Recent Advances in Machine Learning for Physics Analysis at ATLAS
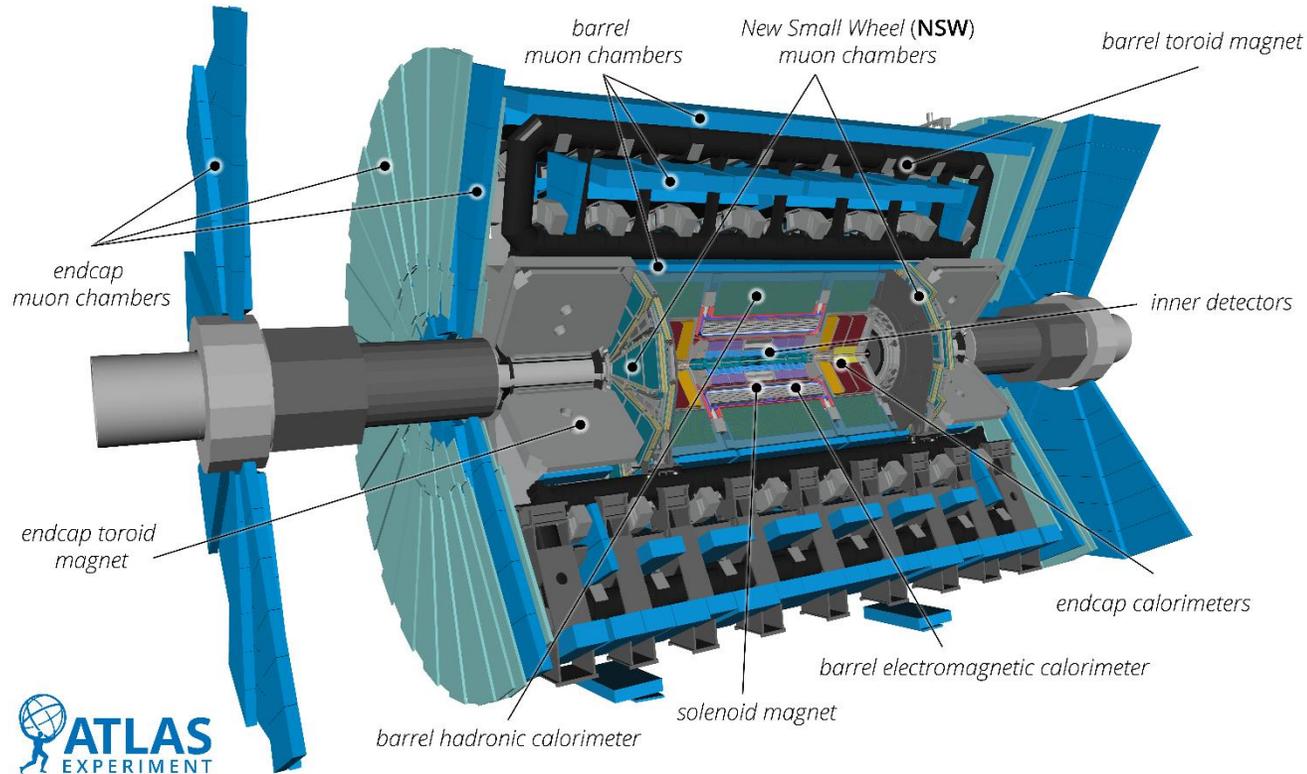
Nicholas Luongo

on behalf of the ATLAS Collaboration

CIPANP 2025

June 9, 2025
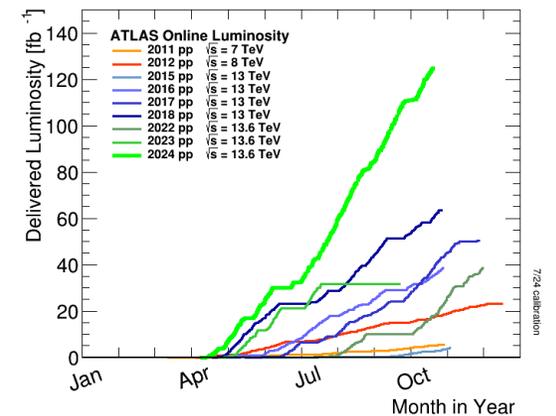
ATLAS Experiment

High-energy experiment studying proton-proton collisions of the Large Hadron Collider at CERN

barrel muon chambers

New Small Wheel (**NSW**) muon chambers

barrel toroid magnet

endcap muon chambers

inner detectors

endcap toroid magnet

endcap calorimeters

barrel electromagnetic calorimeter

solenoid magnet

barrel hadronic calorimeter

General-purpose detector allows for wide-ranging physics program of **Standard Model (SM)** measurements and **Beyond the Standard Model (BSM)** searches in diverse final states

Luminosity recorded to date:
25 fb^{-1} @ 7,8 TeV
147 fb^{-1} @ 13 TeV
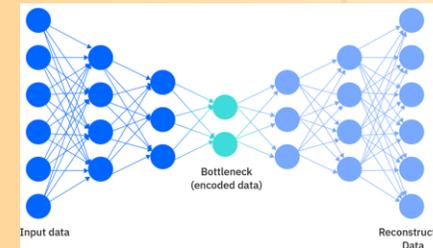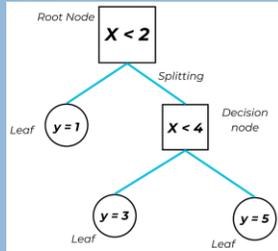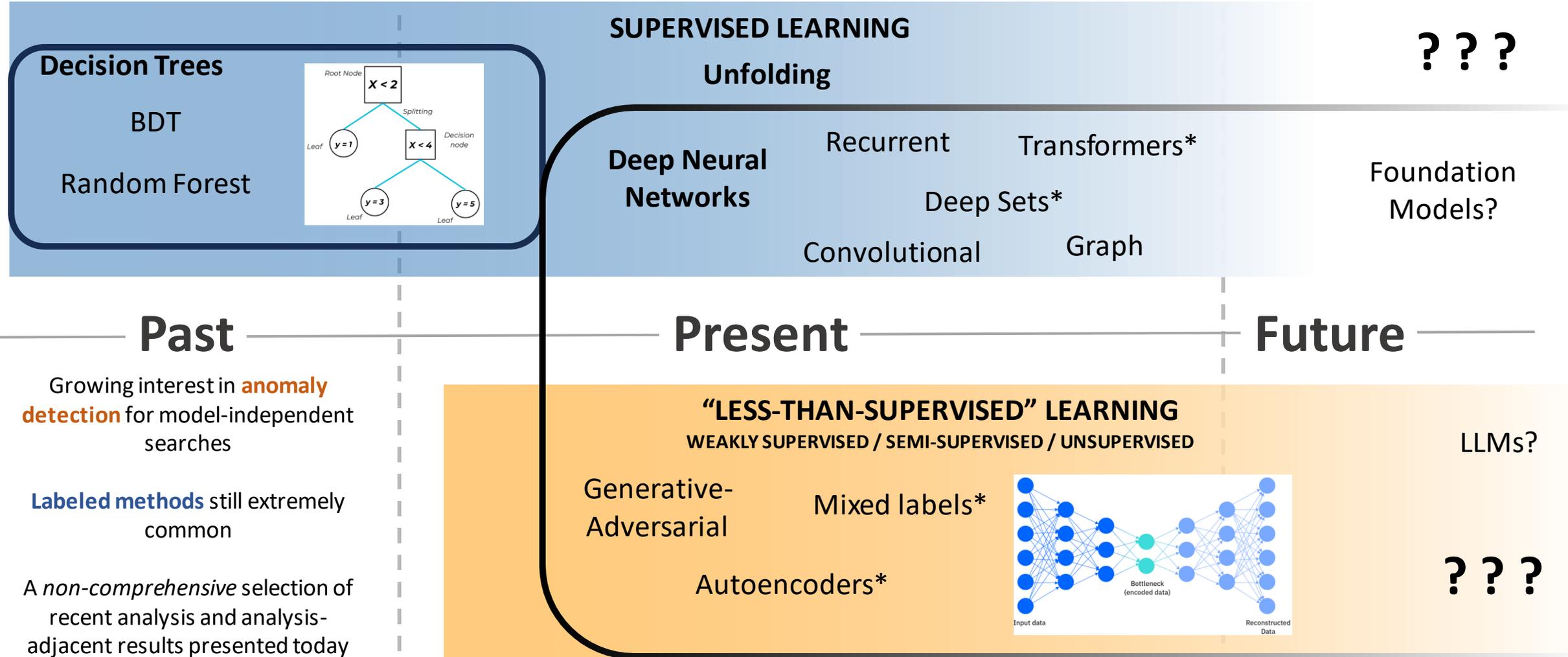183 fb^{-1} @ 13.6 TeV
(and counting)

