Graphing the Dark Sector: Anomalous Shower Detection with GNNs in the ATLAS Calorimeters

Scientific Computing Seminar
20.06.2025, DESY

Lukas Bauckhage[1,2]
[1]Deutsches Elektronen-Synchrotron DESY
[2]Physikalisches Institut Universität Bonn

Previous Talk

- Talk at last year's SciComp Workshop

FH SciComp Workshop 2024

Jul 1, 2024, 2:00 PM → Jul 2, 2024, 2:00 PM Europe/Berlin

Seminar Room 4a/b (DESY Campus Hamburg)

8. CNNs and GNNs for tagging anomalous showers with ATLAS

Lukas Bauckhage (ATLAS (ATLAS Upgrade))

7/2/24, 11:00 AM

Scientific Computing III

This talk will discuss recent work towards developing a ML (CNN/GNN) tagger to distinguish anomalous showers caused by the decays of long-lived particles from QCD jets with the ATLAS detector

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⇒ Loads of updates!

Previous Talk

(in this Seminar)

(indico)

CaloClouds: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation

Scientific Computing Seminar
DESY, 23.05.2025

E. Buhmann[2], H. Day-Hall[1], T. Buss[2], F. Gaede[1], G. Kasieczka[2], W. Korcari[2], **A. Korol[1,*]**, K. Krüger[1], P. McKeown[1,3]

[1] Deutsches Elektronen-Synchrotron, DESY
[2] University of Hamburg, UHH
[3] CERN

*anatolii.korol@desy.de

CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE
HELMHOLTZ

Introduction

HEP Data Pipeline

Standard Tools and Methods

Simulation

Reconstruction

Analysis

Matrix-element Calculation

Parton-shower / Hadronization

Detector Simulation

Digitization

Topoclusters & Spacepoints

Track Finding & Fitting

Jet Tagging & Vertexing

Particle ID & Particle Flow

Calibration

Likelihood Fitting

Unfolding

Numerical Integration

Markov Chain Monte Carlo

Topological clustering

Kalman Filtering & Fitting

Conformal Fits & Hough Transform

Statistical Techniques, Bayesian Inference

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Statistical Techniques, Bayesian Inference

ML?

HEP Data Pipeline

ML Edition

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- Unfolding

ML methods:
- Generative Models: GANs, VAEs, Normalizing Flows and Diffusion
- Metric Learning, Object Condensation
- Deep Full Event Reconstruction
- CNNs, Graph Neural Networks & Transformers
- Symmetric ML & Equivariance
- Autoencoders & Anomaly Detection
- Omnifold and Likelihood-free Inference

HEP Data Pipeline

ML Edition

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Metric Learning, Object Condensation

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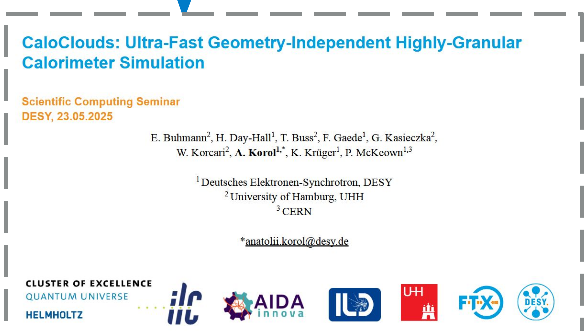
CaloClouds: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation

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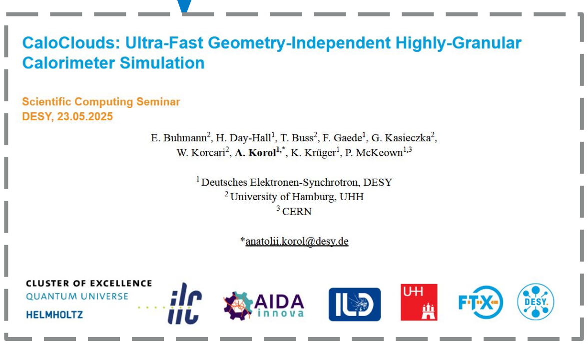
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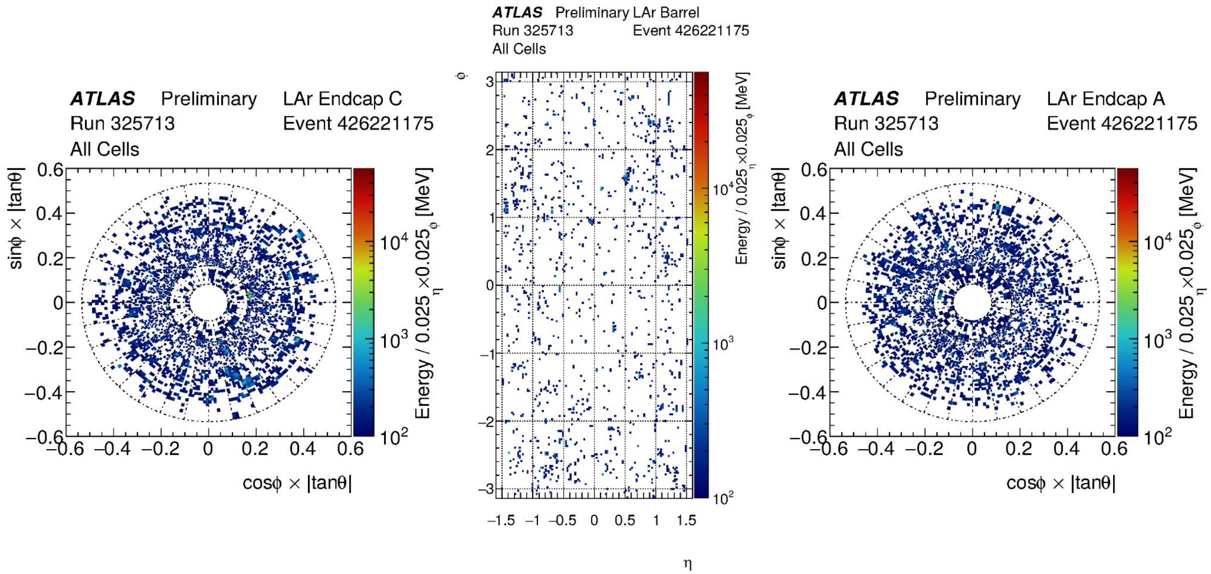
TODAY!

Shower Reconstruction

Particle

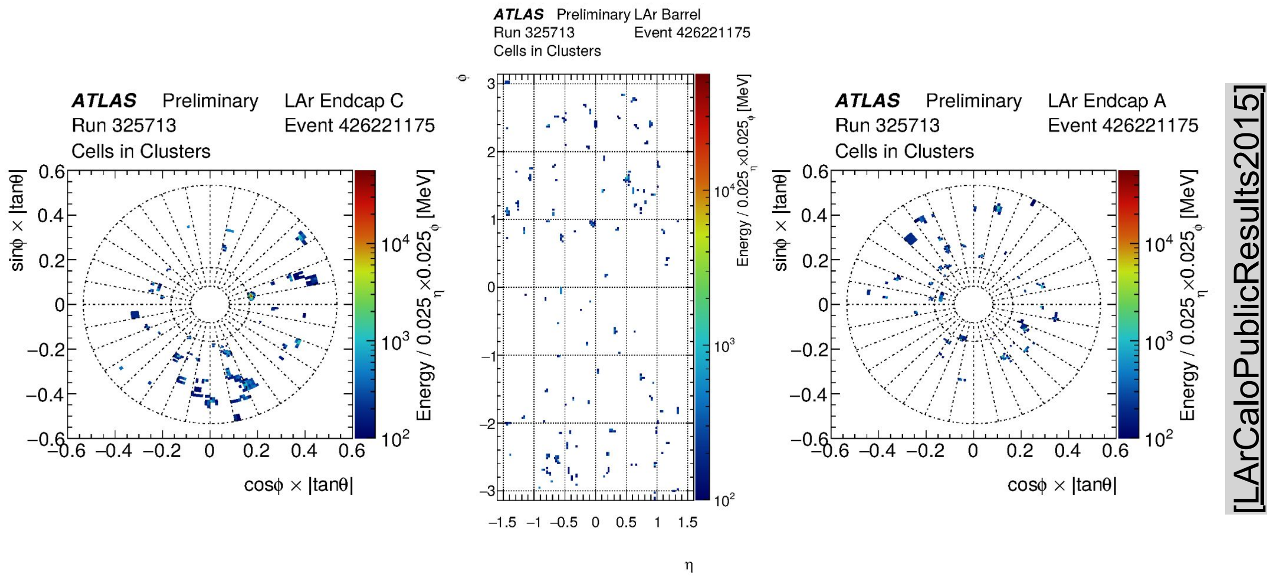
Shower

Energy deposits
cells



[LArCaloPublicResults2015]

Shower Reconstruction



[LArCaloPublicResults2015]

Particle

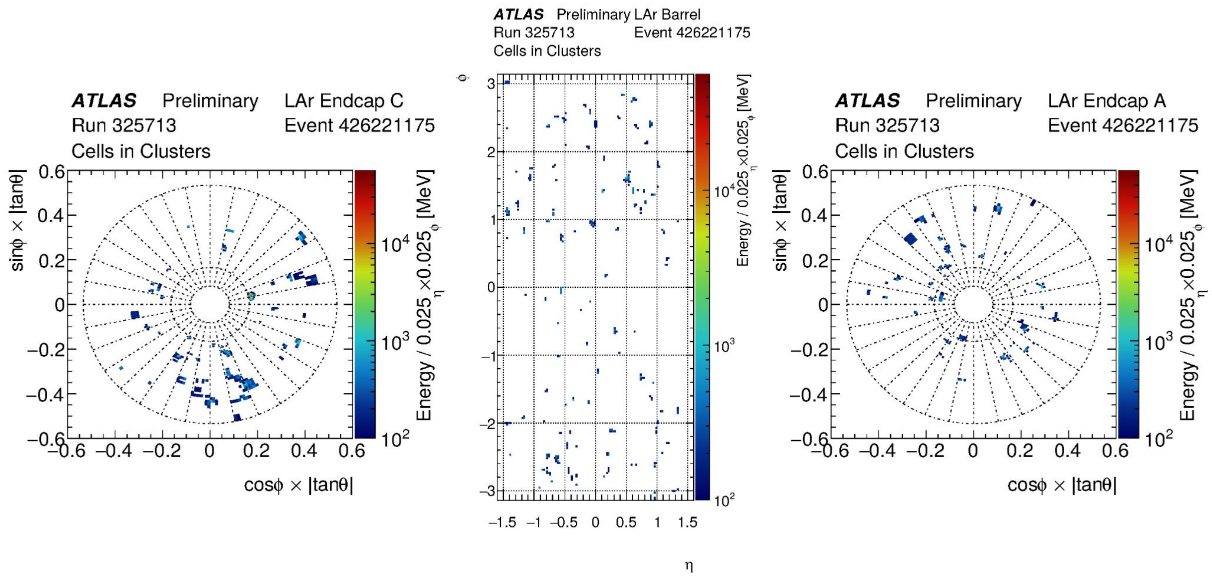
Shower

Topo-Clustering

Energy deposits cells

Clustered cells

Shower Reconstruction



[LArCaloPublicResults2015]

Particle

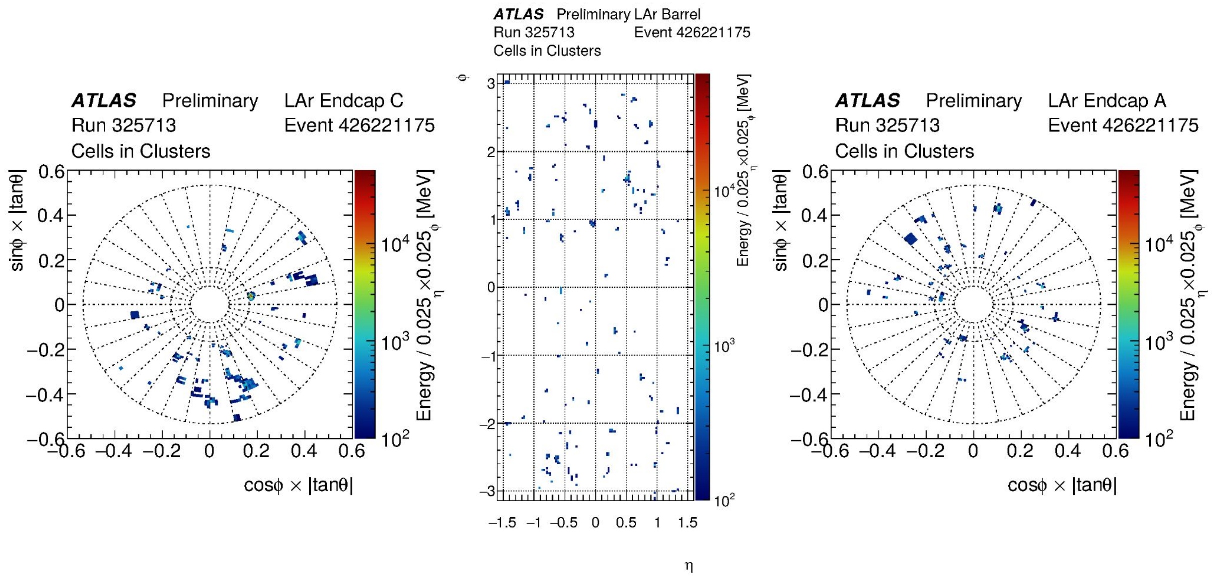
Shower → Topo-Clustering → Object reco

Energy deposits cells

Clustered cells

Jets, Photons, …

Shower Reconstruction



[LArCaloPublicResults2015]

Particle

Shower → Topo-Clustering → Object reco → Corrections & Calibration

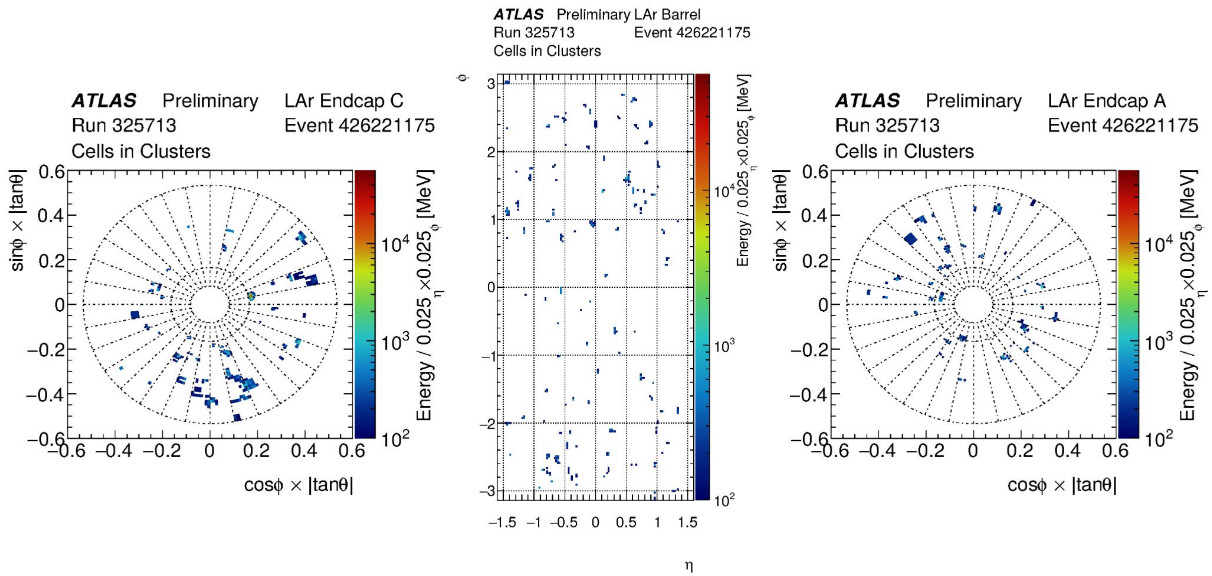
Energy deposits cells

Clustered cells

Jets, Photons, …

Calibrated objects

Shower Reconstruction



[LArCaloPublicResults2015]

Particle

Shower → Topo-Clustering → Object reco → Corrections & Calibration → PID, Analysis

Energy deposits cells

Clustered cells

Jets, Photons, …

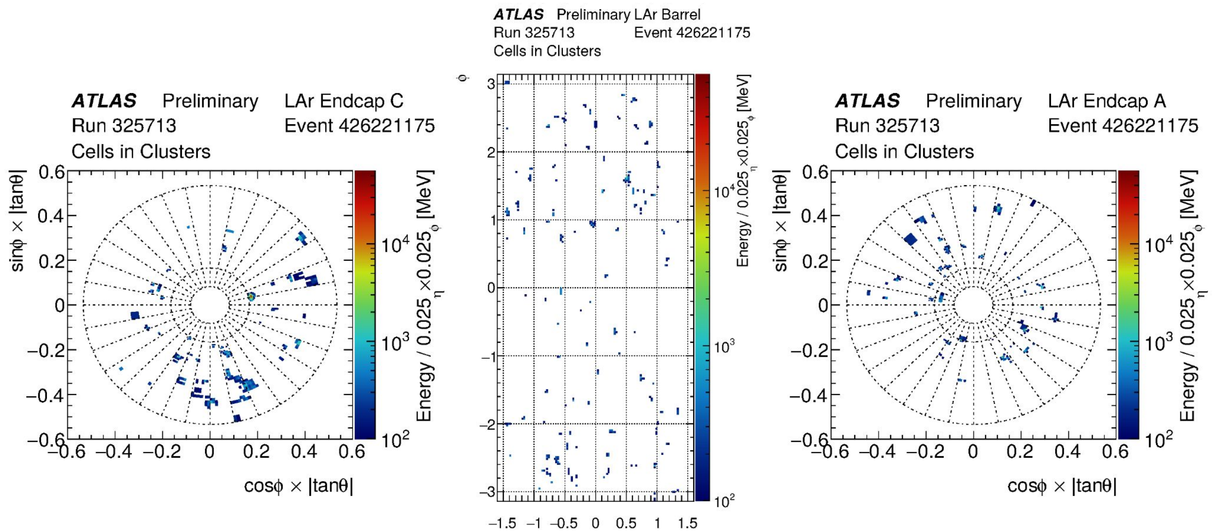
Calibrated objects

Kinematics, shower shape variables

Shower Reconstruction

BSM Physics, LLPs, …

Particle



[LArCaloPublicResults2015]

Shower → Topo-Clustering → ~~Object reco~~ → ? → Corrections & Calibration → PID, Analysis

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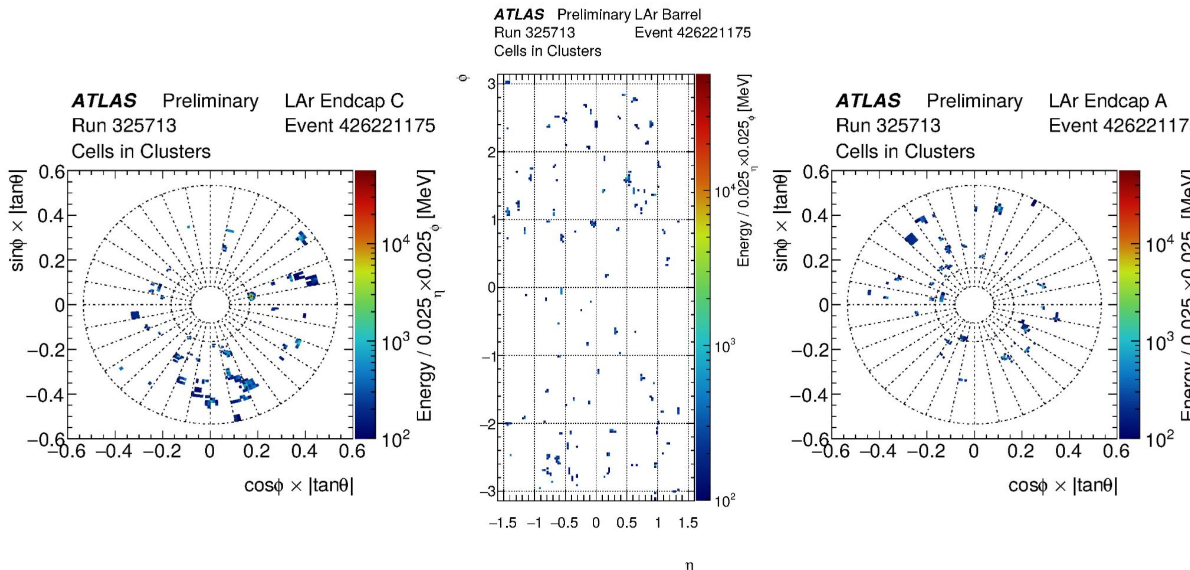
Particle

Shower



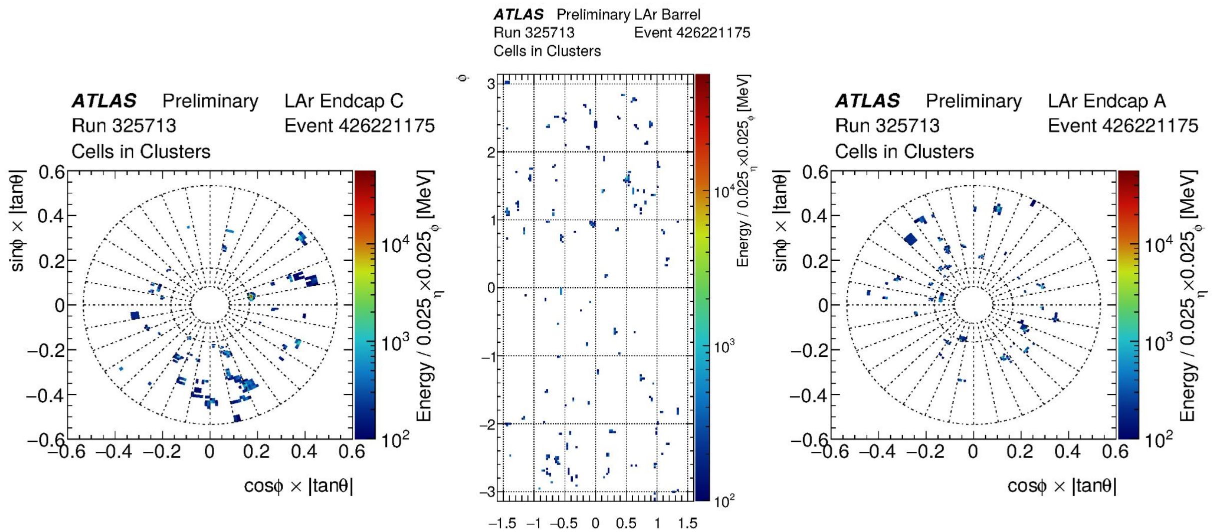
[LArCaloPublicResults2015]

Shower	Topo-Clustering	~~Object reco~~	Corrections & Calibration	PID, Analysis
Energy deposits cells	Clustered cells	Jets, Photons, …	Calibrated objects	Kinematics, shower shape variables

?

