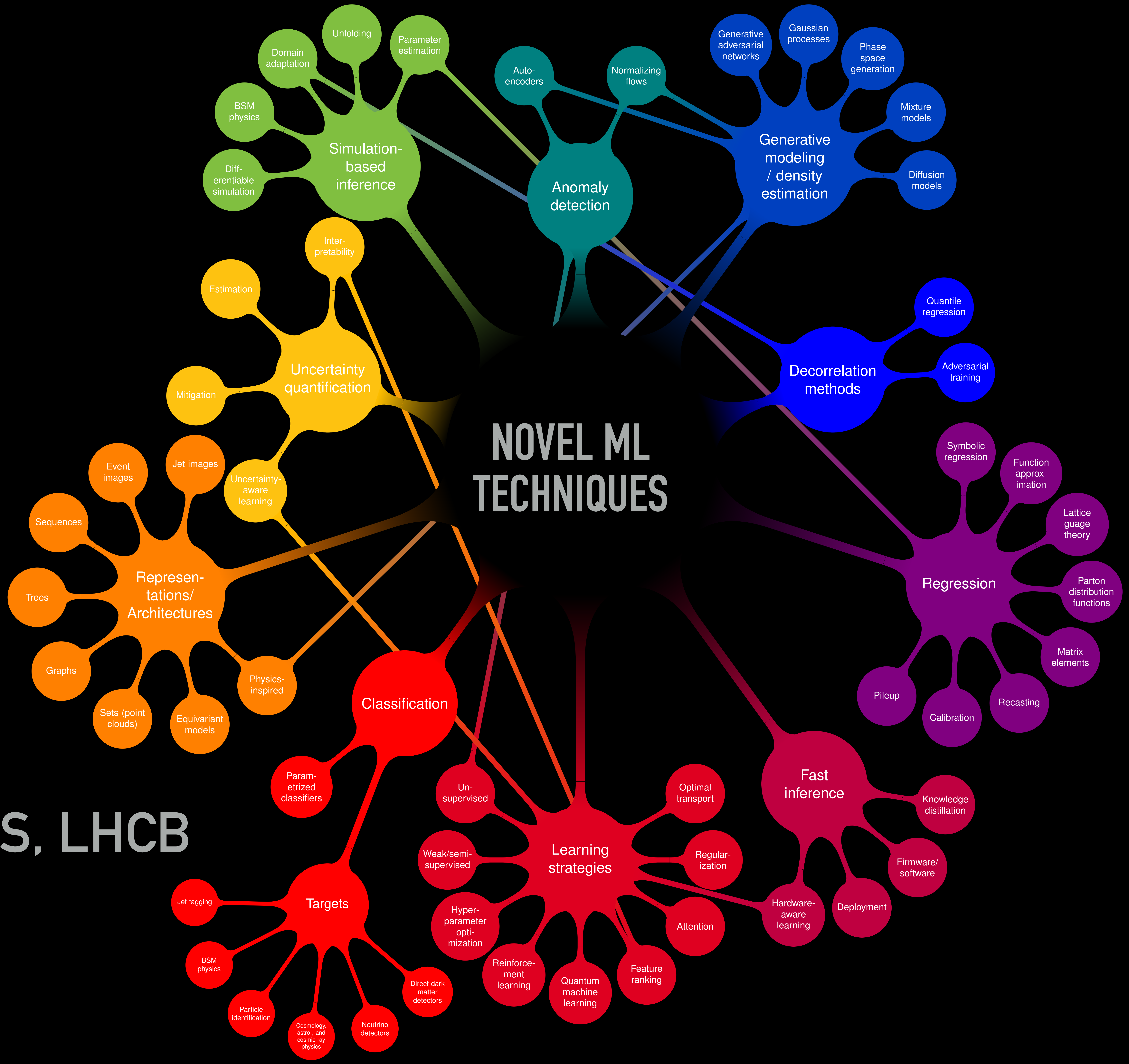


JAVIER DUARTE

ON BEHALF OF ALICE, ATLAS, CMS, LHCB

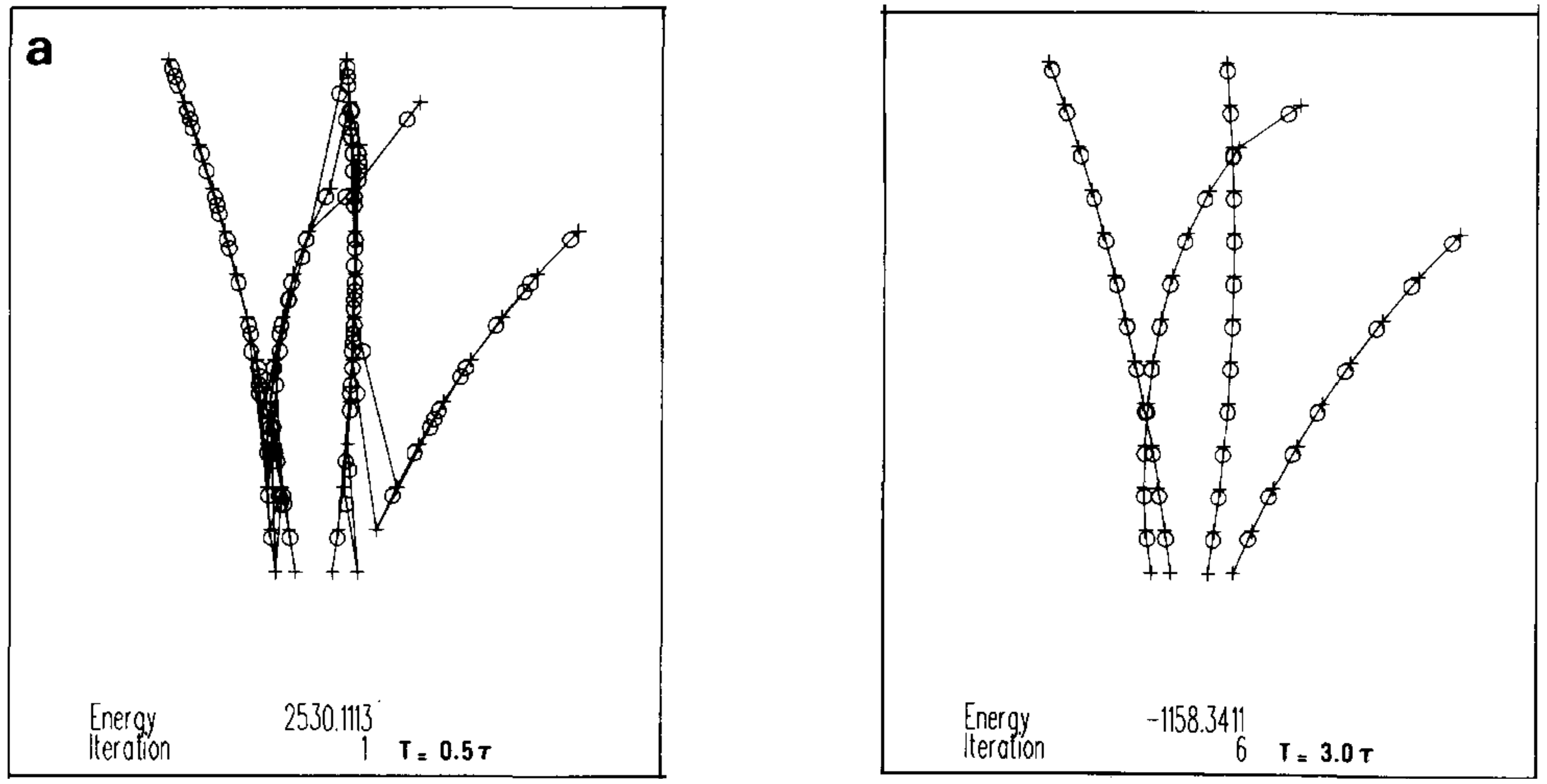
ICHEP 2024

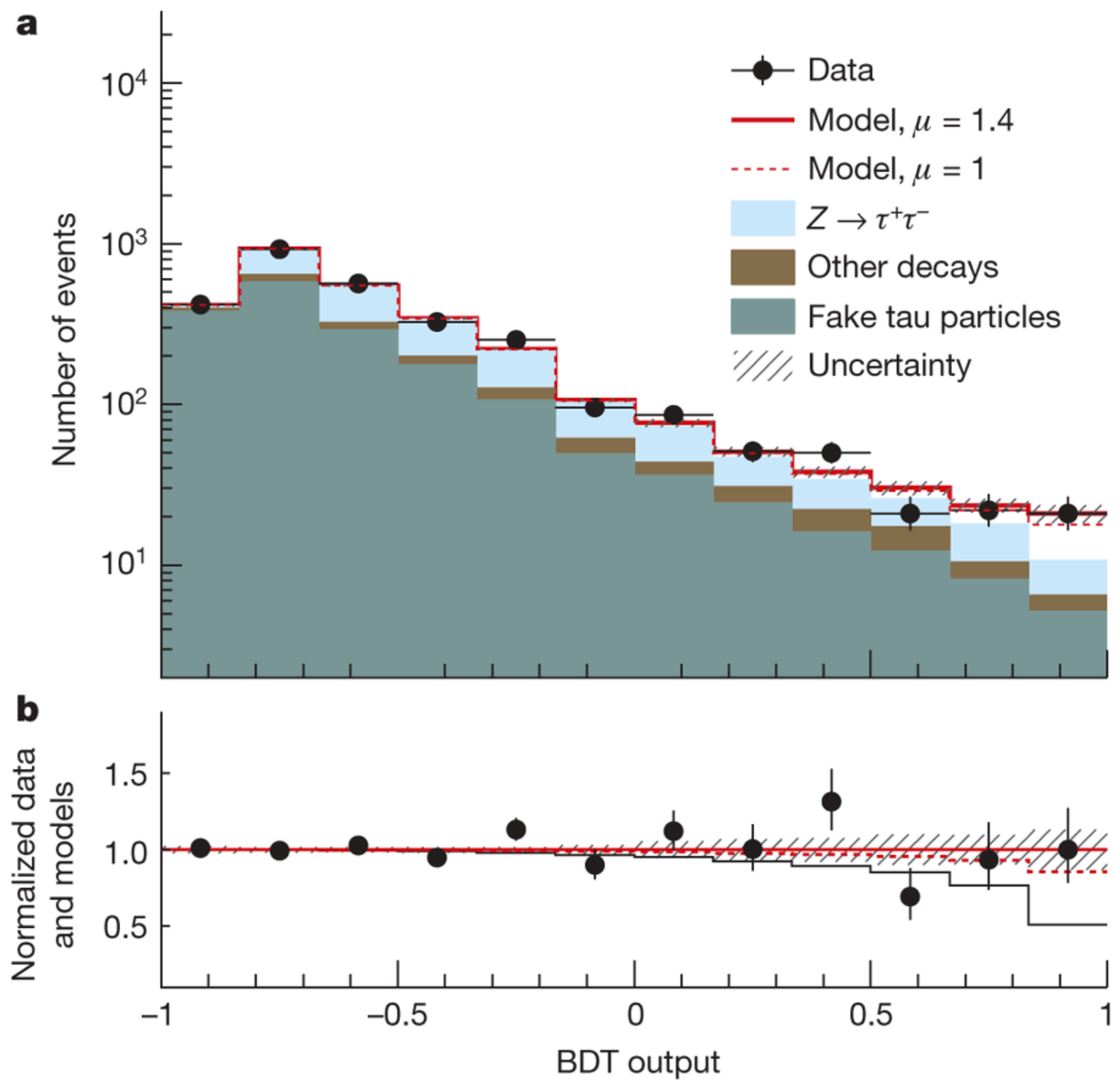
JULY 23, 2024

PARTICLE PHYSICS + MACHINE LEARNING

Comp. Phys. Comm. 49, 429 (1988)
Nature 560, 41 (2018)

- Particle physics has a long history of applying machine learning
  - From the early days in the 1980s applying neural networks to tracking
  - To the Higgs boson discovery in 2012 applying boosted decision trees to identify $H \to \tau\tau$

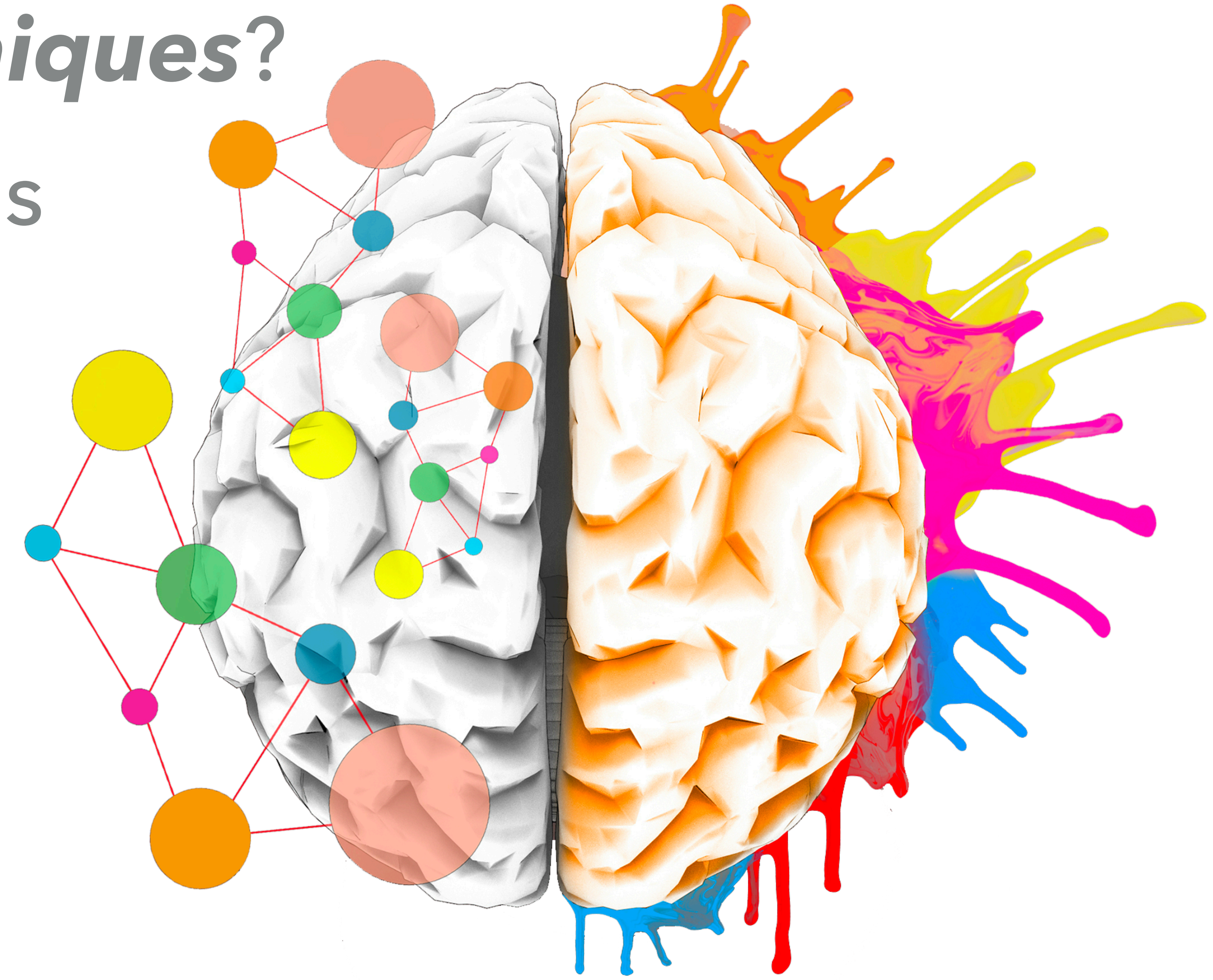




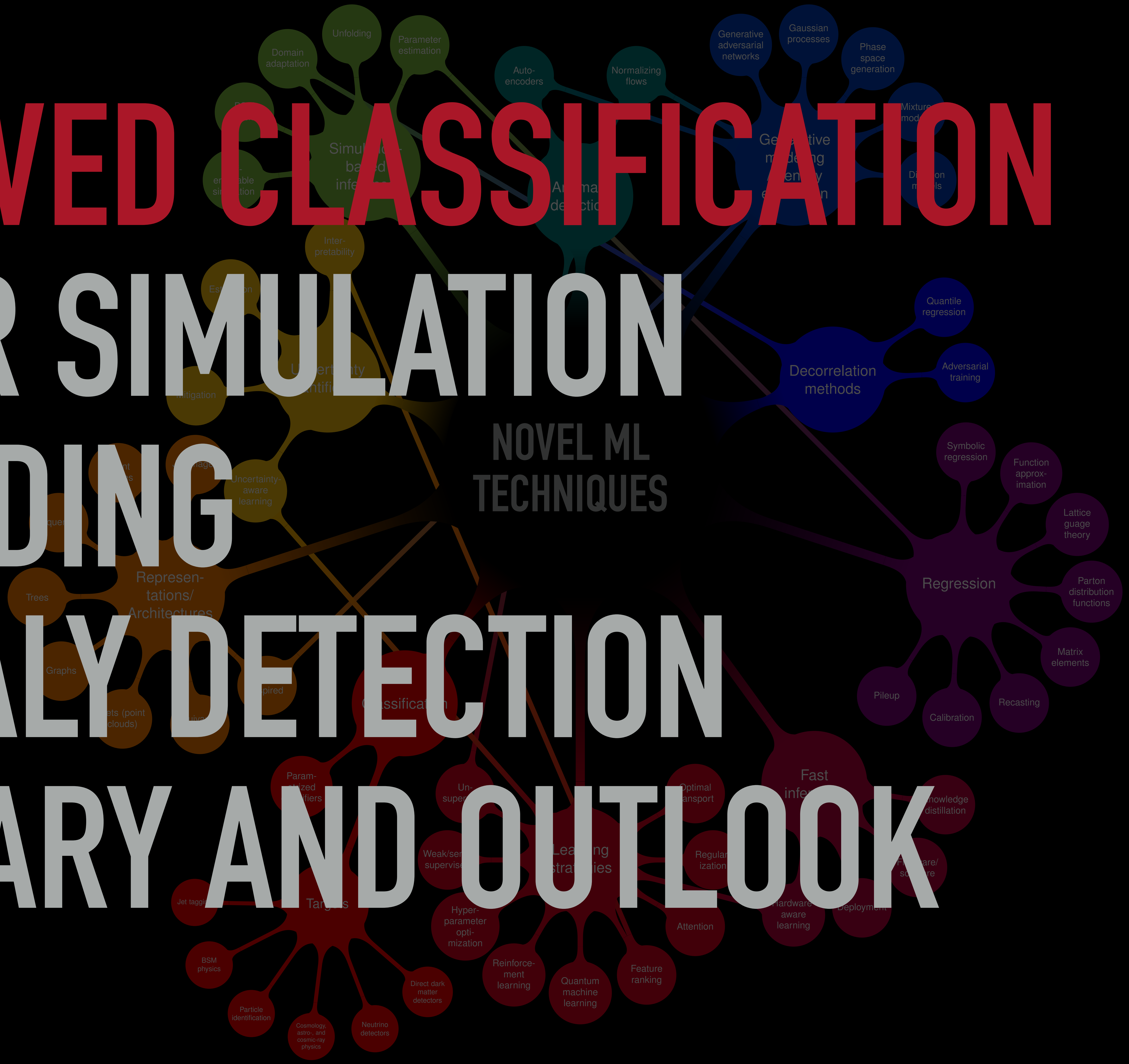
INTRODUCTION & OUTLINE

- ML has changed the way we do physics searches and measurements
  - It is an essential and versatile tool that we use to improve existing approaches
  - It enables fundamentally new approaches

- How are LHC experiments applying ***novel ML techniques***?
  - Improved classification, calibration, & uncertainties
  - Faster simulation
  - Unfolding
  - Anomaly detection
  - Summary and outlook

