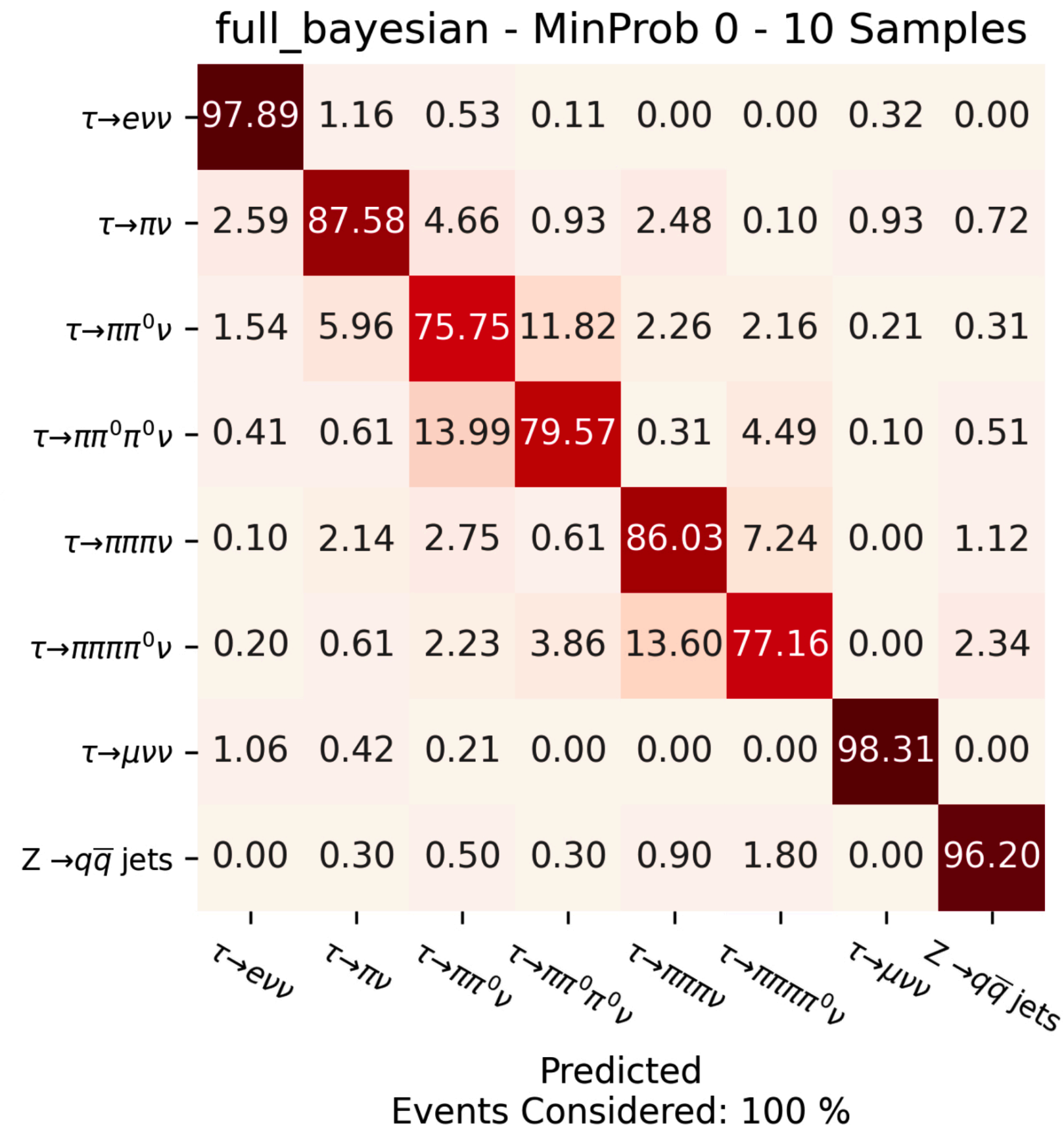


# BAYESIAN-DGCNN

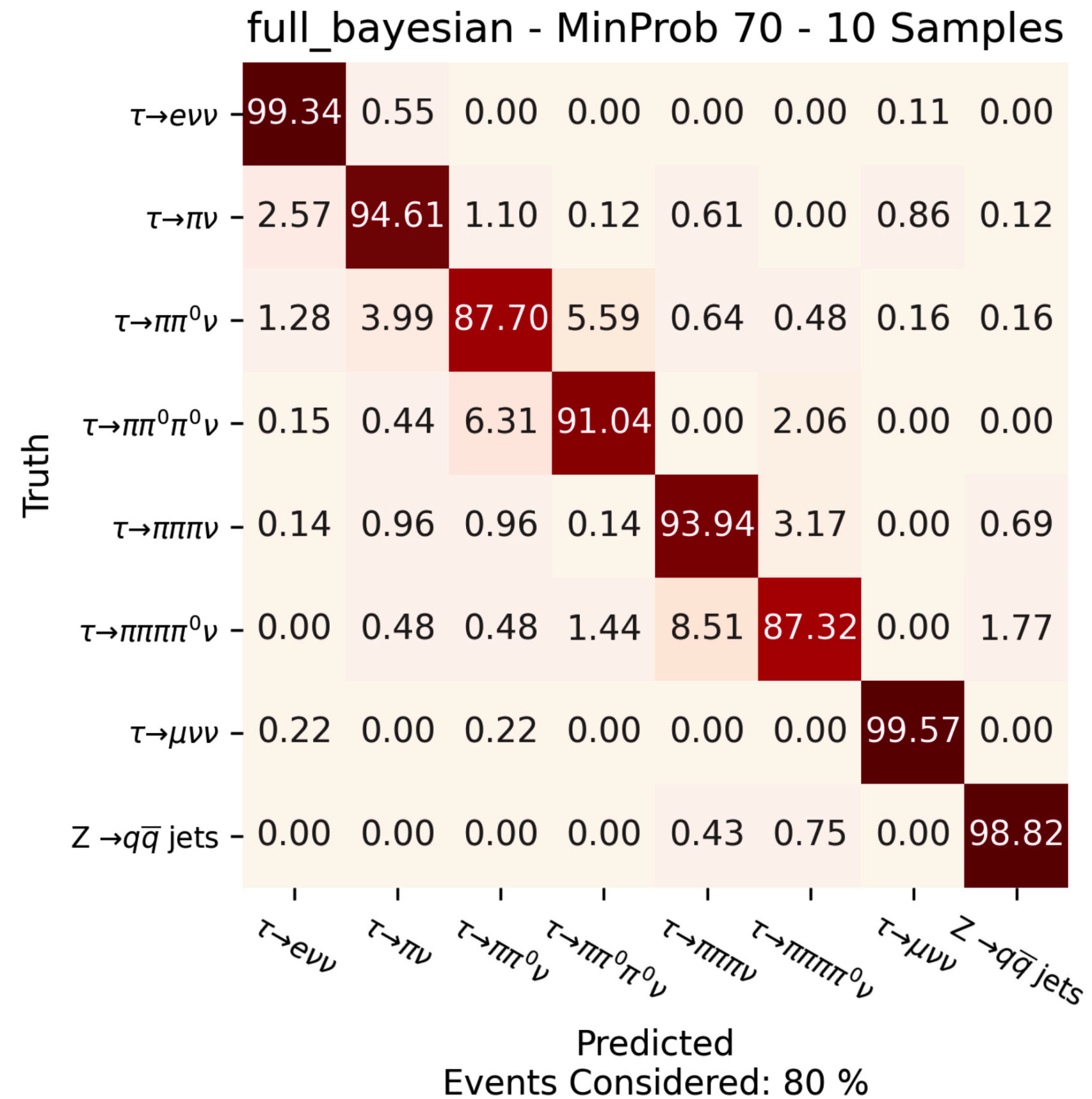


ROC / AUC

# BAYESIAN-DGCNN



B-DGCNN:10 samples per prediction  
no threshold on minimum confidence

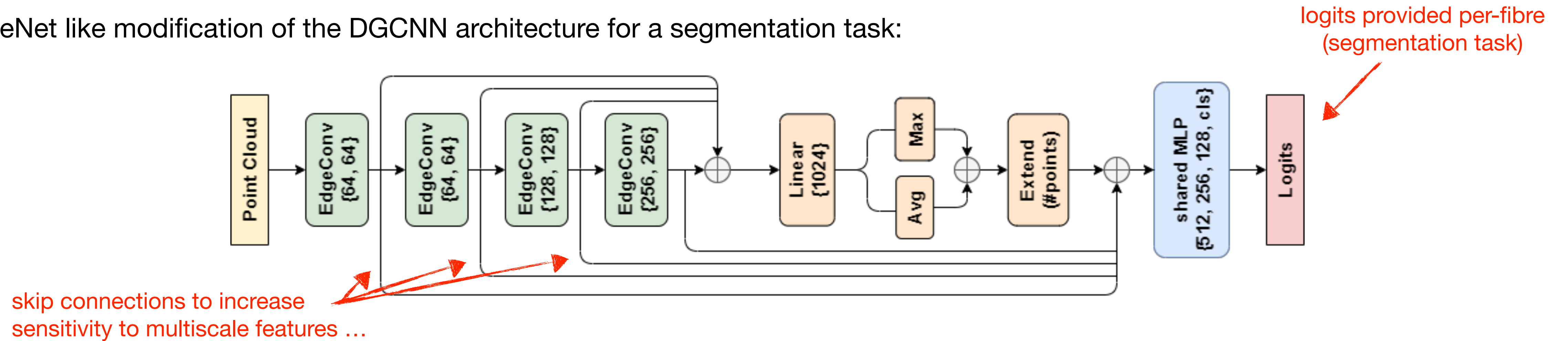


B-DGCNN:10 samples per prediction  
minimum threshold on confidence 0.7

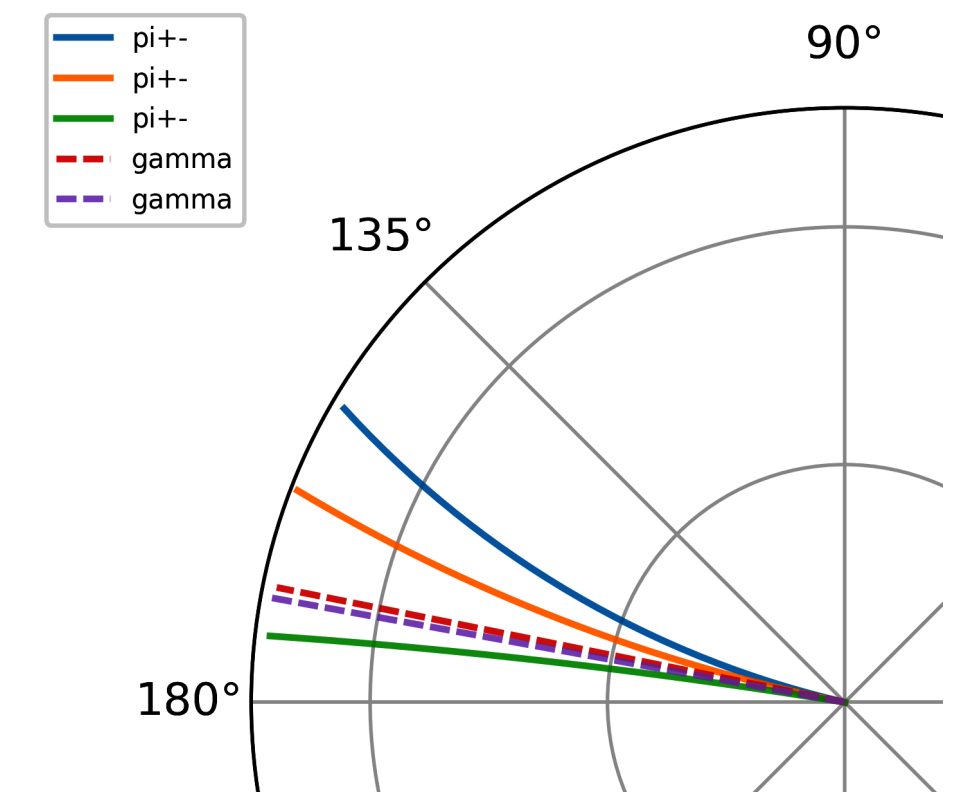
Number of Samples	Minimum Confidence	Events Considered	Test Accuracy
1	0.0	100 %	0.854
	0.7		0.873
	0.9		0.869
3	0.5	94.83 %	0.896
	0.7	80.33 %	0.943
	0.9	62.27 %	0.977
10	0.5	94.72 %	0.900
	0.7	79.82 %	0.947
	0.9	60.52 %	0.981

# JET CONSTITUENTS ID

- DGCNN and dual-readout calorimeter high granularity can be exploited for object (particle) detection inside taus and jets
  - a proto-step for a particle flow algorithms
  - can be implemented with a similar approach as in segmentation tasks (eg pixel/node/fiber-level classification)
- DenseNet like modification of the DGCNN architecture for a segmentation task:



- identify the particle associated to the larger energy deposit in each fibre
- label each fibre by extrapolating Monte Carlo truth particles from production to the DRC into the IDEA magnetic field
- train the DGCNN to predict the label associated to each fibre
- **Initial study:** using point DGCNN only