Can we use something more “low-level”?

Shower Reconstruction



[LArCaloPublicResults2015]

BSM Physics, LLPs, …

Particle

Shower → Topo-Clustering → ~~Object reco~~ → ? → Corrections & Calibration → PID, Analysis

Energy deposits cells

too expensive

Clustered cells

Jets, Photons, …

Calibrated objects

Kinematics, shower shape variables

Can we use something more “low-level”?

Shower Reconstruction

BSM Physics, LLPs, …

Particle

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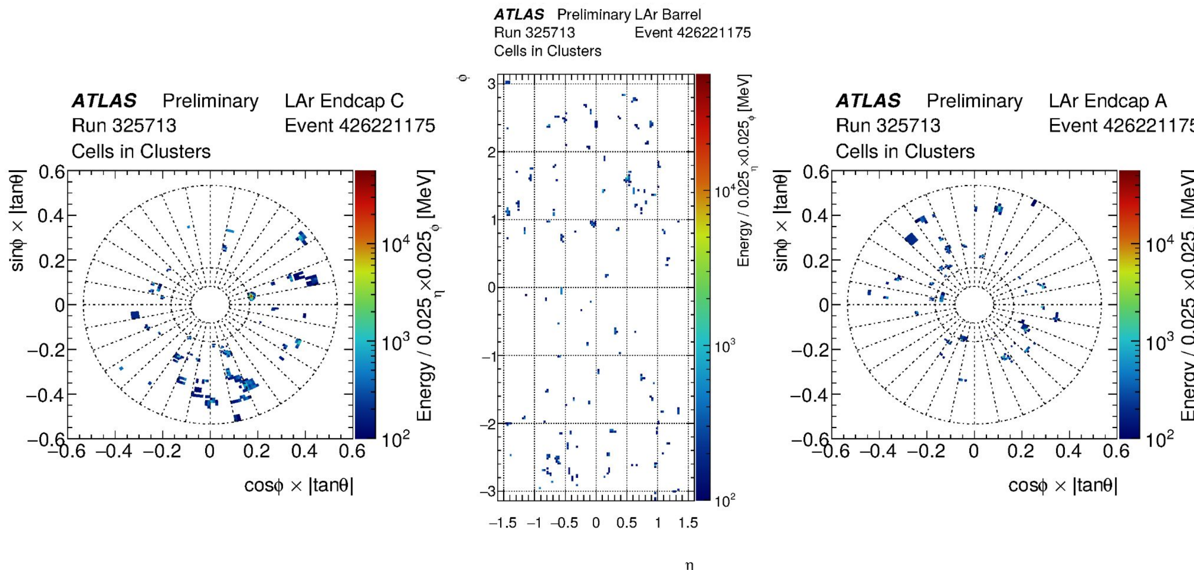

[LArCaloPublicResults2015]

Energy deposits cells

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Clustered cells

(ML) Tagger based on clusters?

Jets, Photons, …

Calibrated objects

Kinematics, shower shape variables

Can we use something more “low-level”?

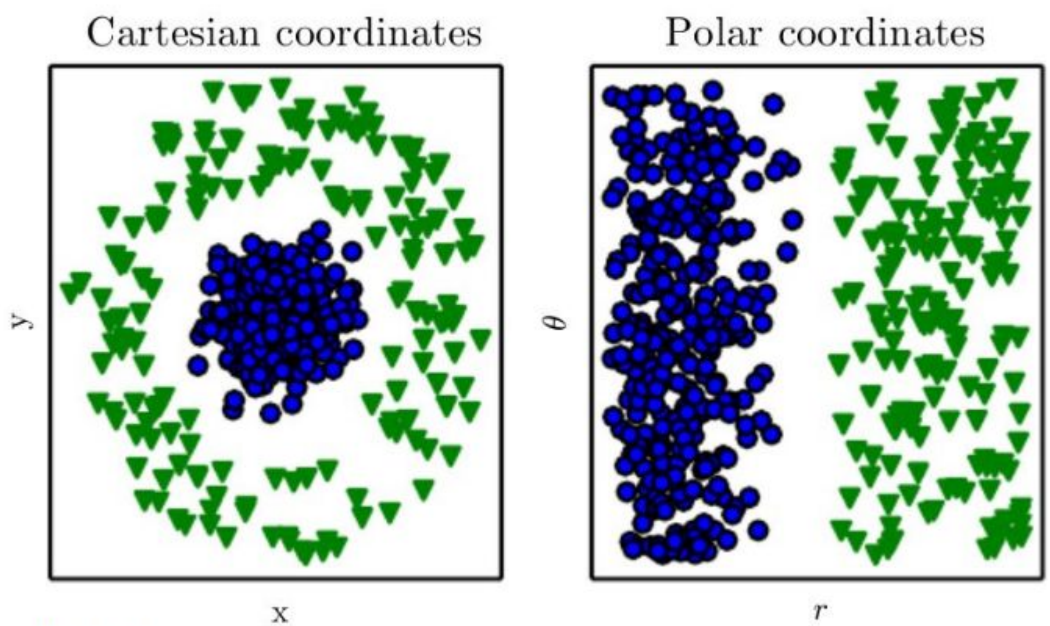
Clusters and Representation of Showers

How to represent calorimeter showers in data?

(indico)

The Right Data Representation Can Turn an Impossible Problem into an Easy One

impossible task for linear model

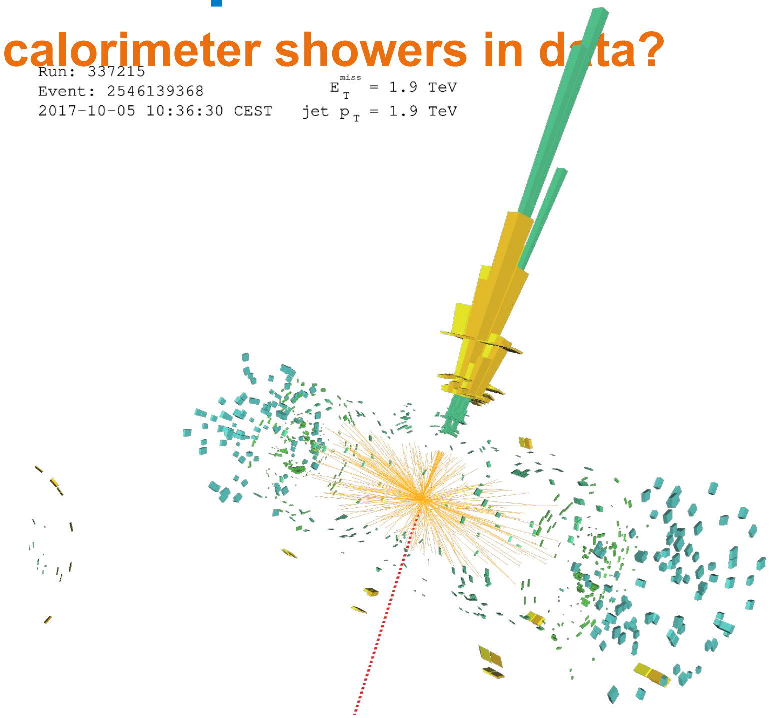


easy to solve with vertical line

Figure from:
Deep Learning, Ian Goodfellow and Yoshua Bengio and Aaron Courville,
https://www.deeplearningbook.org/

Clusters and Representation of Showers

How to represent calorimeter showers in data?



[EXOT-2018-06]

Clusters and Representation of Showers

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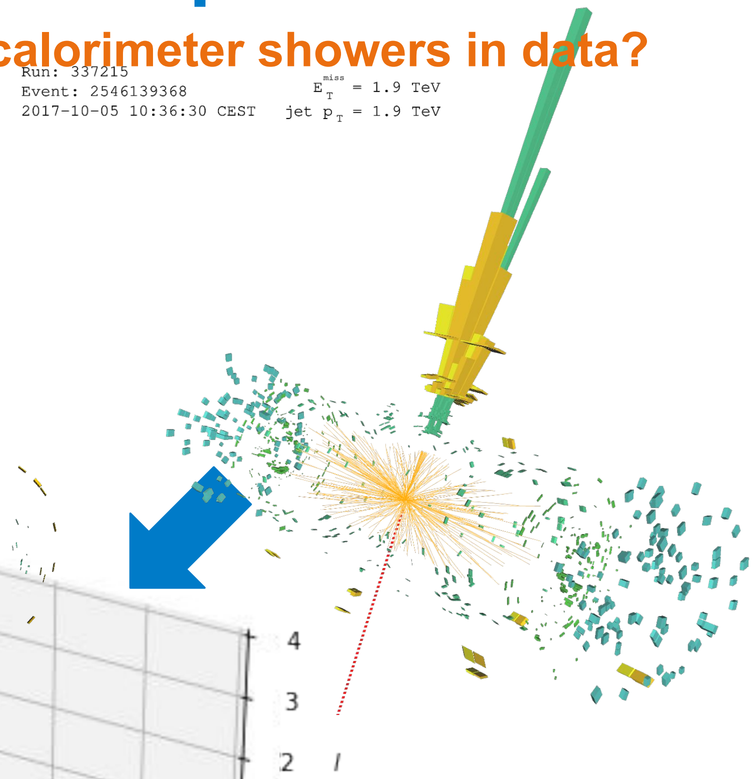

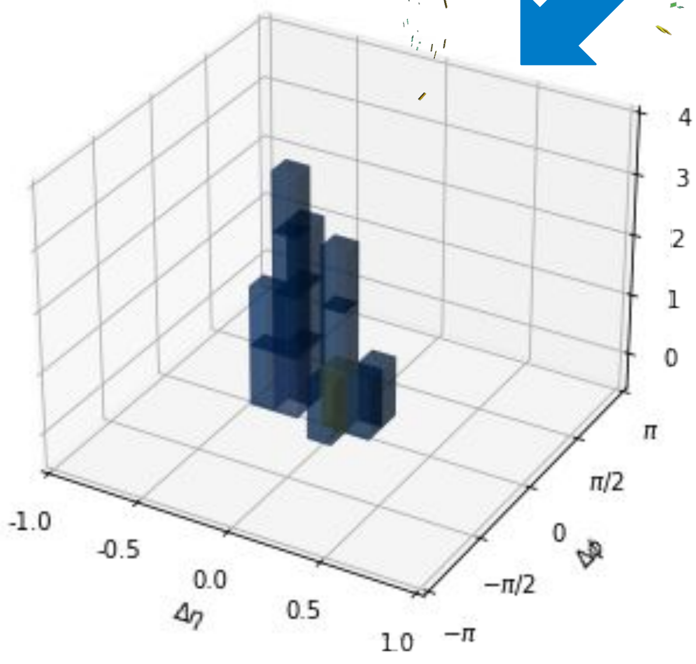

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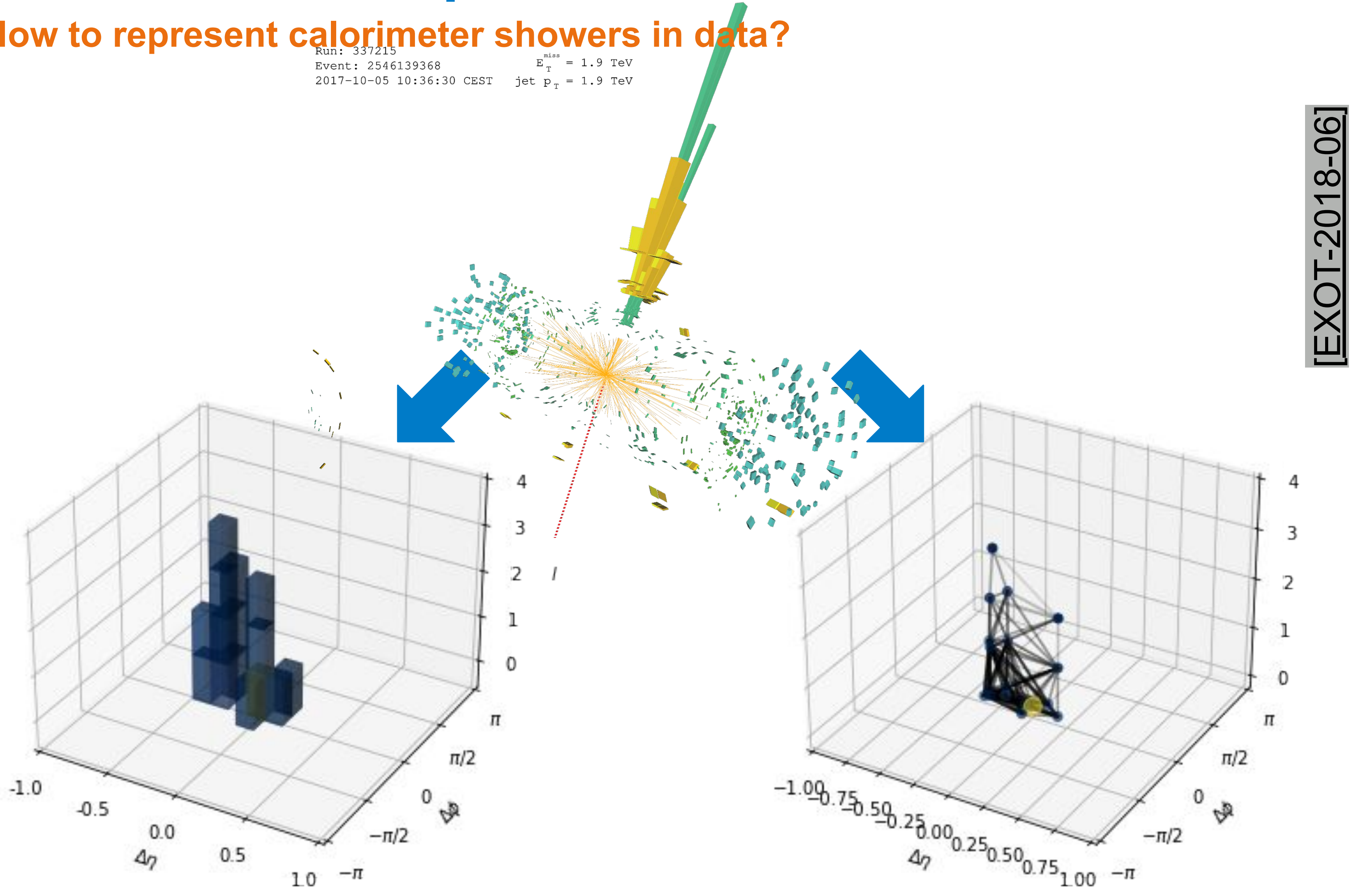

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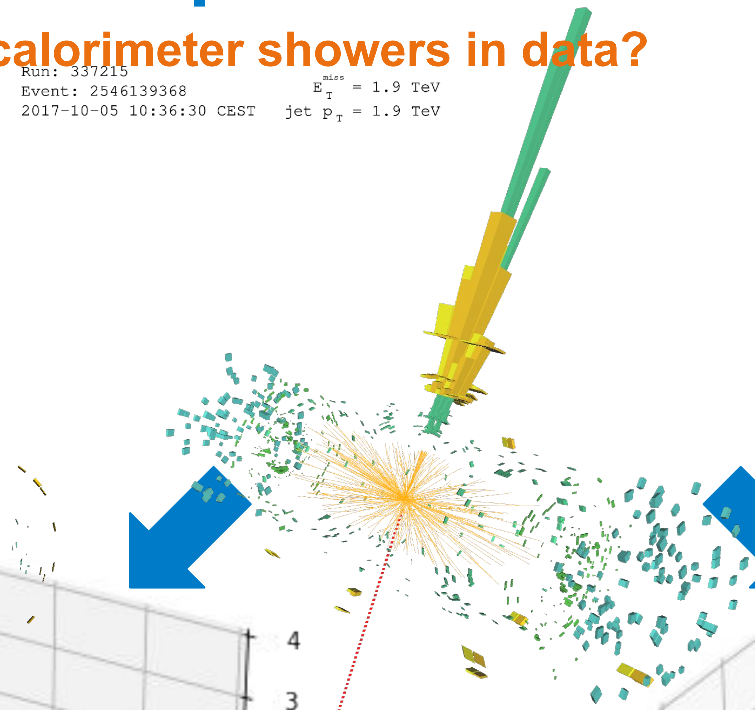
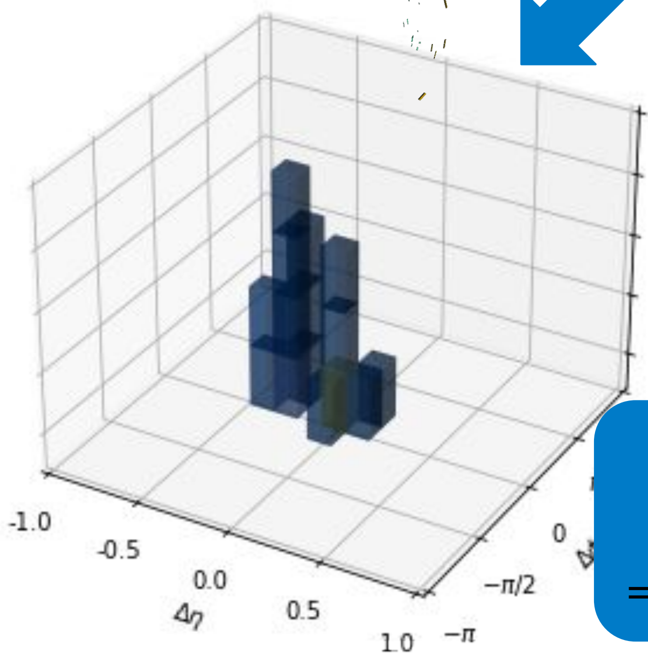
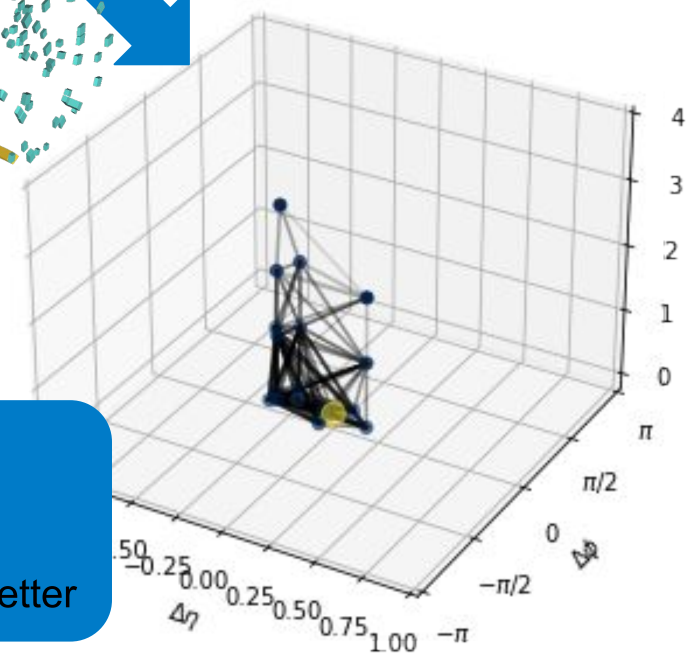






[EXOT-2018-06]

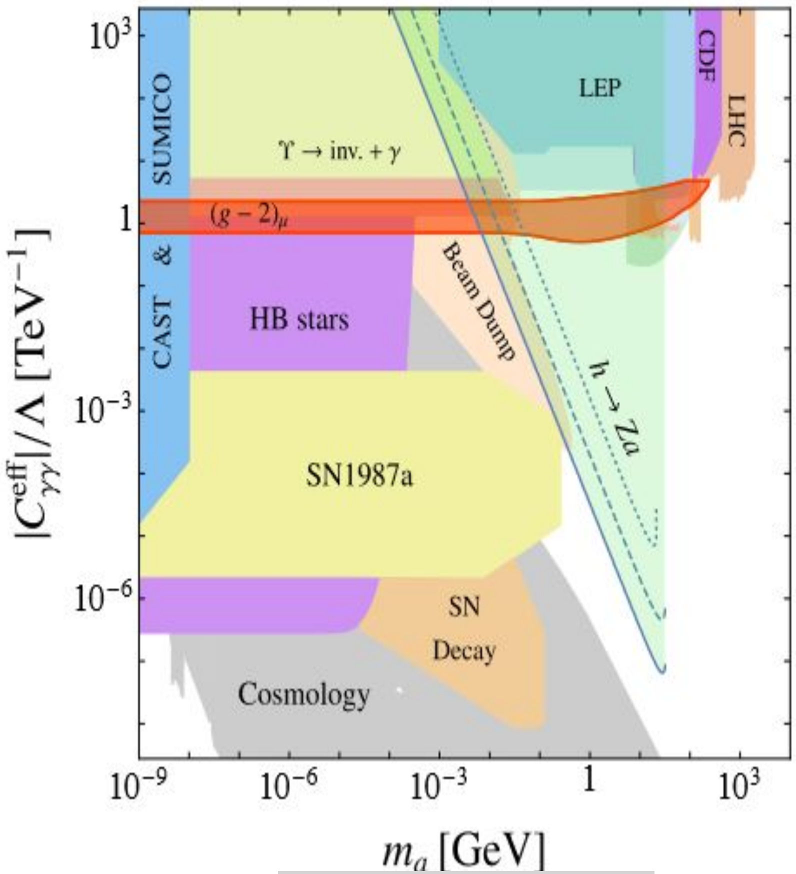
- Binning
- Empty bins
- Size limitations