Machine Learning at ATLAS

ML component now present in most ATLAS analyses (and beyond!)

*Featured in this talk

SUPERVISED LEARNING

Unfolding

Decision Trees

BDT

Random Forest

Deep Neural Networks

Recurrent Transformers*

Deep Sets*

Convolutional Graph

Foundation Models?

? ? ?

Pre-ML Times

Past **Present** **Future**

Growing interest in **anomaly detection** for model-independent searches

Labeled methods still extremely common

A *non-comprehensive* selection of recent analysis and analysis-adjacent results presented today

"LESS-THAN-SUPERVISED" LEARNING
WEAKLY SUPERVISED / SEMI-SUPERVISED / UNSUPERVISED

Generative-Adversarial Mixed labels*

Autoencoders*

LLMs?

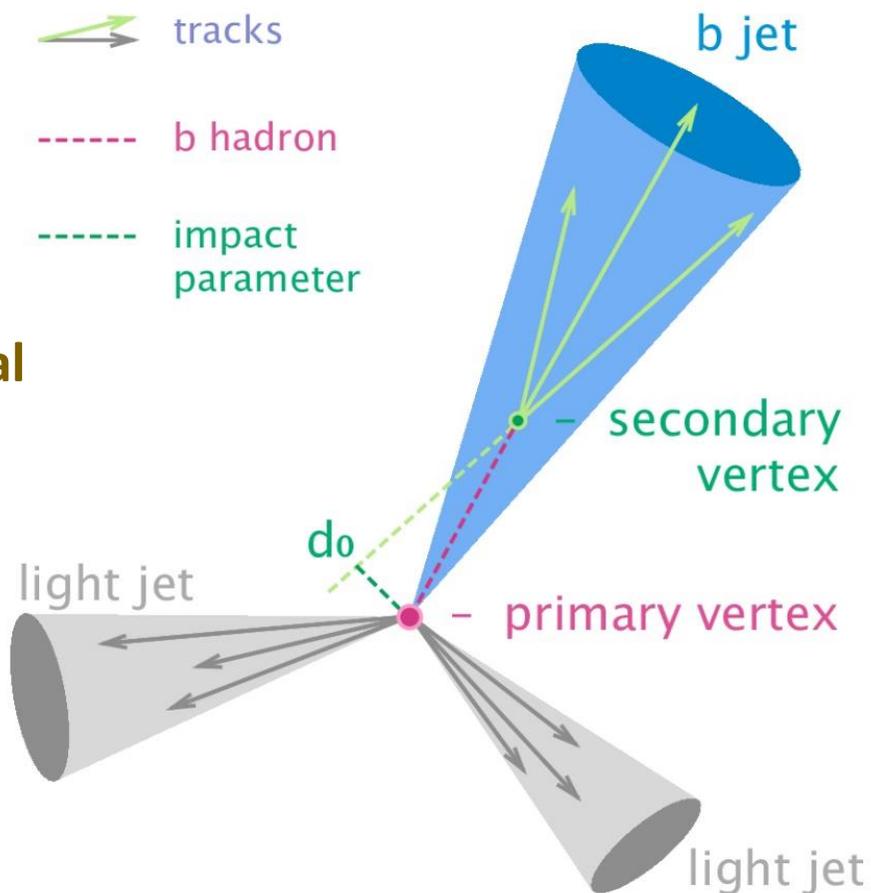? ? ?

Flavor Tagging (FTAG)

Classifying a jet according to the particle from which it originated

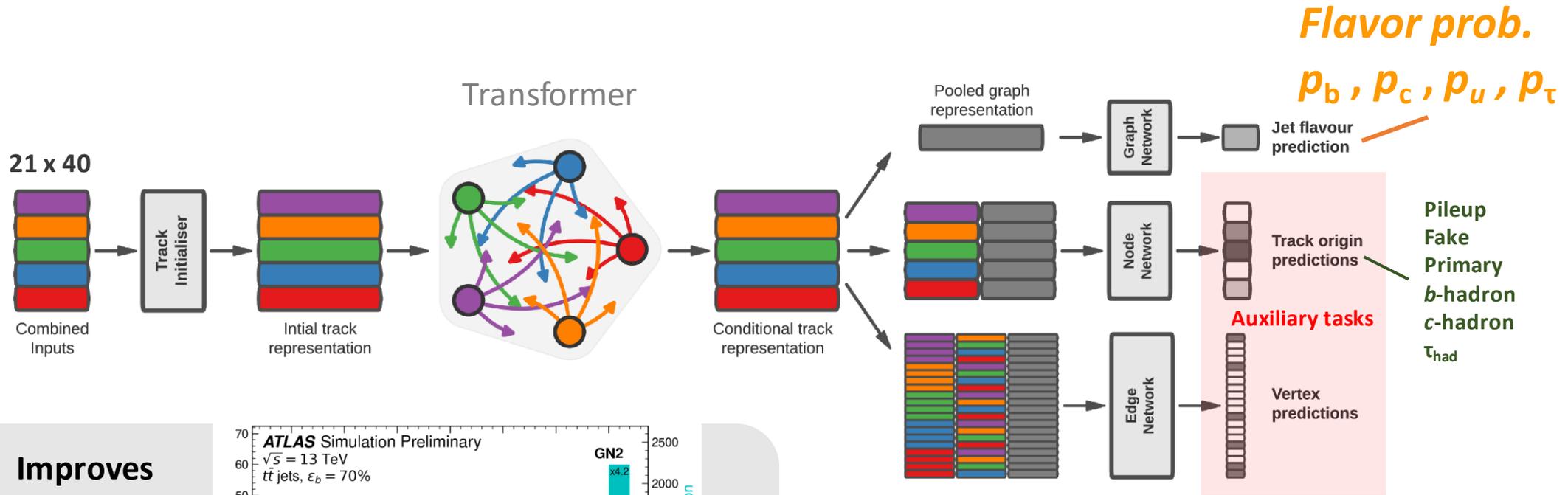**Heavy flavor jets contain secondary vertices, additional tracks, and higher jet mass compared to light jets**