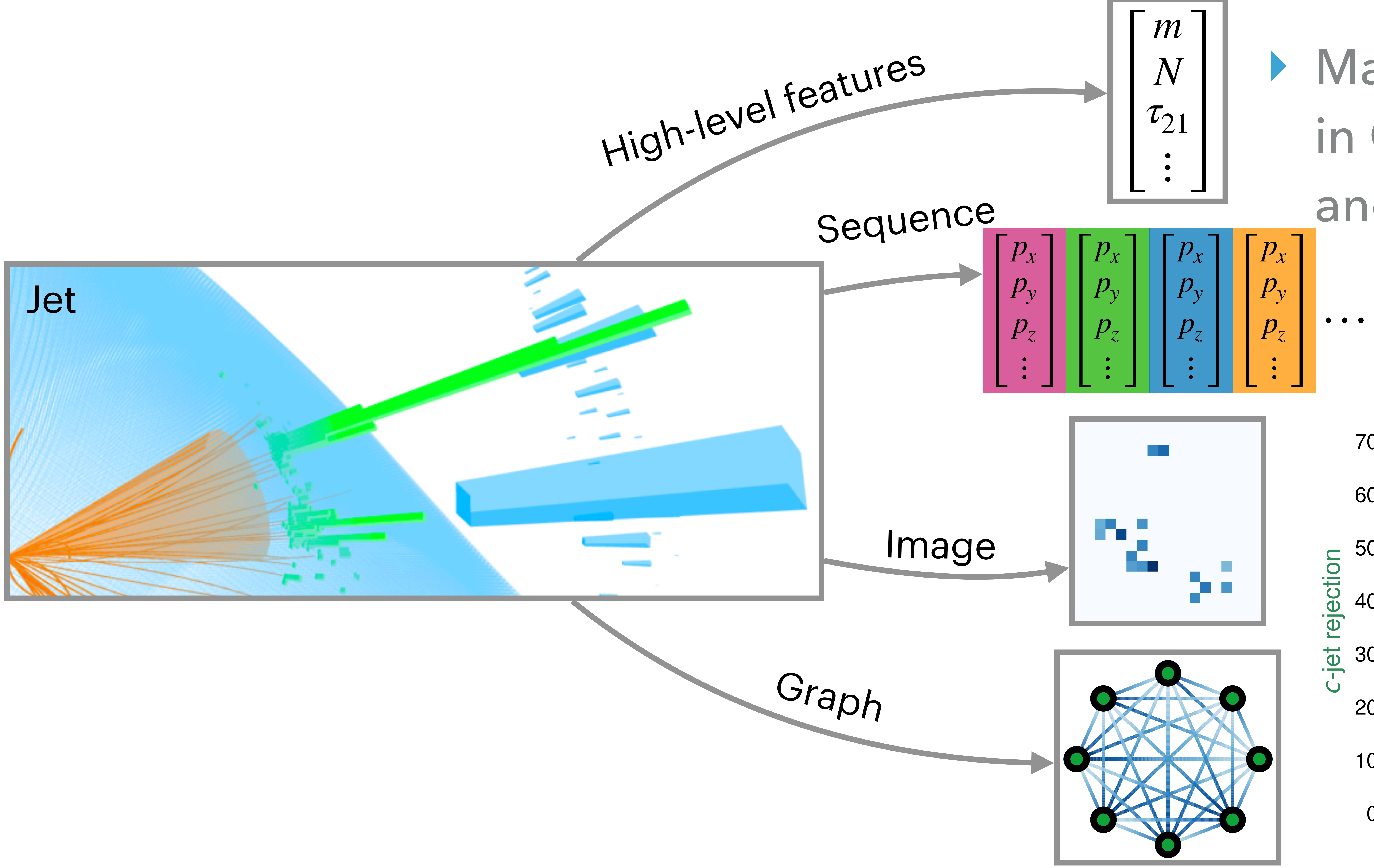


IMPROVED CLASSIFICATION
FASTER SIMULATION
UNFOLDING
ANOMALY DETECTION
SUMMARY AND OUTLOOK

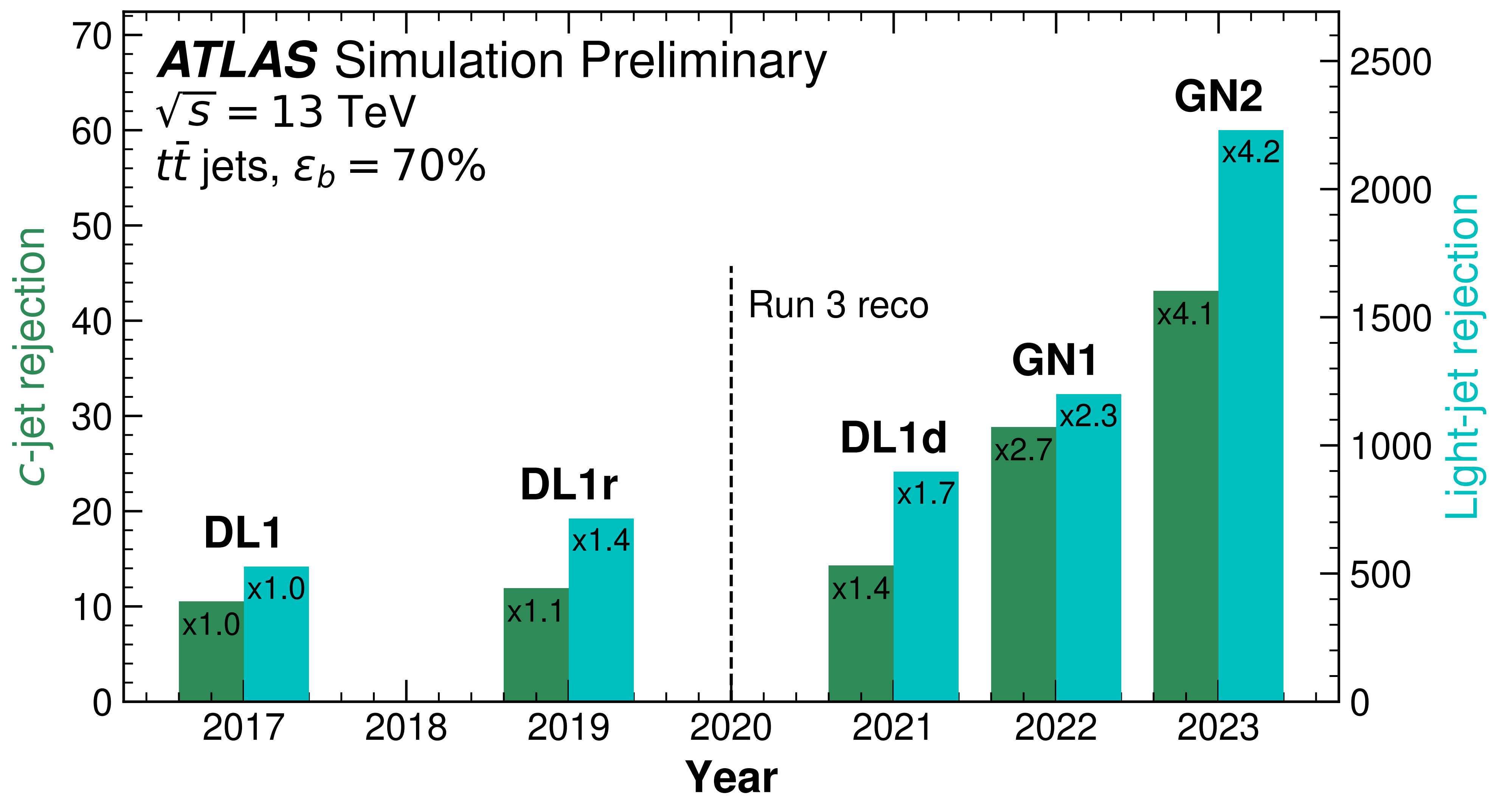


FROM BDTS TO GNNS AND TRANSFORMERS

- Great strides made to leverage **rich low-level information** with **graph neural networks** and **transformers** for a variety of tasks including **jet classification**



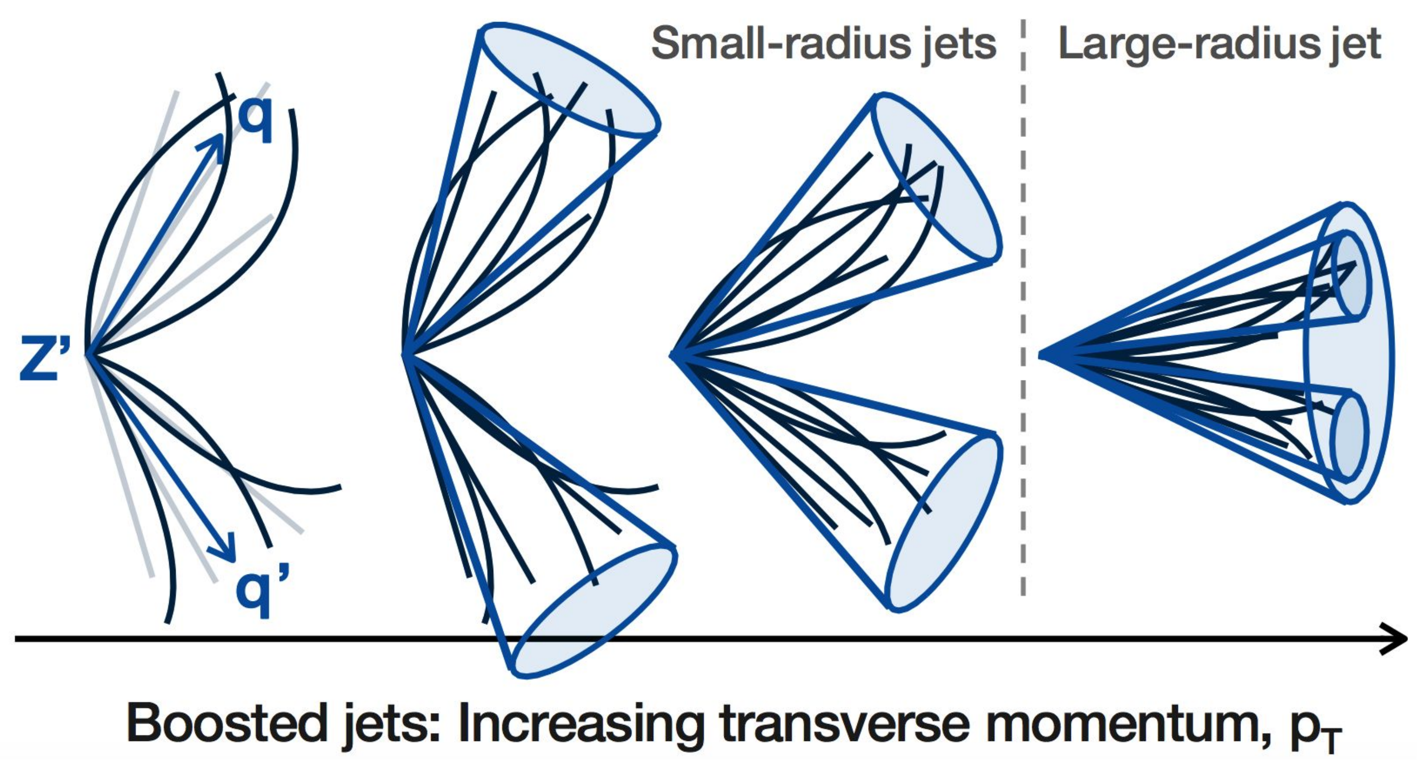
- Major improvements demonstrated in CMS (ParticleNet/Transformer) and **ATLAS (GN1/GN2)**

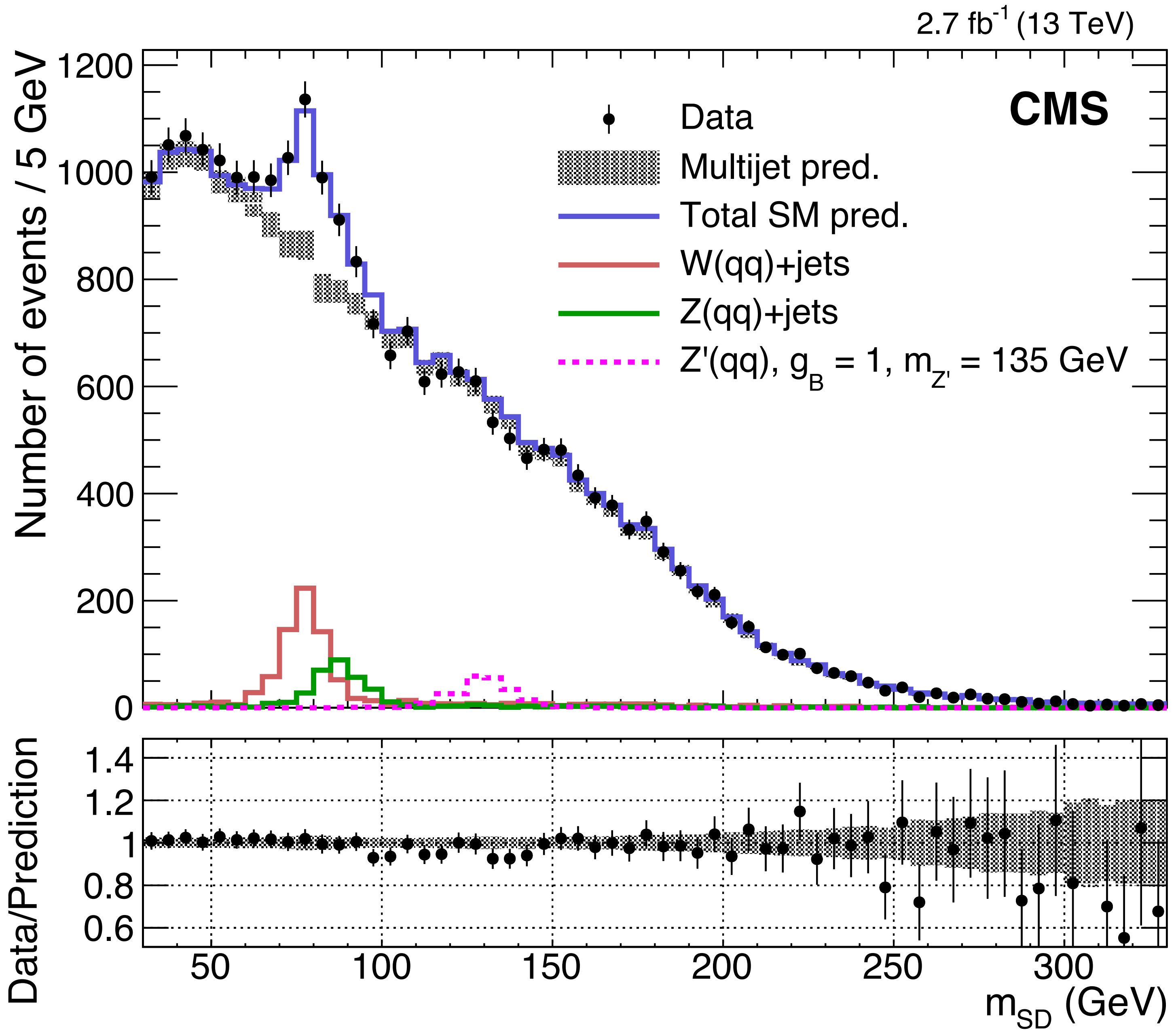


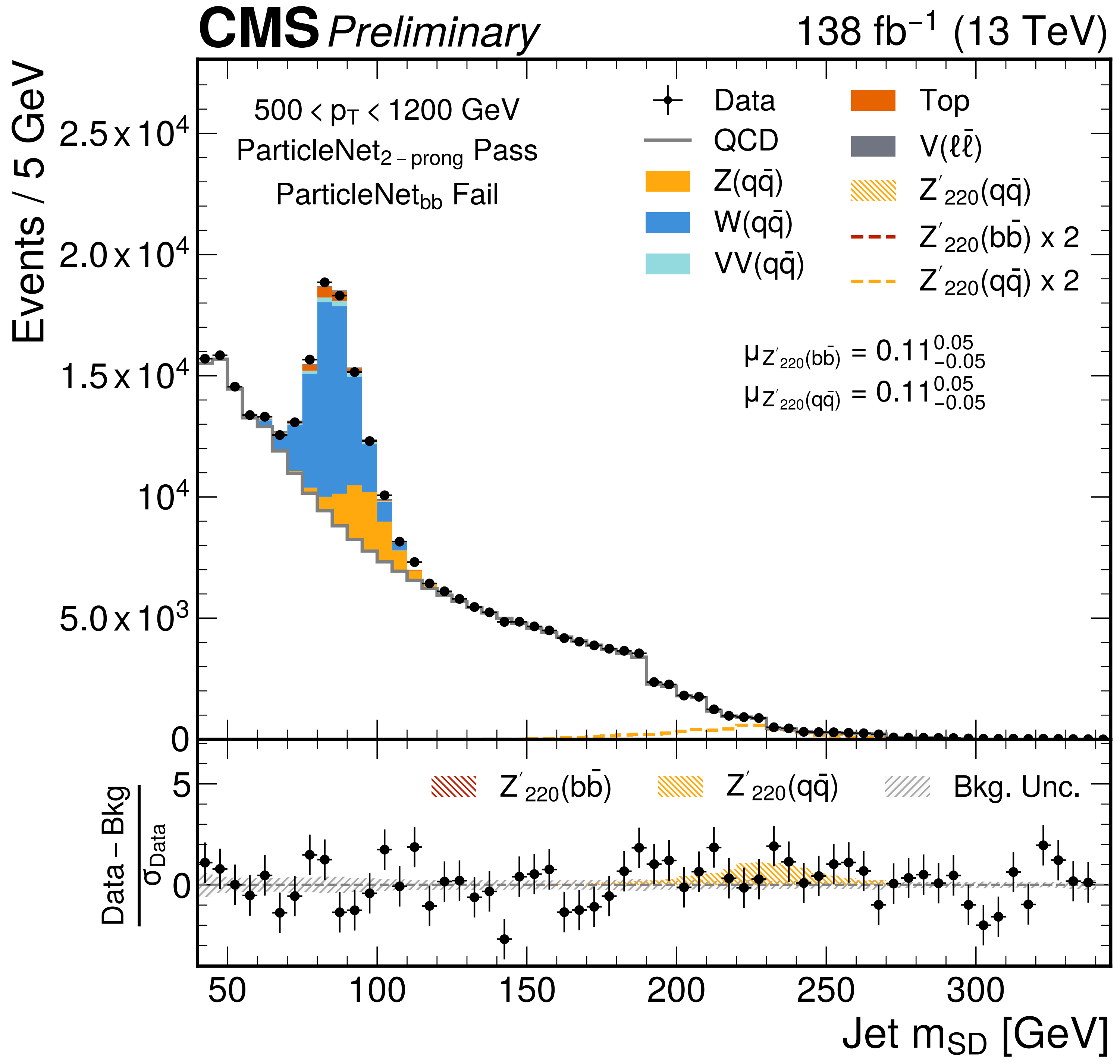
IMPACT OF GNN TAGGING

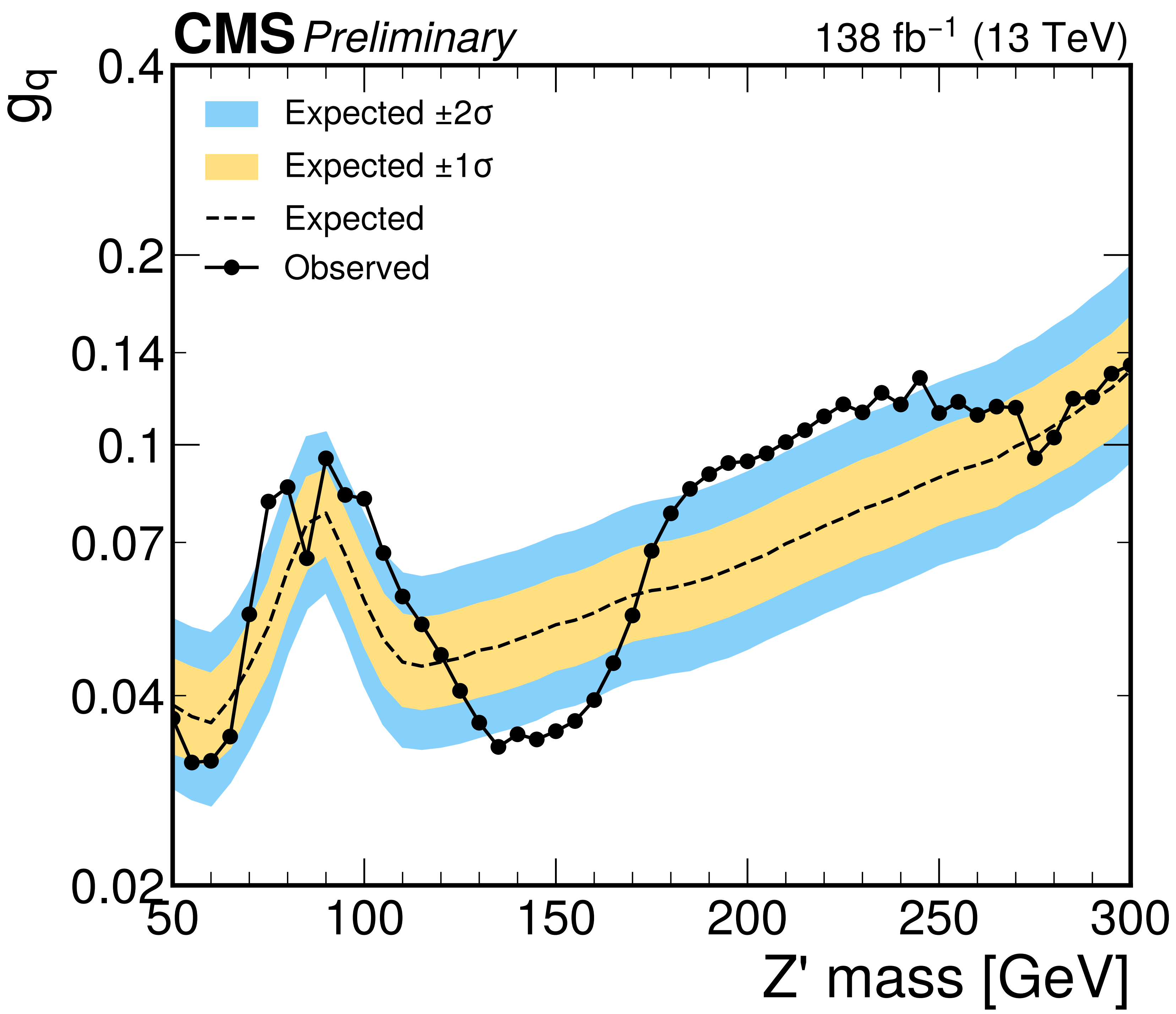
PRL 119 (2017) 111802
CMS-PAS-EXO-24-007