⇒ Not clear which is better

Selected Benchmark Study

Axion-Like Particles (ALPs)

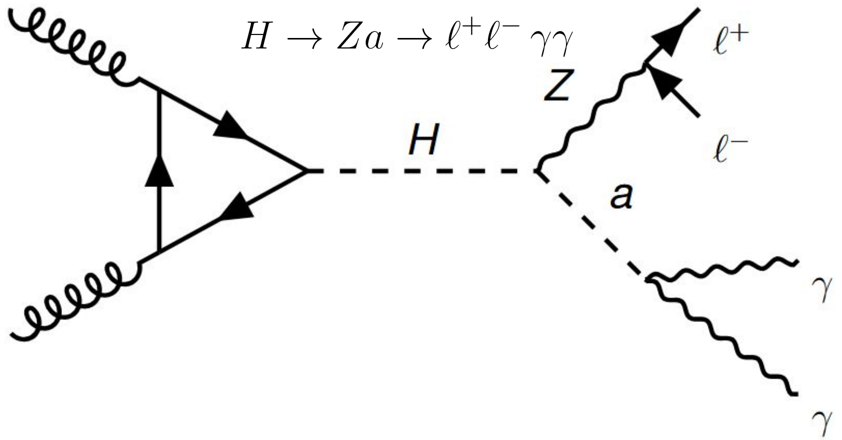
- $g_{a\gamma\gamma}, m_a$ free parameters
- Dark Matter candidate:
  non-thermally in early universe
- Mediator in Dark Sector theories
- Produced in H decays
  (Higgs portal theories)



arXiv:1704.08207

ALPs in Higgs Decays

- $Z \rightarrow ll$: simple and clean signature
- Main background:
  Z + jets or Z + photons



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- $Z \rightarrow ll$: simple and clean signature
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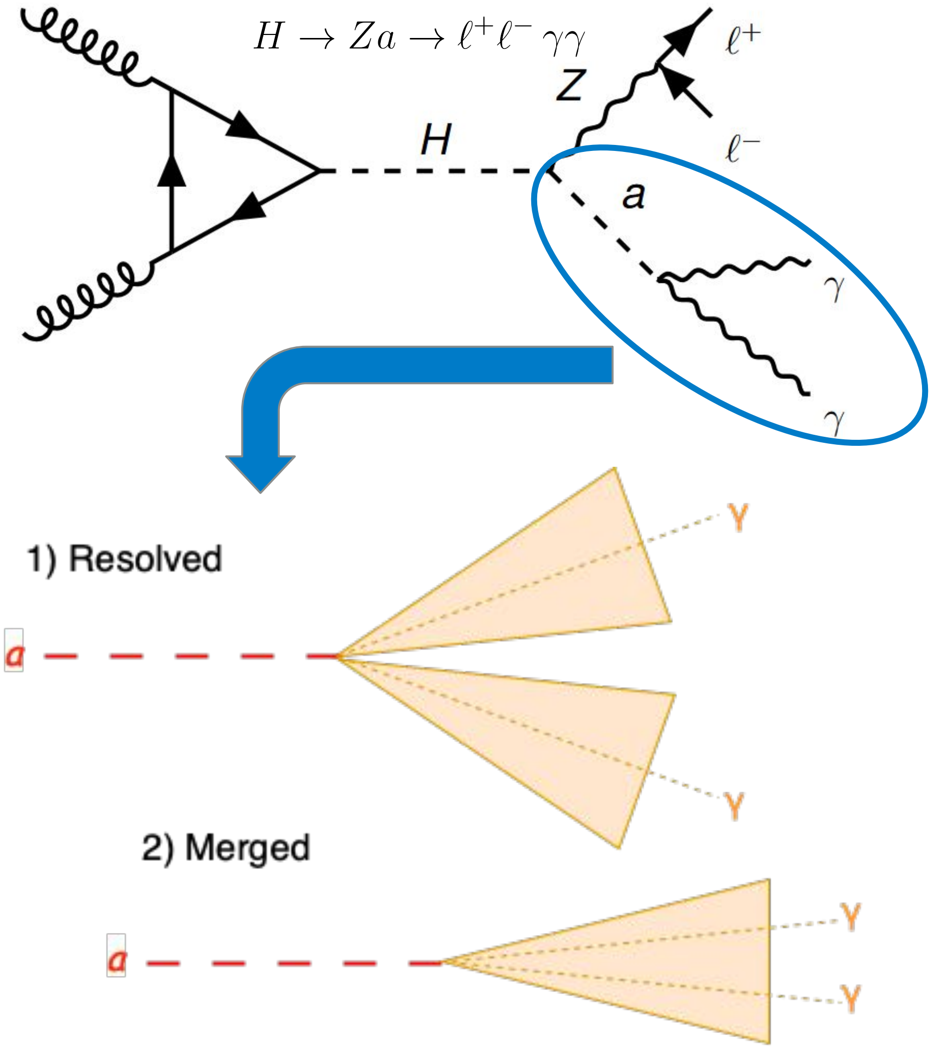
- 2 categories:
  - "Resolved"/Separated:
    high ALP mass
  - "Merged"/Collimated:
    low ALP mass



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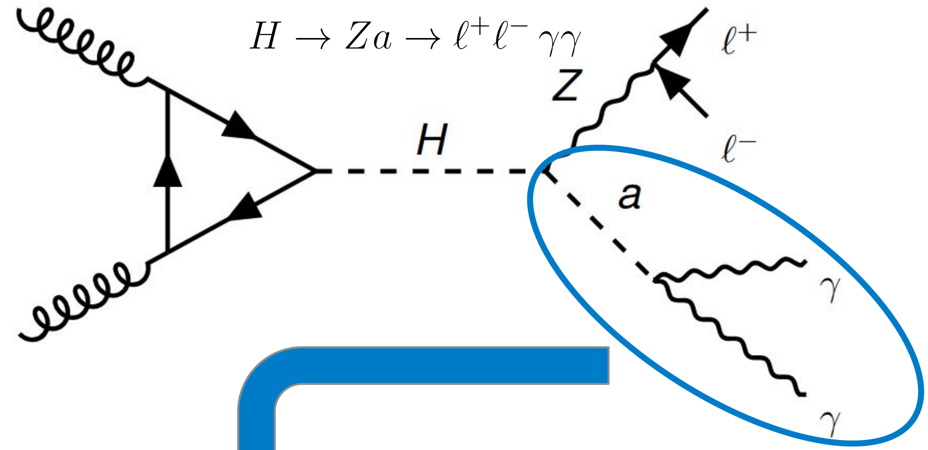
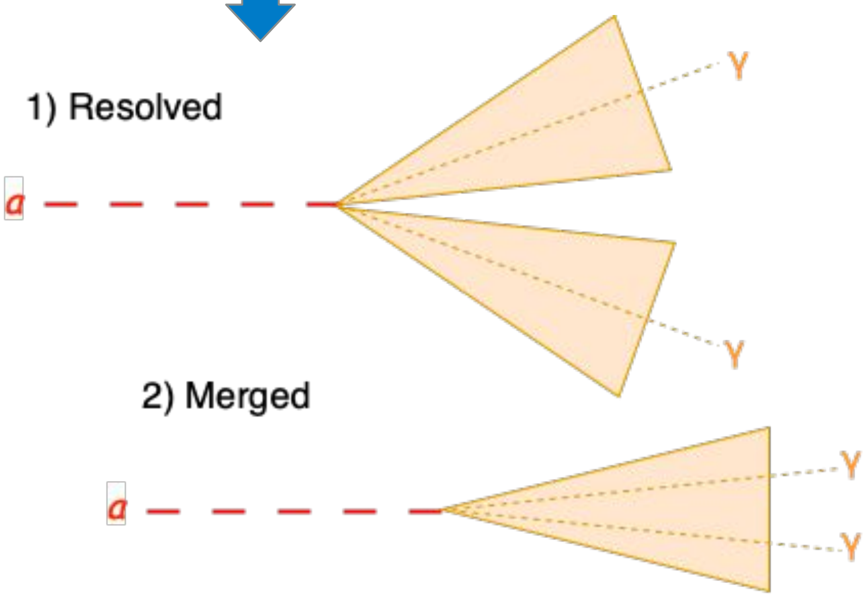
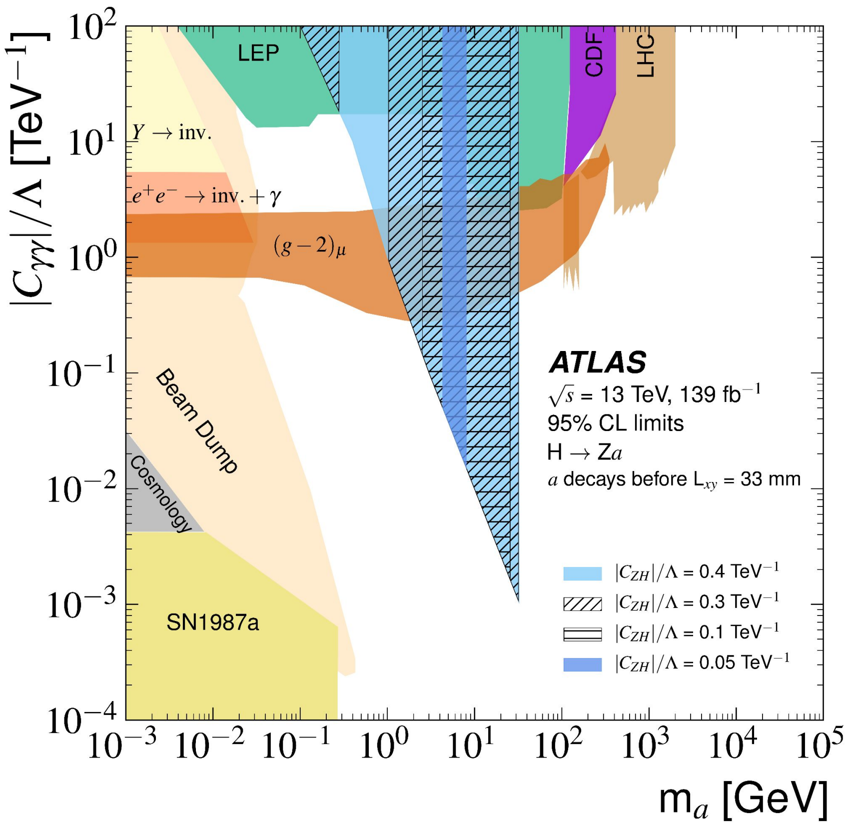
- $H \to 2a \to 4\gamma$ at ATLAS:
  arXiv:2312.03306





Prompt Decay Analysis

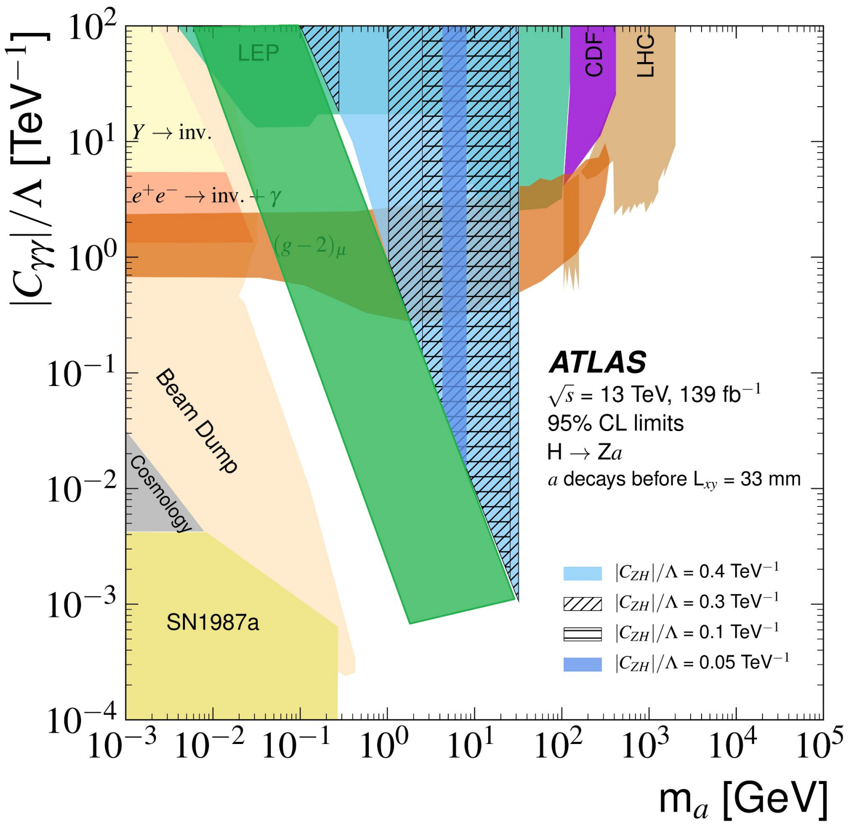
- Search for H → Za in Run 2 data
- Promptly decaying ALP
- Trigger on Z decay leptons
- $m_a \in [0.1, 31]\,\mathrm{GeV}$



arXiv:2312.01942

Prompt Decay Analysis

- Search for H → Za in Run 2 data
- Promptly decaying ALP
- Trigger on Z decay leptons
- $m_a \in [0.1, 31]\,\mathrm{GeV}$
- m_a/$C_{a\gamma\gamma}$ also allow for long-lived ALPs



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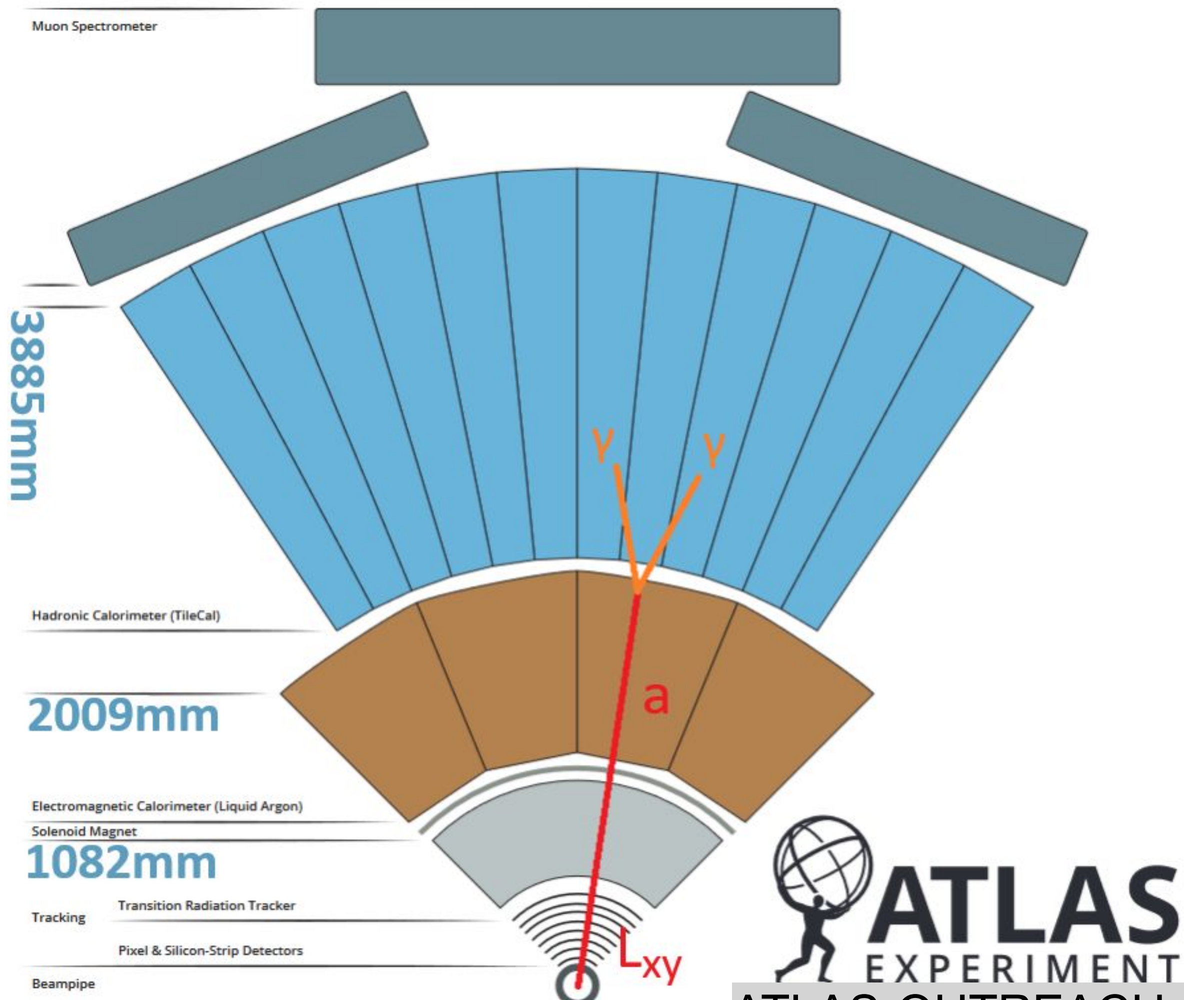
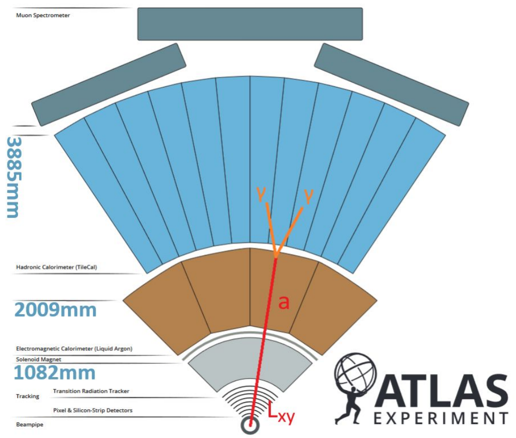
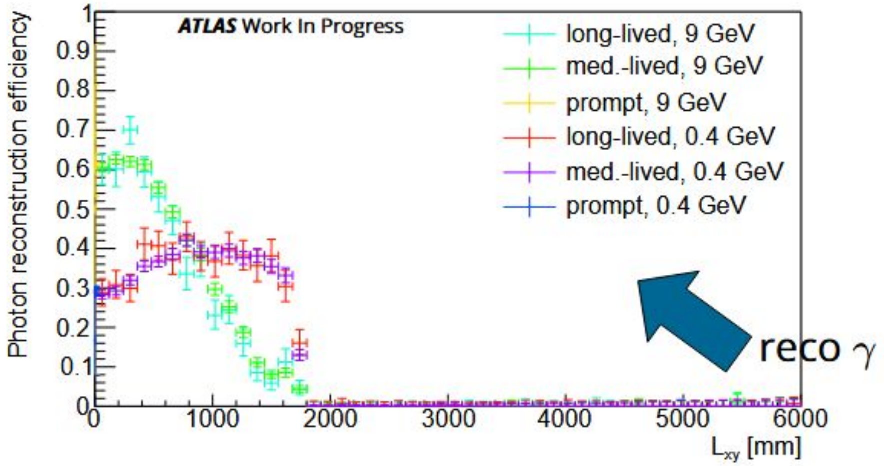
Displaced Showers in the ATLAS Detector



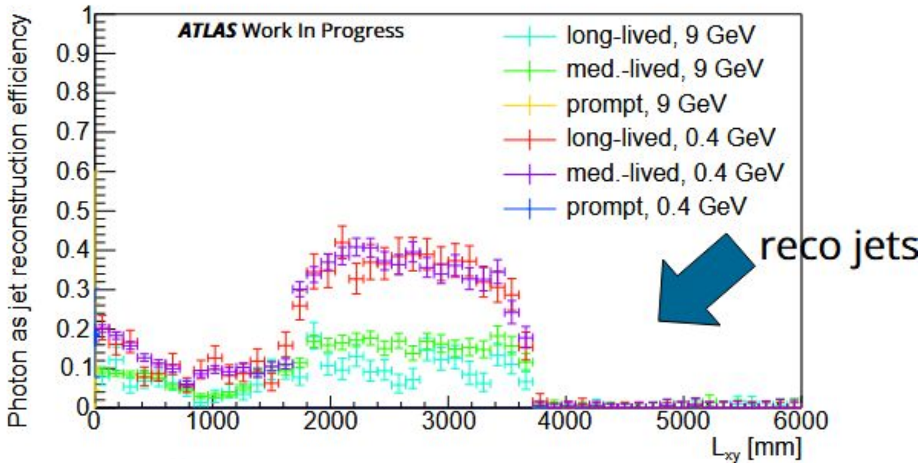
ATLAS-OUTREACH-2021-052

Photon Reconstruction Efficiency





- Reconstruction efficiency of ALP decay photons as function of L_{xy}
- At HCAL: photon reco efficiency = 0