Important for many ATLAS efforts e.g. H→bb in di-Higgs analyses

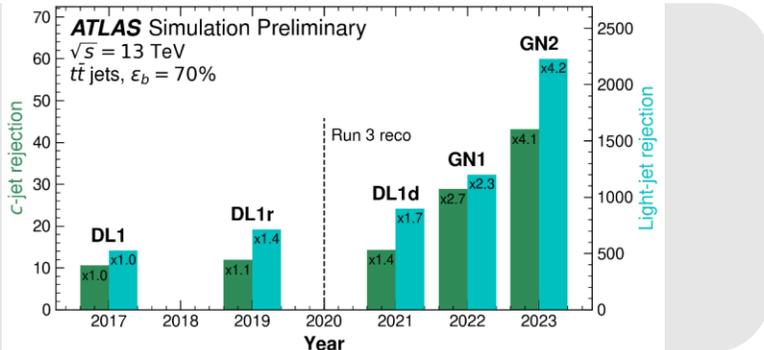**Complex correlations among jet components make this an excellent use case for ML**

GN2

State-of-the-art ATLAS flavor-tagging algorithm with neural network architecture

Jet p_T, η + 19 track variables

Max 40 tracks per jet

Transformer

Flavor prob.
p_b, p_c, p_u, p_τ

Pooled graph representation

Graph Network → Jet flavour prediction

Node Network → Track origin predictions

Pileup
Fake
Primary
b-hadron
c-hadron
τ_{had}

Auxiliary tasks

Edge Network → Vertex predictions

21 x 40

Combined Inputs

Track Initialiser

Intial track representation

Conditional track representation

Improves significantly over previous algorithms

Will improve many analyses throughout ATLAS that rely on flavor-tagging e.g.
HH -> bbyy ATLAS-CONF-2025-005

Argonne NATIONAL LABORATORY

ATLAS EXPERIMENT

Emerging Jets

Search for jets from Z' -> $q_D q_D$ containing dark matter particles in a "hidden sector" decaying to SM after macroscopic flight distance
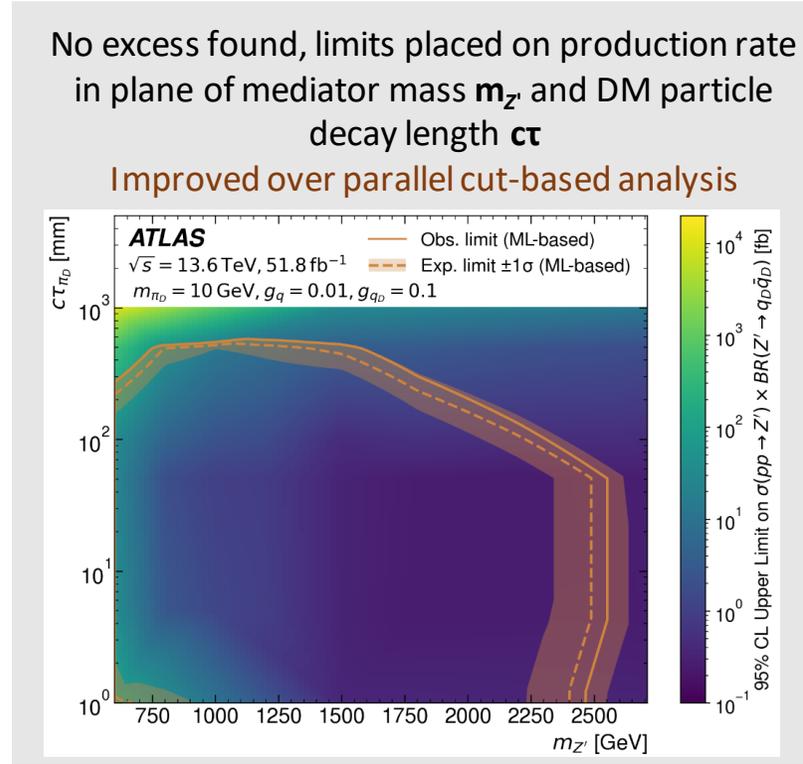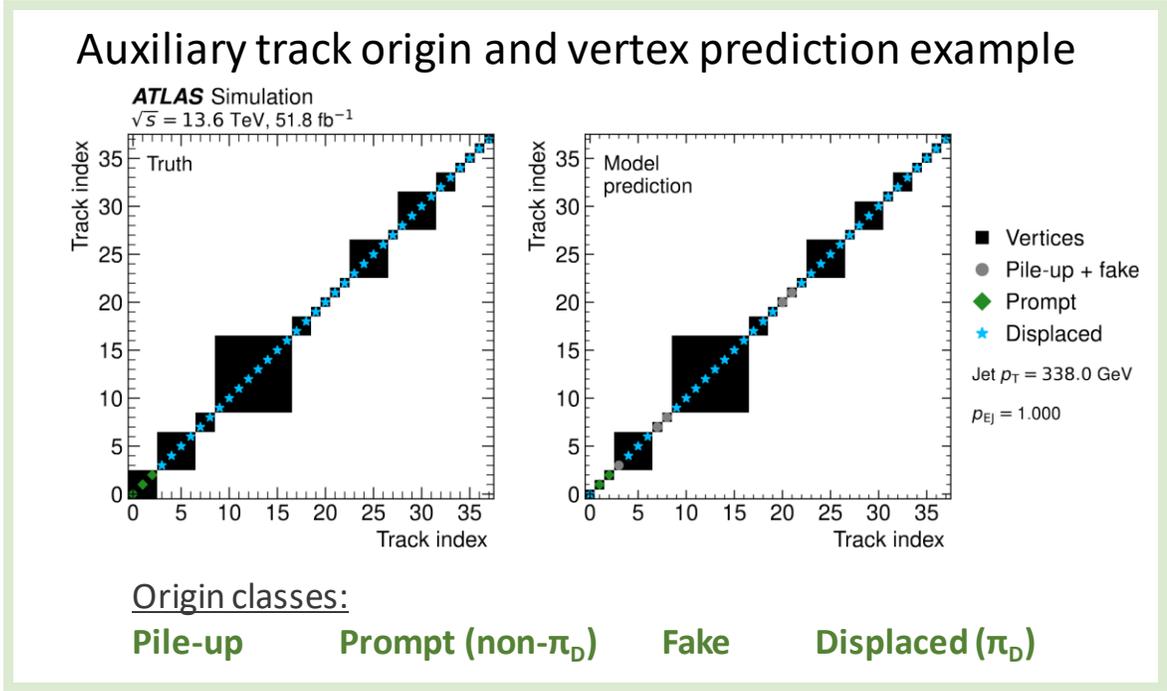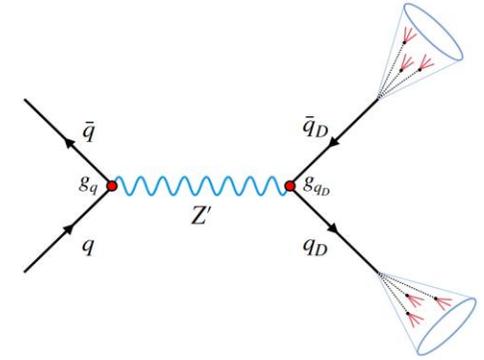
q_D **hadronize** into π_D