- Previously search for boosted $Z' \rightarrow qq$ resonances reconstructed as large-radius jets with substructure
- Now signal distinguished from the backgrounds using **ParticleNet GNN** discriminants
  - Stringent limits on universal g_q coupling







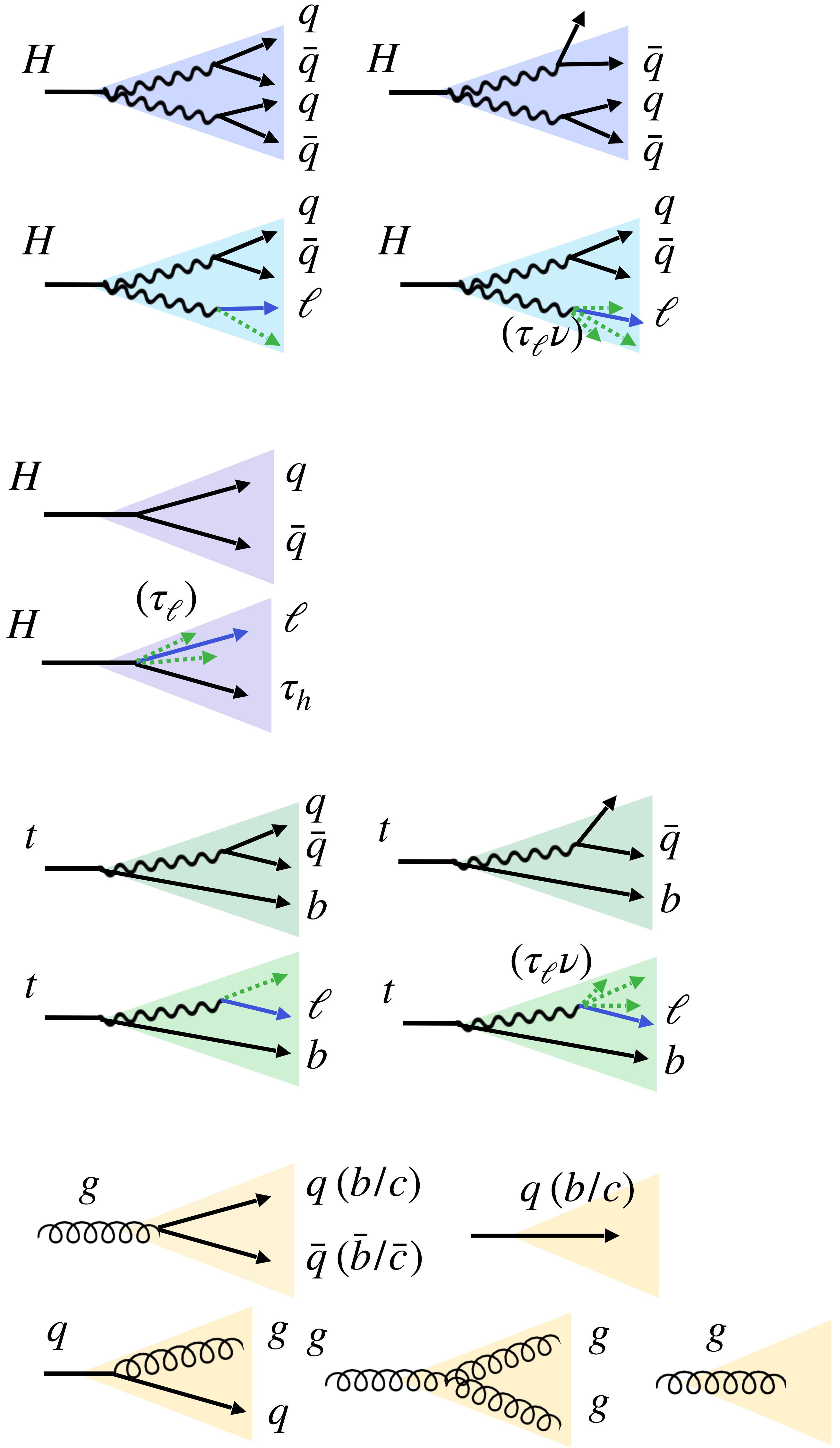


LANDSCAPE OF BOOSTED HIGGS BOSON FINAL STATES

CMS-PAS-HIG-23-012

- CMS ParticleNet has been successfully deployed to identify H→qq vs. QCD large-radius jets in mass-agnostic way using a highly granular multiclassifier
- Extend this same approach to a large array of final states, including H→VV, all-hadronic (3- or 4-prong), and semi-leptonic modes

Process	Final state/ prongness	heavy flavour	# of classes
H→VV (full-hadronic)	qqqq	0c/1c/2c	3
	qqq		3
H→WW (semi-leptonic)	eνqq	0c/1c	2
	μνqq		2
	τ_eνqq		2
	τ_μνqq		2
	τ_hνqq		2
H→qq		bb	1
		cc	1
		ss	1
		qq (q=u/d)	1
H→ττ	$\tau_e\tau_h$		1
	$\tau_\mu\tau_h$		1
	$\tau_h\tau_h$		1
t→bW (hadronic)	bqq	1b + 0c/1c	2
	bq		2
t→bW (leptonic)	beν	1b	1
	bμν		1
	bτ_eν		1
	bτ_μν		1
	bτ_hν		1
QCD		b	1
		bb	1
		c	1
		cc	1
		others (light)	1

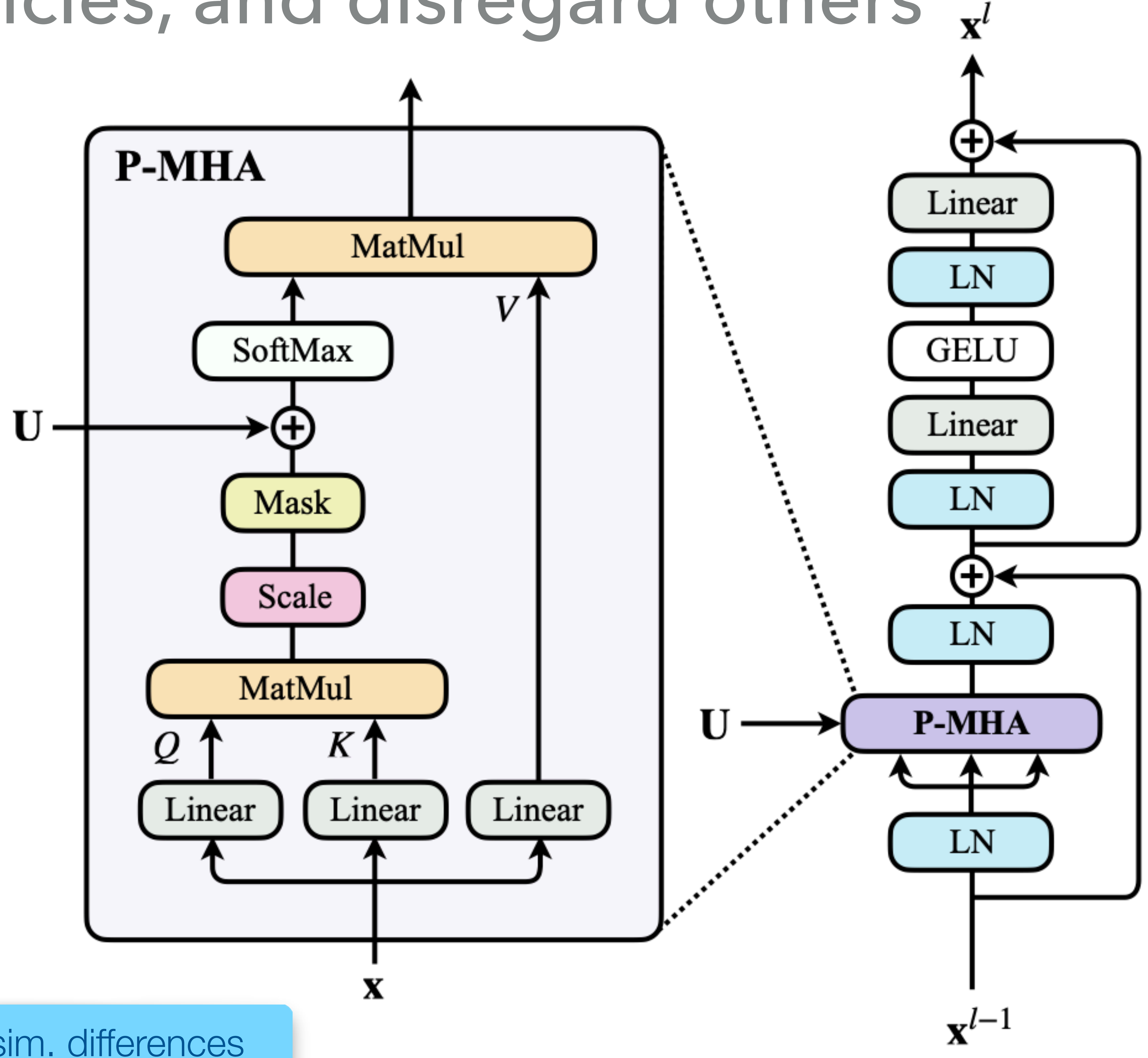


GLOBAL PARTICLE TRANSFORMER

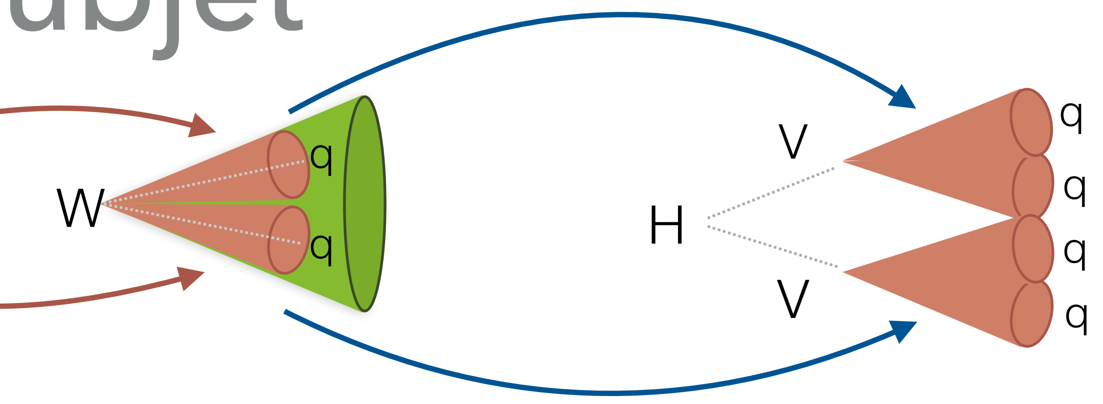
arXiv:2202.03772
CMS-DP-2023-046

- Global Particle Transformer algorithm uses learned "attention" (and pairwise features) to give more weight to certain particles, and disregard others in order to infer the origin of jets

- Challenge to calibrate these taggers when there is no SM analogue for the signal we can isolate
  - New technique uses Lund jet plane for calibration
  - Effectively **measure scale factors** per quark subjet



Measure tagger efficiency per-quark

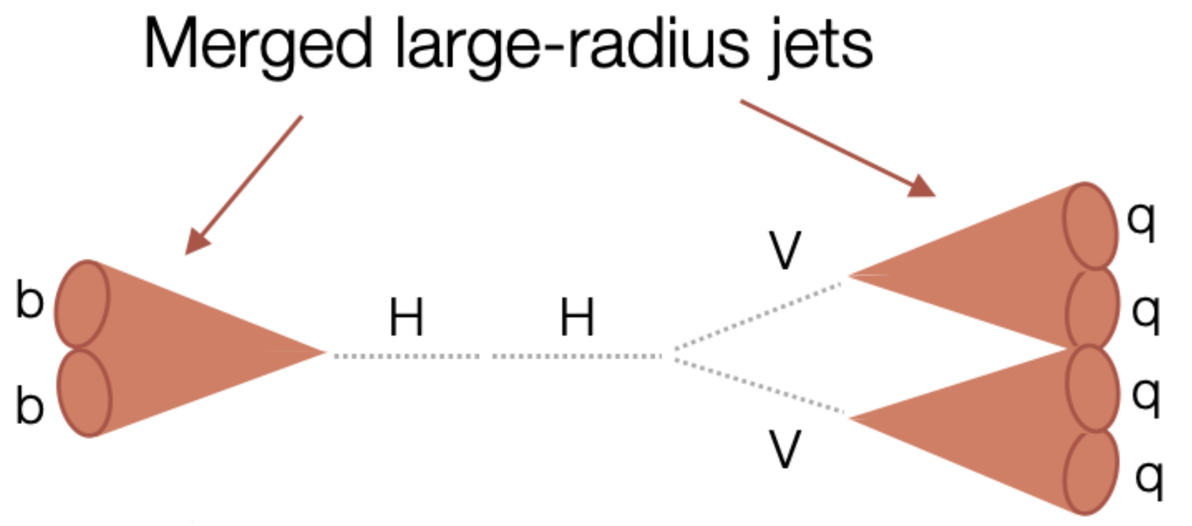


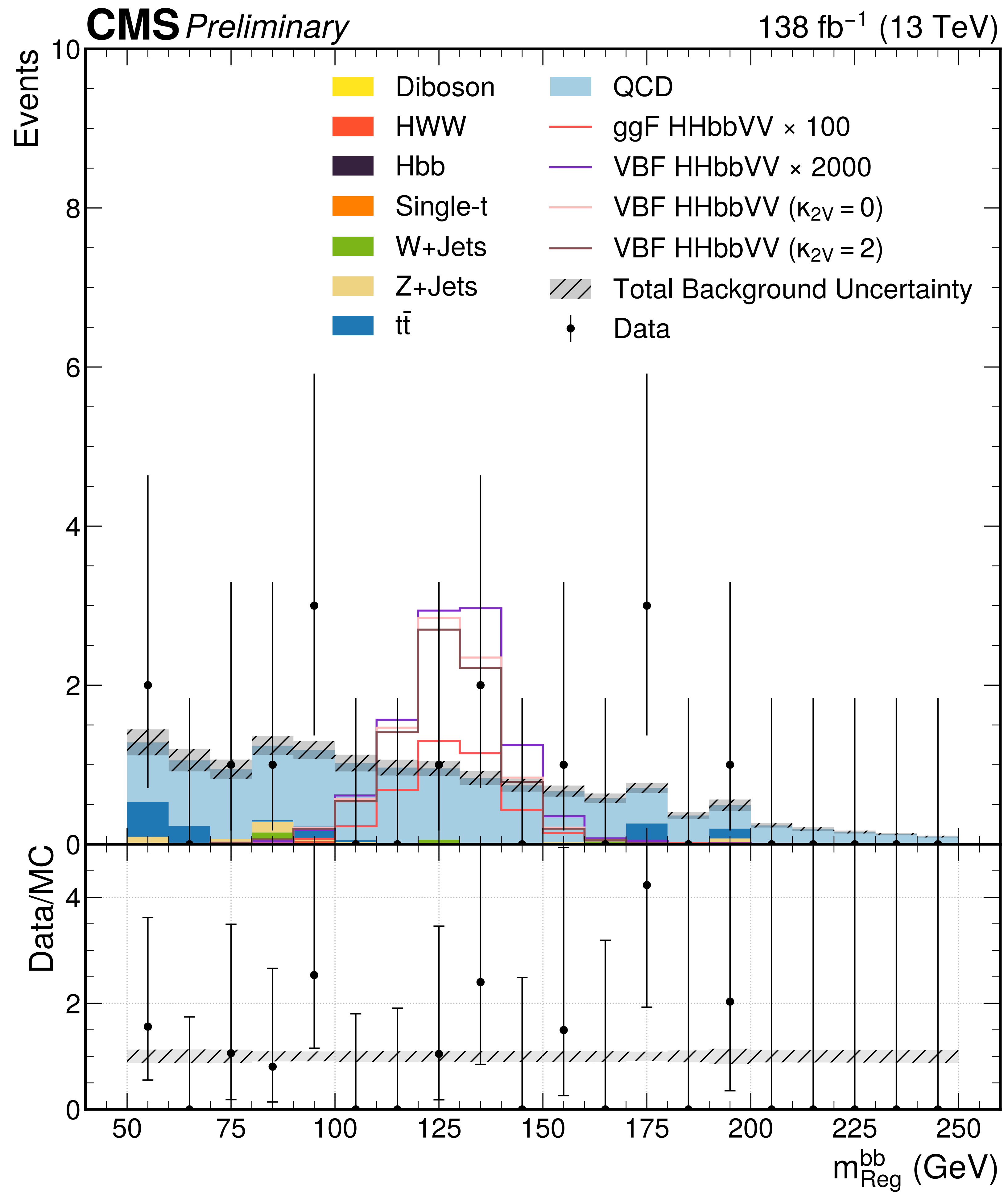
Product of per-quark data / sim. differences
⇒ SF + uncertainty on HVV(4q) tagging

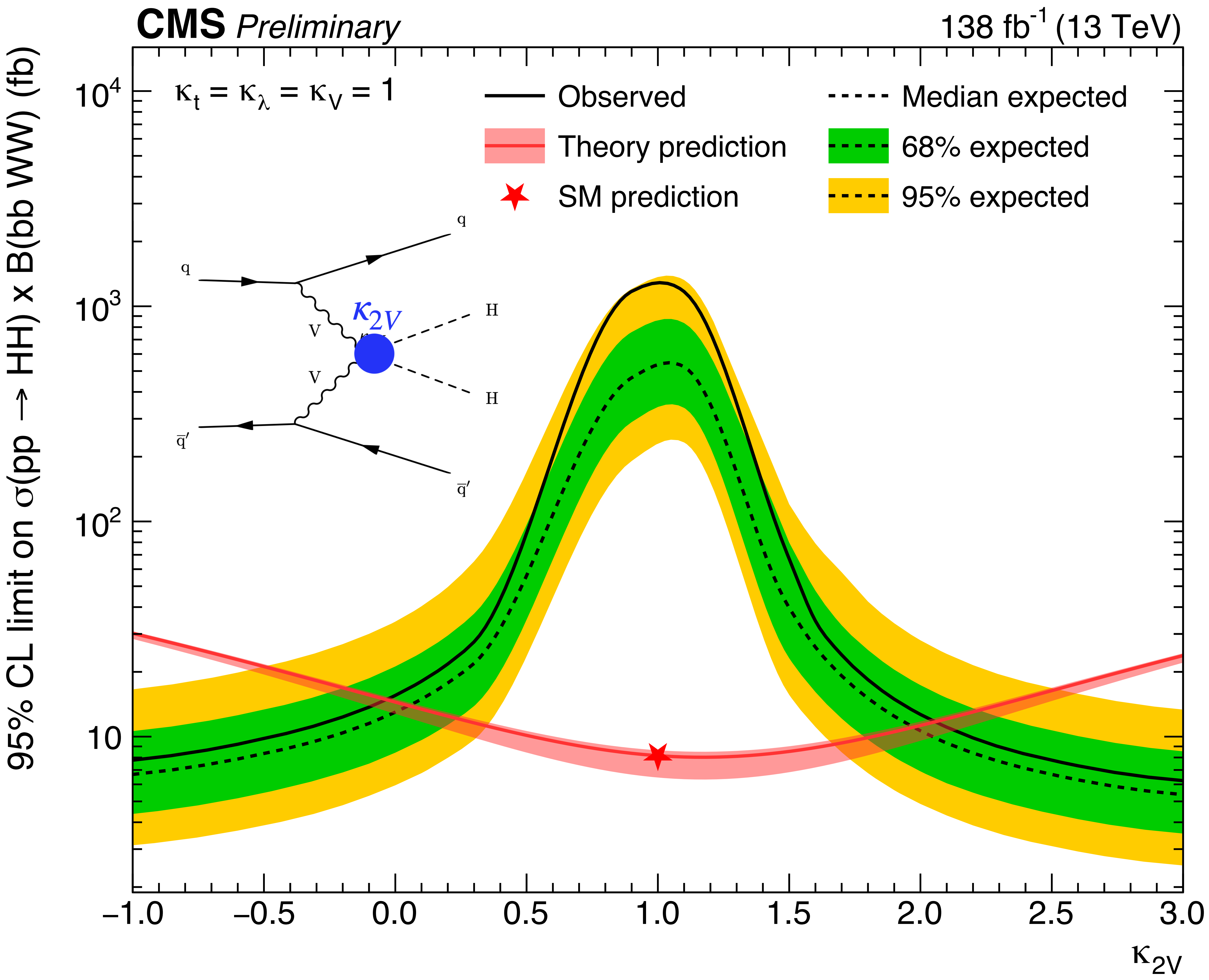
$$\mathrm{softmax}\left(\frac{QK^{\intercal}}{\sqrt{d_k}} + U\right)V$$