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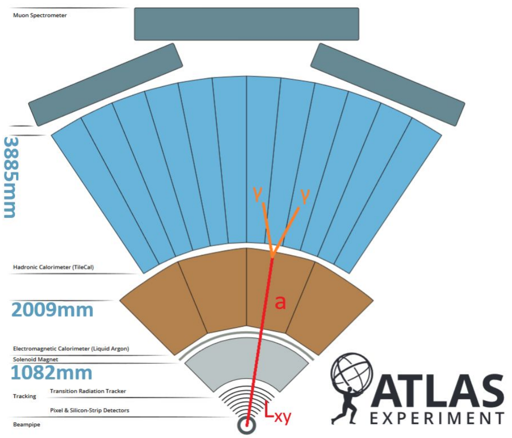
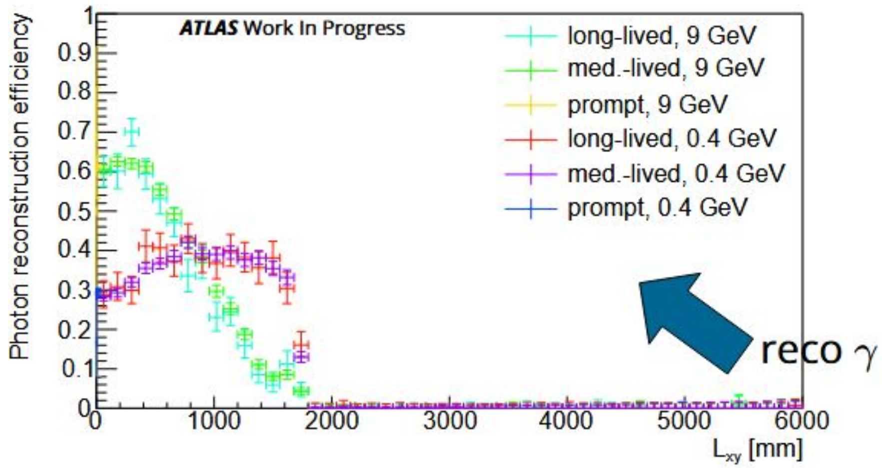
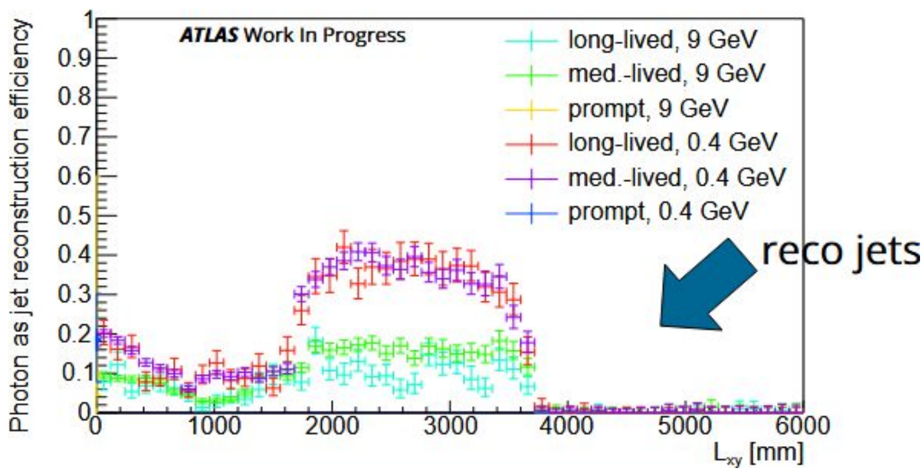


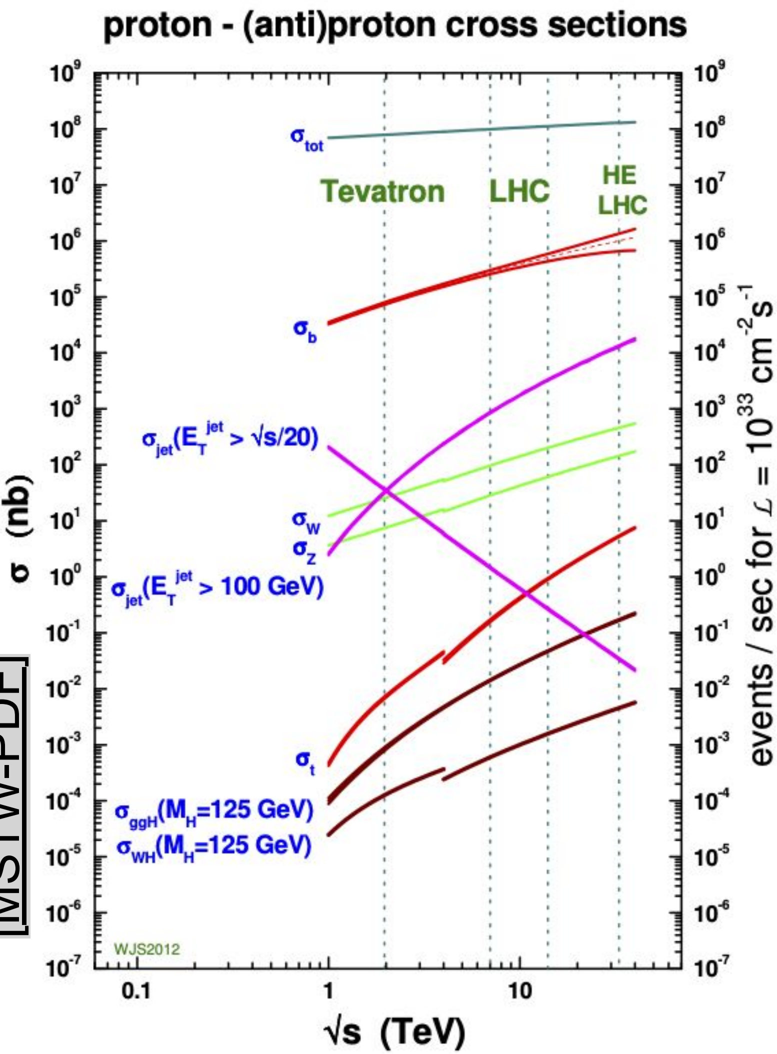


- Reconstruction efficiency of ALP decay photons as function of L_{xy}
- At HCAL: photon reco efficiency = 0

For large L_{xy} we need jets!

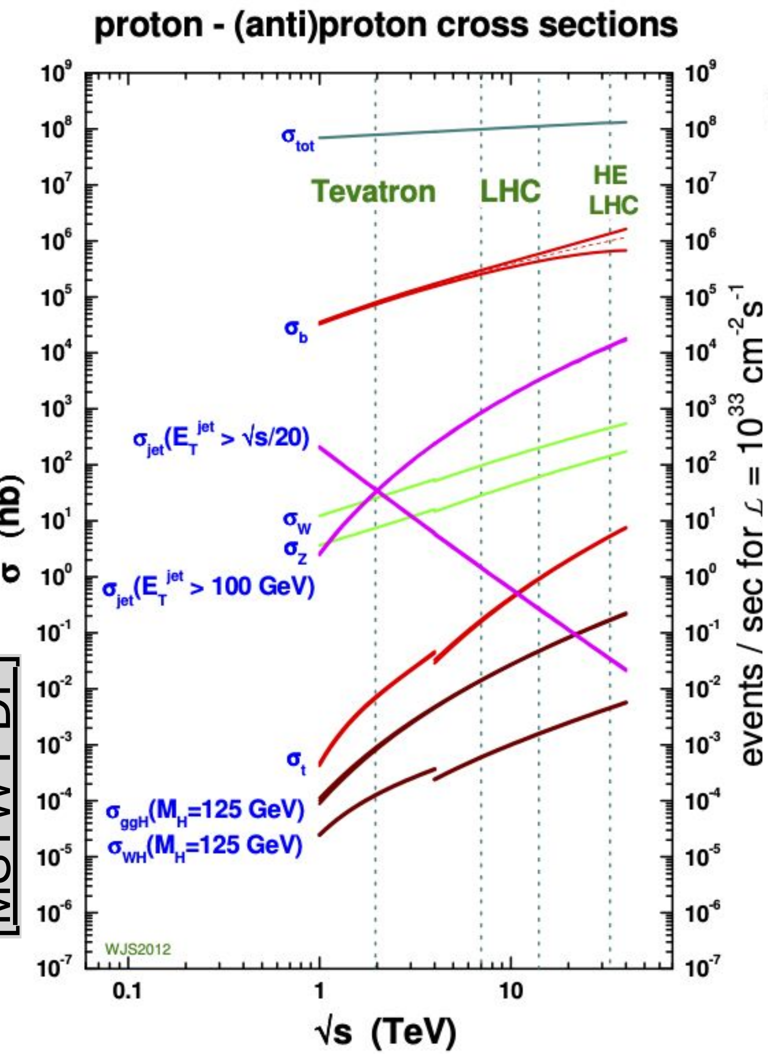


Background Jets

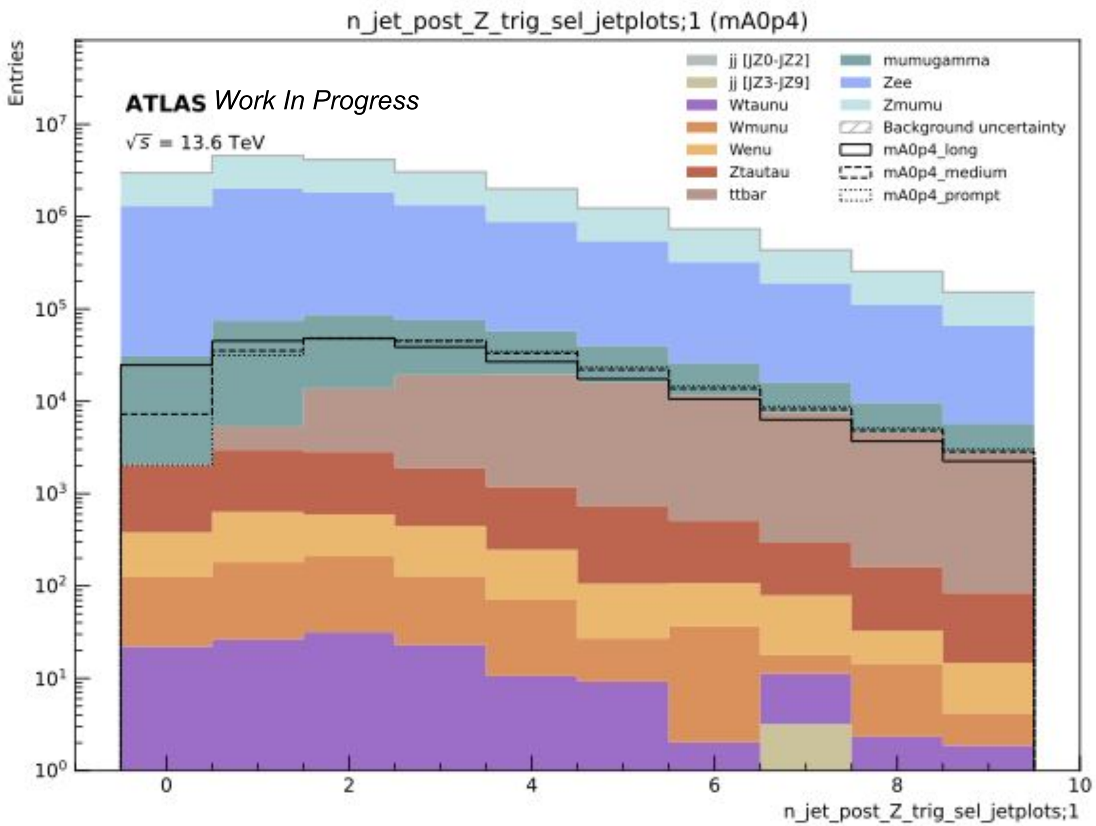


[MSTW-PDF]

Background Jets



[MSTW-PDF]



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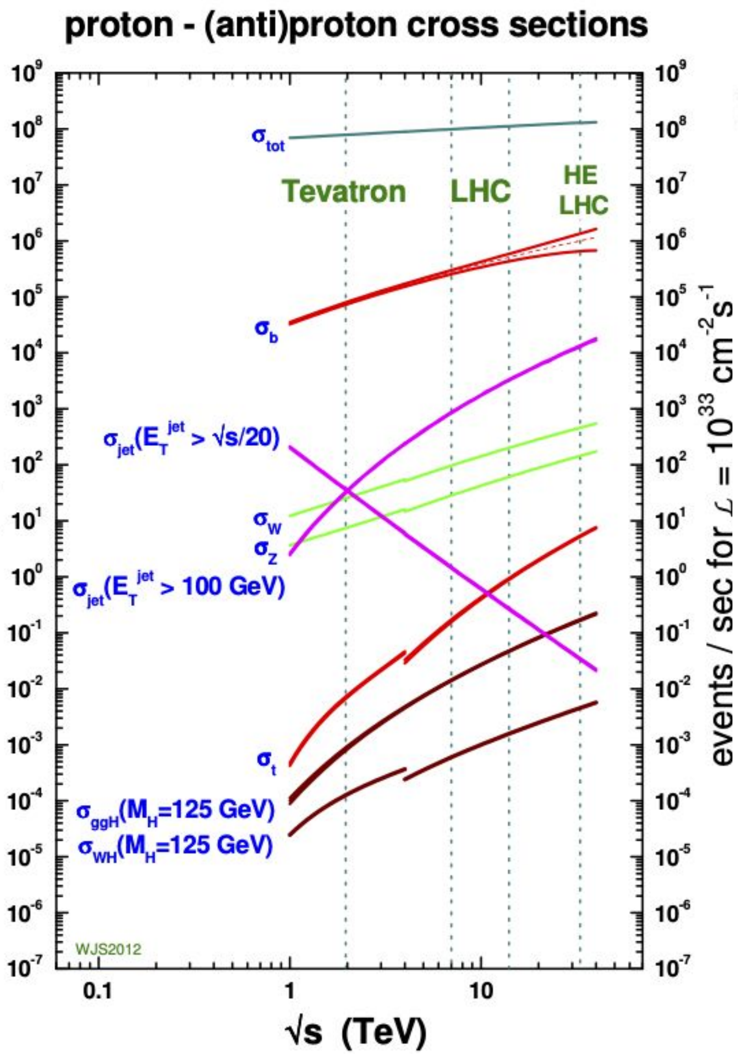
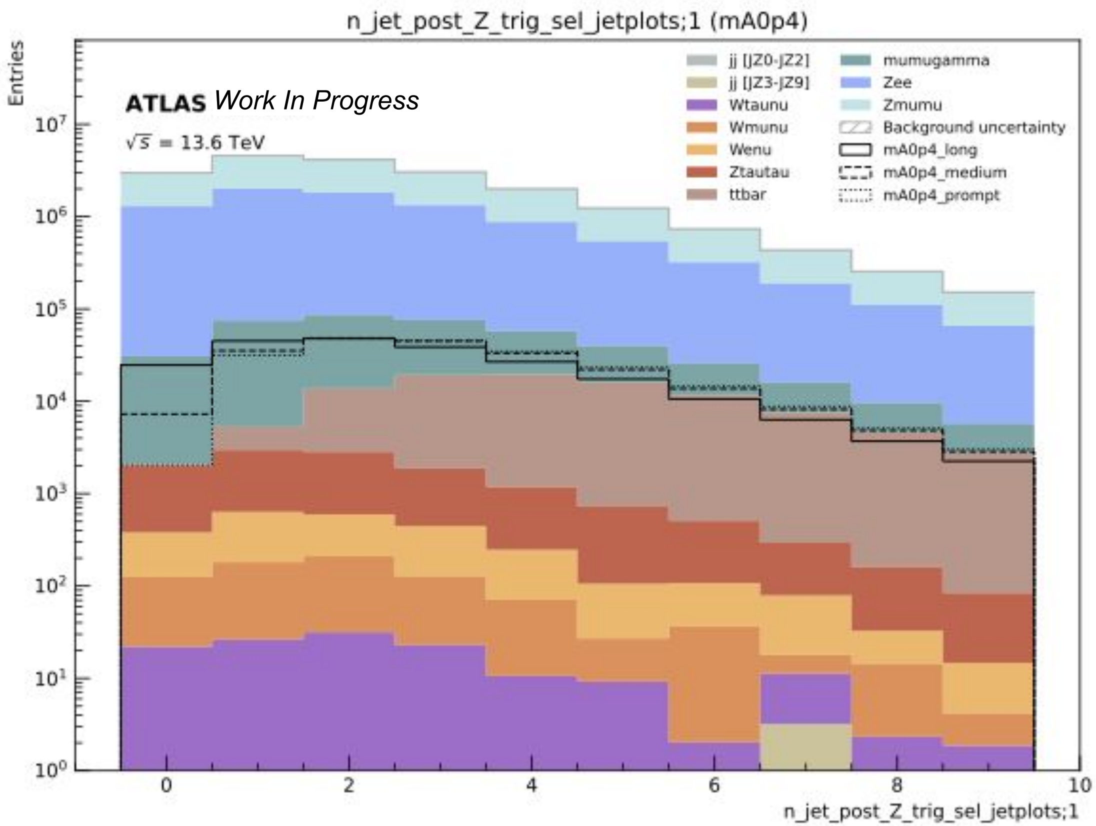


[MSTW-PDF]



<u>Lots</u> of background jets!

Jet Tagging with CNNs and GNNs

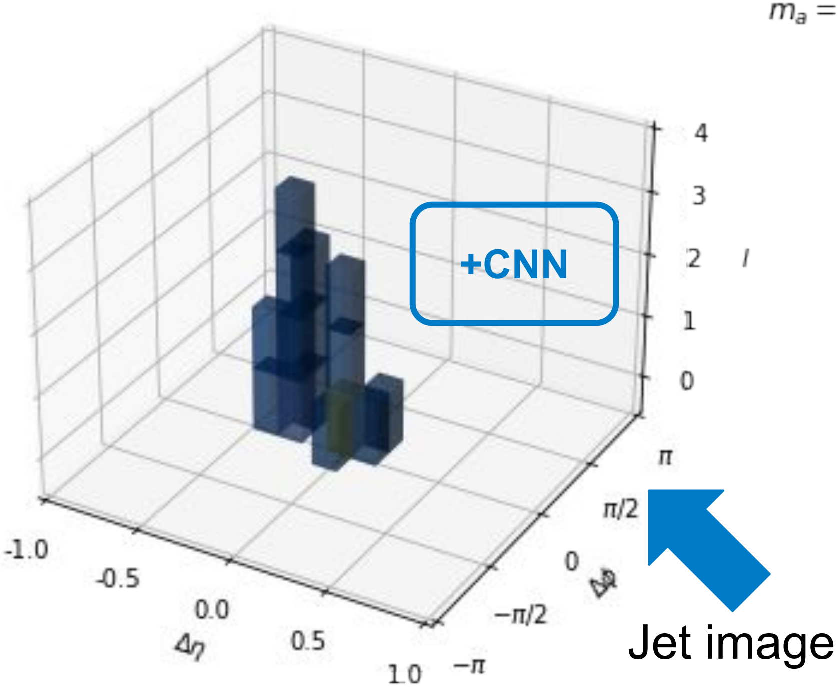
How to identify displaced photons as jets?

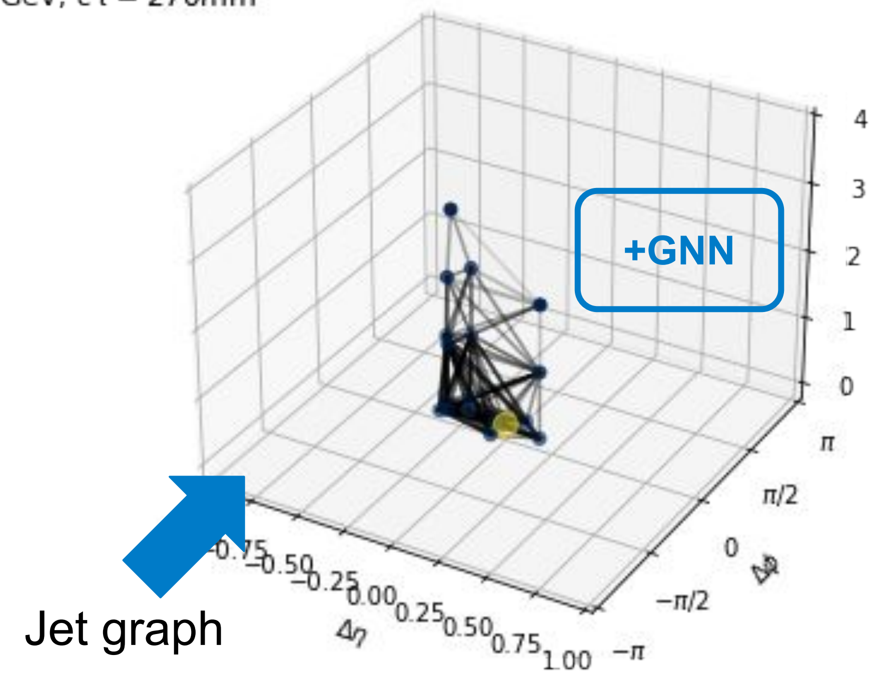
2 approaches

How to identify displaced photons as jets?