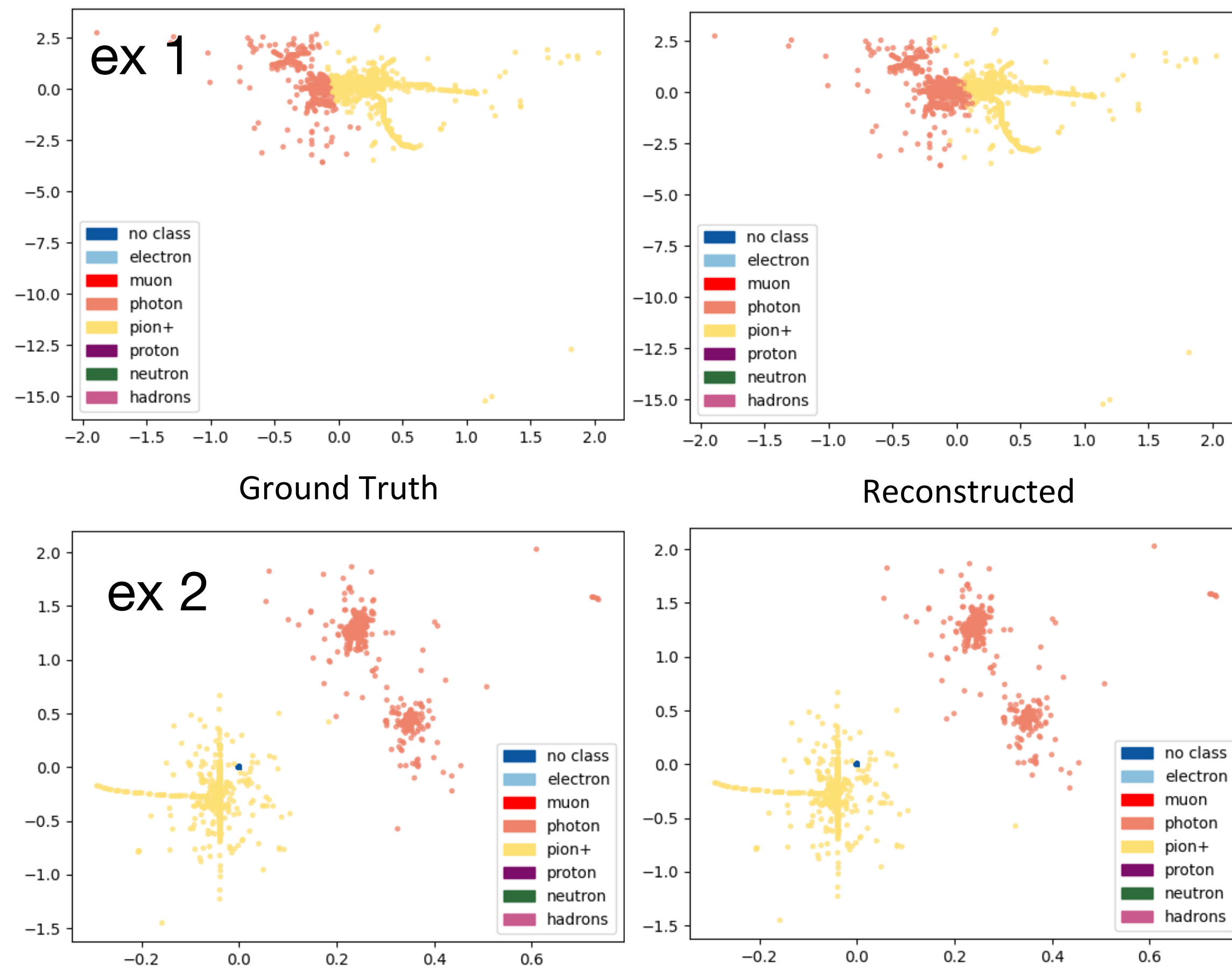


# RESULTS SEGMENTATION

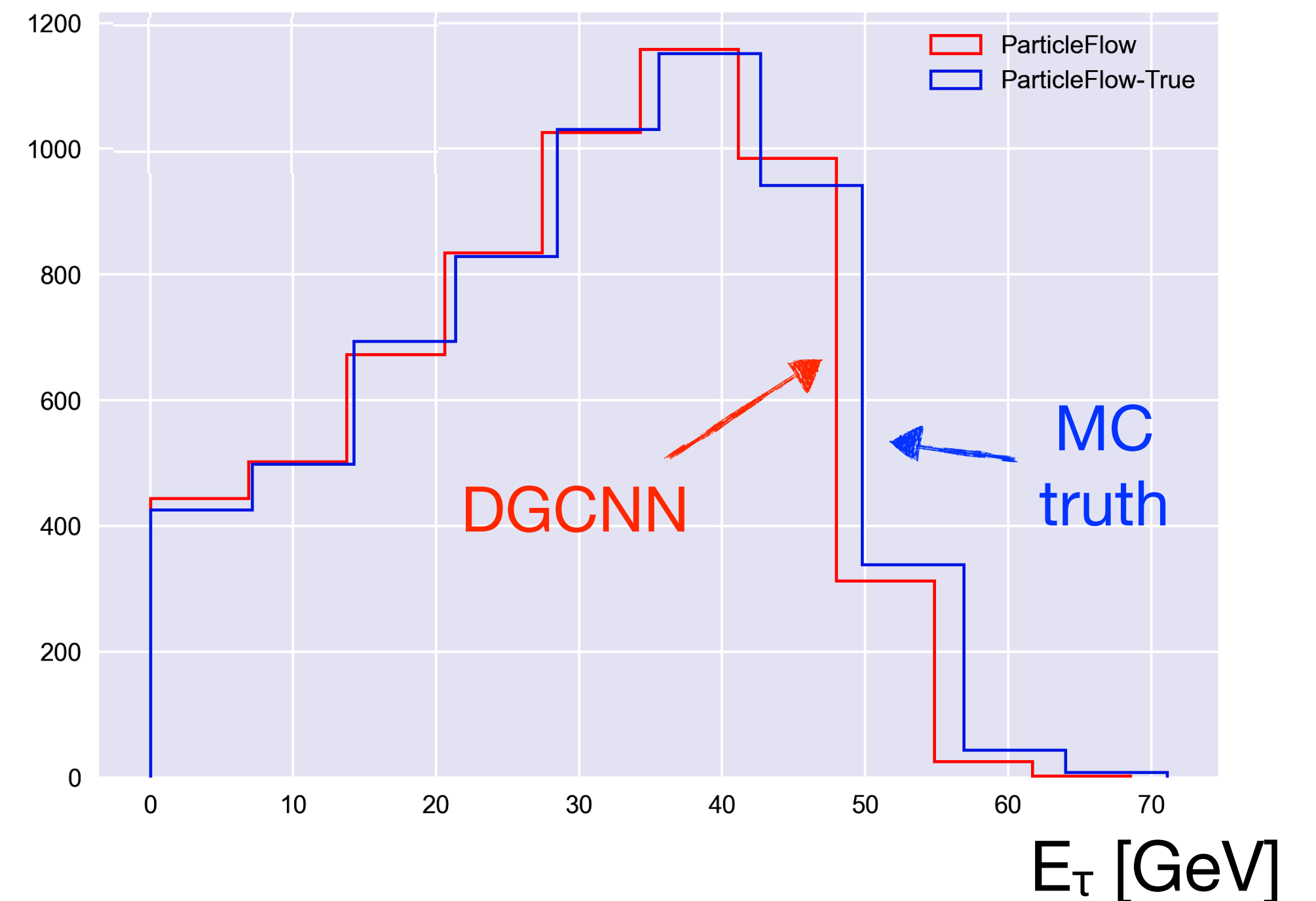
Two nice examples:  $\tau^\pm \rightarrow \pi^\pm \pi^0 \nu_\tau \rightarrow \pi^\pm \gamma \gamma \nu_\tau$

tau visible energy reconstructed using:

- DRC for photons
- MC truth for other particles



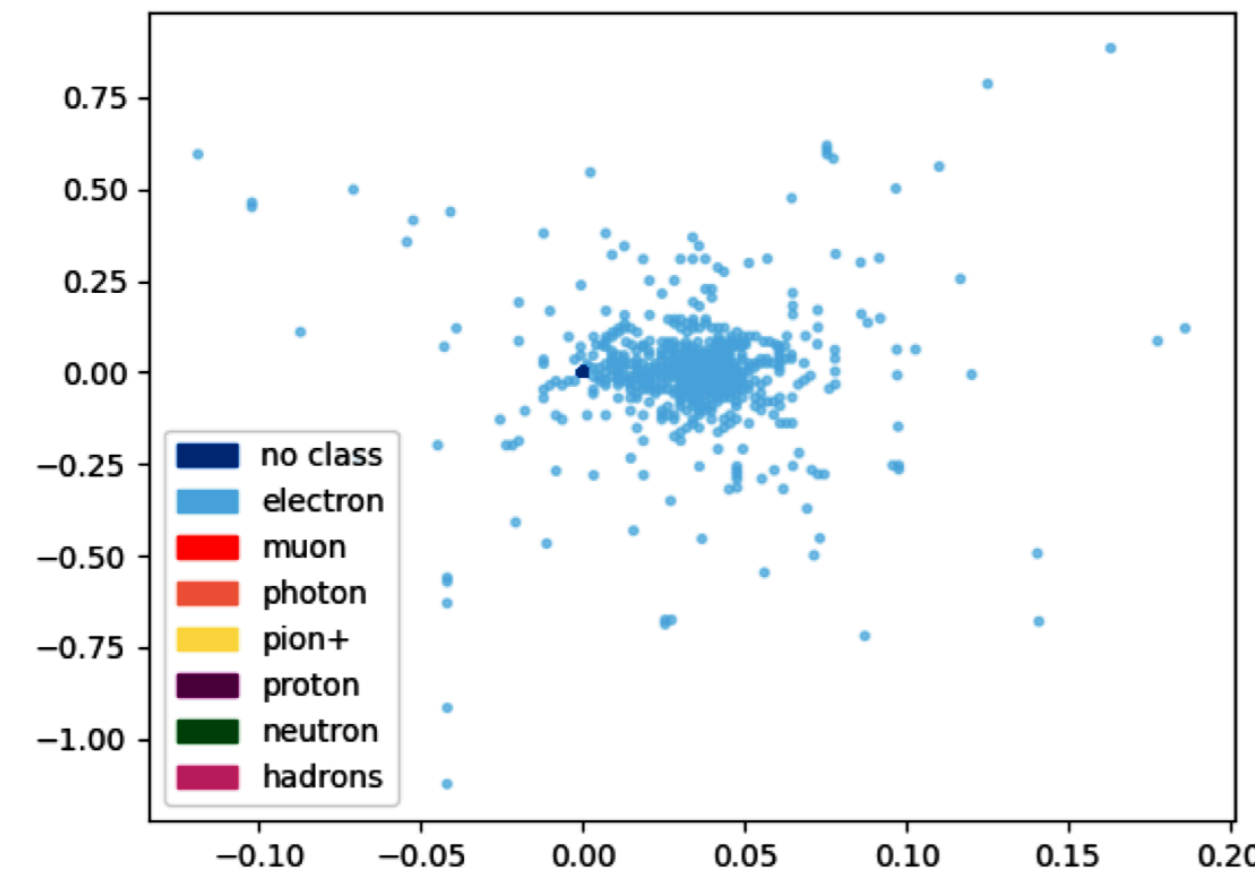
comparison of the visible energy distributions obtained when photons are identified by the DGCNN and when using the MC truth