Visible signatures appear **displaced** from the interaction point as dark matter **does not** interact with detector

Transformer architecture inspired by **GN2** used to classify jets from SM multijet vs Z' -> $q_D q_D$
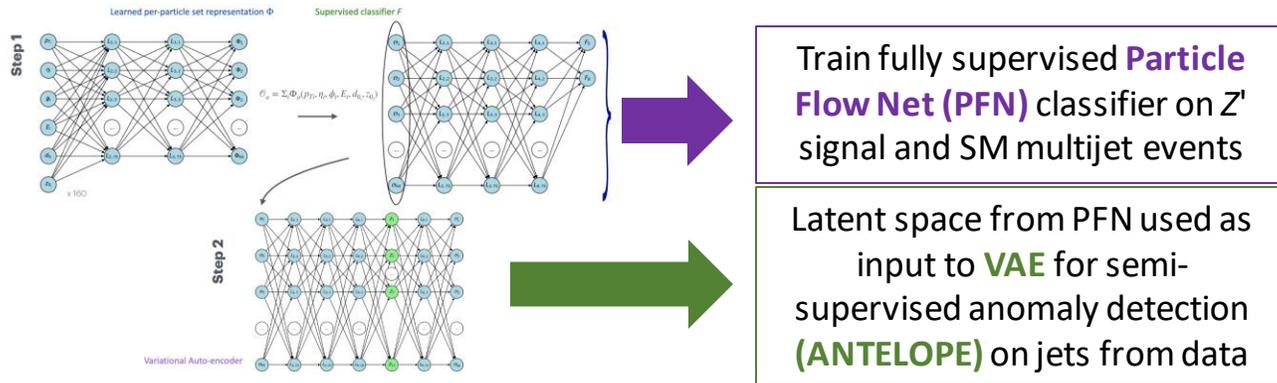
- 200 tracks per jet
- 1 jet + 14 track inputs

Auxiliary track origin and vertex prediction example

ATLAS Simulation
$\sqrt{s} = 13.6$ TeV, 51.8 fb^{-1}

Truth

Model prediction

Track index

■ Vertices
● Pile-up + fake
◆ Prompt
★ Displaced

Jet $p_T = 338.0$ GeV
$p_{EJ} = 1.000$

Origin classes:
Pile-up   **Prompt (non-π_D)**   **Fake**   **Displaced (π_D)**

No excess found, limits placed on production rate in plane of mediator mass **$m_{Z'}$** and DM particle decay length **$c\tau$**
Improved over parallel cut-based analysis

ATLAS
$\sqrt{s} = 13.6$ TeV, 51.8 fb^{-1}
$m_{\pi_D} = 10$ GeV, $g_q = 0.01$, $g_{q_D} = 0.1$

— Obs. limit (ML-based)
--- Exp. limit ±1σ (ML-based)

$c\tau_{\pi_D}$ [mm]

$m_{Z'}$ [GeV]

95% CL Upper Limit on $\sigma(pp \to Z') \times BR(Z' \to q_D \bar{q}_D)$ [fb]
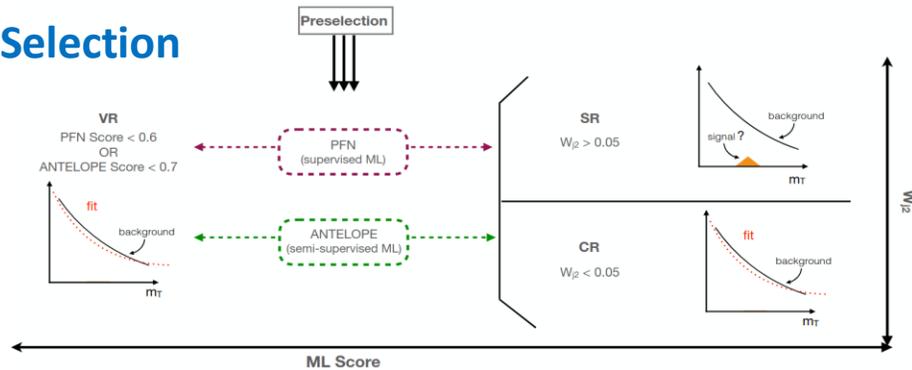
Semi-visible or Anomalous Jets

Two-pronged search for jets from Z' -> $q_D q_D$ containing both SM and non-interacting DM particles, leading to partially visible jets

R_{inv} – fraction of jet invisible

Inputs: (pT, η, ϕ, E, d_0, z_0) of 80 leading tracks for leading and sub-leading jets

R_{inv}

Architecture

Train fully supervised **Particle Flow Net (PFN)** classifier on Z' signal and SM multijet events

Latent space from PFN used as input to **VAE** for semi-supervised anomaly detection **(ANTELOPE)** on jets from data

Selection

PFN S-plus-B fit

ANTELOPE Bump Hunt

Comparison of limits between PFN and ANTELOPE

PFN fit allows for setting of limits parametrized by $m_{Z'}$ and R_{inv}

CWoLa (Classification Without Labels)

Search for narrow-width resonance decaying to two large-R jets using background estimation and weakly-supervised classifier

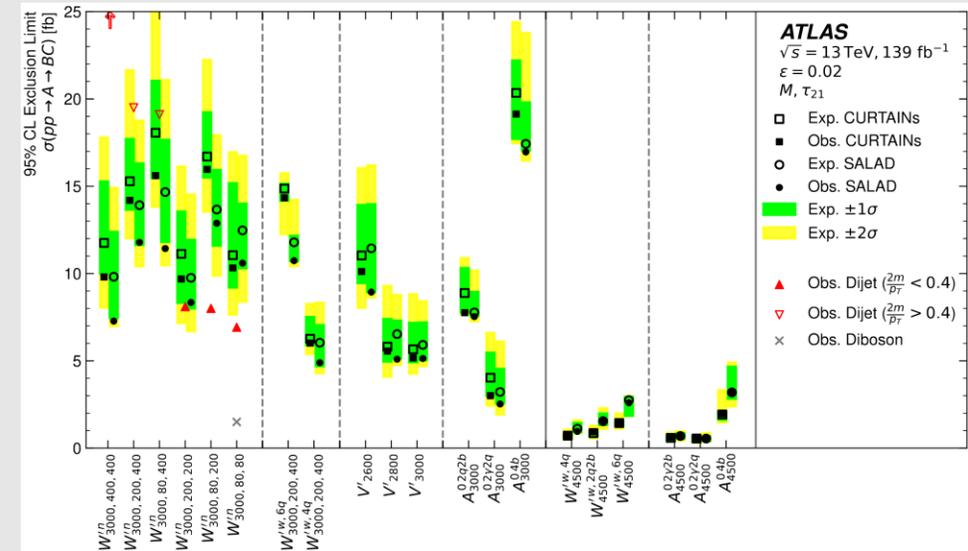| Observable	Selection
leading jet p_T [GeV]	> 500
subleading jet p_T [GeV]	> 200
jet $|\eta|$ (both)	< 2.0
jet mass, M [GeV] (both)	$30 < M < 500$
$|\Delta Y| = |y_1 - y_2|$	< 1.2