CMS BOOSTED HADRONIC HHBBVV SEARCH

- Enables a new search for boosted $HH \rightarrow bbVV \rightarrow bb4q$
- Provides second-best constraint on $HHVV$ coupling κ_{2V}



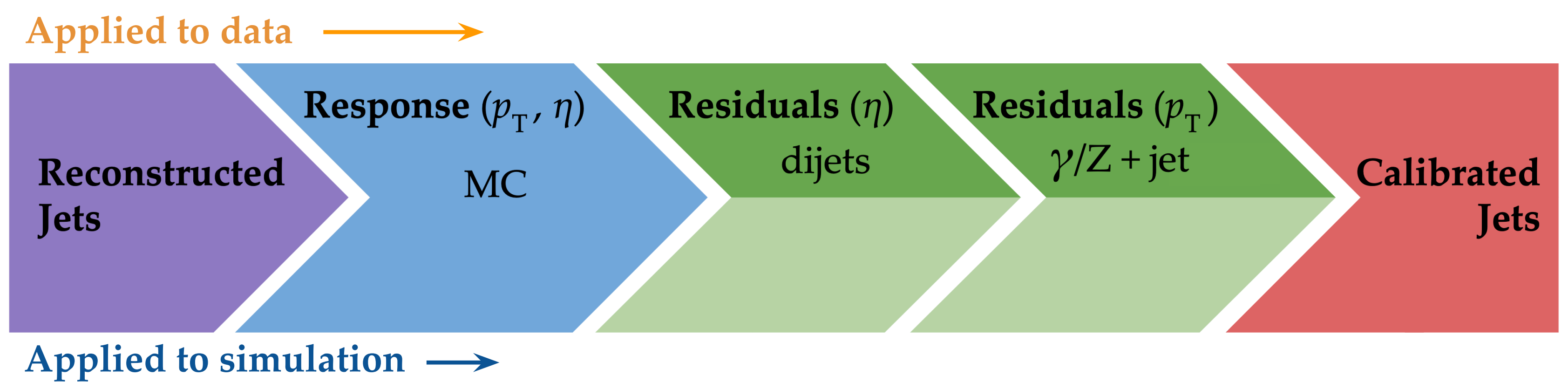


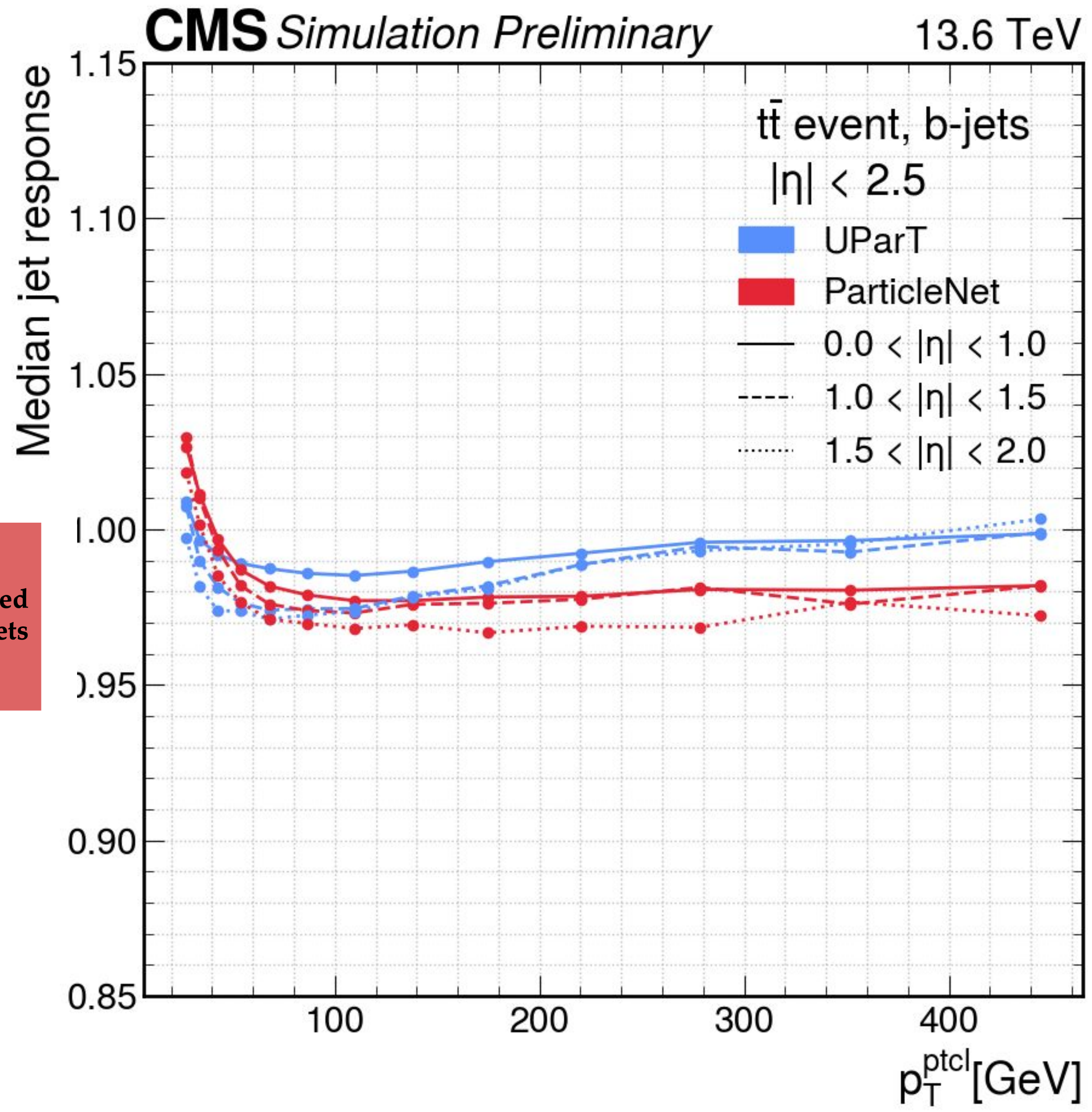


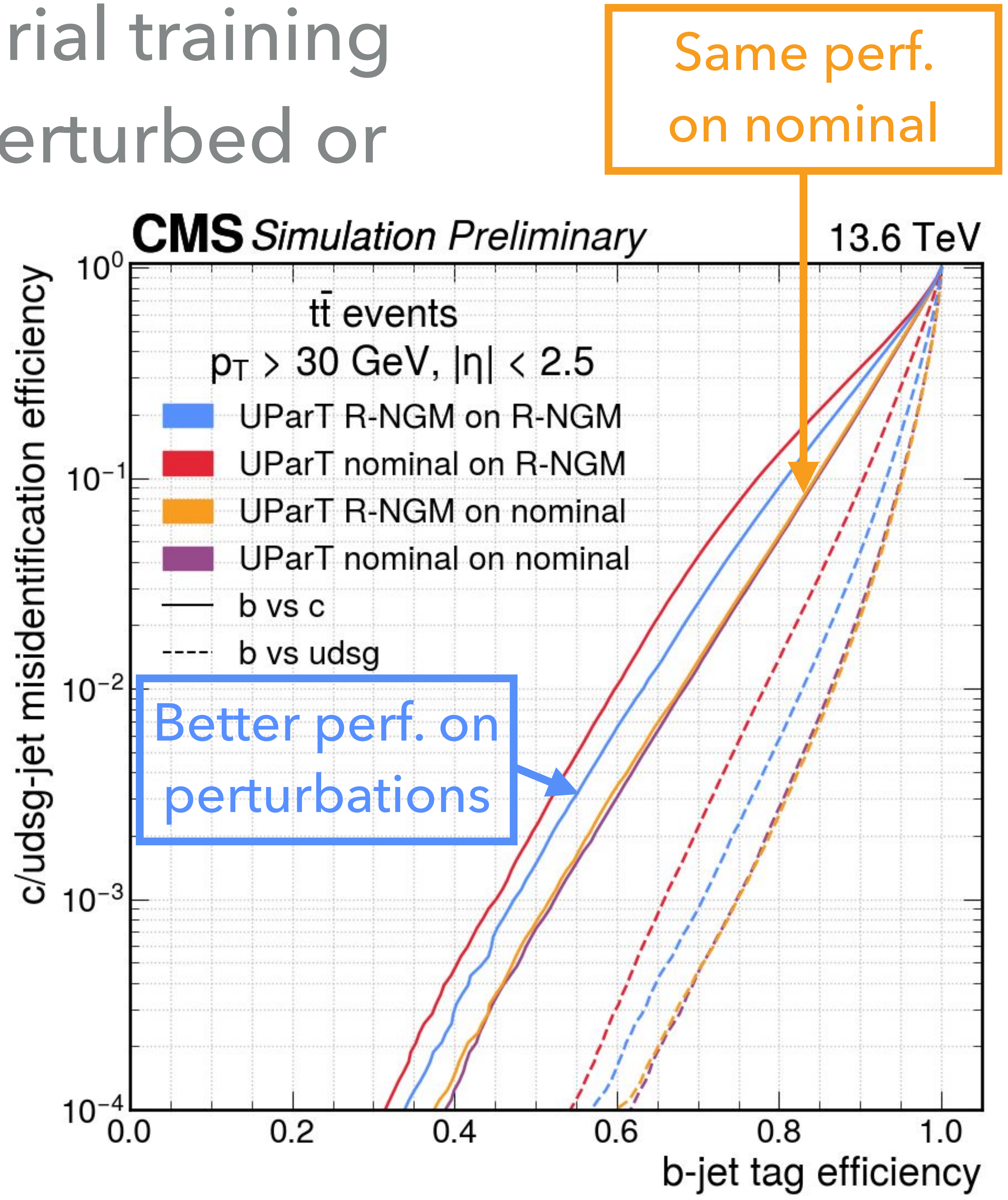
UNIFIED PARTICLE TRANSFORMER SMALL-RADIUS JETS

CMS-DP-2024-066
CMS-DP-2024-064

- Unified approach using same architecture to tag heavy flavor, tag hadronic taus, **regress jet energy**, and estimate jet energy resolution
- Rectified normed gradient method (R-NGM) adversarial training used improve model robustness even when facing perturbed or mismodeled inputs
- Calibration in progress for 2022+2023 data



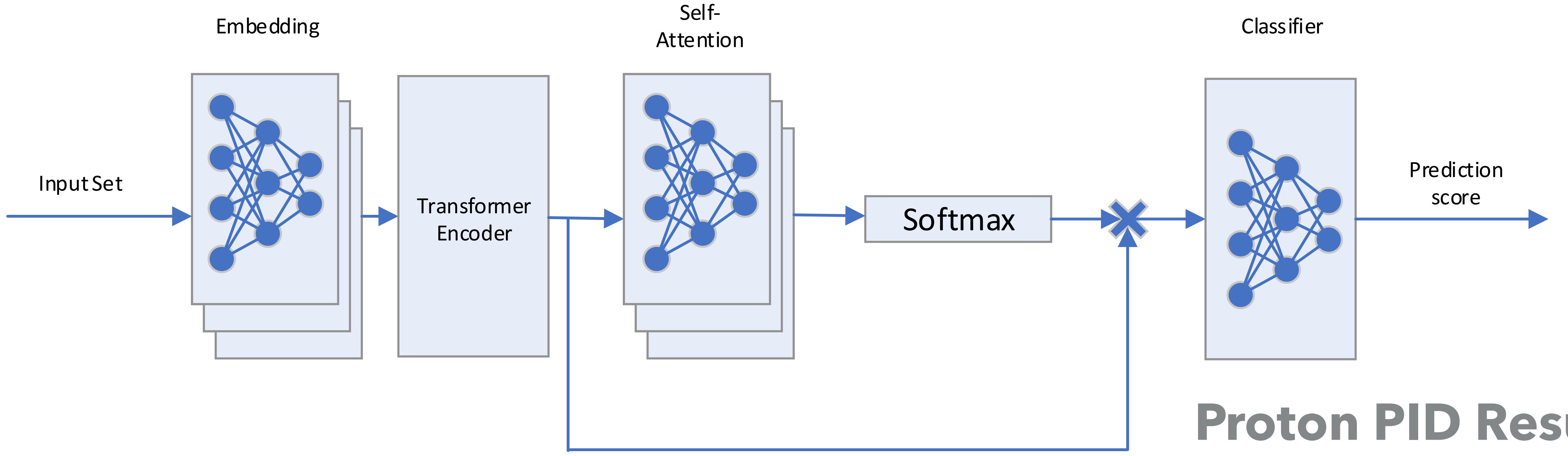


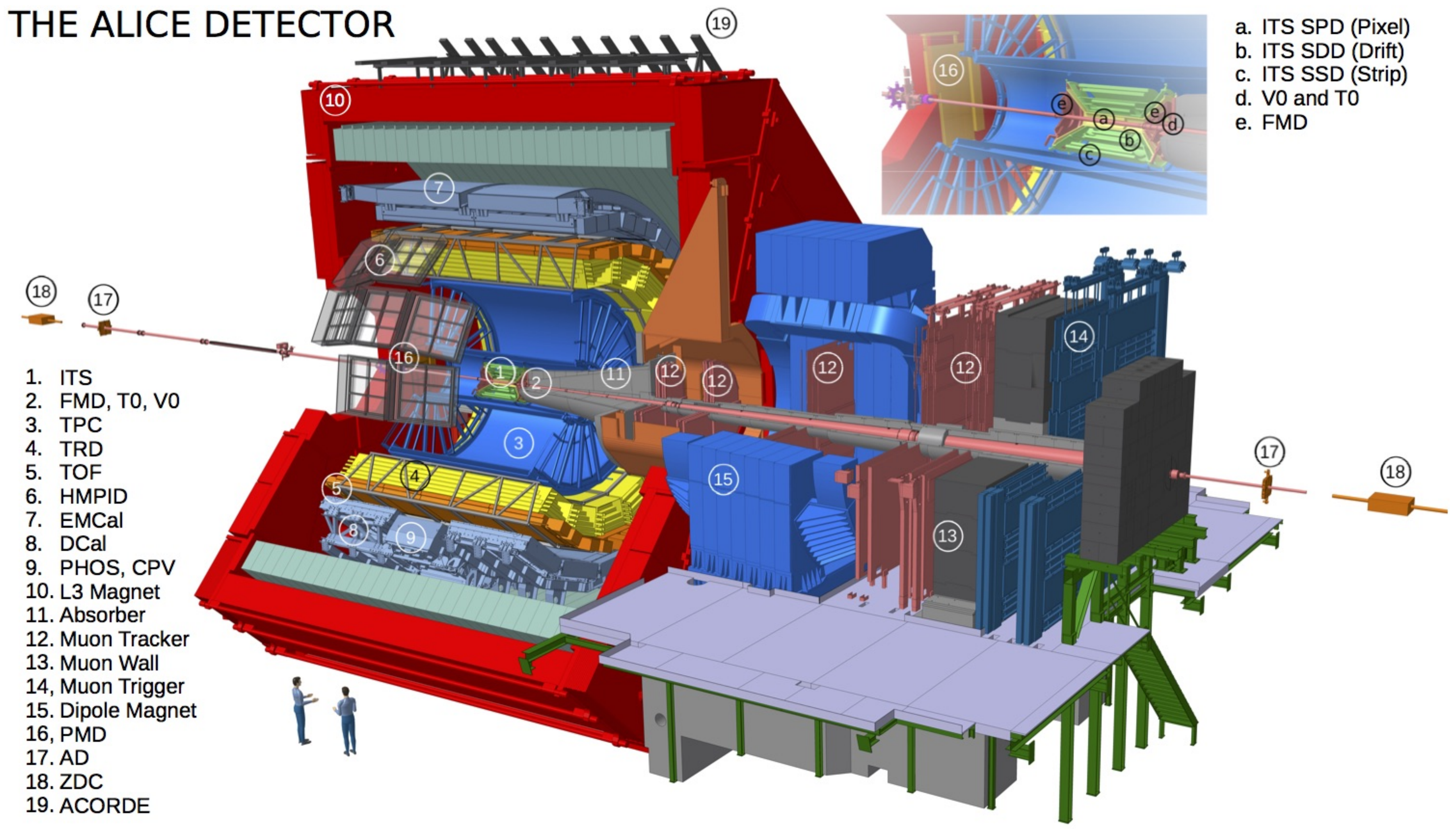


PARTICLE ID WITH TRANSFORMER

arXiv:2403.17436
arXiv:2401.01905

- **Transformer** for particle ID in ALICE can result in higher purity and efficiency than standard methods
- Use **domain adversarial neural networks** to mitigate data-simulation differences