2 approaches

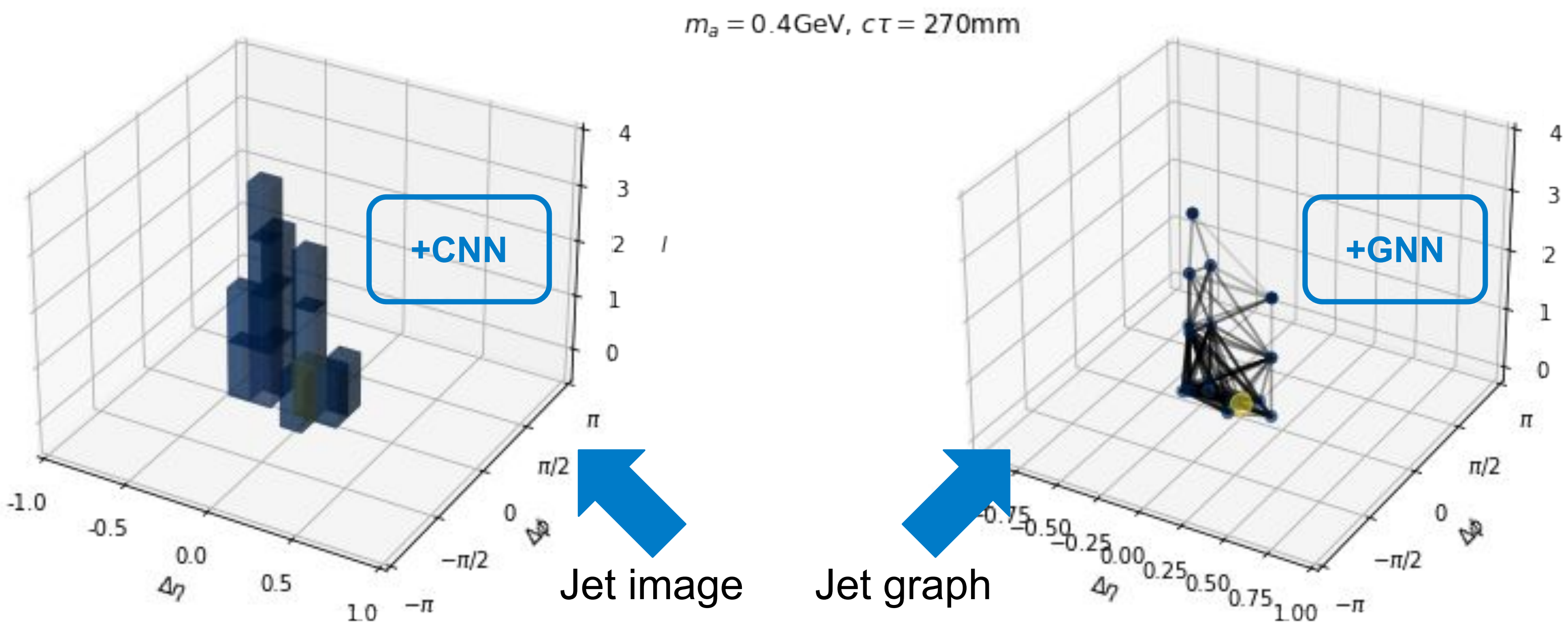
$m_a = 0.4\text{GeV},\ c\tau = 270\text{mm}$





How to identify displaced photons as jets?

2 approaches



Which one performs better on the task?

Input Processing

Common Pre-Transformation

Truth Matching
resolved: ALP
merged: γ

Jet

Calo Clusters

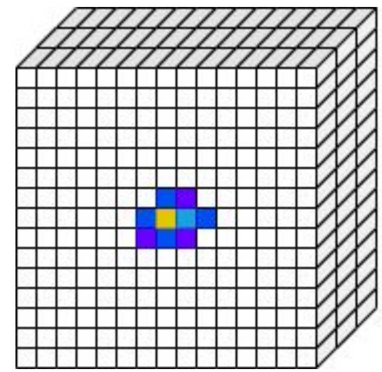
E

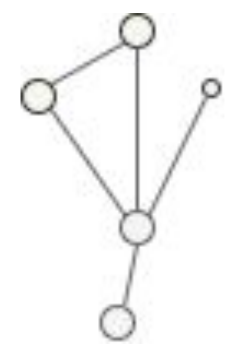
$\eta, \ \phi$

Layer

<u>Common</u> Cluster Pre-Transformation

1. Remove clusters E < 400MeV
2. Rescale $E \rightarrow [0,1]$
3. $\eta, \phi \rightarrow$ rel. coords





Input Processing Recipe

Common Pre-Transformation

Truth Matching
resolved: ALP
merged: γ

Jet

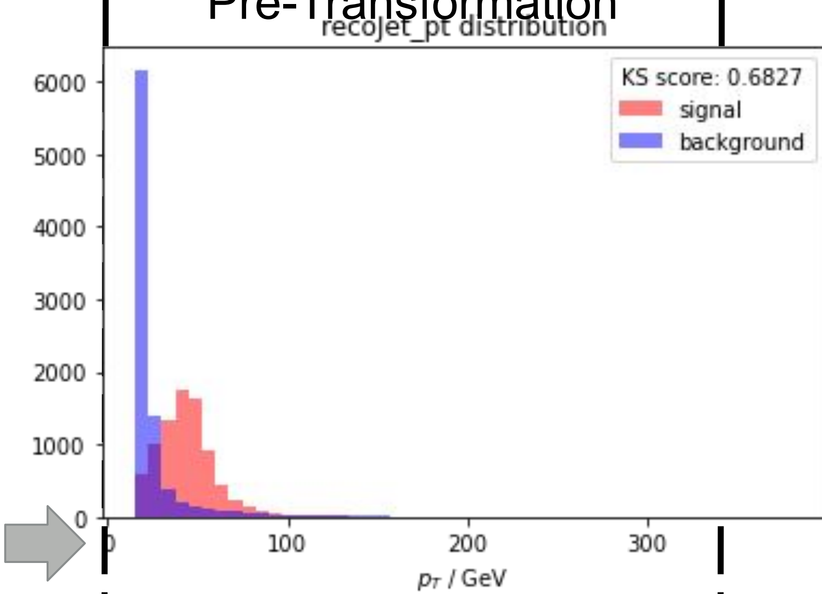
Calo Clusters

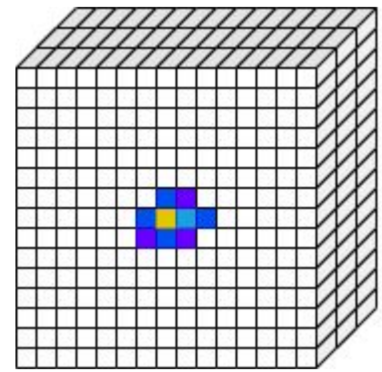
E

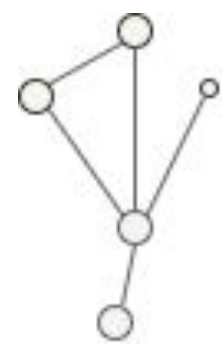
$\eta,\ \phi$

Layer

<u>Common</u> Cluster Pre-Transformation







Input Processing

Common Pre-Transformation

Truth Matching
resolved: ALP
merged: γ

Jet

Calo Clusters

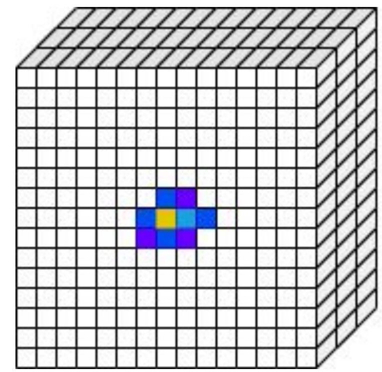
E

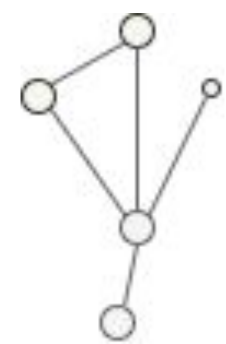
η, ϕ

Layer

Common Cluster Pre-Transformation

1. Remove clusters E < 400MeV
2. Rescale $E \rightarrow [0,1]$
3. $\eta, \phi \rightarrow$ rel. coords

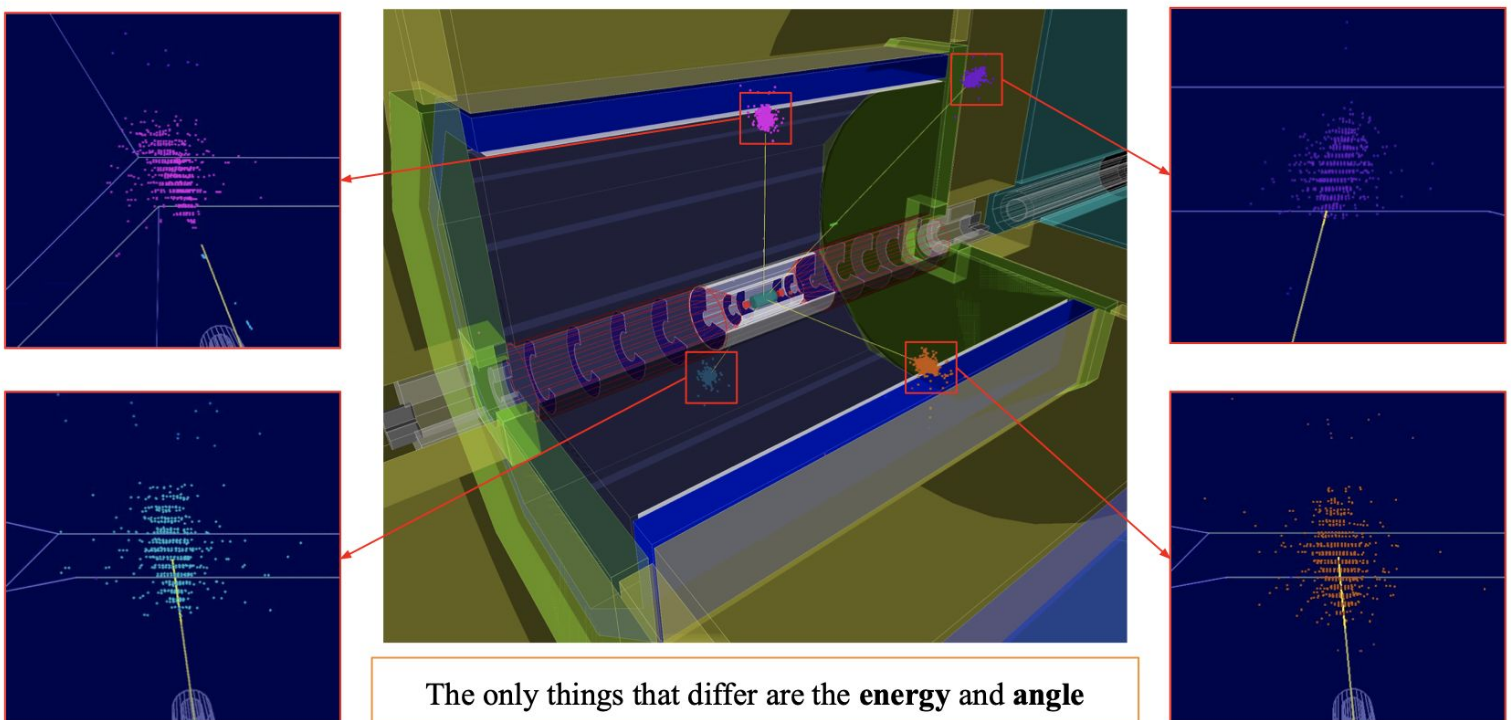




Input Processing

Common Pre-Transformation

Shower Development is Consistent Across Regions with Identical Material Structure



The only things that differ are the **energy** and **angle**

DESY. | Scientific Computing Seminar, 23.05.25 | Anatolii Korol

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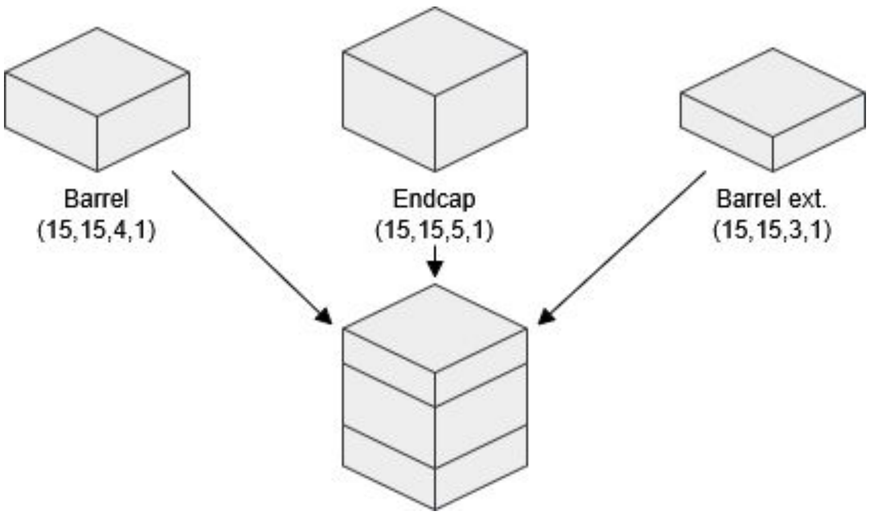
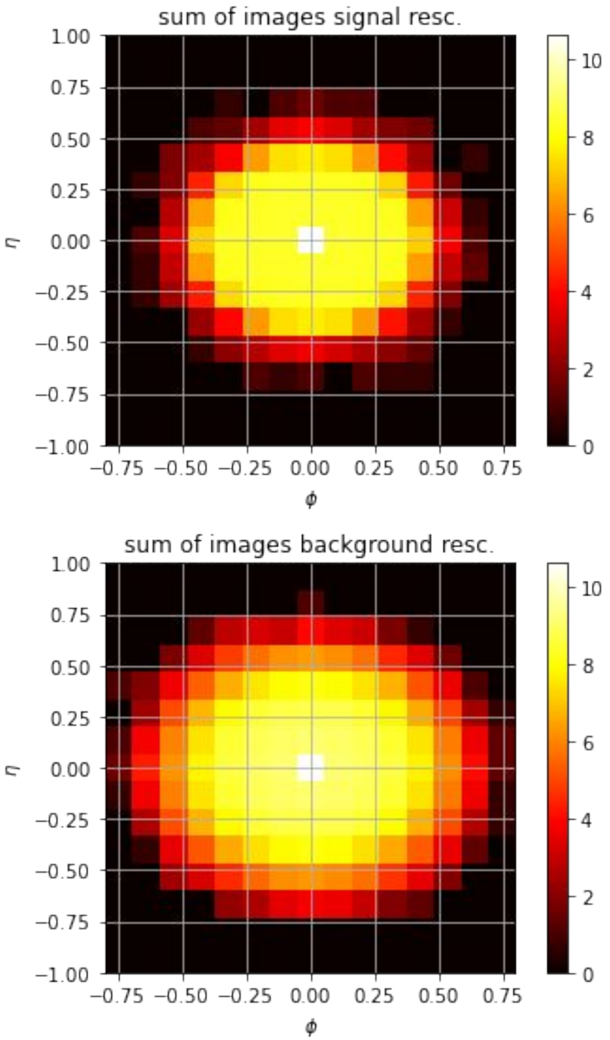
Image Building



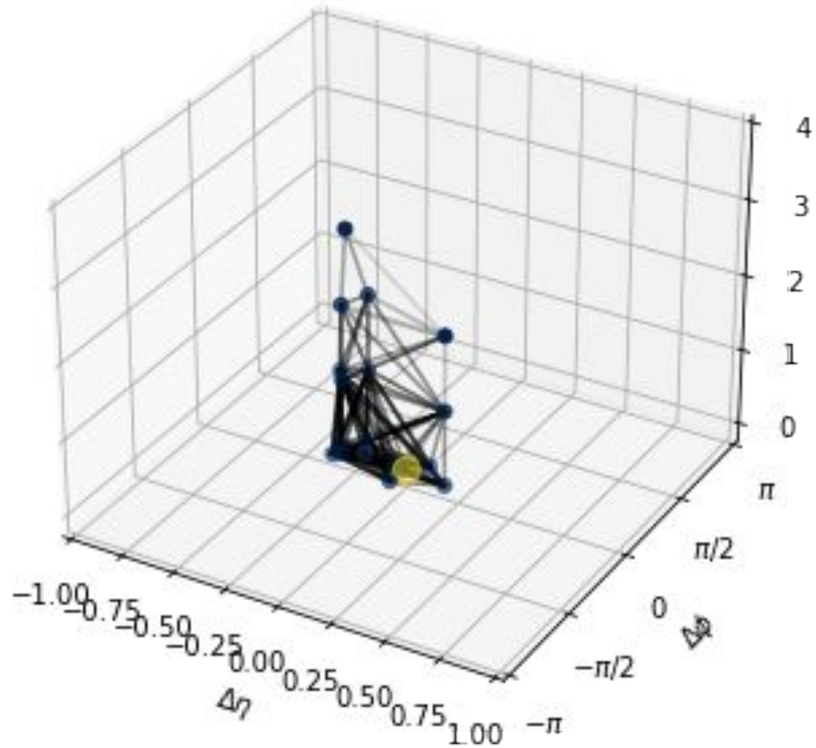


- Images binned in $\eta \times \phi = 15 \times\ 15$ bins
- Sph. symmetry, high E in center ✅
- Bound to fixed-size inputs
- Barrel, Endcap, Barrel ext. stacked

Graph Building

- Nodes = [E, η, ϕ, ℓ] of clusters

- Edges = ΔR between clusters
  - $\Delta\ell$ = 0: if $\Delta R \leq 0.6$
  - $\Delta\ell$ = 1: if $\Delta R \leq 0.6$



Model Architectures

CNN:

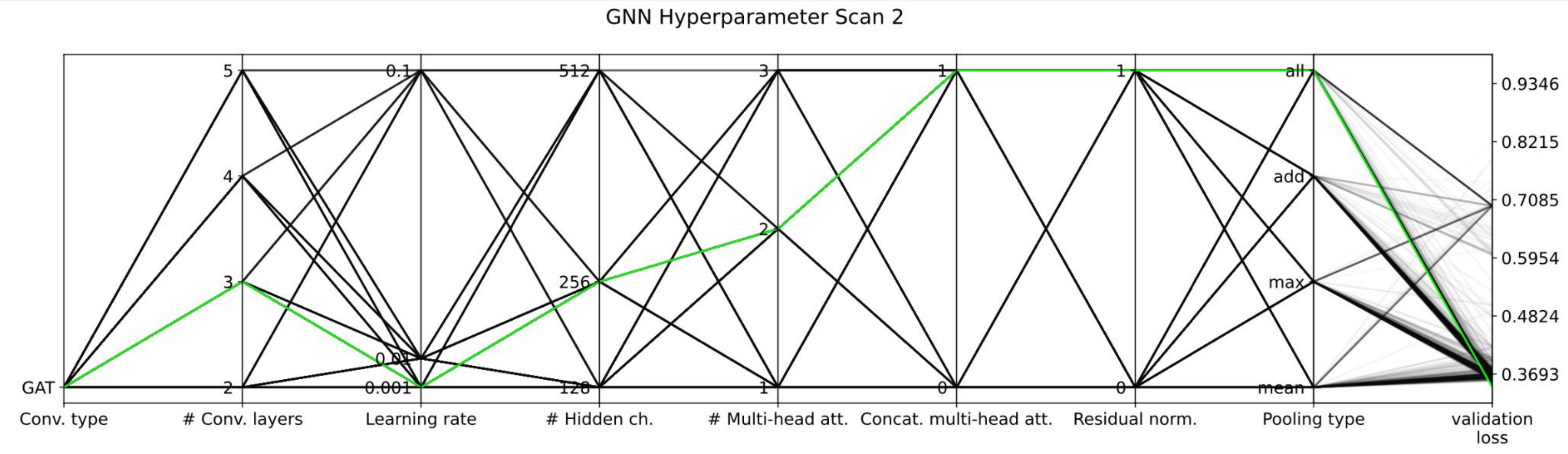
- Tensorflow
- Based on CNN developed for dark photon analysis (arXiv:2206.12181)
- Conv3D + Pooling, Dense layers

GNN:

- PyTorch + `pytorch_geometric`
- Based loosely on `jetgraphs` library
- Convolution/Attention Graph Filters + Pooling

Hyperparameter Optimization

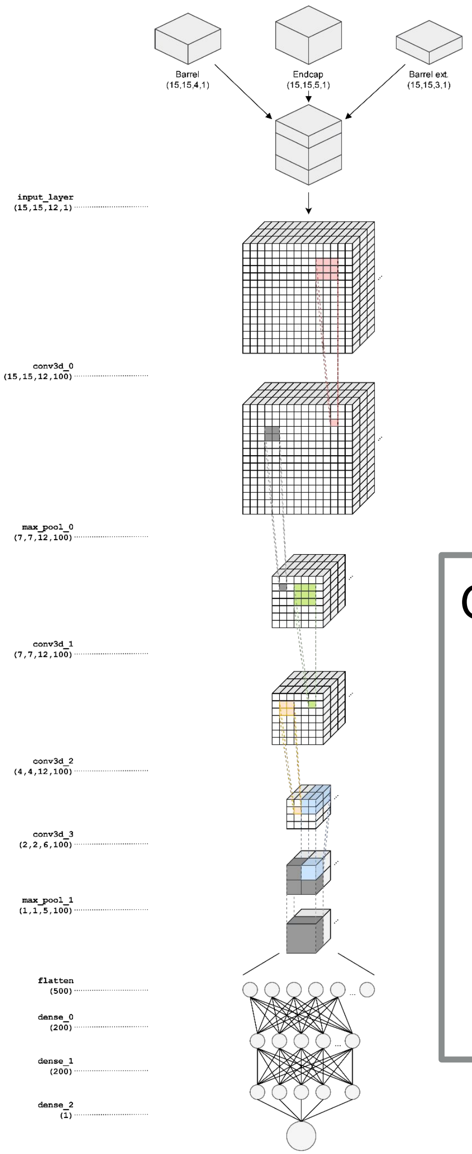
- Fully parallelized grid scans performed for CNN+GNN
- For 1 benchmark signal (0.4GeV, medium lifetime)



green line: best hyperparam configuration

& similar for the CNN

Model Architectures after Optimization

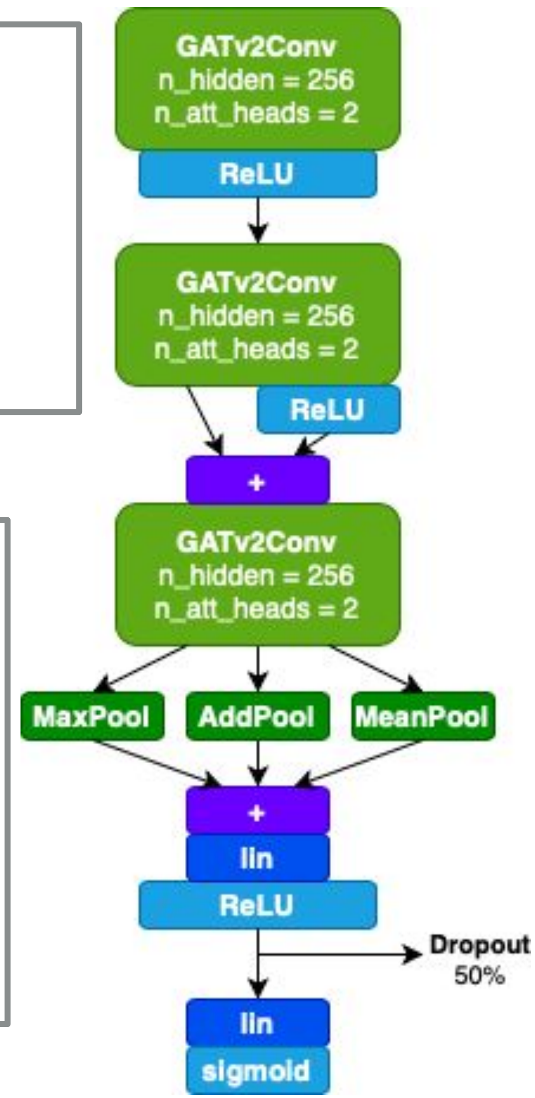


← CNN

- input [15,15,12,1]
- 3× Conv3D
- MaxPooling
- 3× Dense (n_nodes=200)
- ~1M parameters

GNN →

- 3× GATv2Conv (2 att. heads, 256 hidden ch.)
- Feed-forward at every 2nd layer
- Max+Mean+Add pooling combined
- ~1.3M parameters



Deploying to Analysis

C++ Framework Integration

- **Python** framework good for training & evaluation
- For analysis big scale inference: Implement model into ATLAS data processing framework (**`TopCPToolkit`**) **C++**
- CaloClusters can be **huge** in data! (esp. for backgrounds with many jets)
  → Only save output score for each jet & drop clusters afterwards!