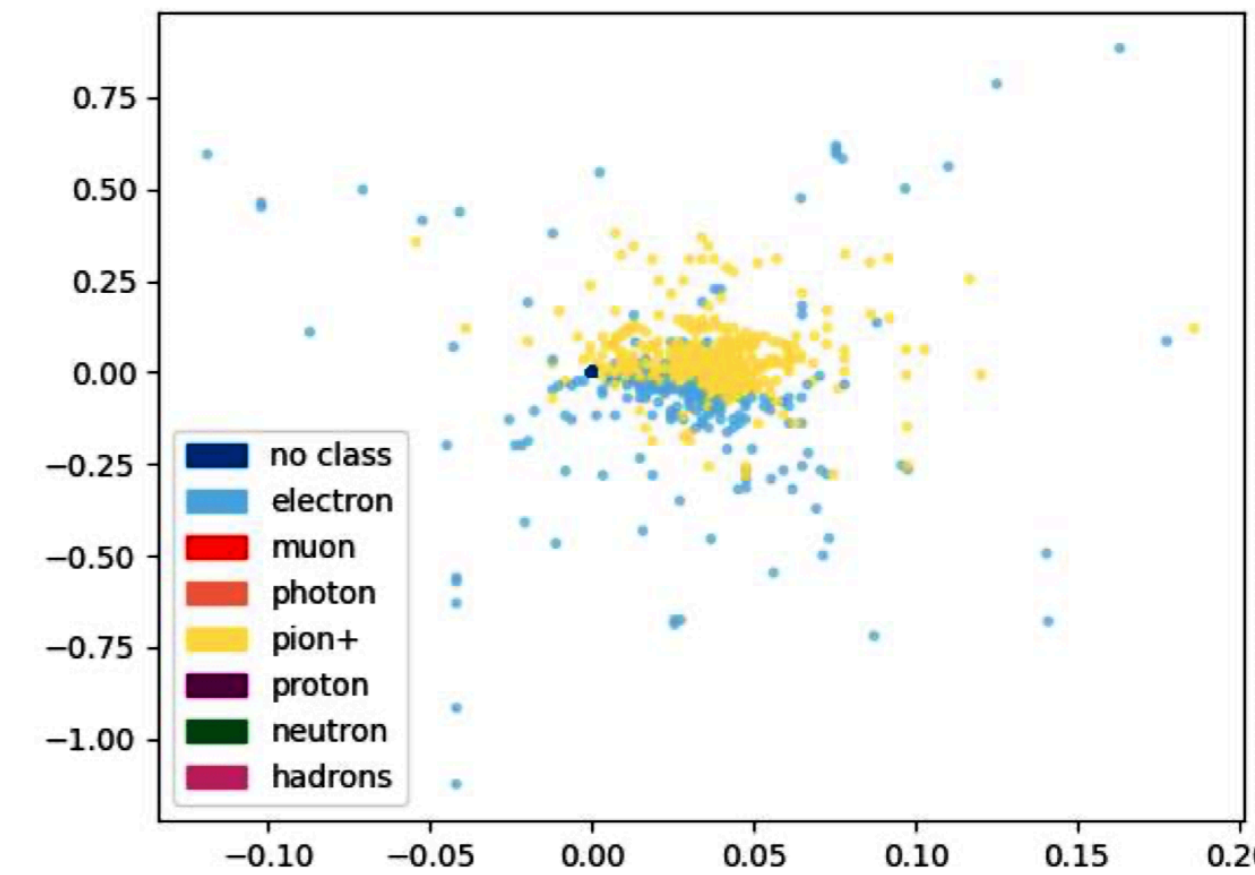
# RESULTS SEGMENTATION

Two “less nice” results:

ex 1

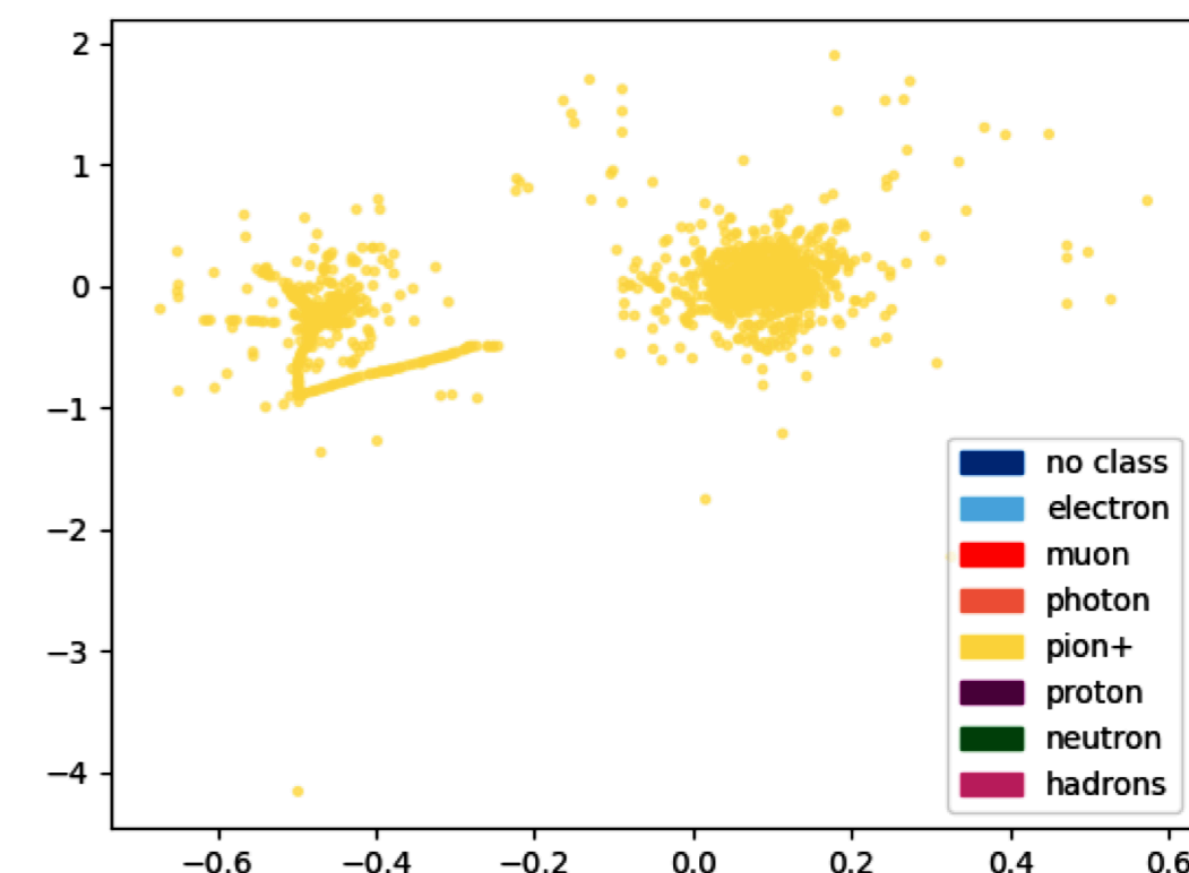
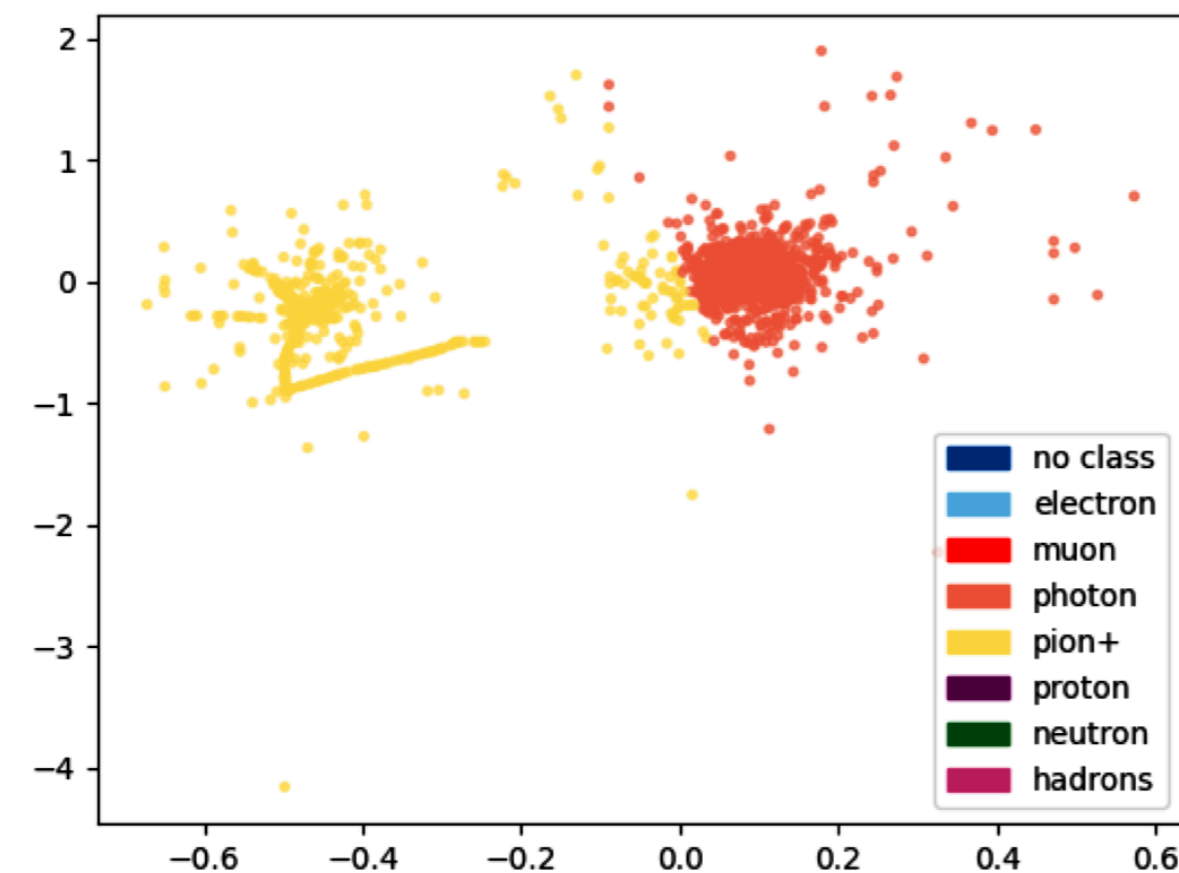
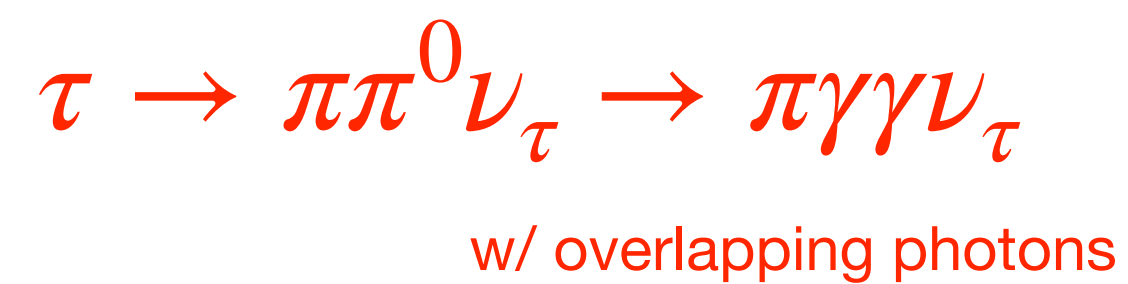


Ground Truth



Reconstructed

ex 2



# ONGOING DEVELOPMENTS

- improve jet constituents ID by moving from DGCNN segmentation to Graph-Transformer object detection
- **hybrid architecture**: GNN → high-level representation → Transformed encoder/decoder → bounding box predictions
  - GNN encode the graph for the transformed architecture and **extracts compact representation of the global graph structure**
  - the **transformer encoder** process this data to produce an **embedding context** representing the whole graph
  - this embedding is passed to a **transformer decoder** that takes as input a small fixed of **learned positional embeddings** (object queries) and attends to the encoder output
  - the self-attention and the encoder-decoder attention over the embedding and the object queries allows the model to analyse all objects together using pair-wise relations between them, and to independently decode it into box coordinates and class labels by a FFN head
  - the FFN head is a **shared MLP that predict class and bounding box for each object**
- results will be ready in time for the fall meetings/conferences ...