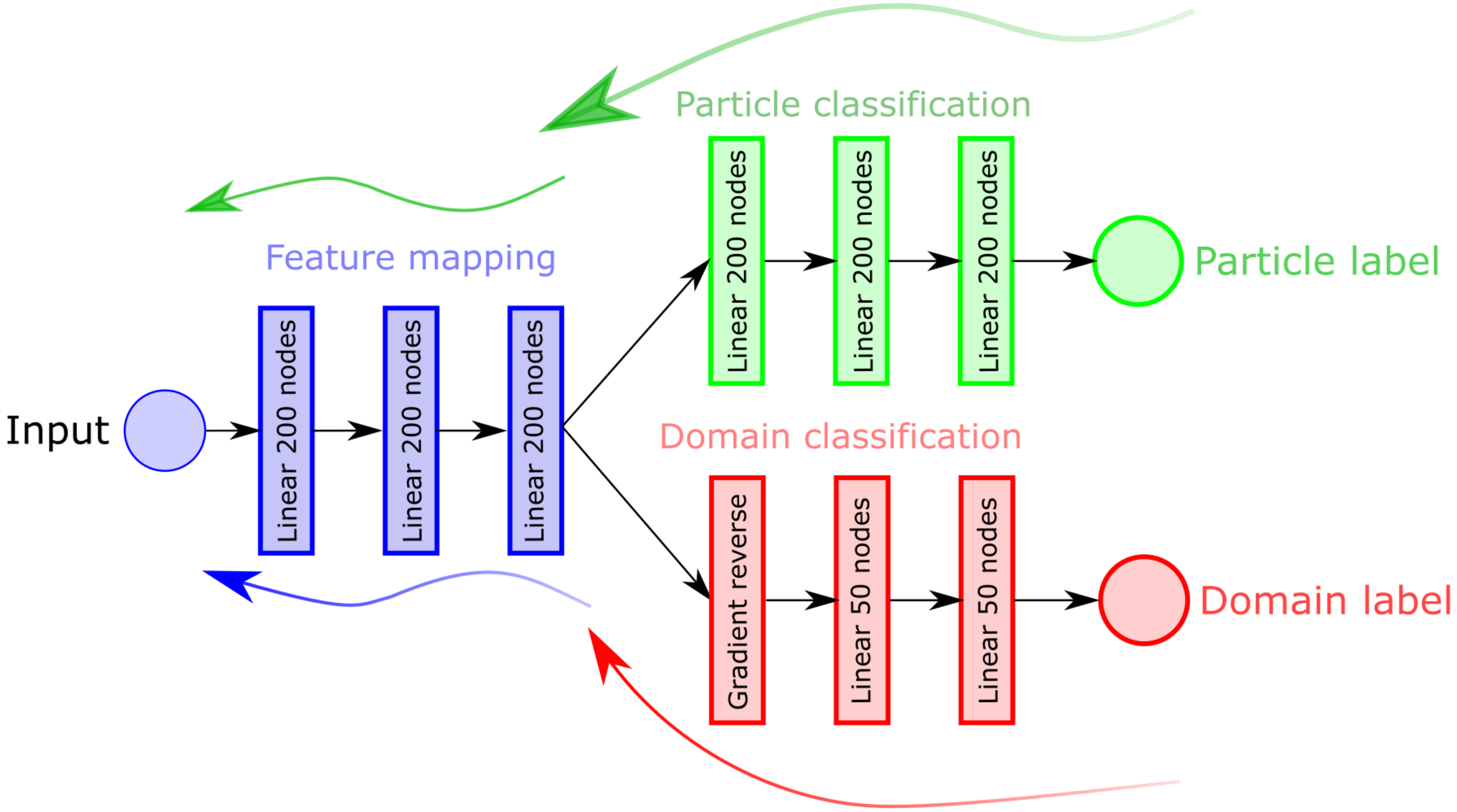




Proton PID Results

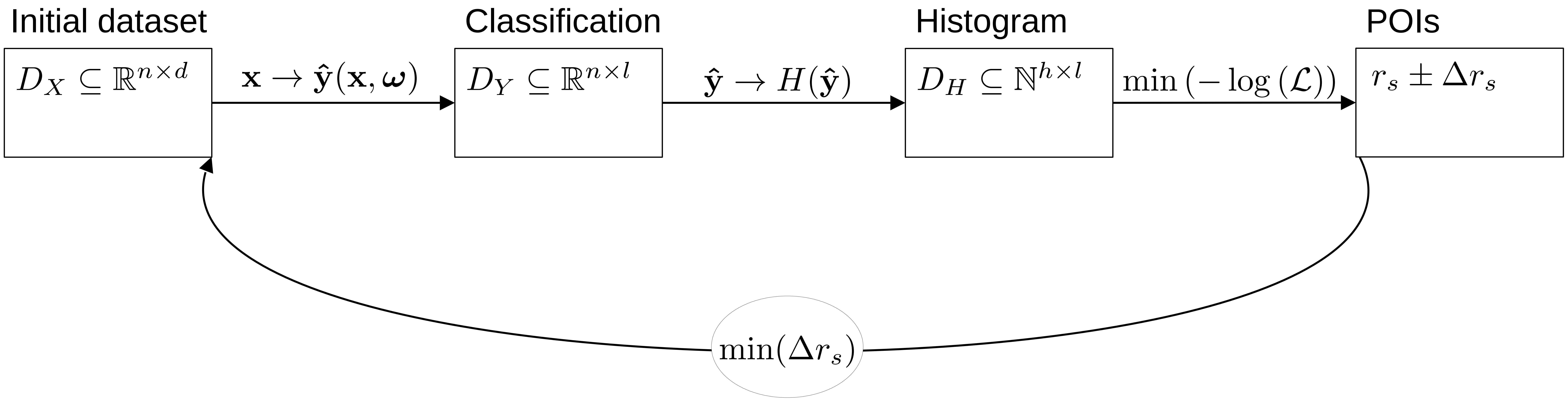
Transformer

Model	Precision	Recall	F_1
Standard	**99.40 ± 0.01**	59.72 ± 0.03	74.61 ± 1.88
Ensemble	97.16 ± 0.46	93.74 ± 0.30	95.42 ± 0.12
Mean	97.85 ± 0.41	93.34 ± 0.32	95.54 ± 0.06
Proposed	97.80 ± 0.44	**93.86 ± 0.27**	**95.79 ± 0.07**
Regression	97.38 ± 0.40	93.67 ± 0.38	95.49 ± 0.15



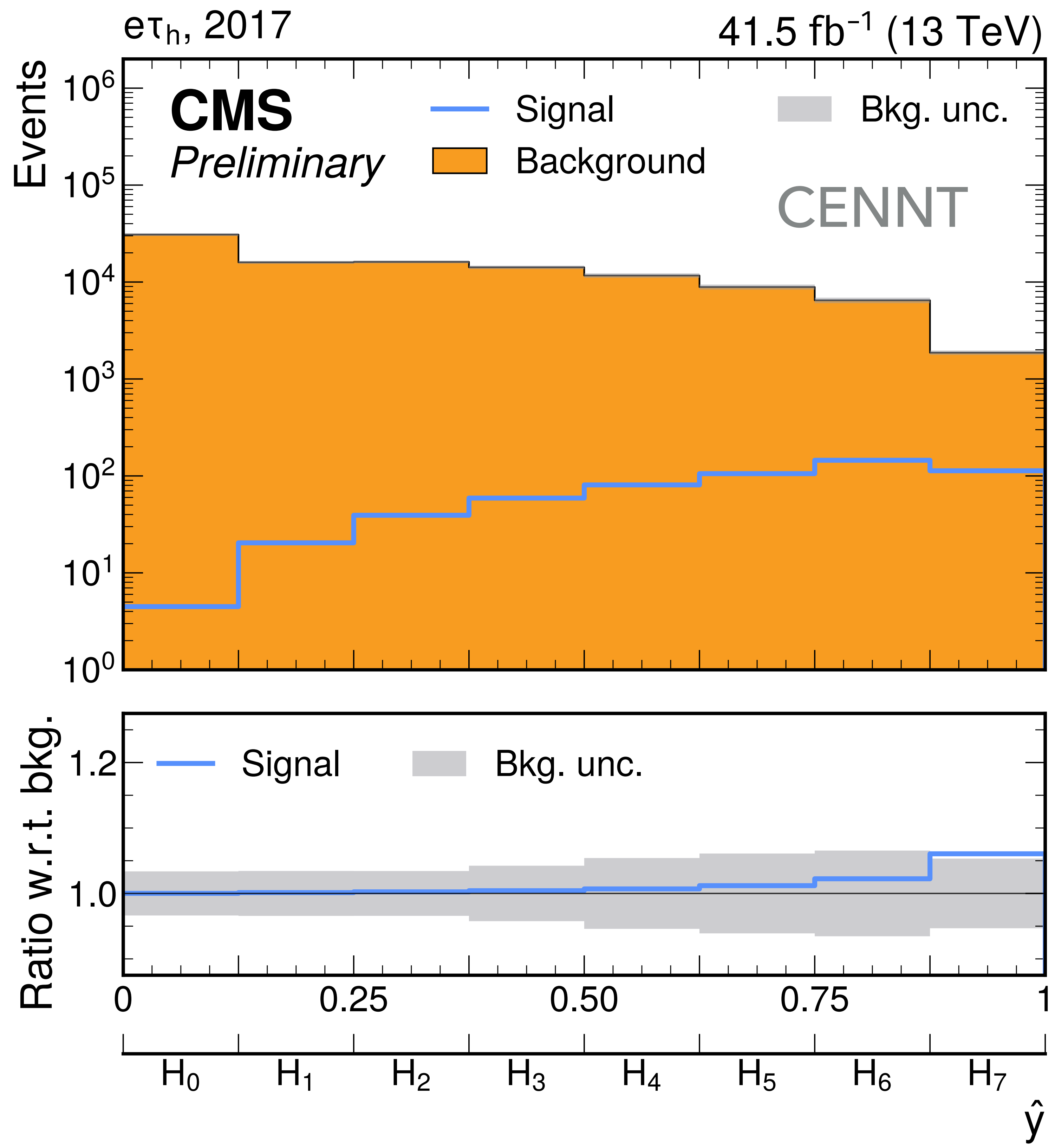
SYSTEMATIC-AWARE LEARNING

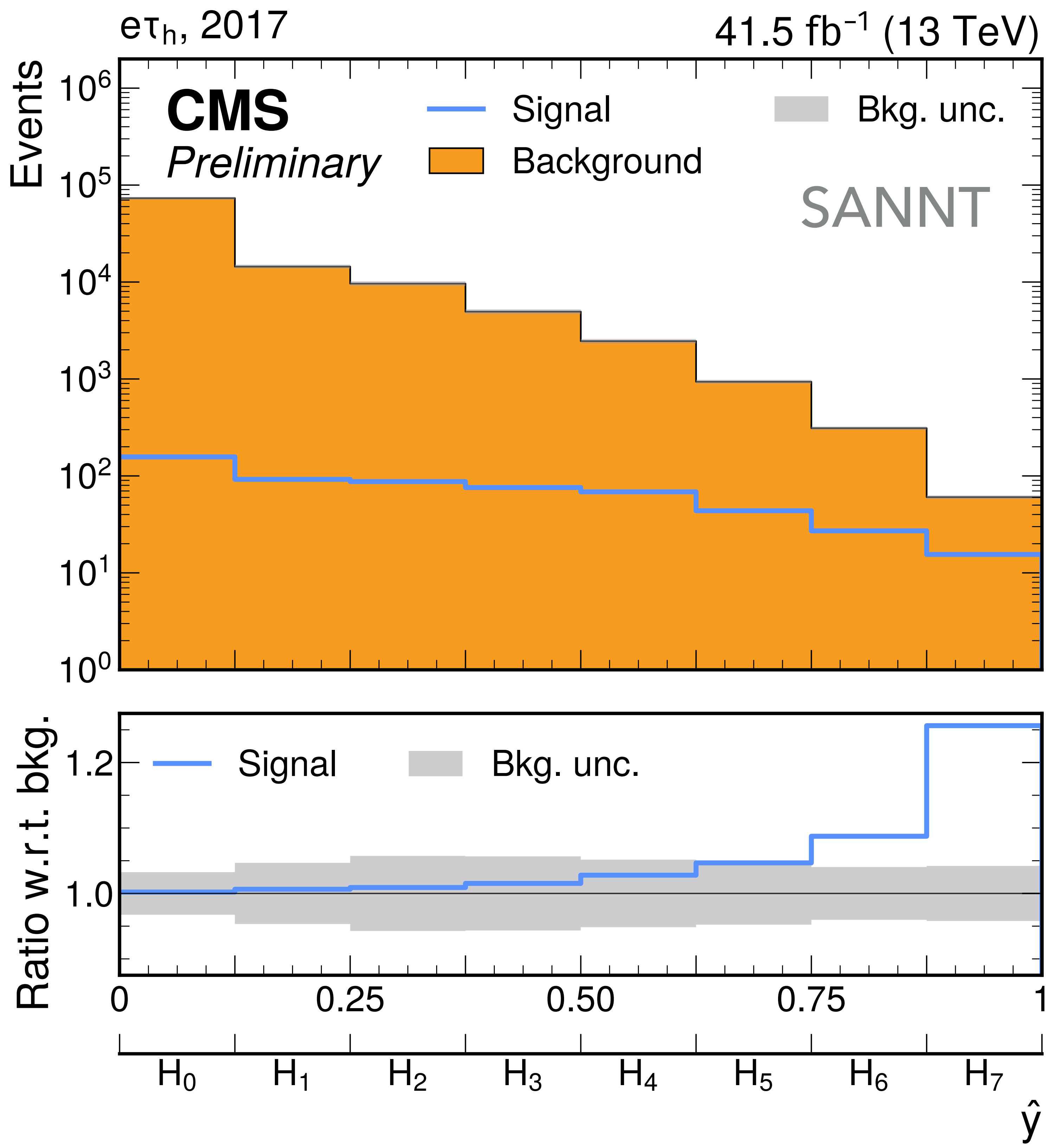
- Standard classifier training (CENNT) optimizes for signal vs. background discrimination without considering systematics and other effects that affect the ultimate figure: uncertainty Δr_s on a physics parameter r_s
- By implementing the analysis chain (including systematics) in a **differentiable way**, we can directly optimize for min. Δr_s in the neural network training!
  - Key choosing gradients for histogram operation $\hat{\mathbf{y}} \rightarrow H(\hat{\mathbf{y}})$

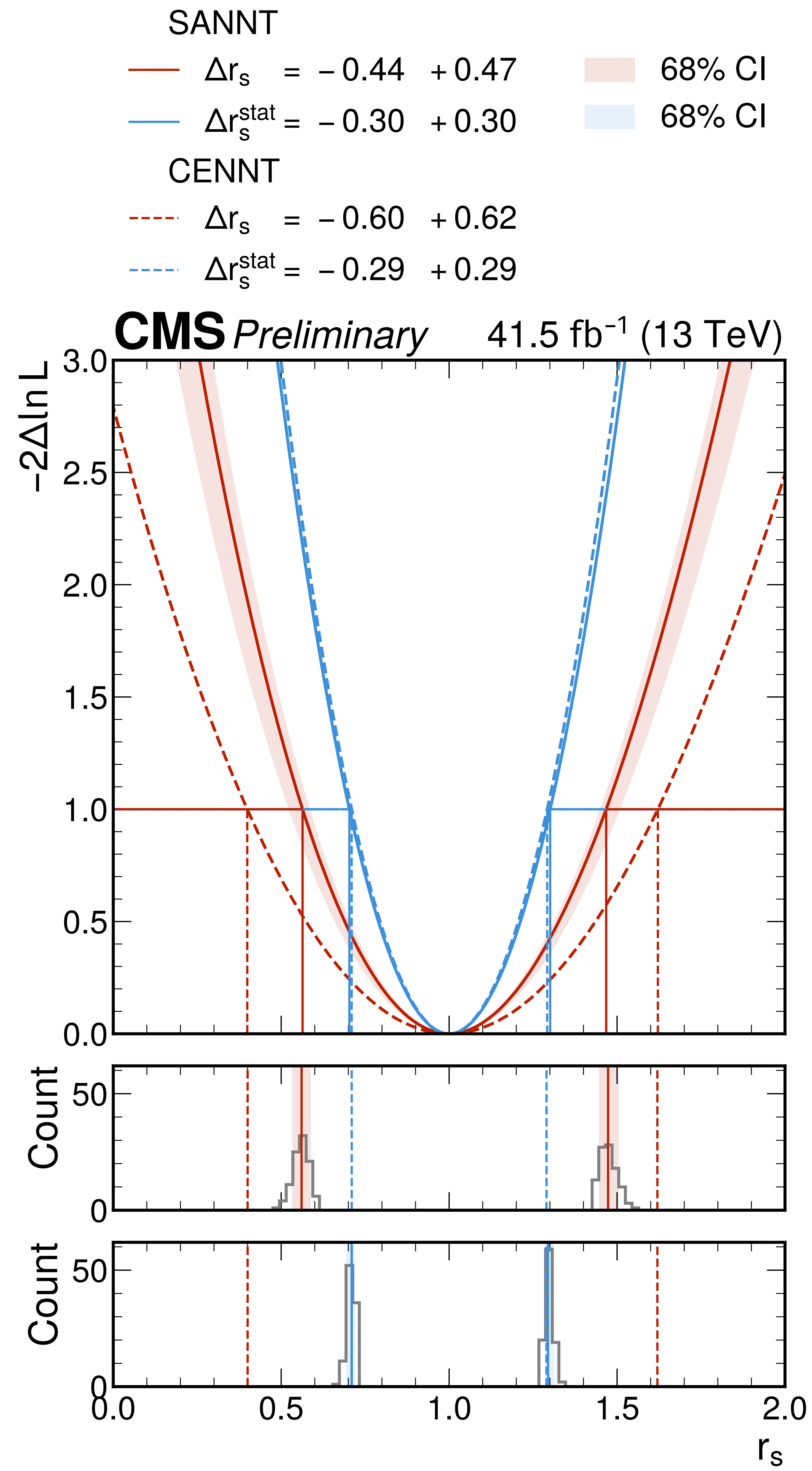


SYSTEMATIC-AWARE LEARNING

- CENNT optimizes for separation, while SANNT (Δr_s) concentrates signal in bins with smaller background uncertainty
- Total uncertainty improves by 25%