(a) Definition of Regions
(b) Background Estimation
(c) Classification of Signal

- SR
- SB
- Background
- Signal
- Estimate

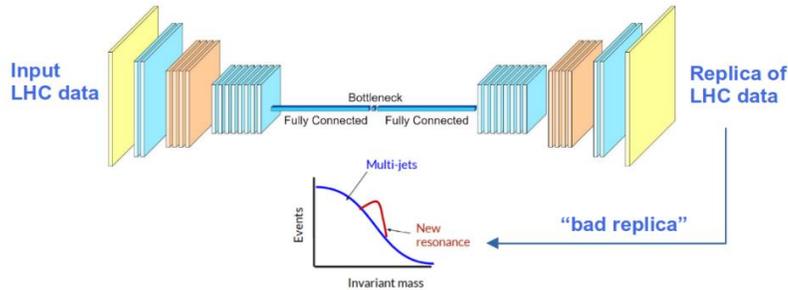m_{JJ} – Invariant mass of two jets $\mathcal{T}$ – other VOI

No excess found, limits placed for several signal models with resonance mass range from **2.6 - 4.5 TeV**

- $W' \rightarrow W''Z''$
- $A^0 \rightarrow H''Z''$
- $V' \rightarrow WV$

<u>Analysis procedure</u>:
1. Divide m_{JJ} spectrum into shifting **signal-enriched** region (SR) and **signal-depleted** sideband (SB) regions
2. Learn background dijet distribution in SR from SBs – SALAD (reweighting MC to data) and CURTAINS (interpolation)
3. Train NN classifier to separate **populations** of data in SR (1) and background estimated events (0) derived from SBs in Step 2
4. After cut on NN score, perform **bump hunt** on remaining events

ATLAS
$\sqrt{s} = 13$ TeV, 139 fb^{-1}
$\varepsilon = 0.02$
M, τ_{21}

□ Exp. CURTAINs
■ Obs. CURTAINs
○ Exp. SALAD
● Obs. SALAD
▬ Exp. ±1σ
▬ Exp. ±2σ
▲ Obs. Dijet ($\frac{2m}{p_T} < 0.4$)
▽ Obs. Dijet ($\frac{2m}{p_T} > 0.4$)
× Obs. Diboson

Unsupervised 2-body Anomaly Detection

Search for resonance in 2-body jet + *X* final states using fully unsupervised method

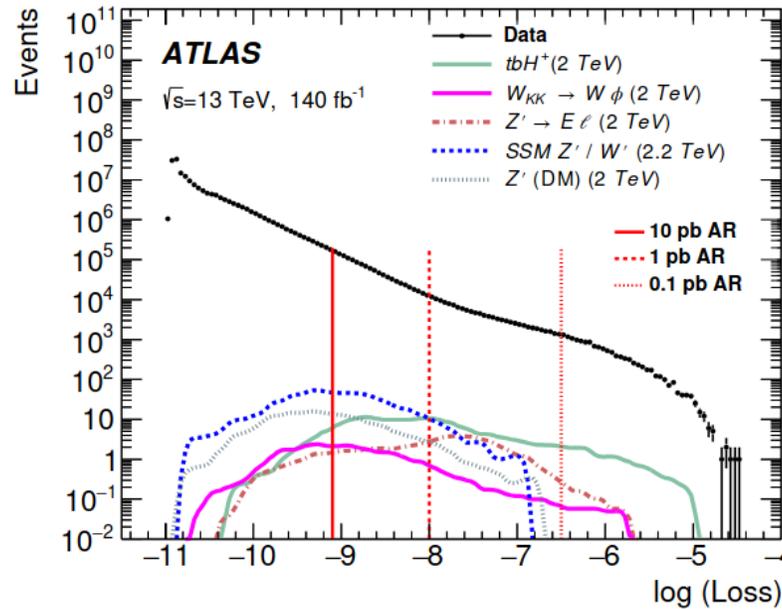**Autoencoder** trained over events passing **single-lepton trigger** and offline p_T cuts

Limits placed on 9 jet+*X* invariant masses with no significant excess found

Kinematics of leading jets and leptons encoded in **rapidity-mass matrix** containing:
- Missing transverse energy of event
- Transverse energies
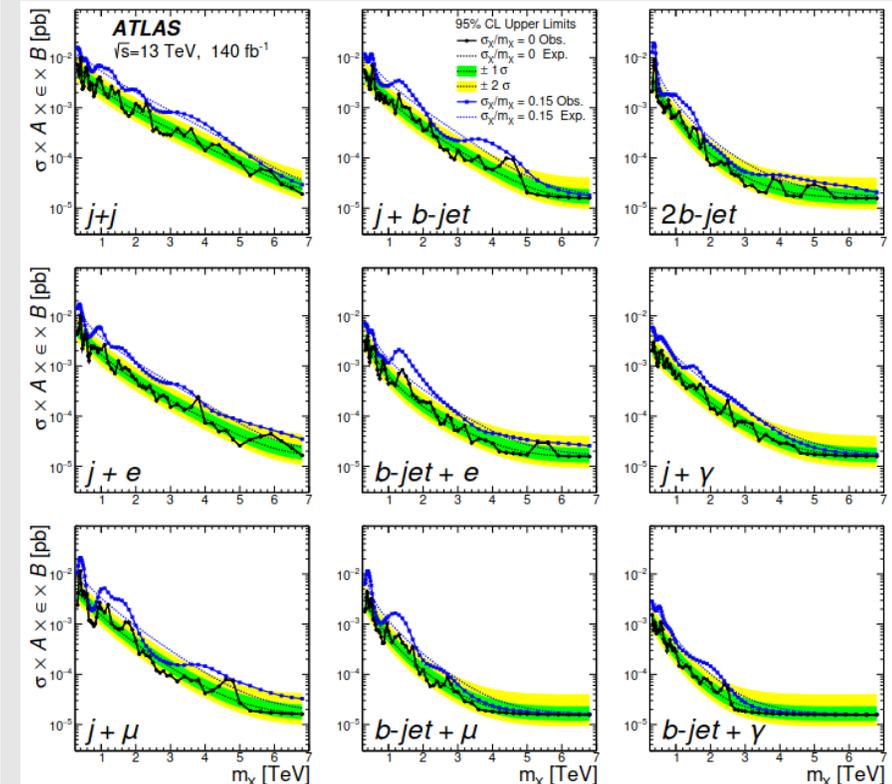- Pairwise rapidity differences and invariant masses