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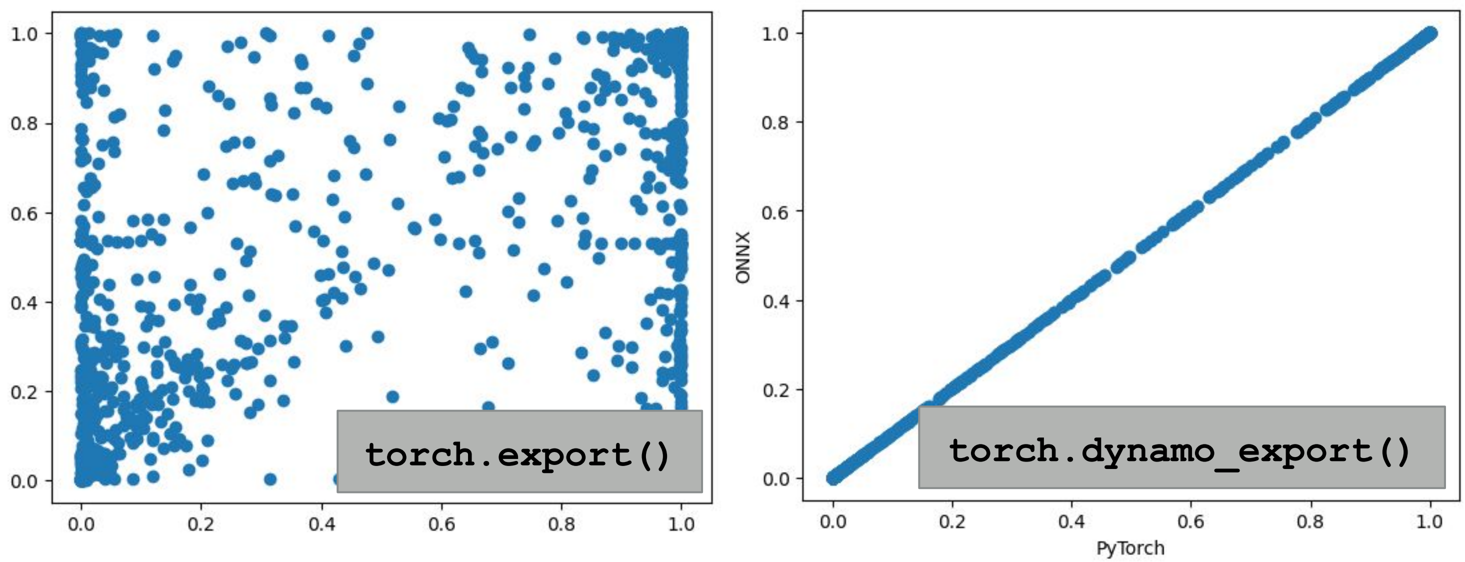
- **`TopCPToolkit`** can talk to ONNX models ✅
- To accomplish:
  1. Export models to ONNX
  2. Rewrite model-inputs processing in C++ Algorithm

ONNX Export

Part I: The scatter_reduce fight

- ONNX does not support **`torch.scatter_reduce`** with **`include_self=False`**
- E.g. GATv2Conv layers in GNN from **`torch_geometric`** use this
- Luckily, there was a long-awaited fix to **`torch_geometric`** lib (commit) ✅

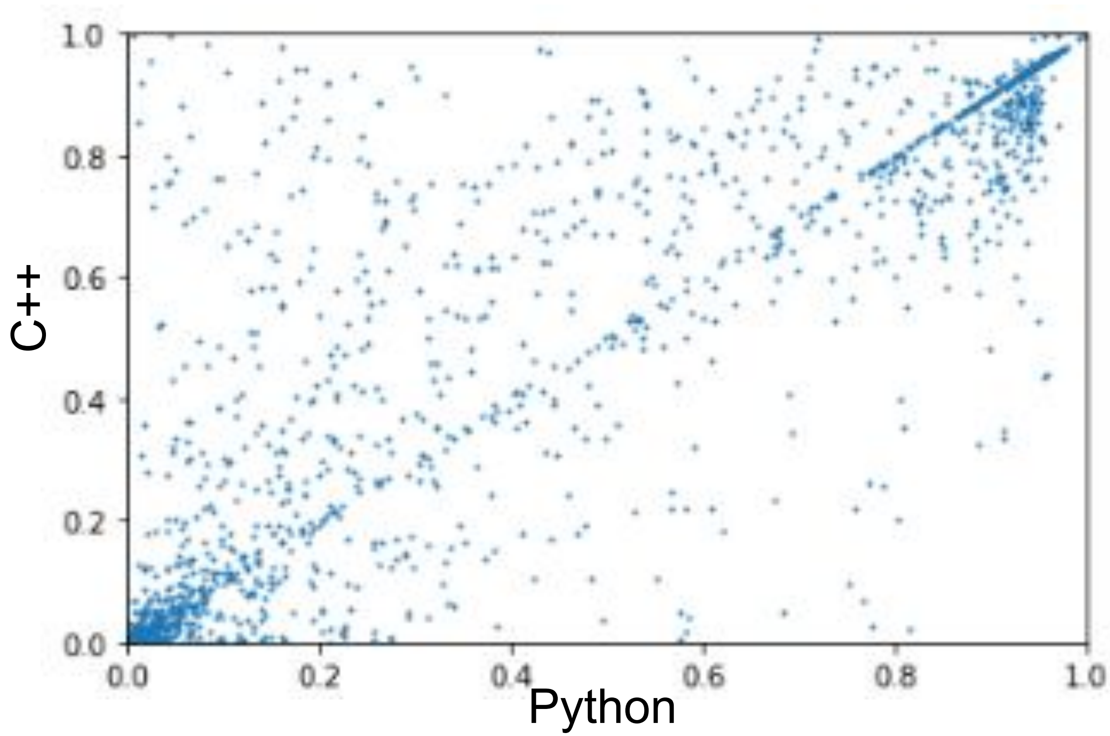
- GNN: variable-sized inputs (“dynamic axes”):



Input Building

Part II: Attack of the <vector<vector<vector<vector<…>>>>>

- No trivial task: Have to mimic exact behavior of e.g. graph building in C++ (incl. special-cases, numerical precision, …)
- Step-by-step align graph building in both frameworks by matching output scores:



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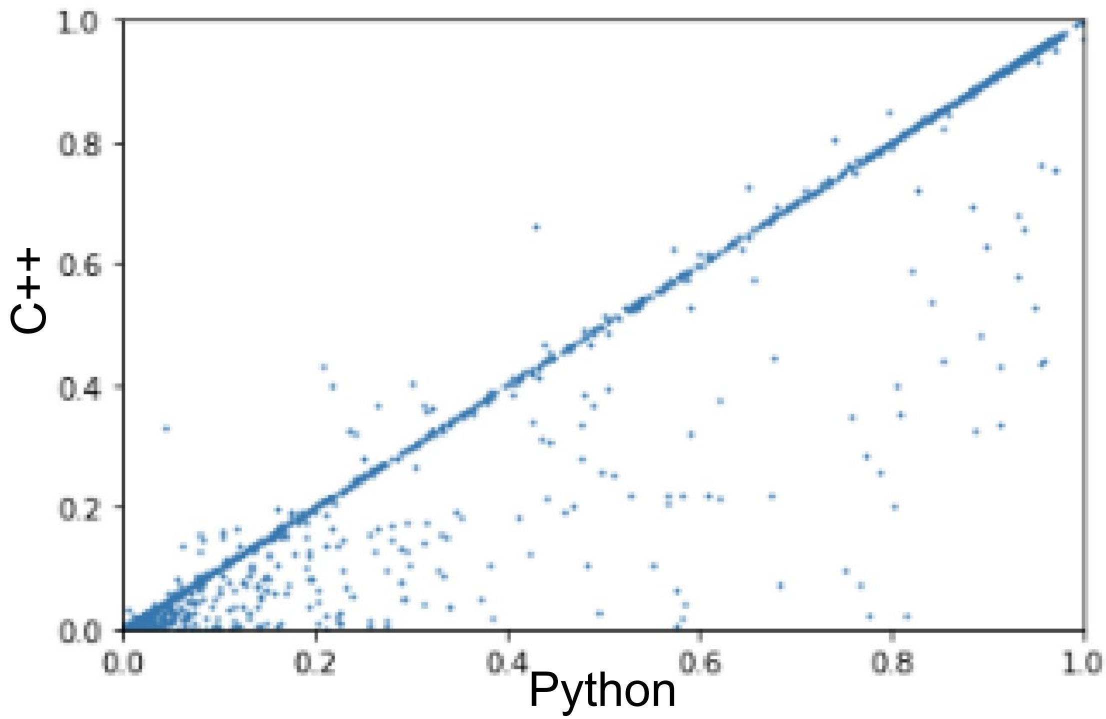

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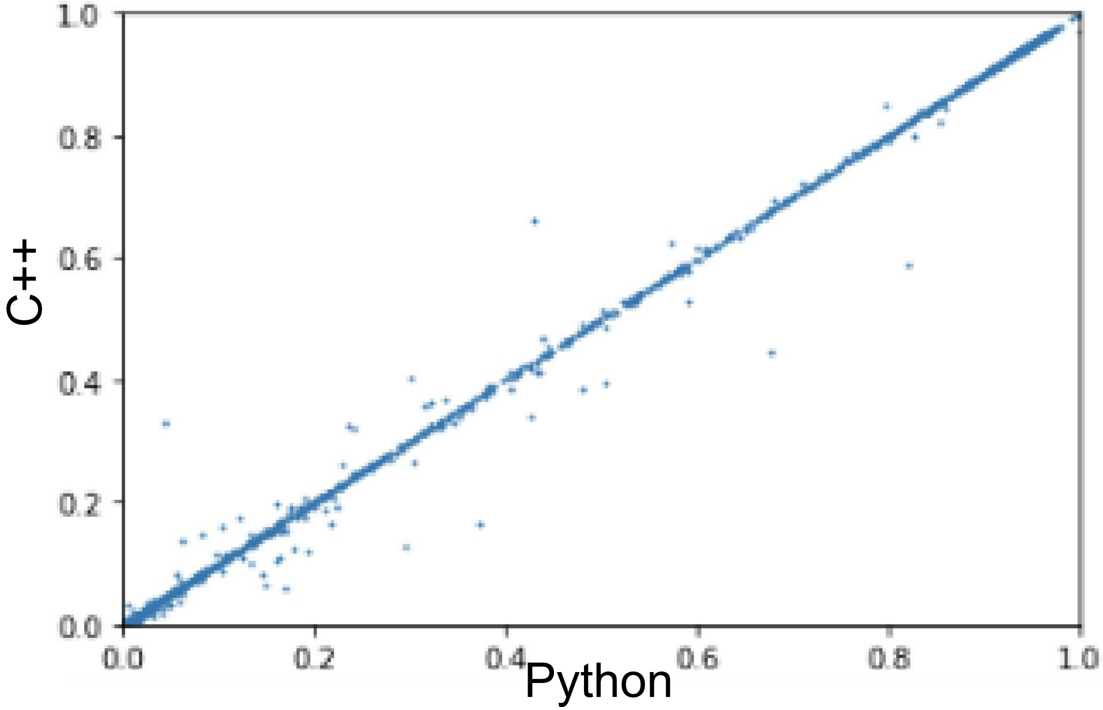

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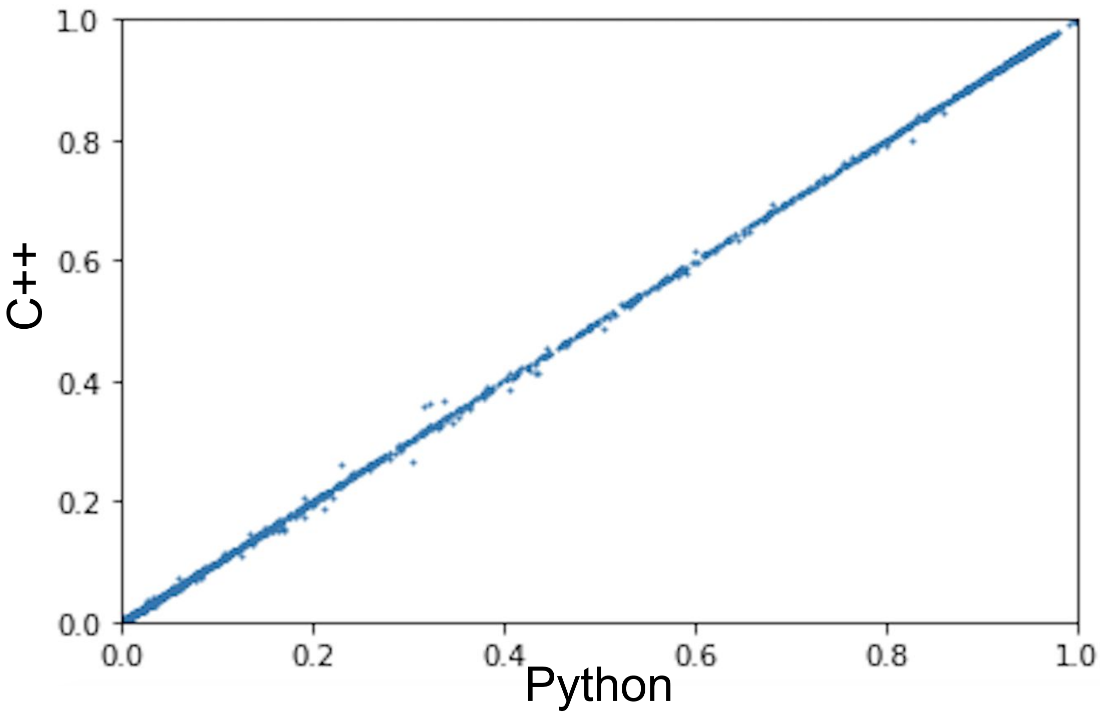

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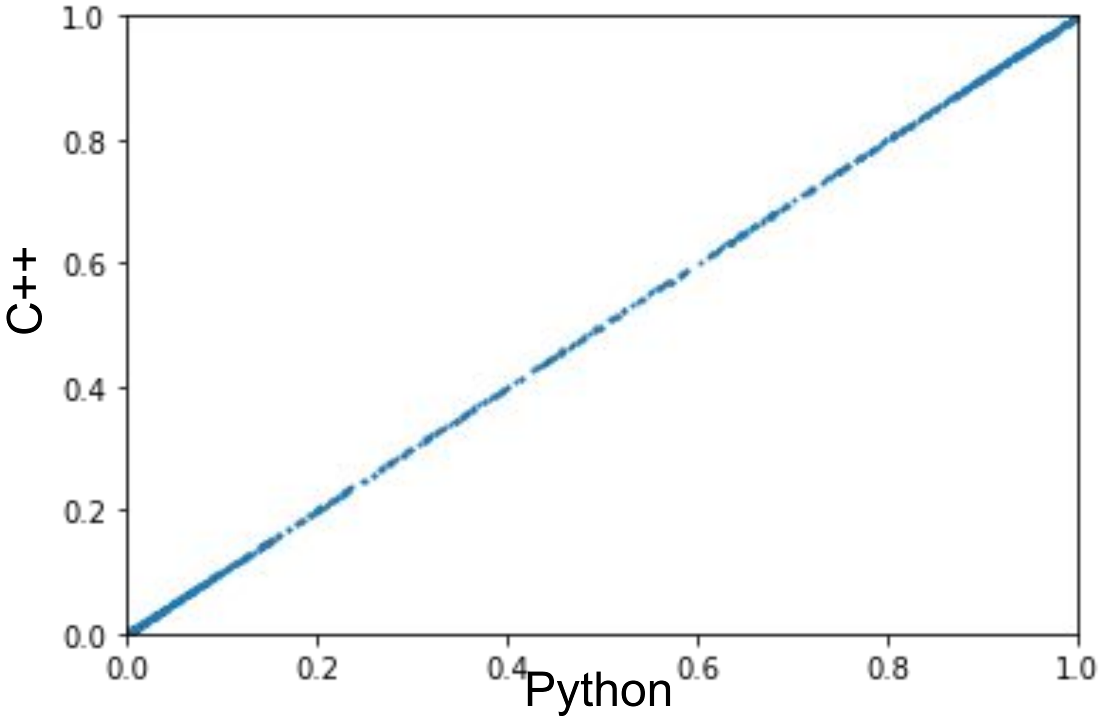
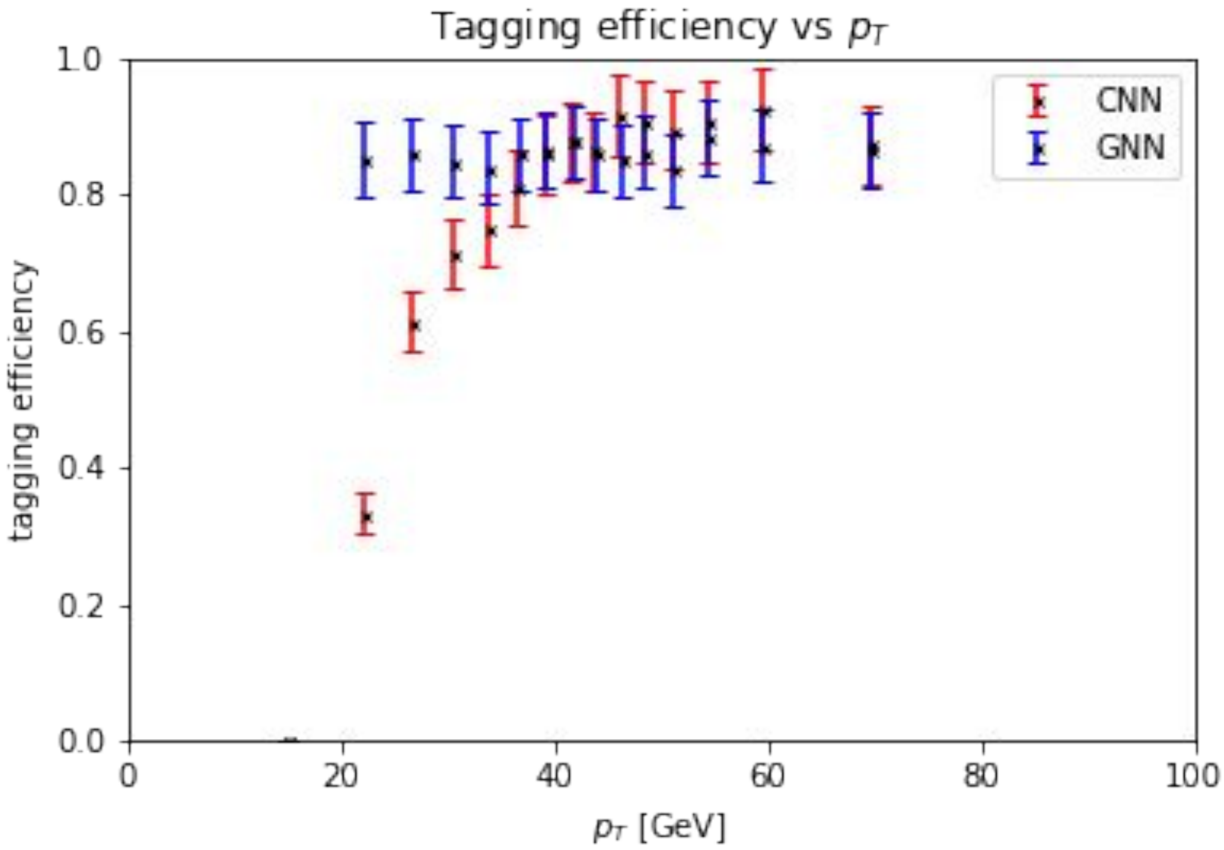