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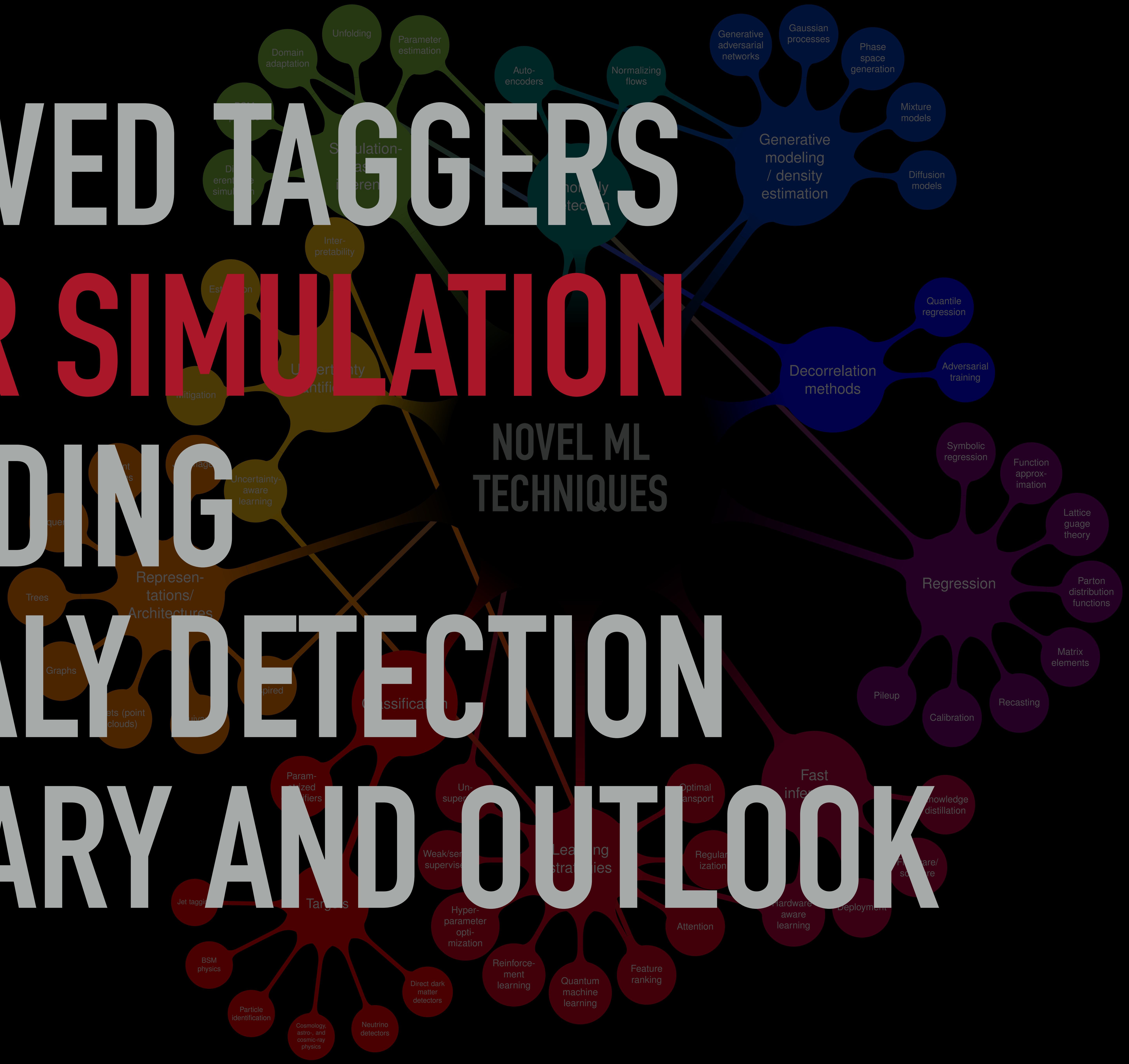
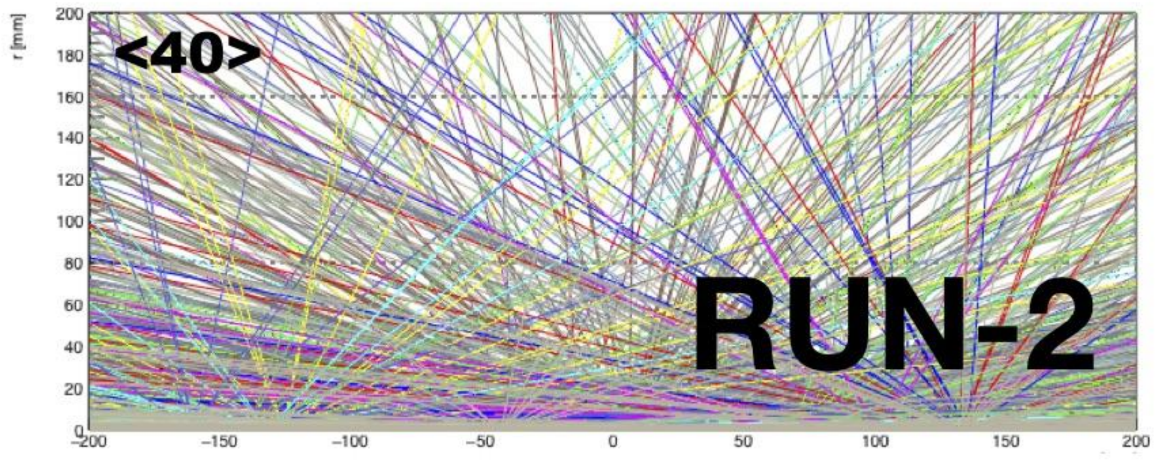
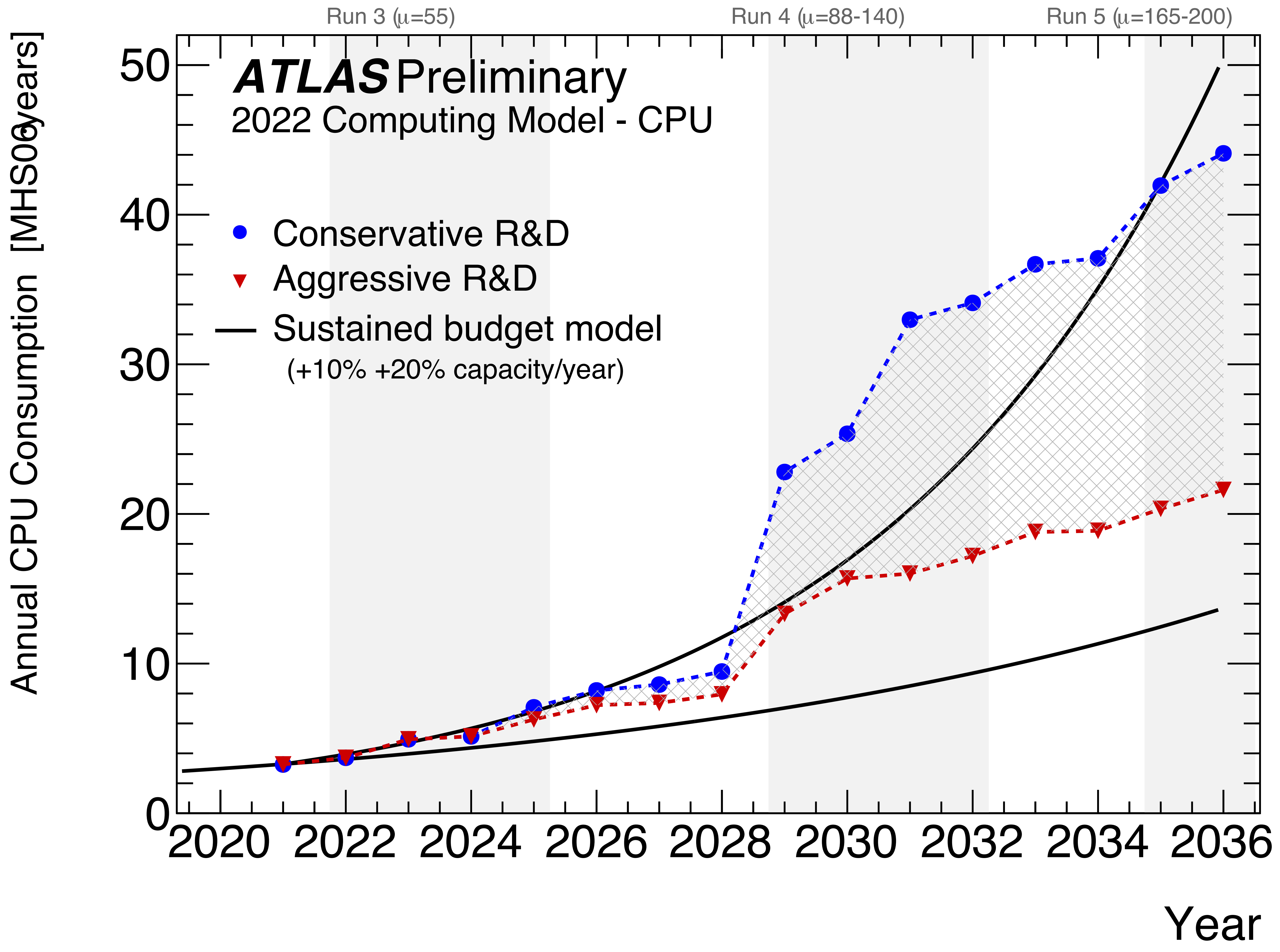
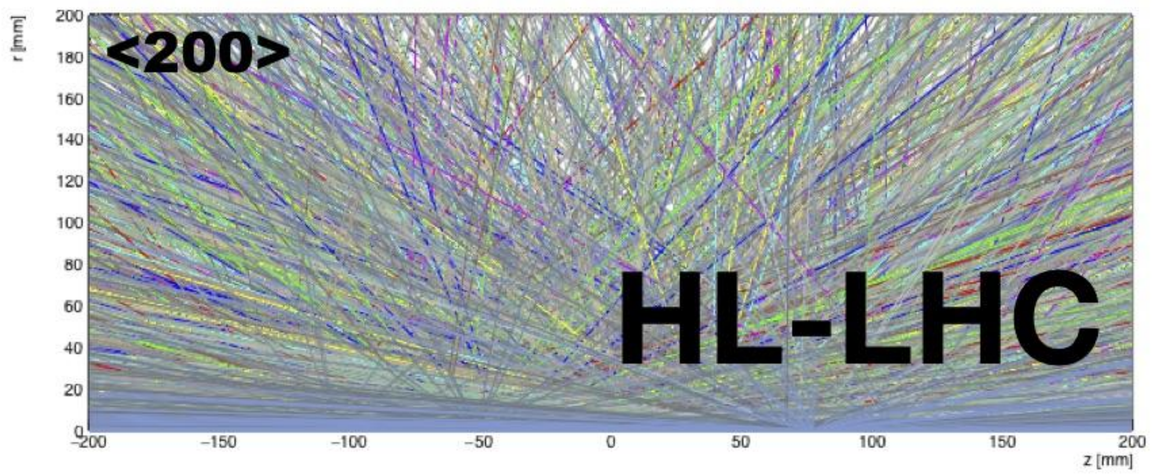
SUMMARY AND OUTLOOK



TOWARD HL-LHC



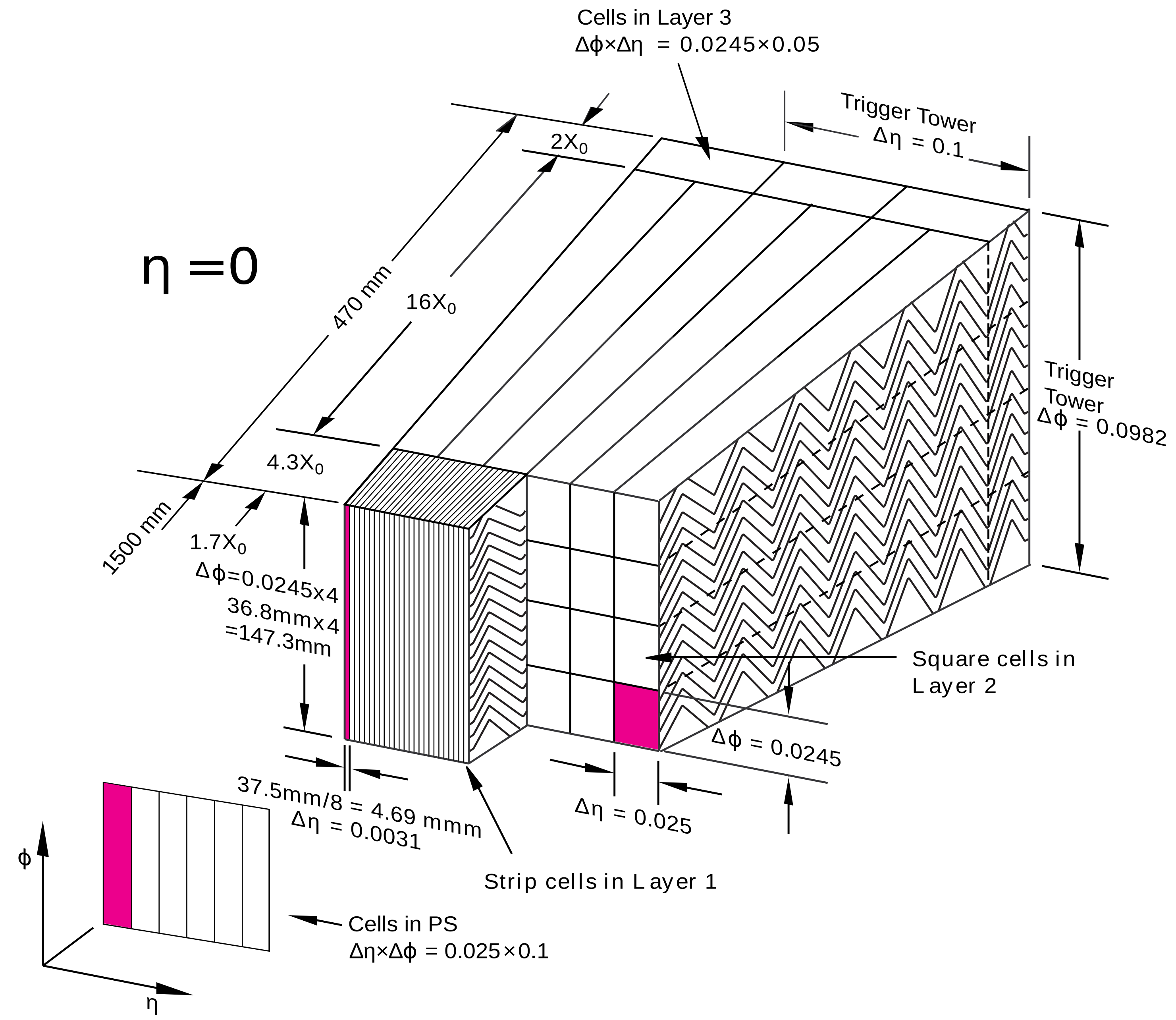




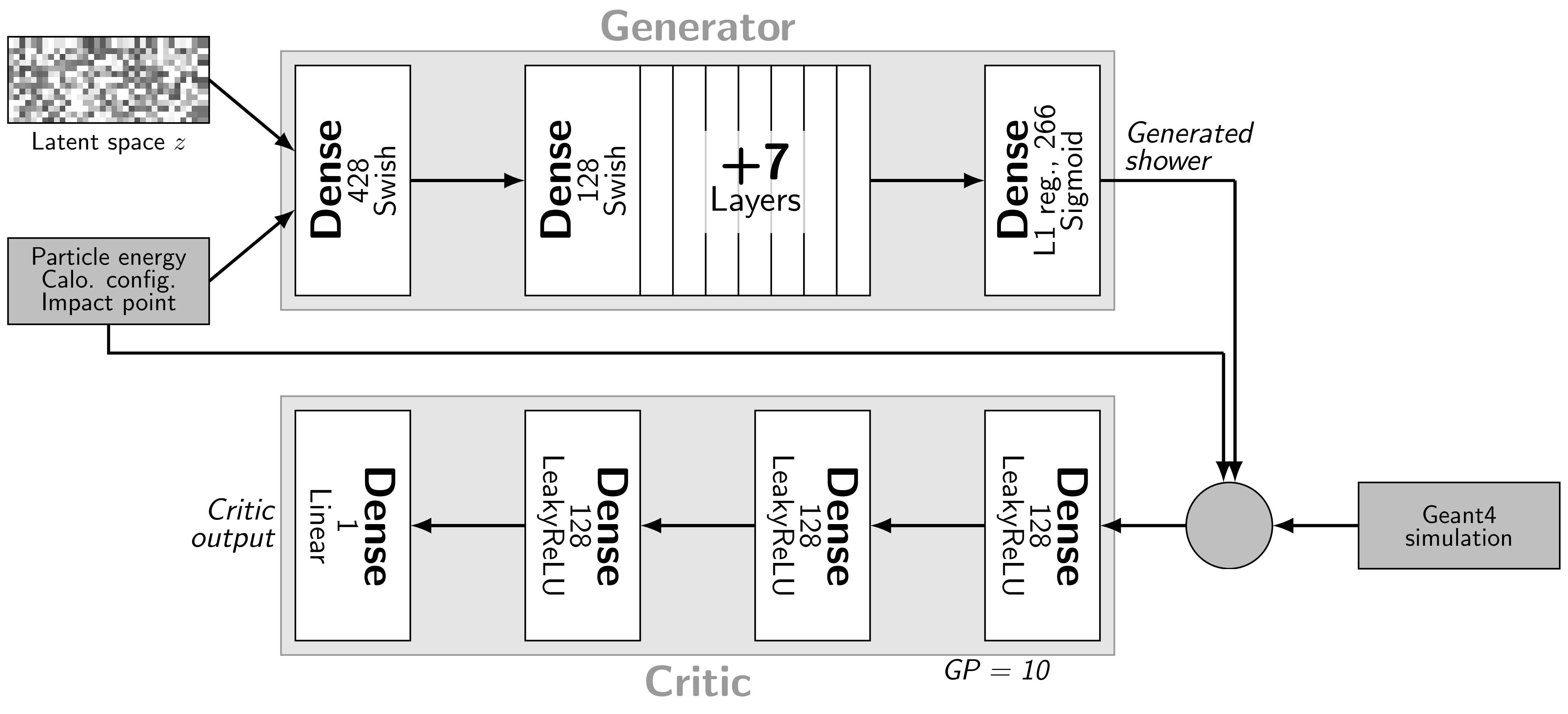
- Simulation is a key driver of CPU needs for the HL-LHC
- ML can be used to "short cut" simulation needs, e.g. additional samples for evaluating systematic uncertainties or higher order corrections

FASTCALOGAN

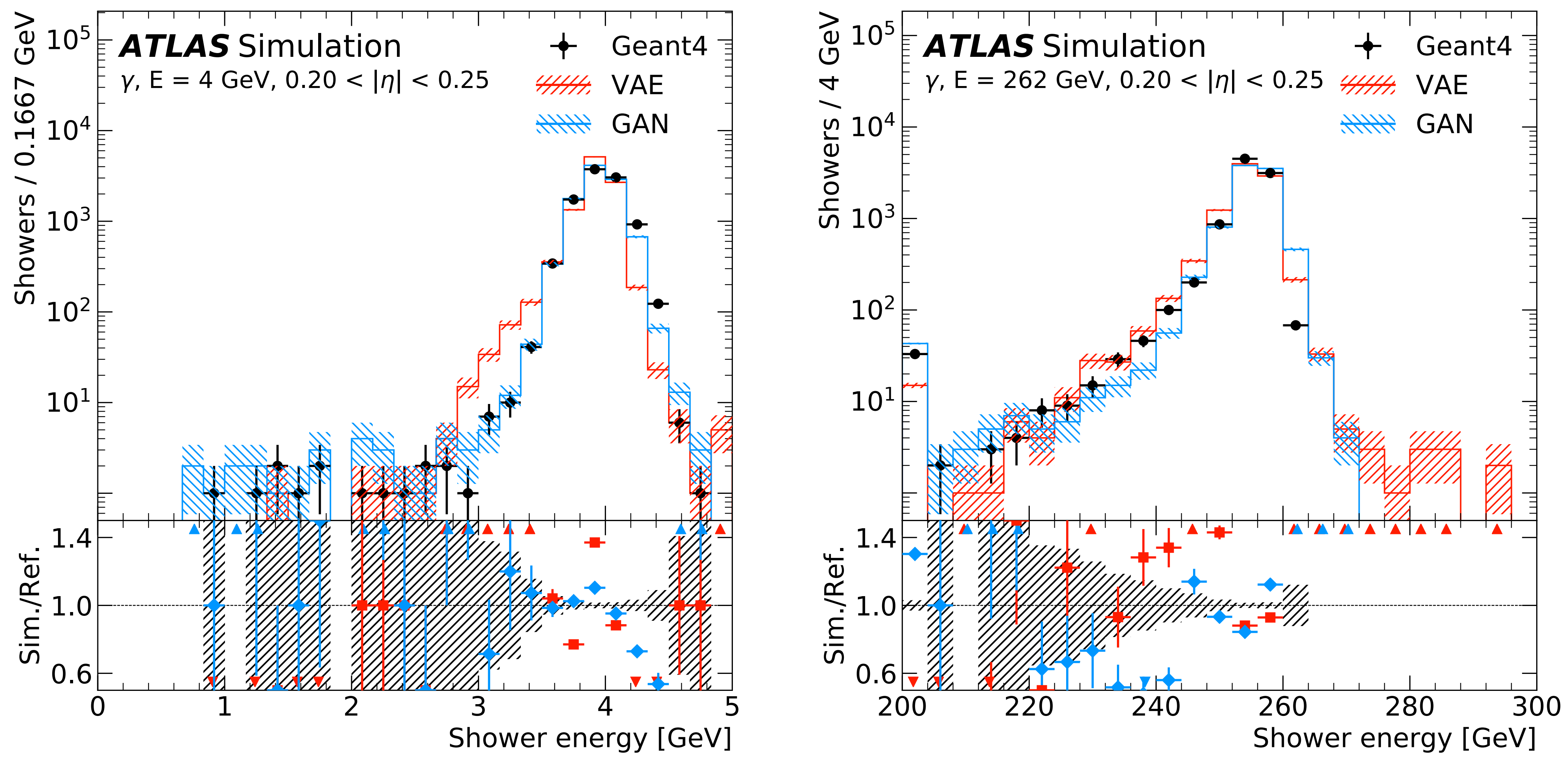
[CSBS 8, 7 (2024)](https://doi.org/)