Anomaly region boundary defined above reconstruction loss cutoff value

Bump hunt performed in signal region (above cutoff) against functional fit derived from control region (below cutoff)

Loss from data compared against panel of BSM samples

Neural Simulation-Based Inference (NSBI)

Method for physics parameter estimation using learned, high-dimensional likelihood ratios with application to H -> ZZ -> 4l production measurement

Standard workflow:

- Reduce data to one-dimensional histograms and perform **likelihood test** for value of physics parameter

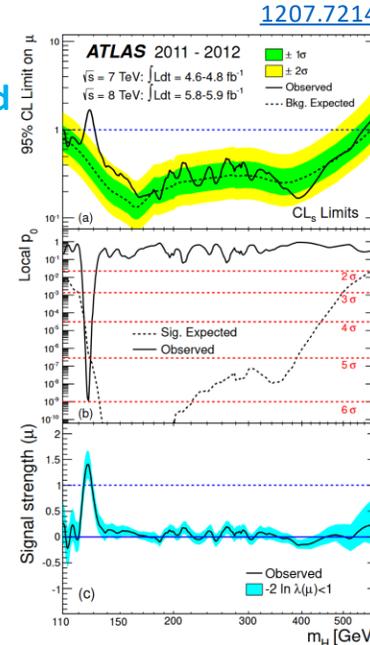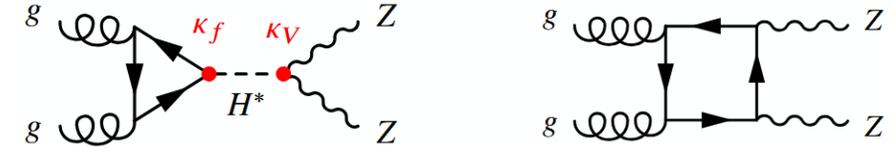Works well for simple **µS + B** scenarios (no interference)

NSBI:

- Construct high-dimensional likelihood ratios, estimated by NNs, which preserve full event information

Ideal for scenarios with S/B interference resulting in **non-linear dependence on µ**

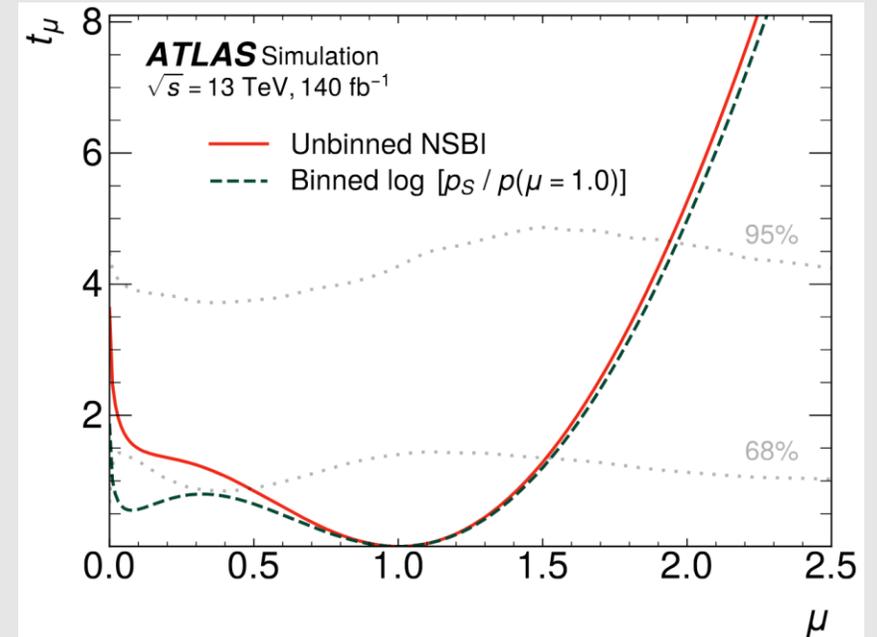Use density ratios inside "**search-oriented mixture model**":

$$\frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_J^{C_{\text{proc}}} f_J(\mu)\, \nu_J \, \frac{p_J(x_i)}{p_{\text{ref}}(x_i)} \quad \longrightarrow \quad \frac{p(x|\mu)}{p_S(x)} = \frac{1}{\nu(\mu)} \left[(\mu - \sqrt{\mu})\, \nu_S + \sqrt{\mu}\, \nu_{\text{SBI}} \frac{p_{\text{SBI}}(x)}{p_S(x)} + (1 - \sqrt{\mu}) \nu_B \frac{p_B(x)}{p_S(x)} \right]$$

Estimated using NN classifiers, **per-event**, then used to calculate likelihood and test statistic t_μ

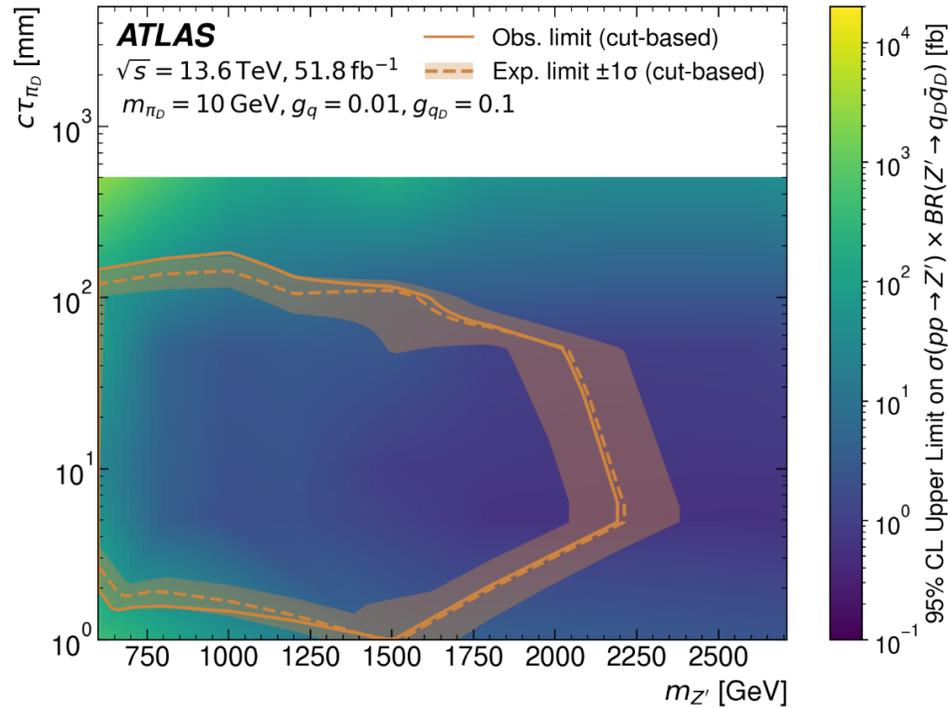**NSBI** limits shown compared with traditional **binned** analysis