Recent Results

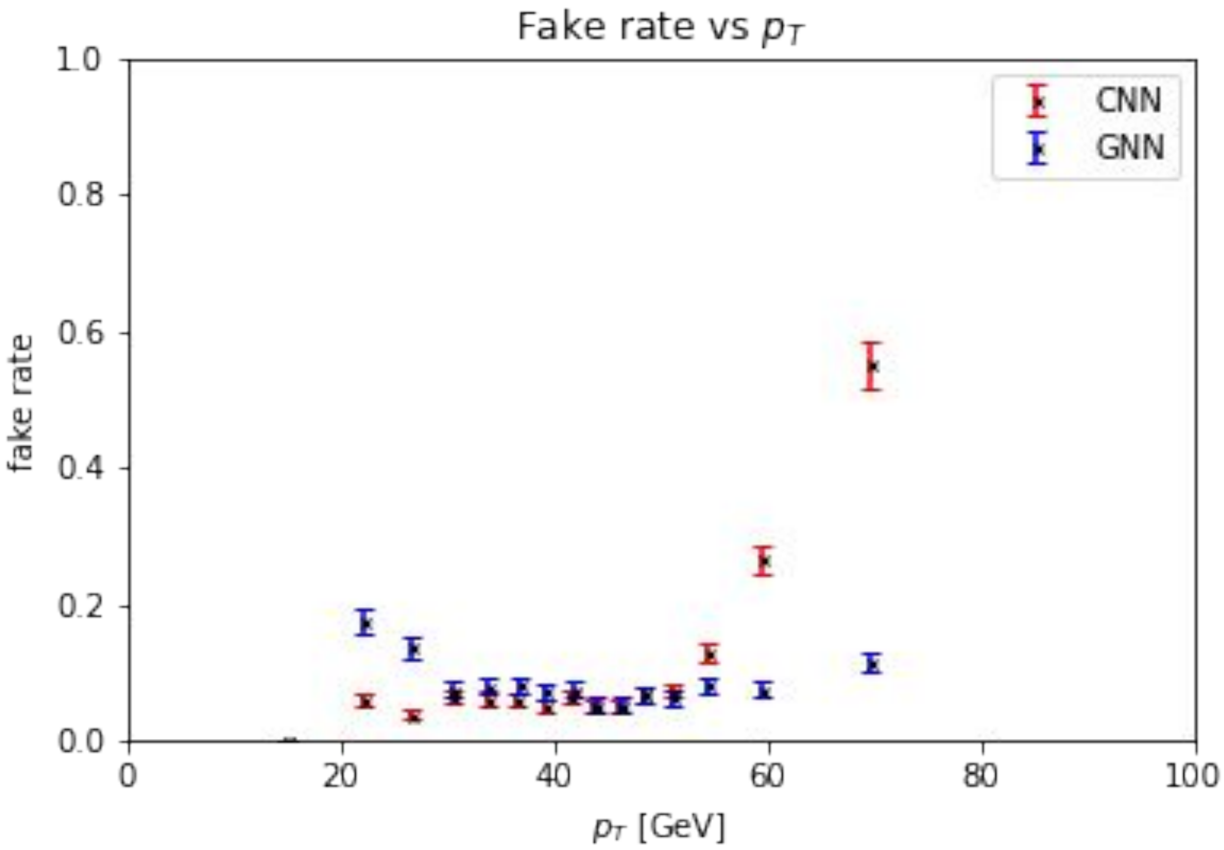
CNN vs. GNN

CNN vs. GNN



- (0.4GeV, medium lifetime sample)

CNN vs. GNN



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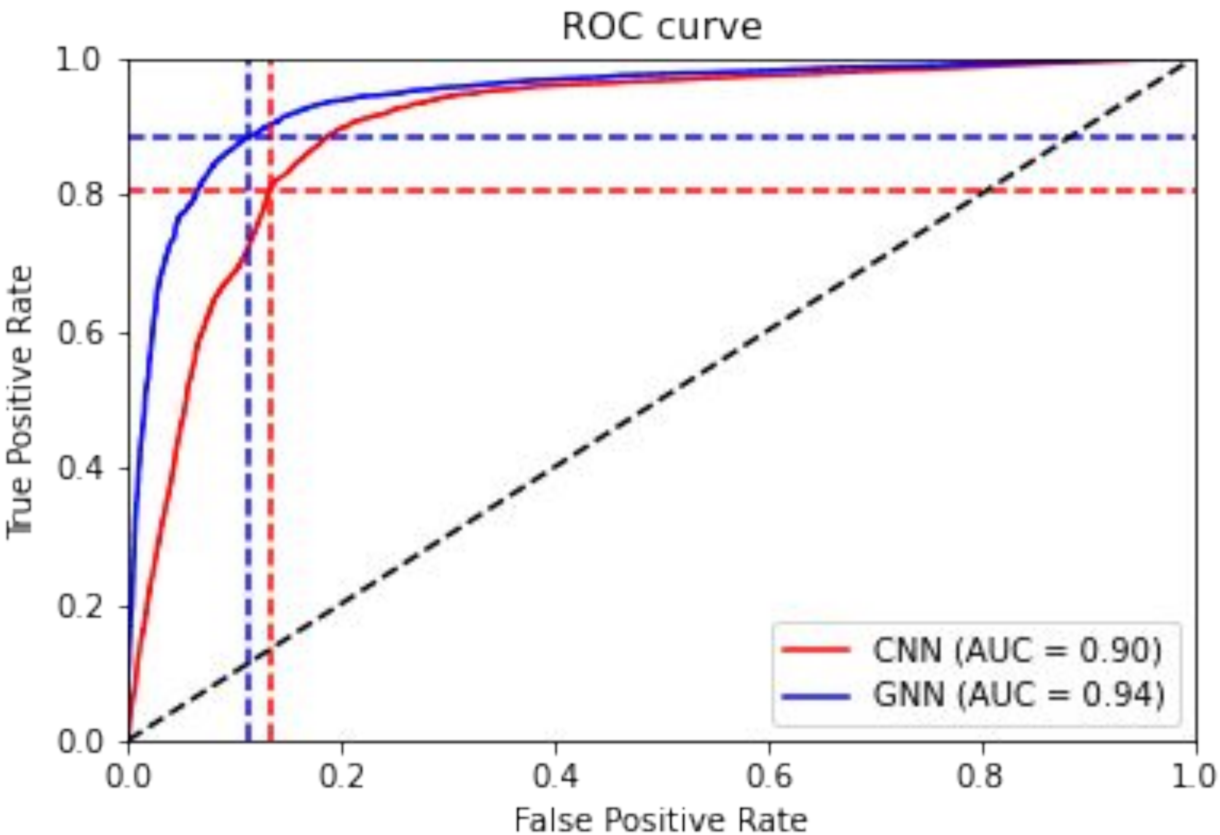

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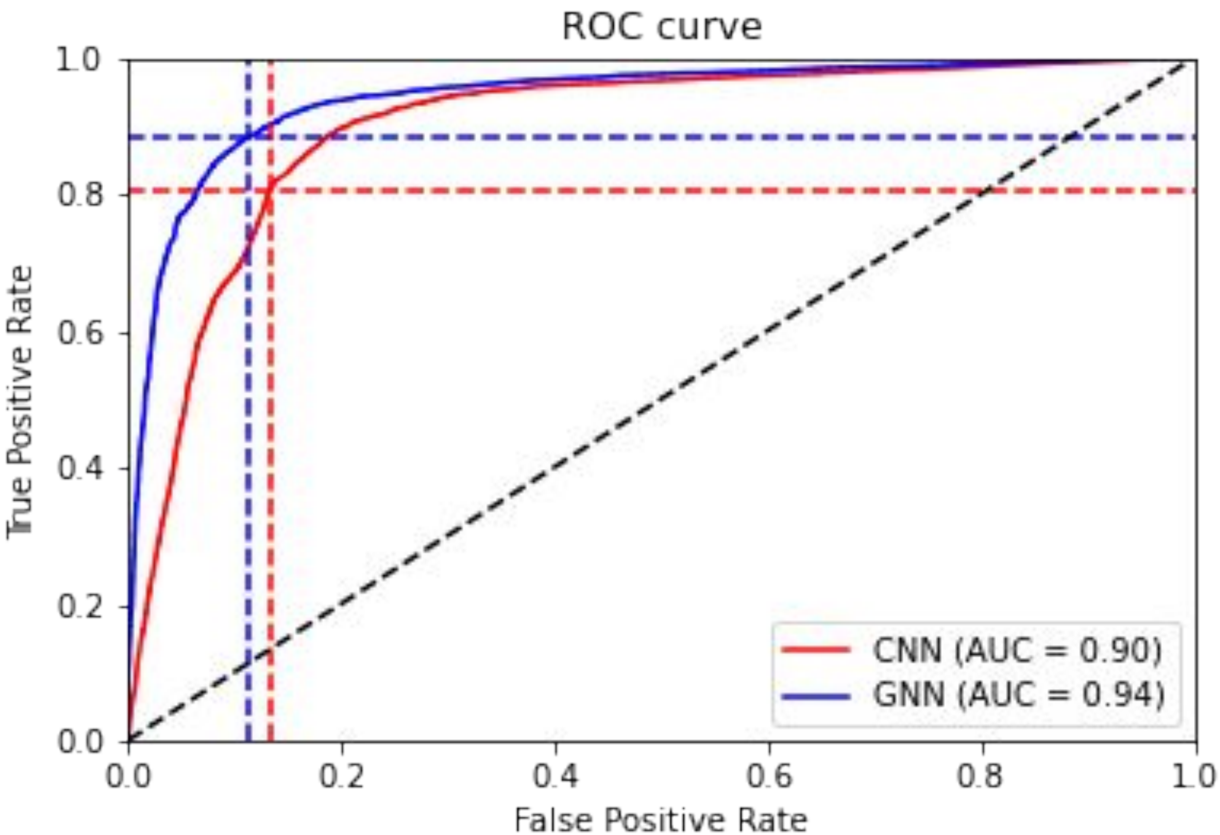
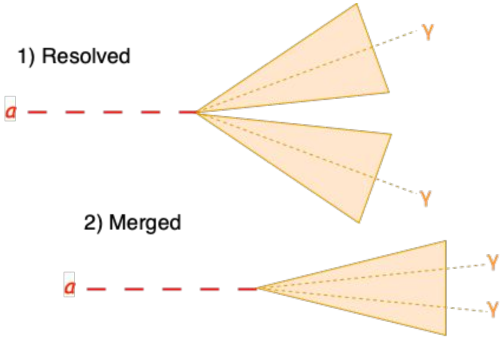


GNN seems to perform better than CNN!

GNN Signal Topology Dependence



- So far only trained on ma=0.4GeV (merged) sample

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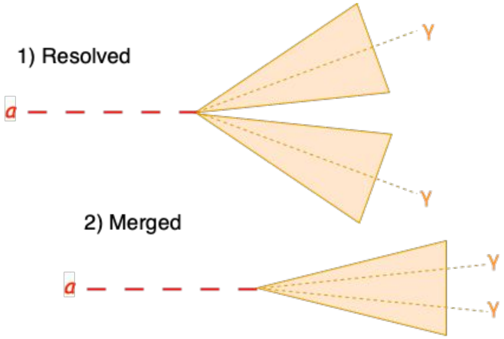
Separate GNNs for merged/resolved topology? 💭



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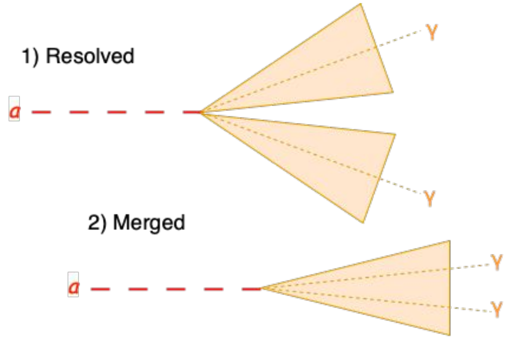

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- Train 2 GNNs on merged (0.4GeV) and resolved (9GeV) scenario → cross-tests!

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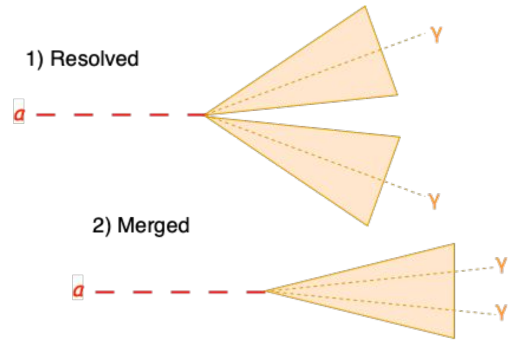

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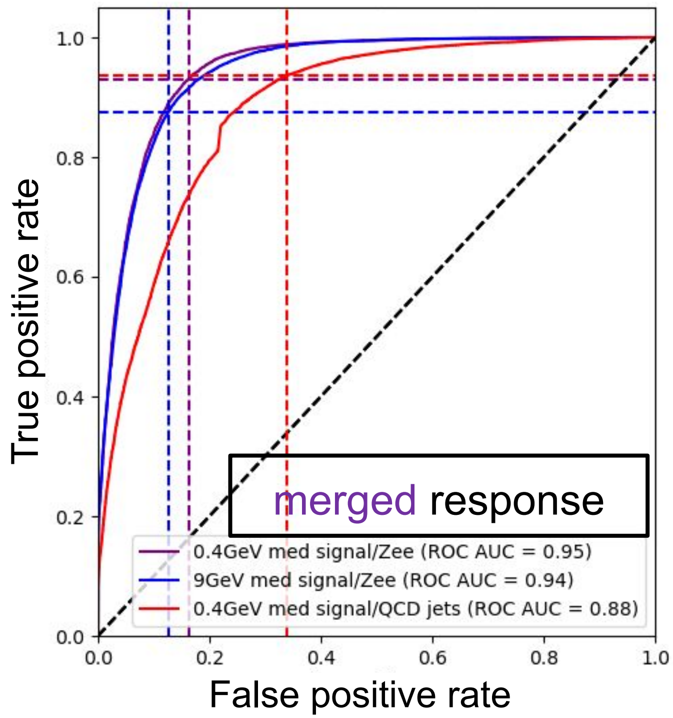

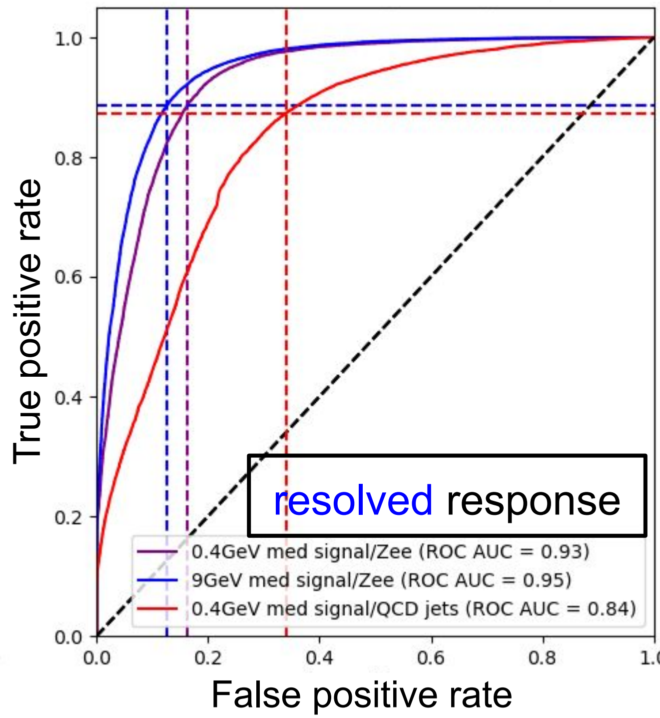

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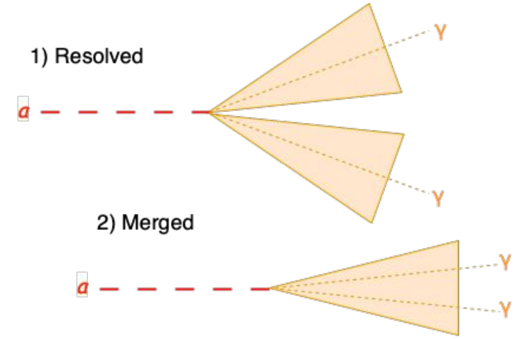

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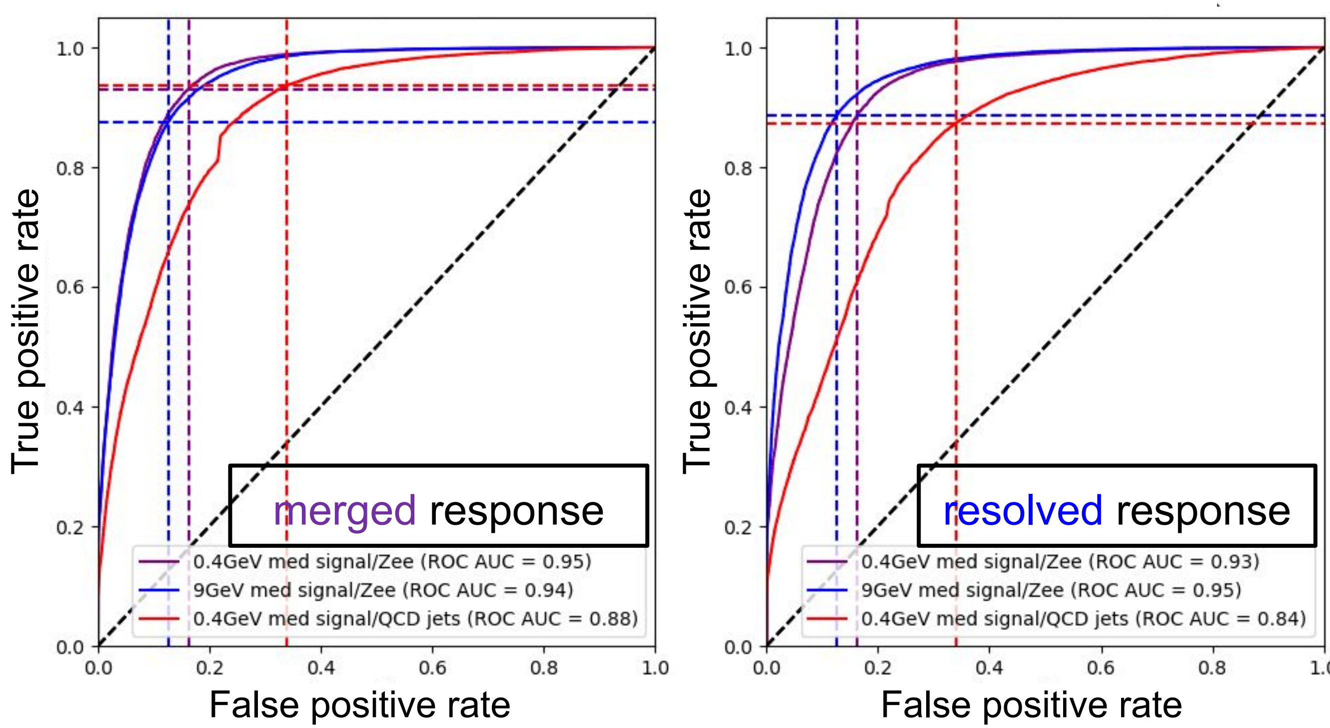

- Both GNNs perform well on both test datasets!
- ⇒ no need for separate GNNs for merged/resolved!

Can train 1 GNN for both scenarios!

GNN Prompt Photon Background

- Other signal topologies: ✅ - what about other backgrounds?