Voxelization

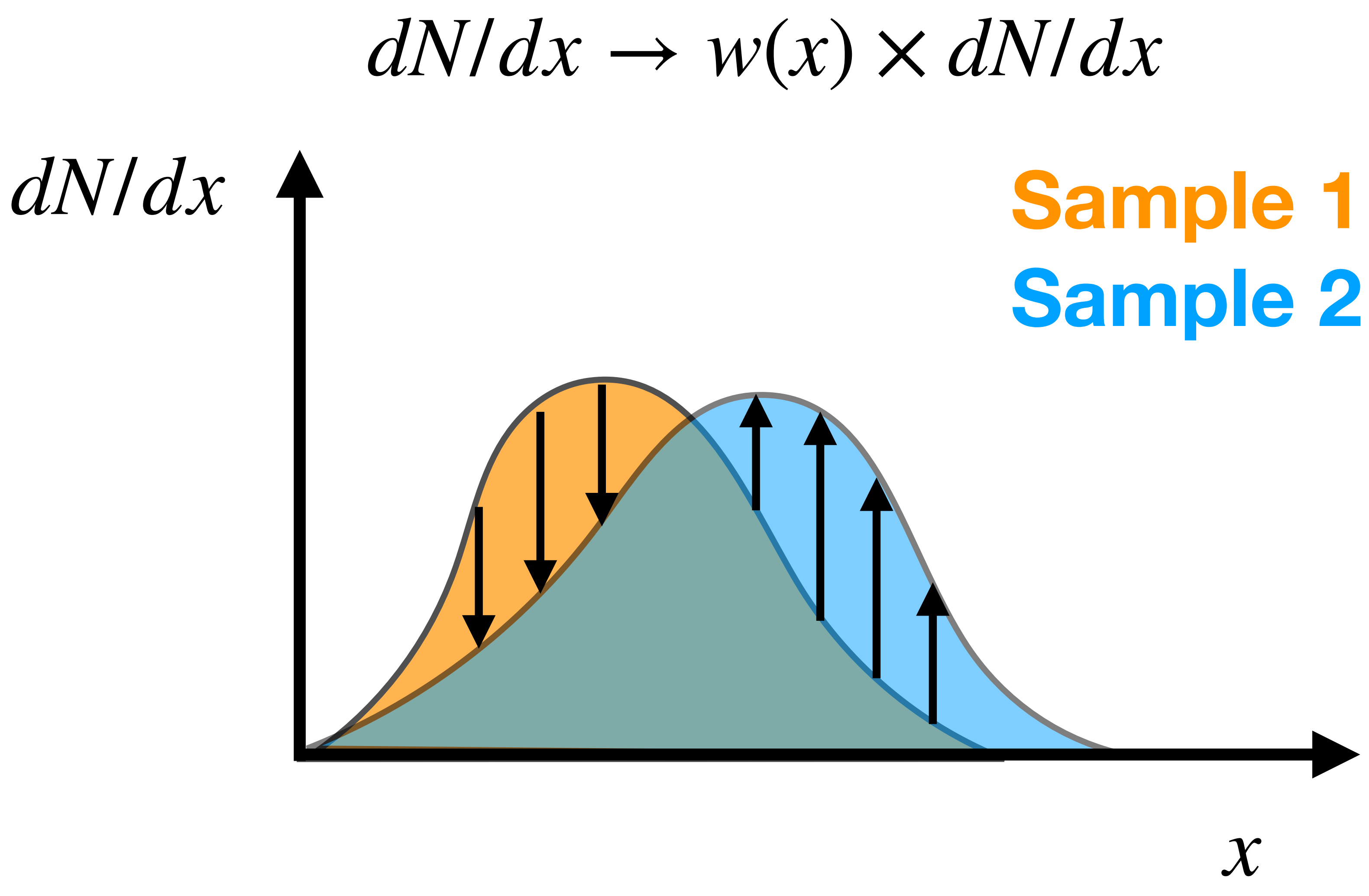


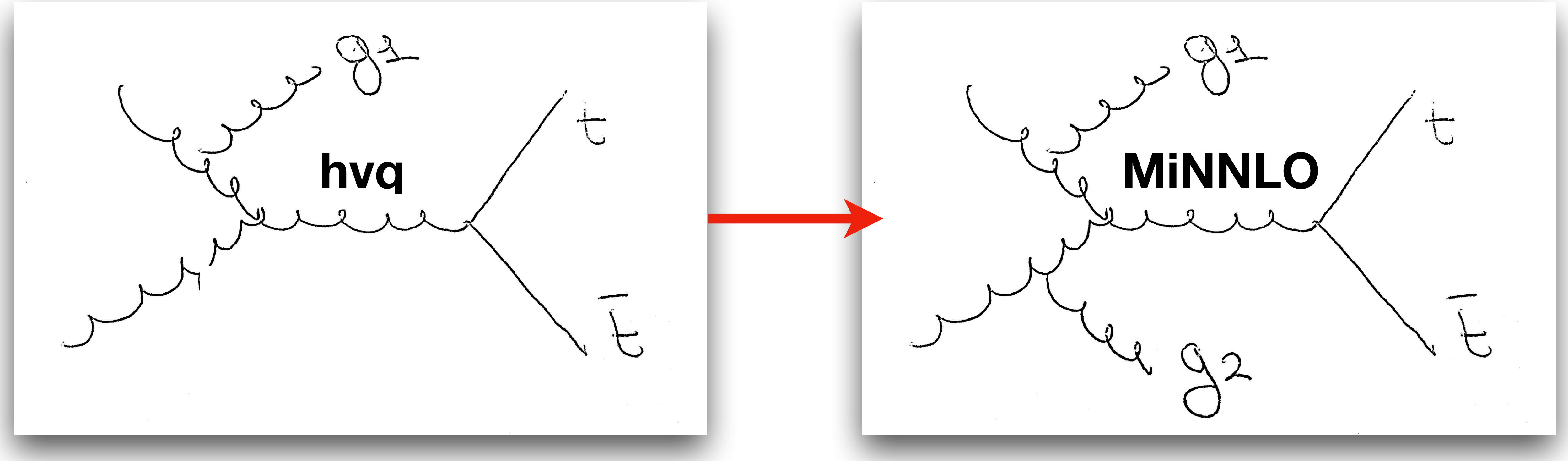
- Can we replace slow Geant4-based simulation of ATLAS calorimeter with fast generative ML?
- GAN/VAEs trained to parametrize the detector response to photons, electrons, and pions
- Good agreement between GAN/VAE and Geant4 for showers of different energies



NEURAL NETWORK REWEIGHTING

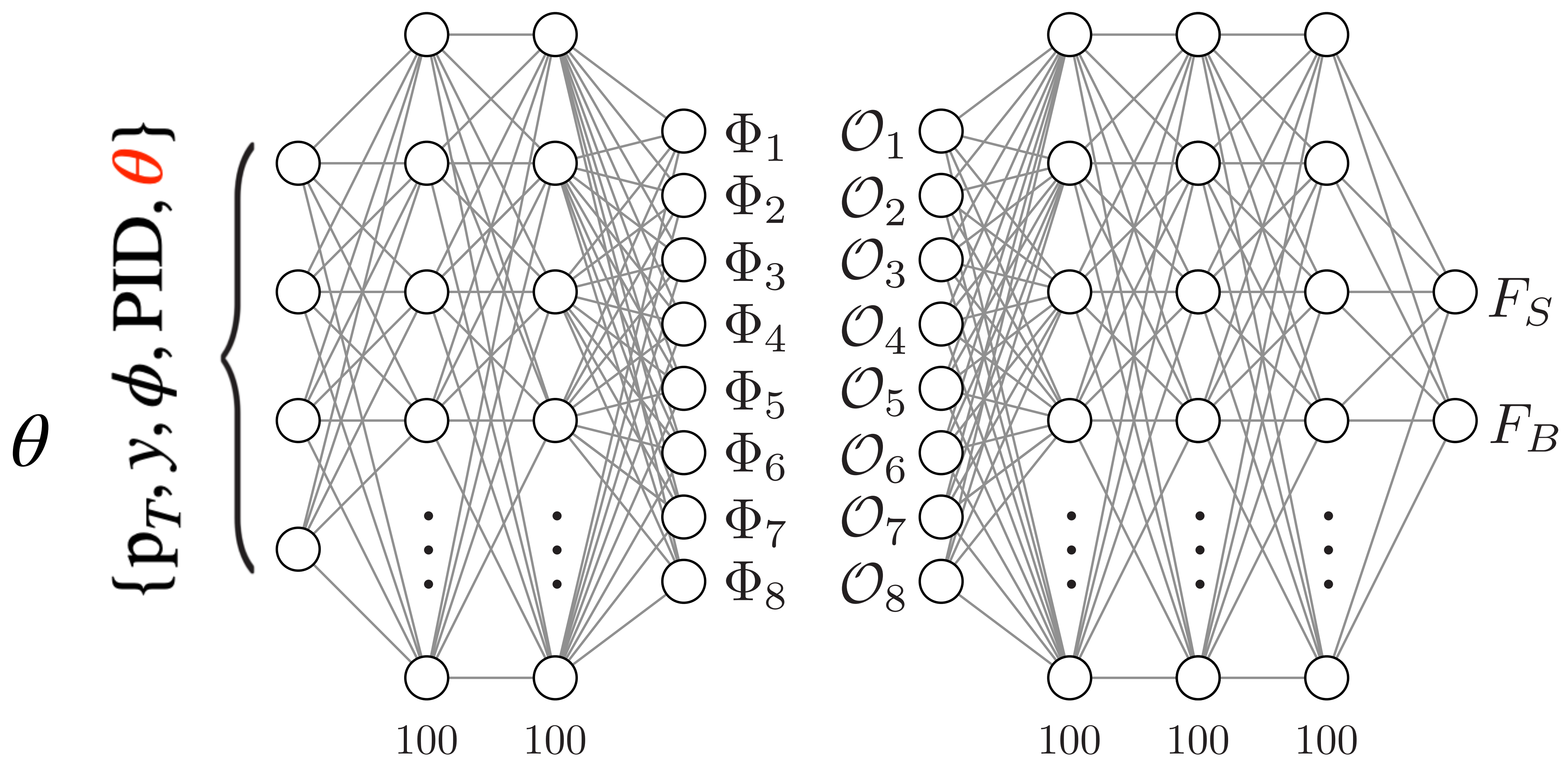
- To reweight sample from $p_1(x)$ to sample from $p_0(x)$ need $w(x) = p_0(x)/p_1(x)$
- **Likelihood ratio trick**: a neural network classifier $f(x)$ trained to distinguish the two samples approximates this ratio: $f(x)/(1 - f(x)) \approx p_0(x)/p_1(x)$
- CMS use cases for top quark physics
  - Reweight MC for evaluation of systematic uncertainties
  - **Reweight MC to higher-order theory predictions**



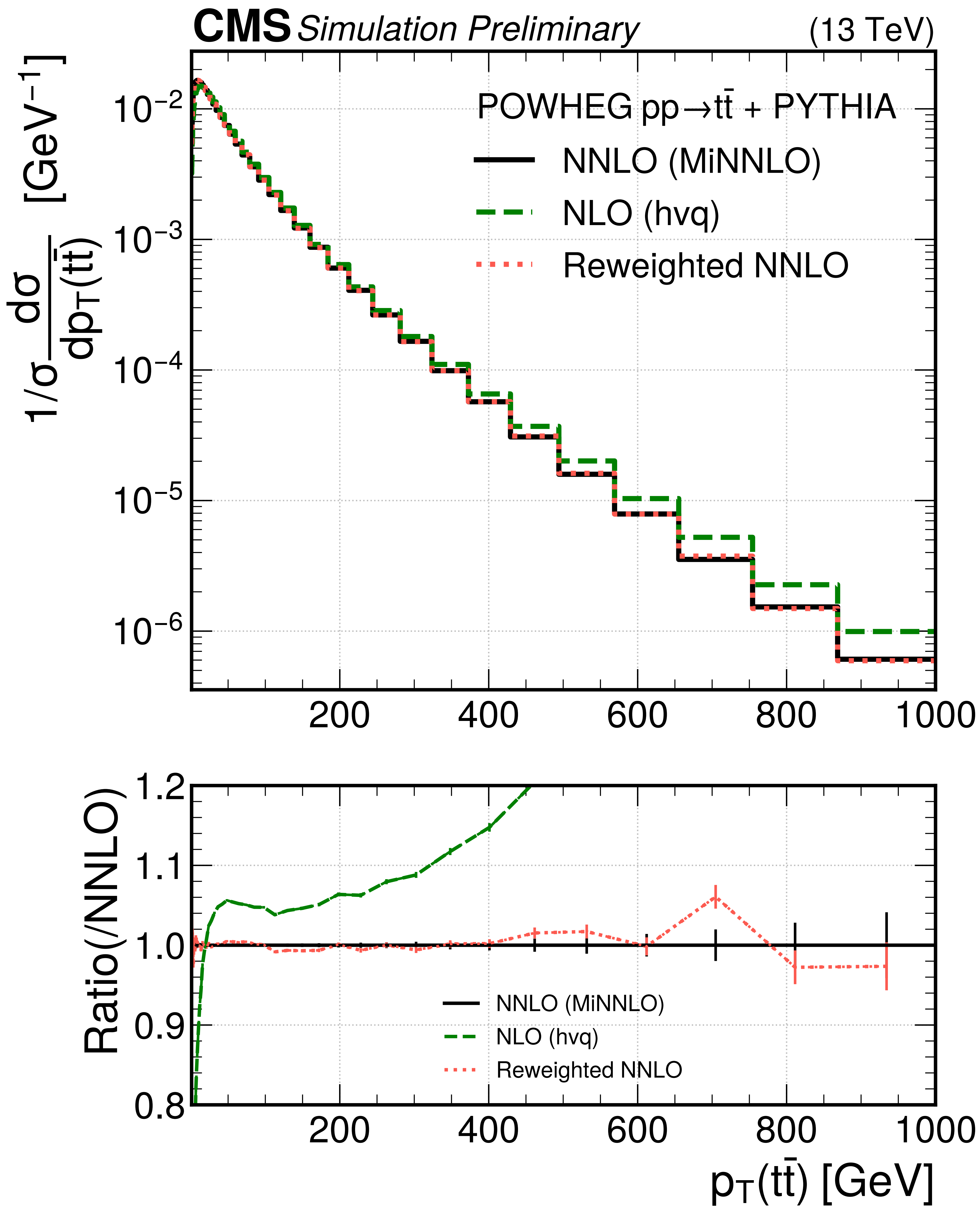


HIGHER ORDER REWEIGHTING RESULTS

- Parton level information input to the Particle Flow Network:
  - 4-vector $(p_{\mathrm{T}}, \eta, \phi, m)$ and PID of $[t, \bar{t}, t\bar{t}]$ system of the showered events



- Method closes within ~2% of target NNLO distribution



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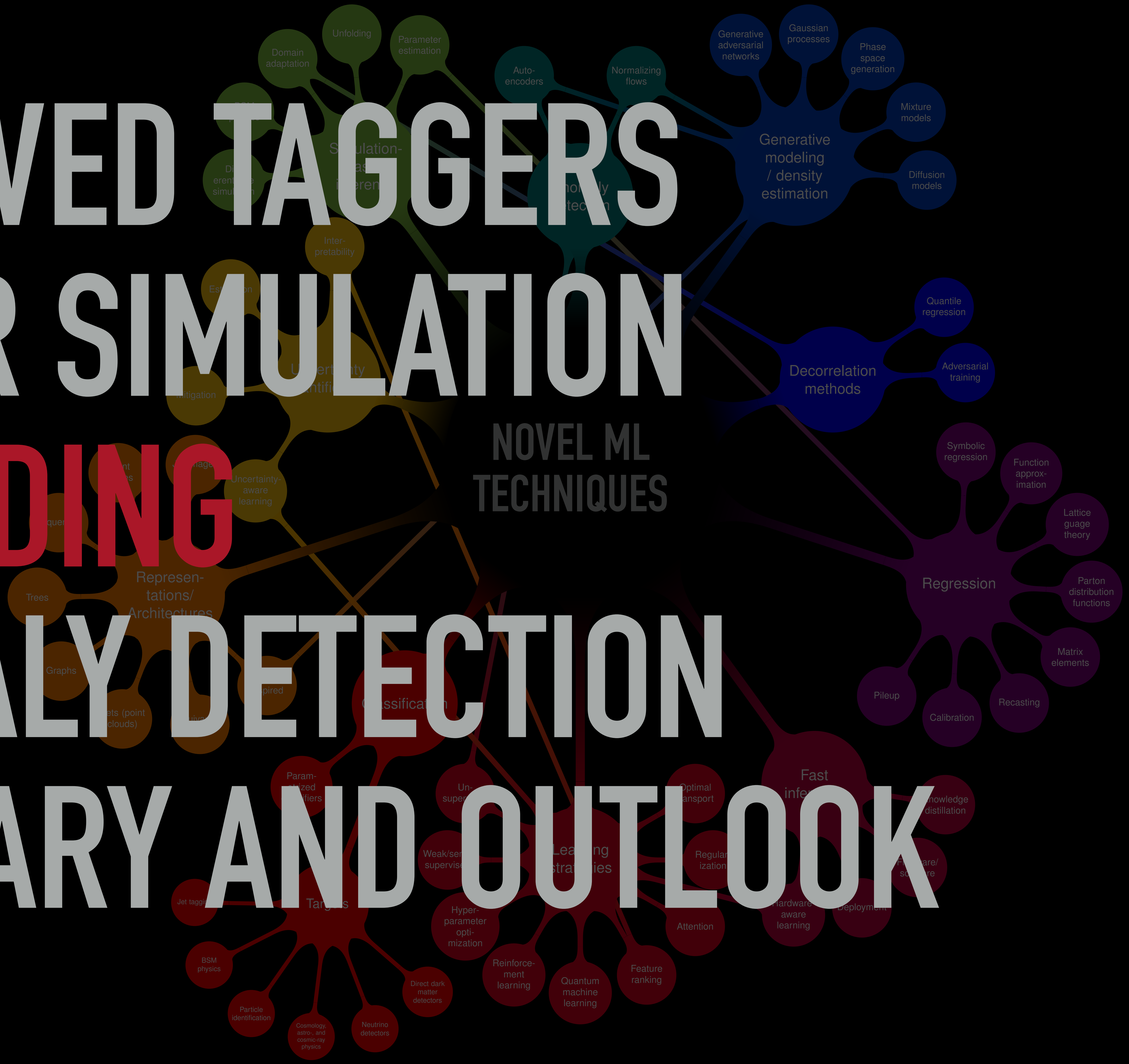
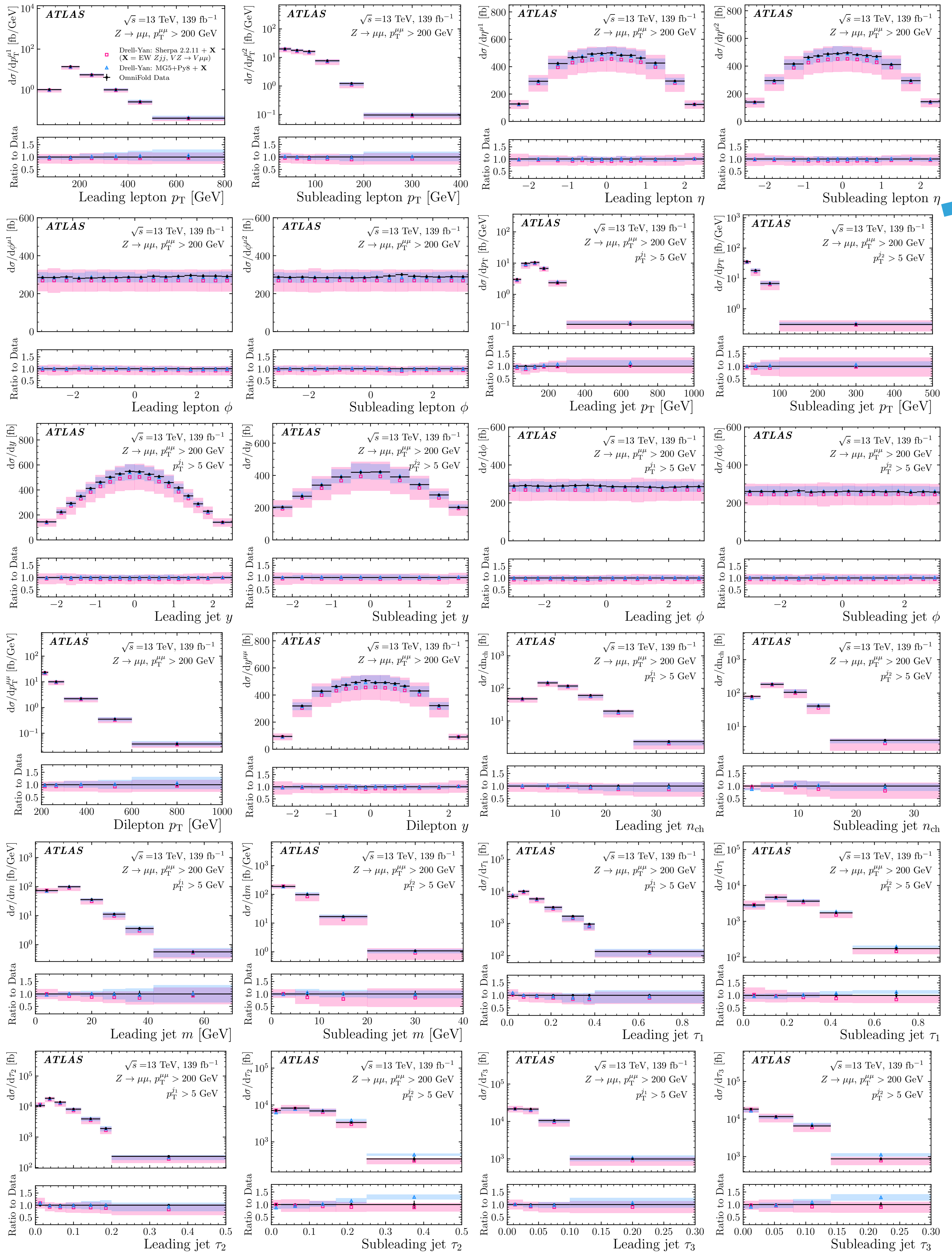