Summary

o Machine learning is an ever more **integral** part of ATLAS analyses, with almost every analysis containing some type of ML component

o **Supervised learning** on labeled data is increasingly joined by **unsupervised learning** for model-independent searches, sometimes within the same analysis

o ATLAS continues to incorporate **cutting-edge ML** methods like Transformers into tools and analyses with impressive performance results
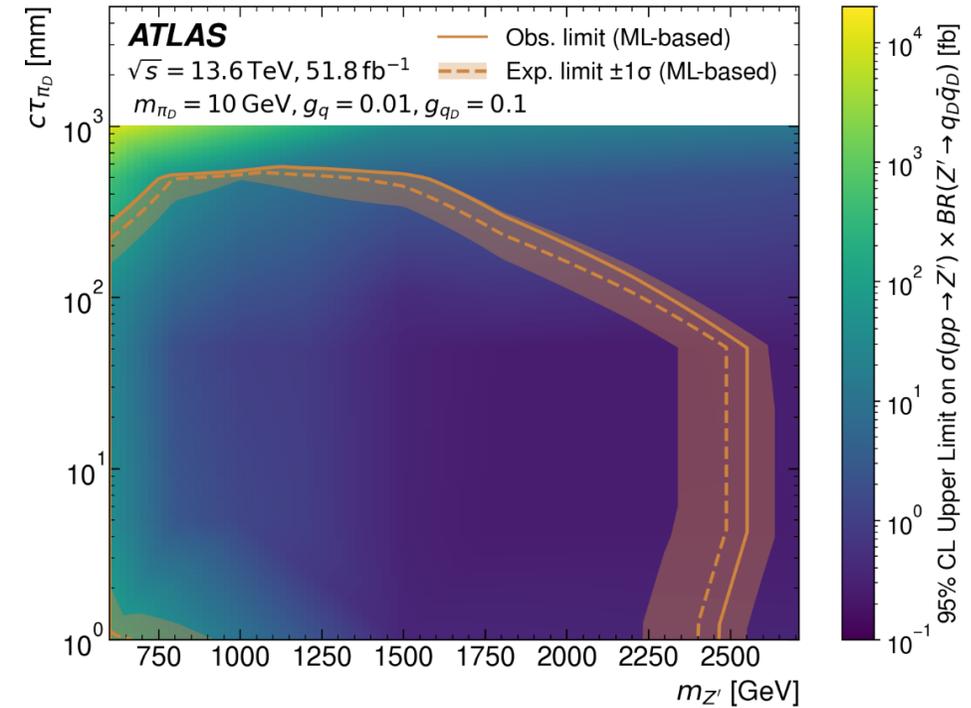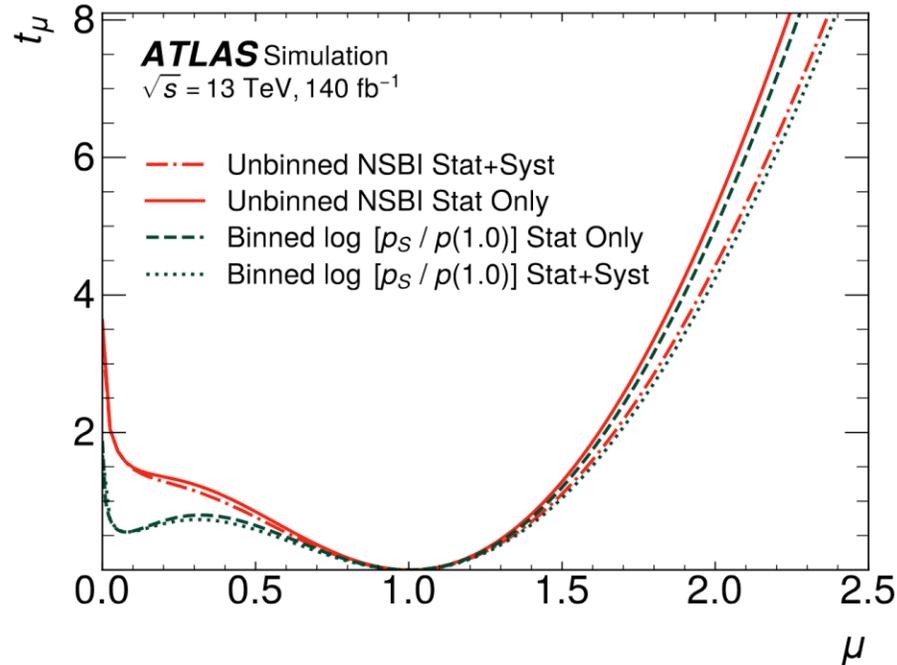
Thank you!

Backup

Emerging Jets

Neural Simulation-Based Inference (NSBI)

Derivation

$$\mu\nu_{\mathrm{S}} + \sqrt{\mu}\nu_{\mathrm{I}} + \nu_{\mathrm{B}} = (\mu - \sqrt{\mu})\nu_{\mathrm{S}} + \sqrt{\mu}(\nu_{\mathrm{S}} + \nu_{\mathrm{I}} + \nu_{\mathrm{B}}) + (1 - \sqrt{\mu})\nu_{\mathrm{B}}$$

Likelihood

t_{μ}

$$\frac{L_{\mathrm{full}}(\mu, \alpha|\mathcal{D})}{L_{\mathrm{ref}}(\mathcal{D})} = \mathrm{Pois}(N_{\mathrm{data}}|\nu(\mu, \alpha)) \prod_{i}^{N_{\mathrm{data}}} \frac{p(x_i|\mu, \alpha)}{p_{\mathrm{ref}}(x_i)} \prod_{k} \mathrm{Gaus}(a_k|\alpha_k, \delta_k)$$

$$t_{\mu} = -2\ln\left(\frac{L_{\mathrm{full}}(\mu, \widehat{\widehat{\alpha}}(\mu))}{L_{\mathrm{full}}(\widehat{\mu}, \widehat{\alpha})}\right)$$