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- Idea: Train separate GNNs on 4 datasets different backgrounds (same signal) (X% photon gun + 1-X% QCD jets)
- Here: Test on 100% QCD jets and 100% photon gun

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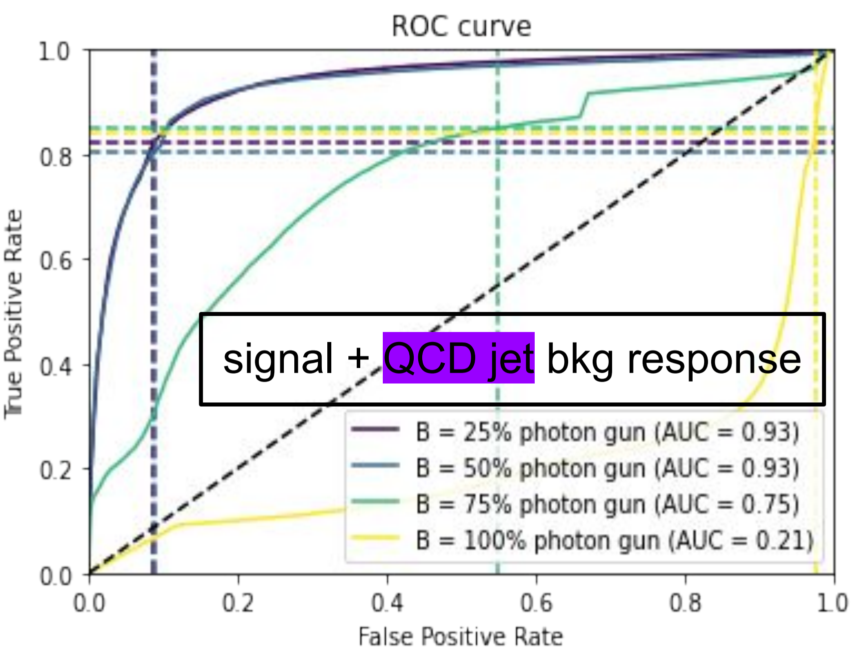

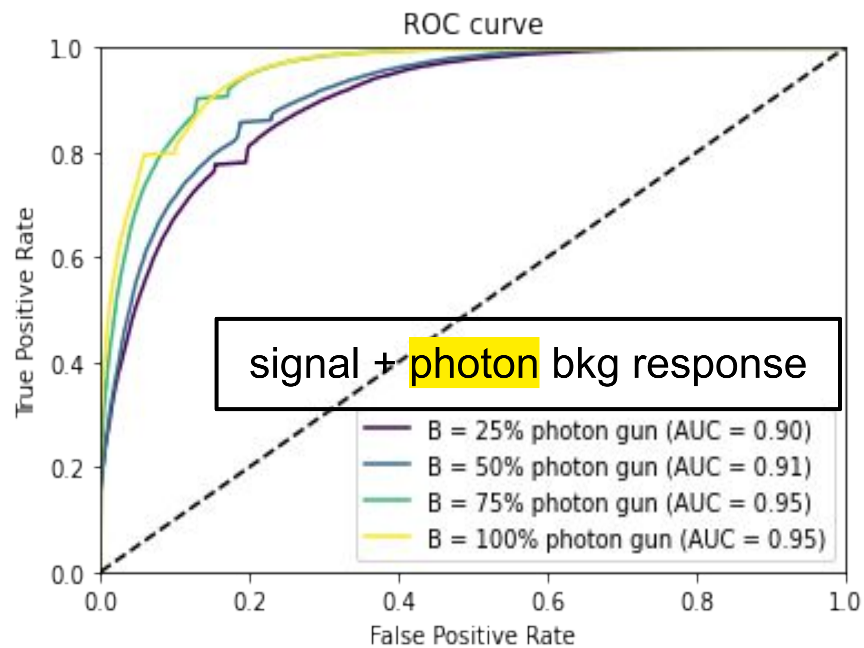

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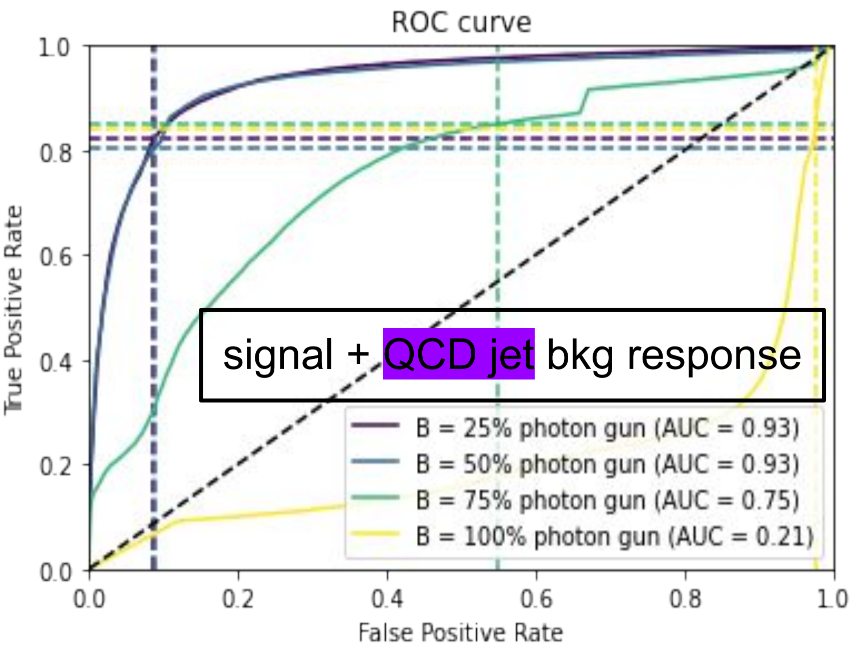
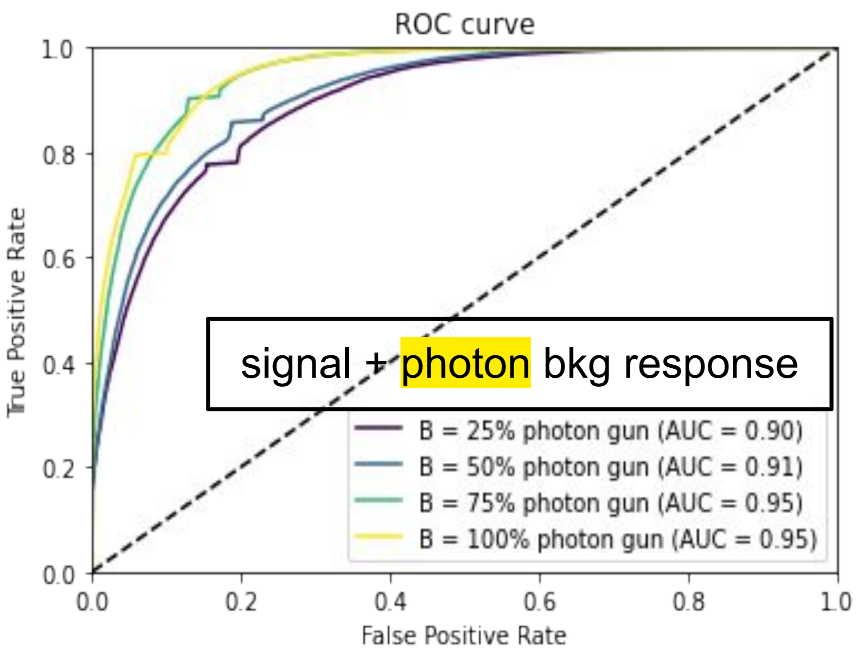


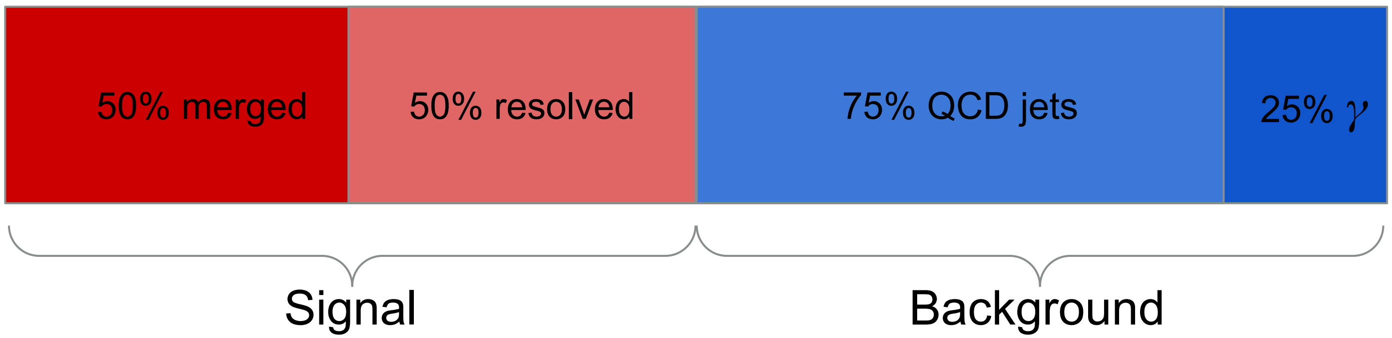


- ⇒Low number of prompt photons to achieve for good separation
- ⇒Trade-off: ✨“Perfect mixture”✨ for training around 25% - 50% prompt γ

Combining what we have learned

The Ultimate Training

- Idea: Train GNN on combined dataset



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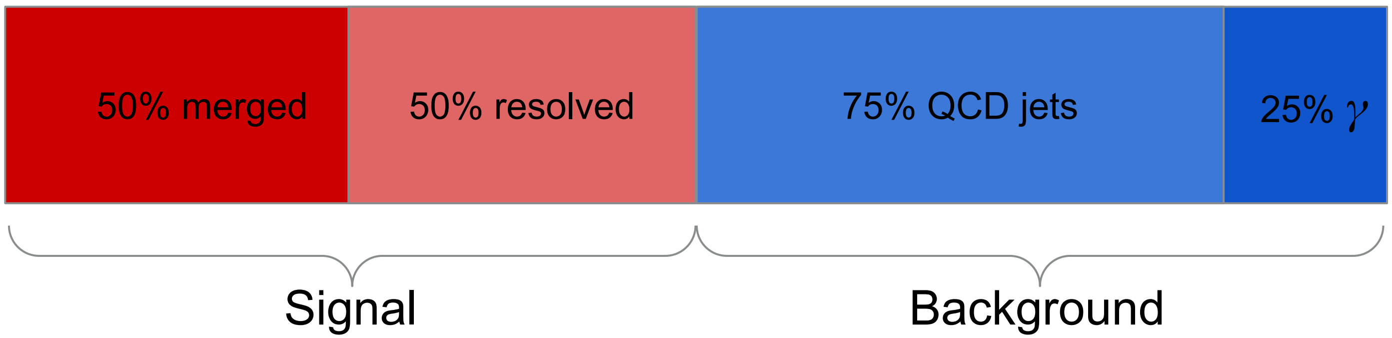

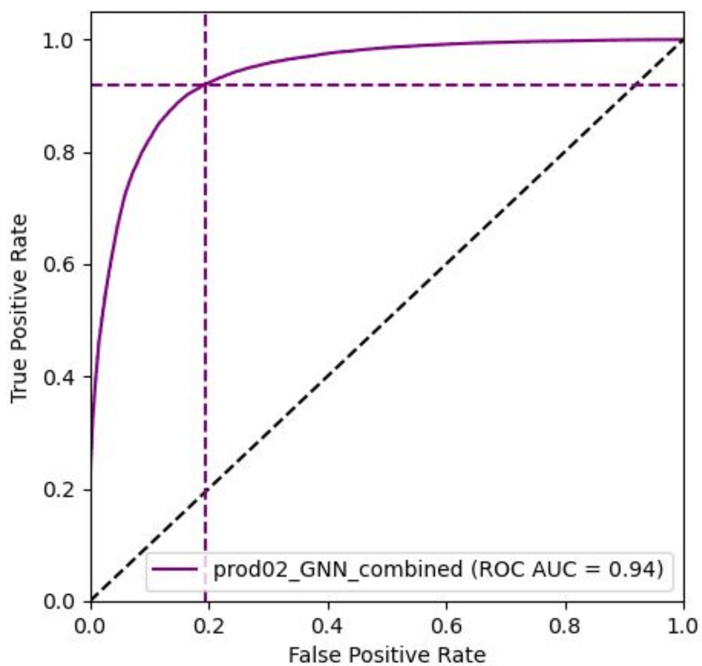

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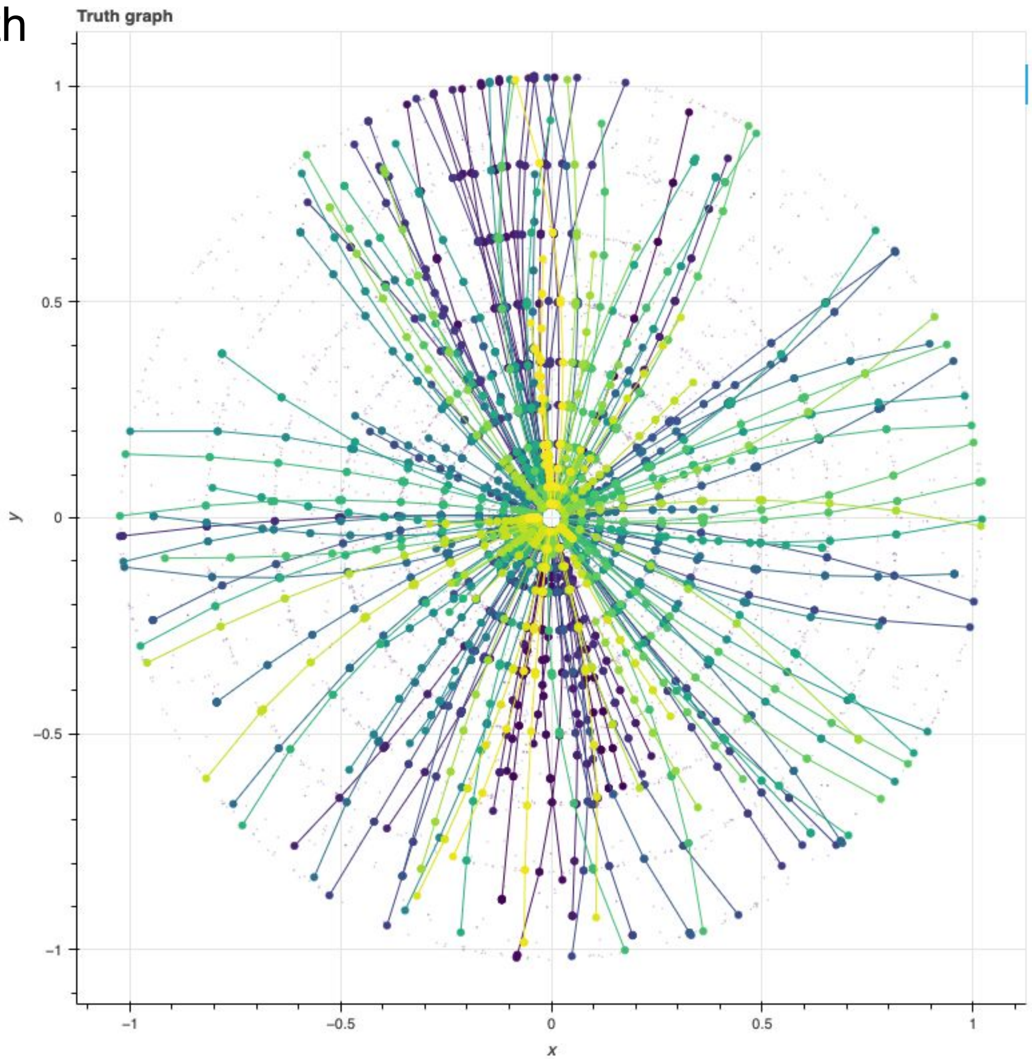
Conclusion

- Cluster images/graphs well suited to identify anomalous (here: displaced photon-) showers
- GNN seems to be preferred solution in terms of performance here
- No need to have separate GNNs for different signal topologies
- With ~low fraction of training data, GNN can achieve good separation against prompt photons
- Next: Evaluating signal model dependence of GNN tagger

What else can you do with GNNs?

(A Cliffhanger)

- Exa.TrkX: advanced tracking with GNNs in HEP
- Side-project with Federico and Thomas
- Tracking at future muon collider experiments (e.g. MAIA)
- Incl. timing (4D Tracking)

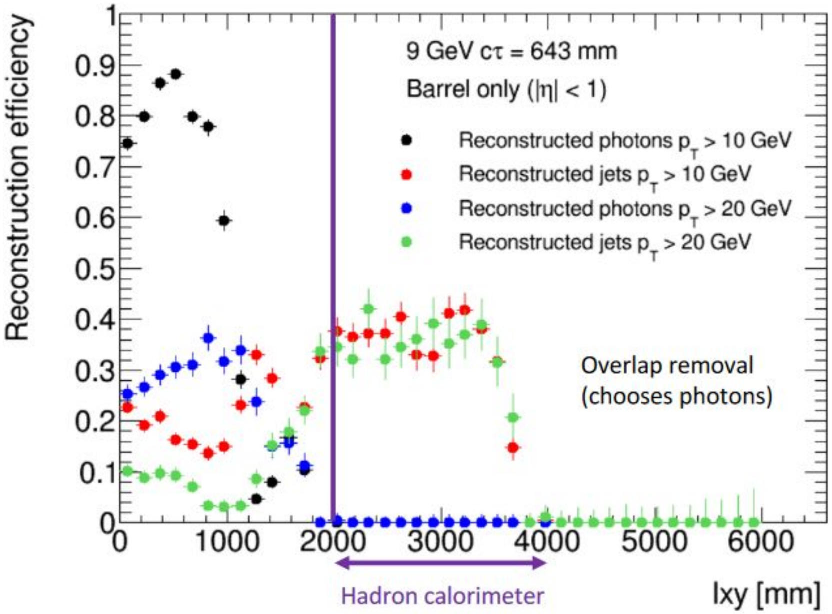


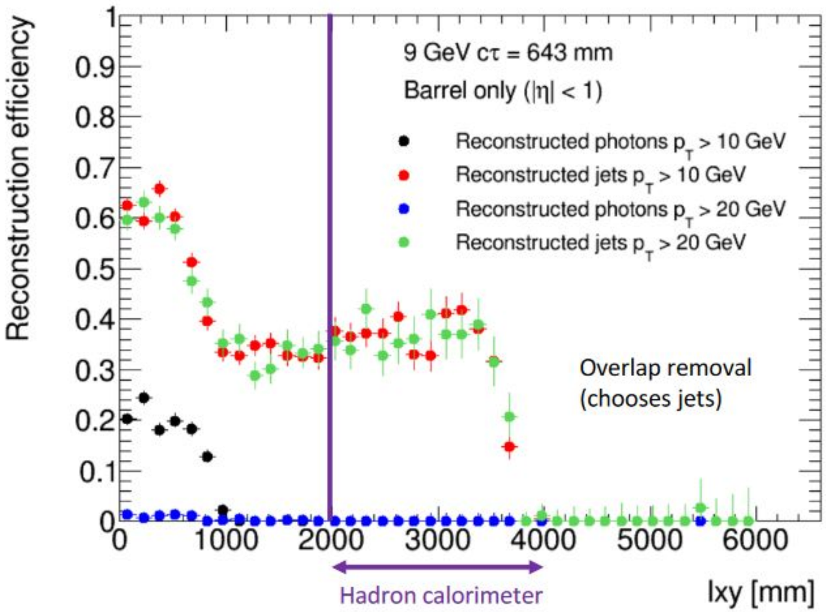
Thank you!

Backup

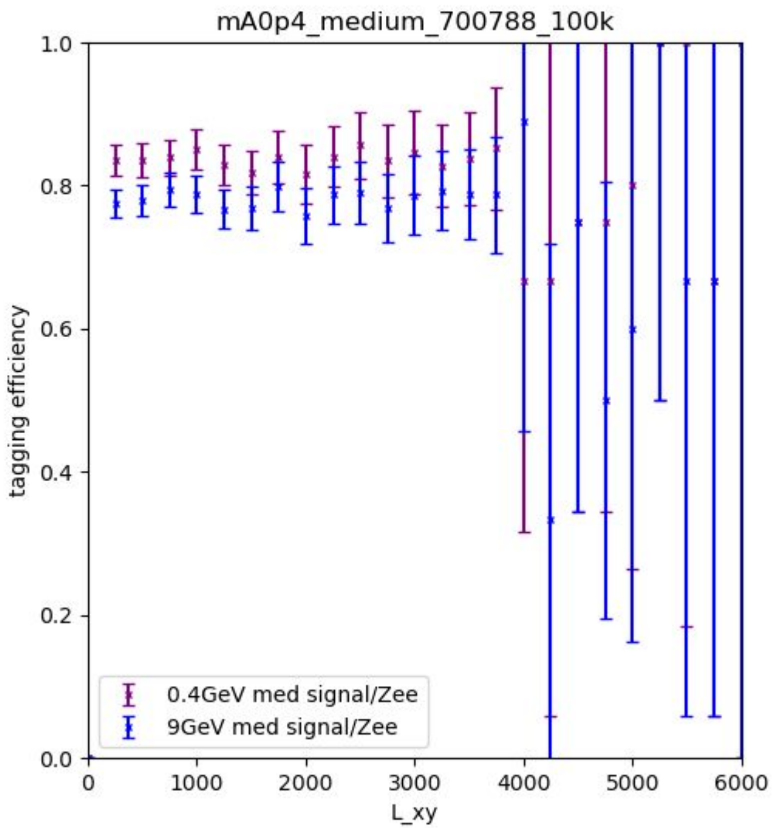
Photon Reconstruction Efficiency

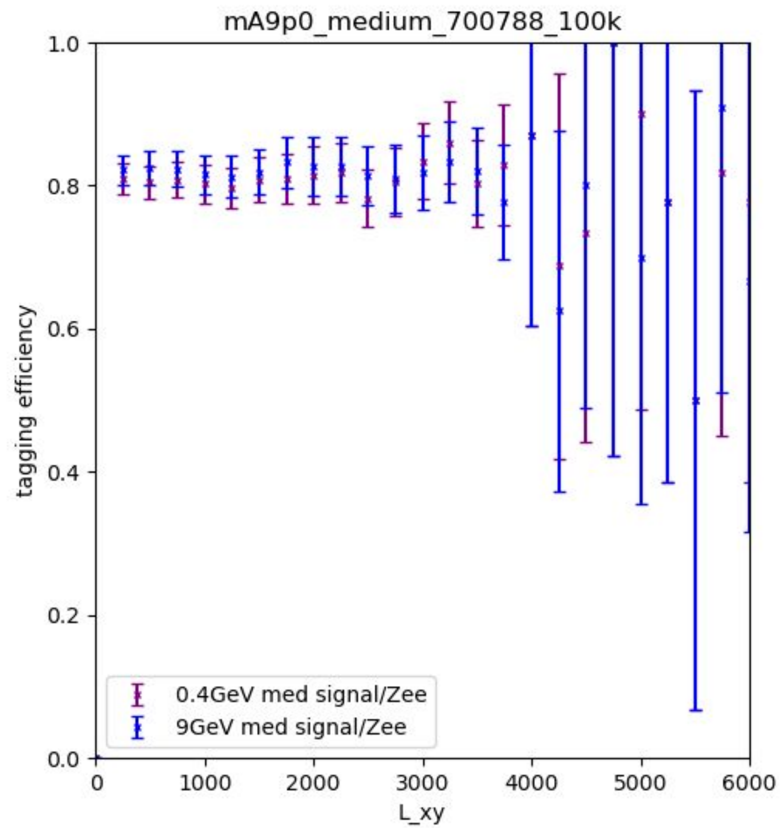
Overlap Removal





Tagging efficiency Lxy





Output Score Distribution Features