Binned histogram method approaches
NSBI as $N_{\mathrm{bin}} \to \infty$

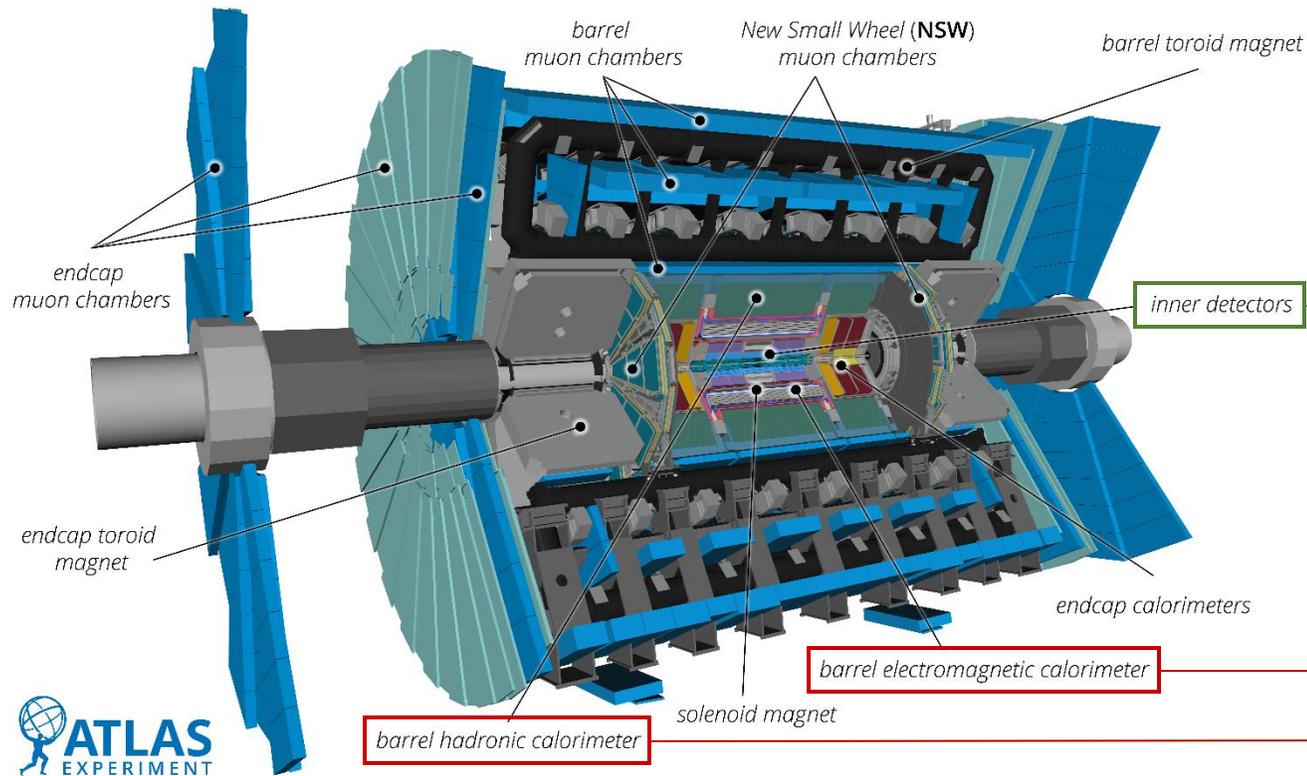With stat. uncertainties

Neural Simulation-Based Inference (NSBI)

SM HH Interference

ATLAS

High-energy experiment studying proton-proton collisions of the Large Hadron Collider at CERN

Labels on diagram:
- barrel muon chambers
- New Small Wheel (**NSW**) muon chambers
- barrel toroid magnet
- endcap muon chambers
- endcap toroid magnet
- inner detectors
- endcap calorimeters
- barrel electromagnetic calorimeter
- solenoid magnet
- barrel hadronic calorimeter

Tracker:
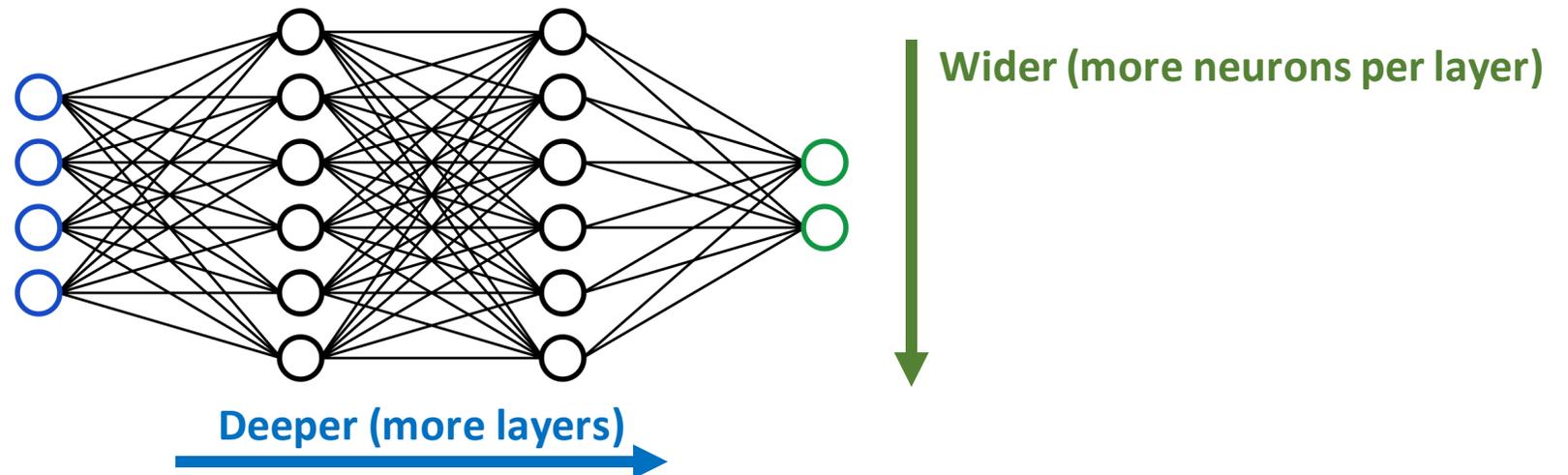Inner detector system that measures **tracks** – paths of charged particles

Calorimeters:
Captures and measures the **energy** of particles through their electromagnetic and hadronic interactions with detector material

Hyperparameter Optimization (HPO)

Determining which values of network architecture properties (width, depth, learning rate, activation) produce the most performant trained network

❖ Most relevant to GN2 successor **GN3**, can use these results as baseline speedup expectation

❖ First interested in seeing how big we can make the GN3 model without seeing evidence of **overtraining**

Wider (more neurons per layer)

Deeper (more layers)

GN2 Inputs

Jet Input	Description
p_T	Jet transverse momentum
η	Signed jet pseudorapidity

Track Input	Description
q/p	Track charge divided by momentum (measure of curvature)
$d\eta$	Pseudorapidity of the track, relative to the jet η
$d\phi$	Azimuthal angle of the track, relative to the jet ϕ
d_0	Closest distance from the track to the PV in the longitudinal plane
$z_0 \sin\theta$	Closest distance from the track to the PV in the transverse plane
$\sigma(q/p)$	Uncertainty on q/p
$\sigma(\theta)$	Uncertainty on track polar angle θ
$\sigma(\phi)$	Uncertainty on track azimuthal angle ϕ
$s(d_0)$	Lifetime signed transverse IP significance
$s(z_0)$	Lifetime signed longitudinal IP significance
nPixHits	Number of pixel hits
nSCTHits	Number of SCT hits
nIBLHits	Number of IBL hits
nBLHits	Number of B-layer hits
nIBLShared	Number of shared IBL hits
nIBLSplit	Number of split IBL hits
nPixShared	Number of shared pixel hits
nPixSplit	Number of split pixel hits
nSCTShared	Number of shared SCT hits
nPixHoles	Number of pixel holes
nSCTHoles	Number of SCT holes
leptonID	Indicates if track was used in the reconstruction of an electron or muon (only for GN1 Lep)