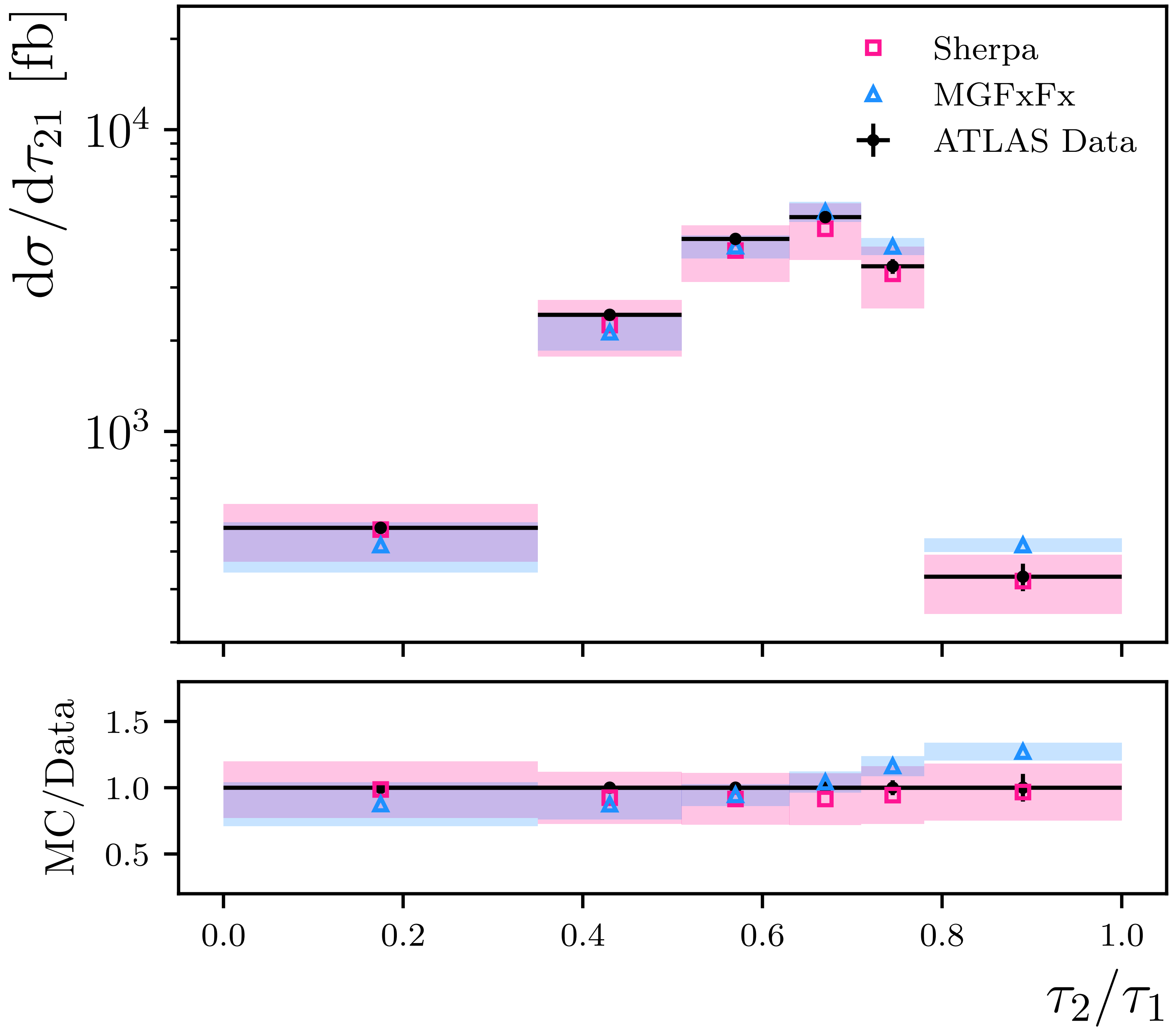
MEASUREMENTS & UNFOLDING WITH OMNIFOLD

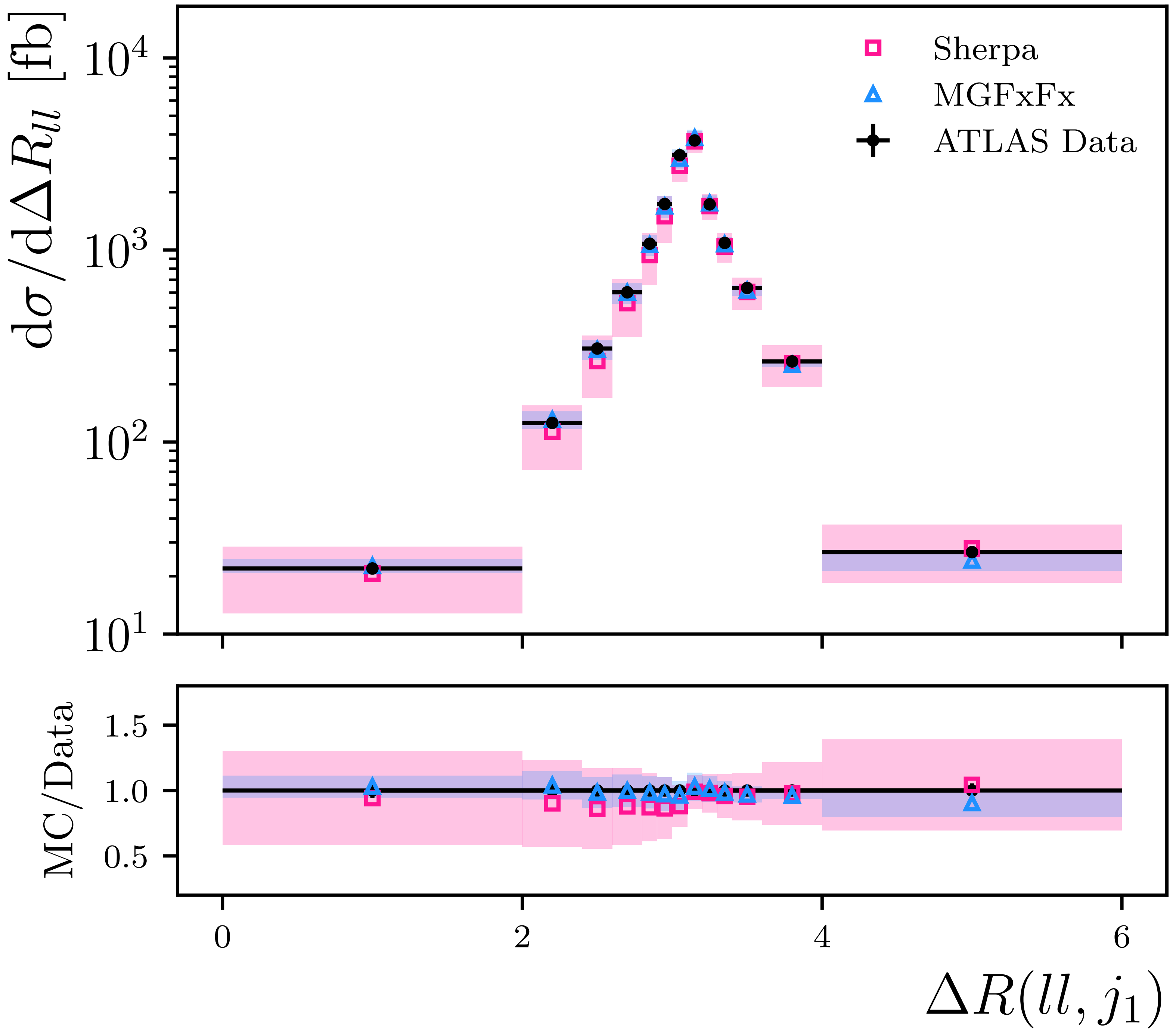
- Omnifold used to unfold 24 Z+jets kinematic observables in ATLAS
  - Detector-level MC corrected by $\omega(\vec{x}_r)$ to match data
  - Particle-level MC corrected by $\nu(\vec{x}_p)$ to match $\omega(\vec{x}_r)$-adjusted MC
  - Method repeated four more times
  - Final measurement is $\nu(\vec{x}_p)$-weighted MC events

MEASUREMENTS & UNFOLDING WITH OMNIFOLD

- Unbinned results provided as 24-dim. dataset on Zenodo and code on GitLab
- Enables measurement of new observables not presented in original paper!







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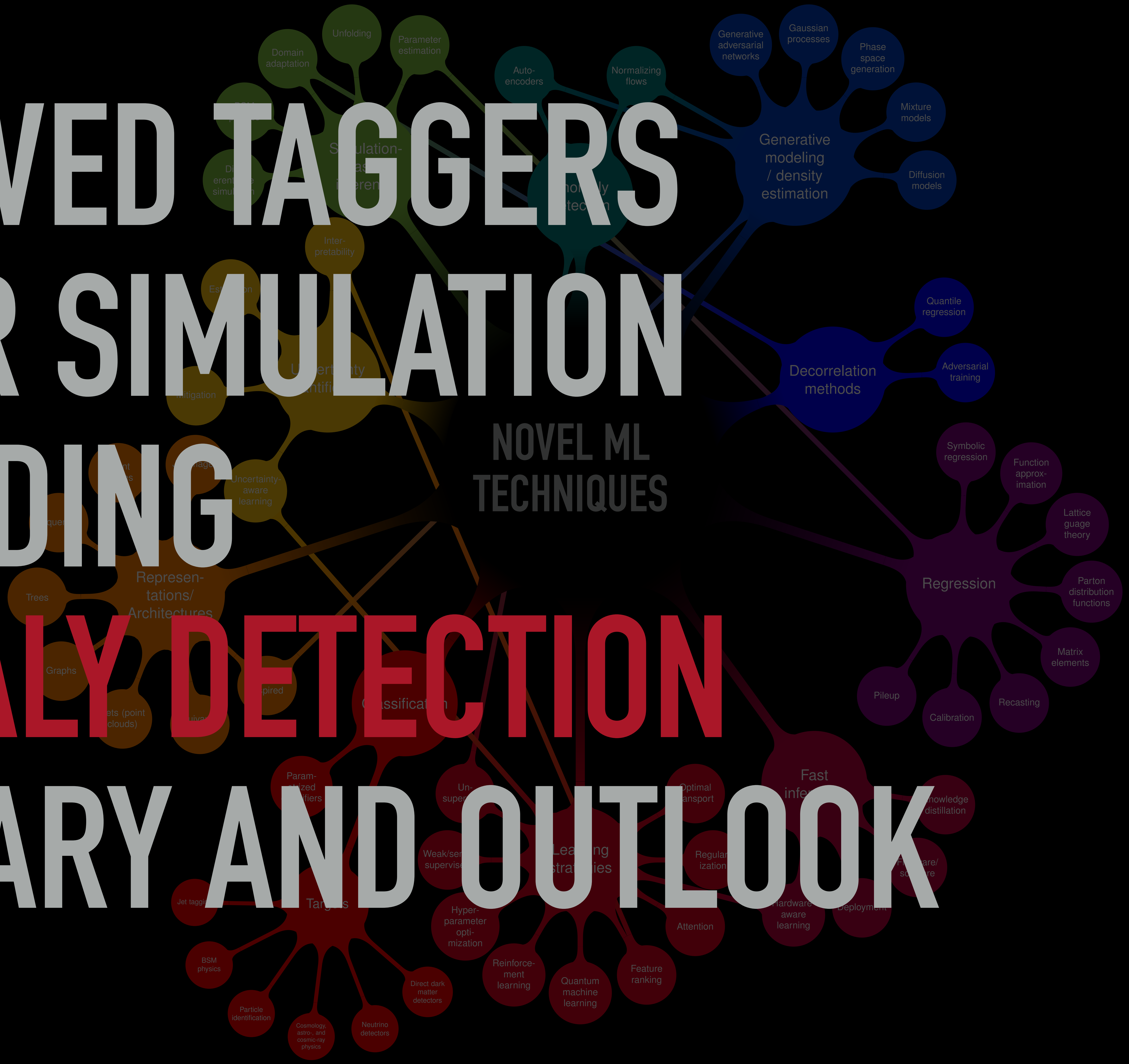
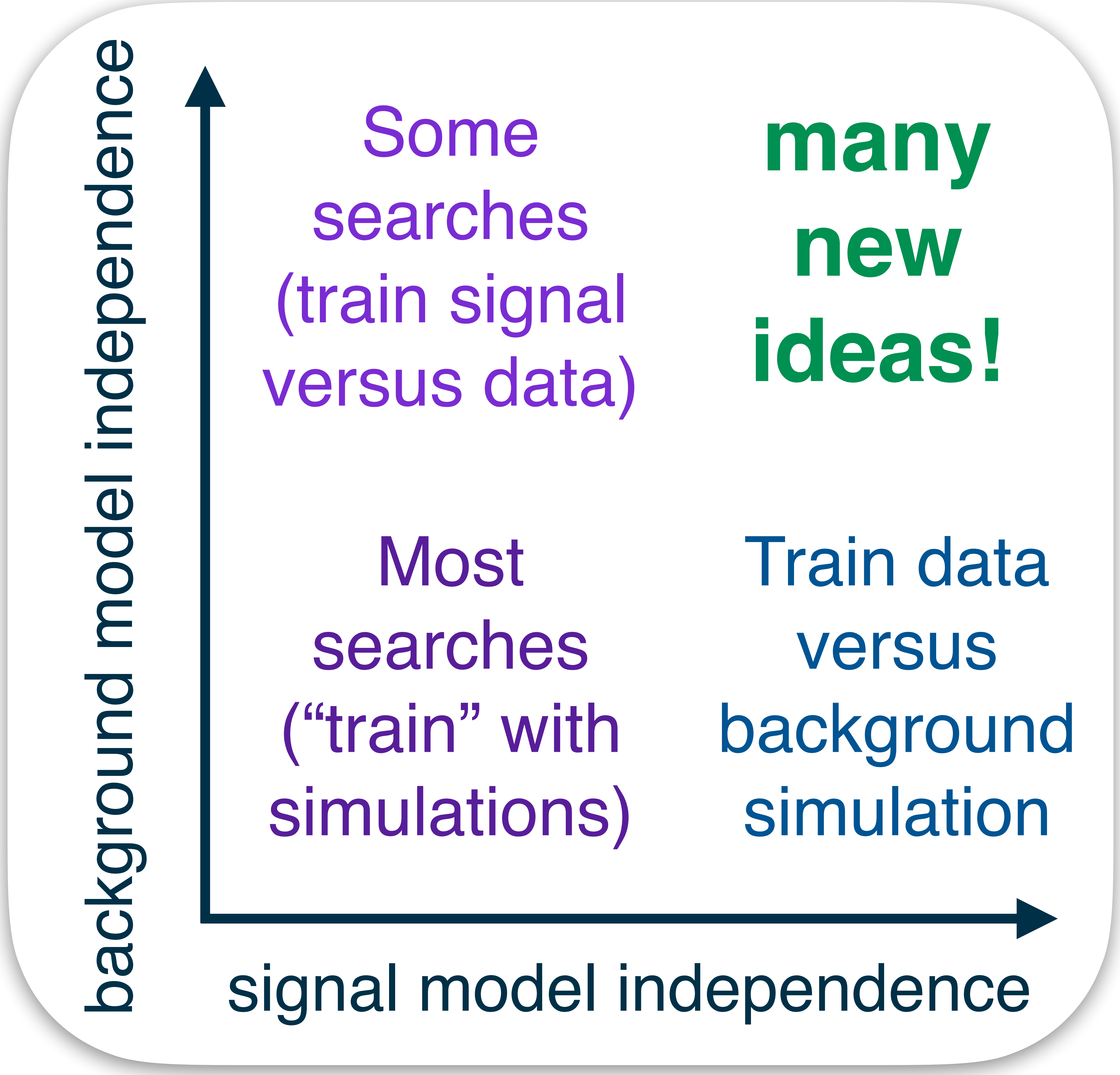
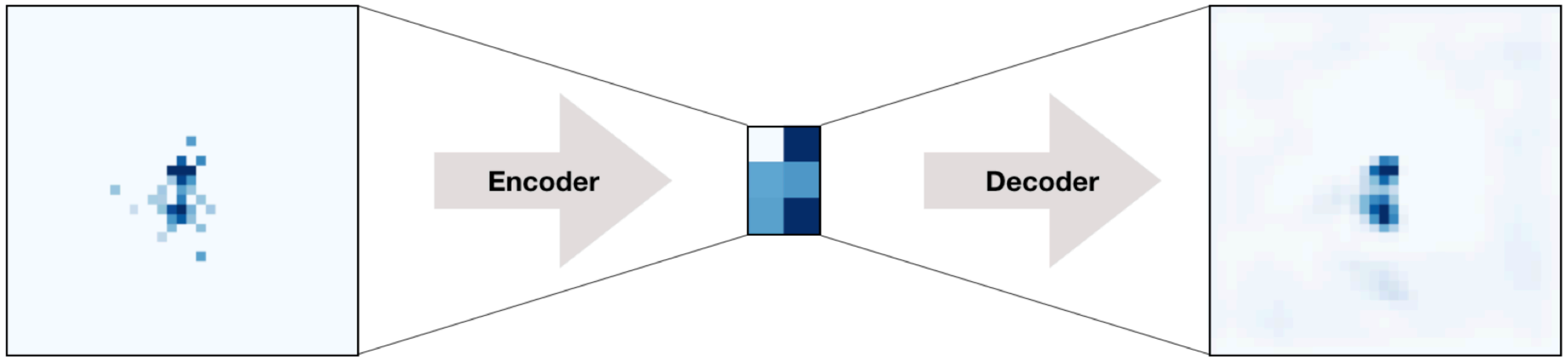


LANDSCAPE OF BSM SEARCHES

Credit: B. Nachman
https://indico.cern.ch/event/1188153/



- Supervised = full label information
- Semi-supervised = partial labels
- Weakly-supervised = noisy labels
- Unsupervised = no labels
  - Example: autoencoders compress data and then uncompress it
  - Assumption: if x is far from $\mathrm{Decoder}(\mathrm{Encoder}(x))$, then x has low $p_{\mathrm{bkgd}}(x)$

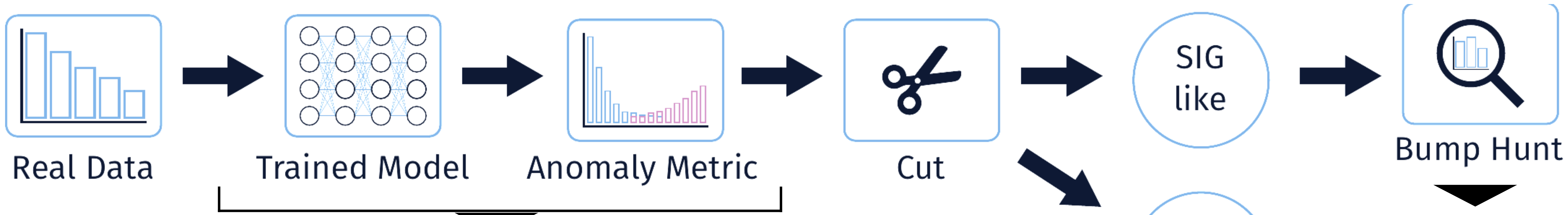


ANOMALY DETECTION: GENERAL STRATEGY

Start from **data**

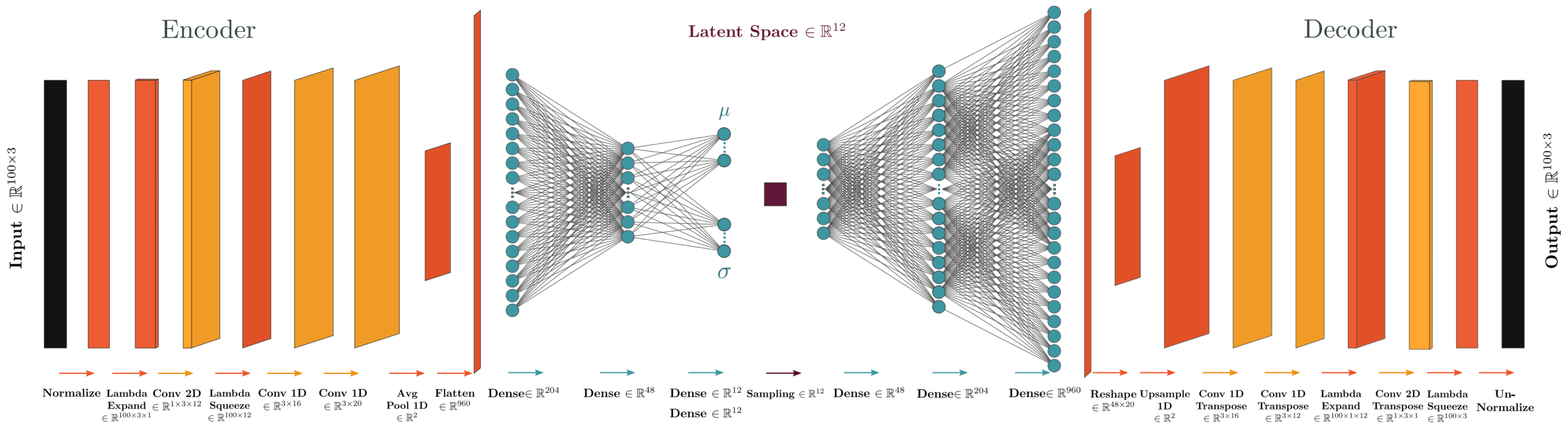
Anti-k_T jets with R = 0.8
Basic selection criteria

Keep ~**1%** most anomalous events



5 different methods

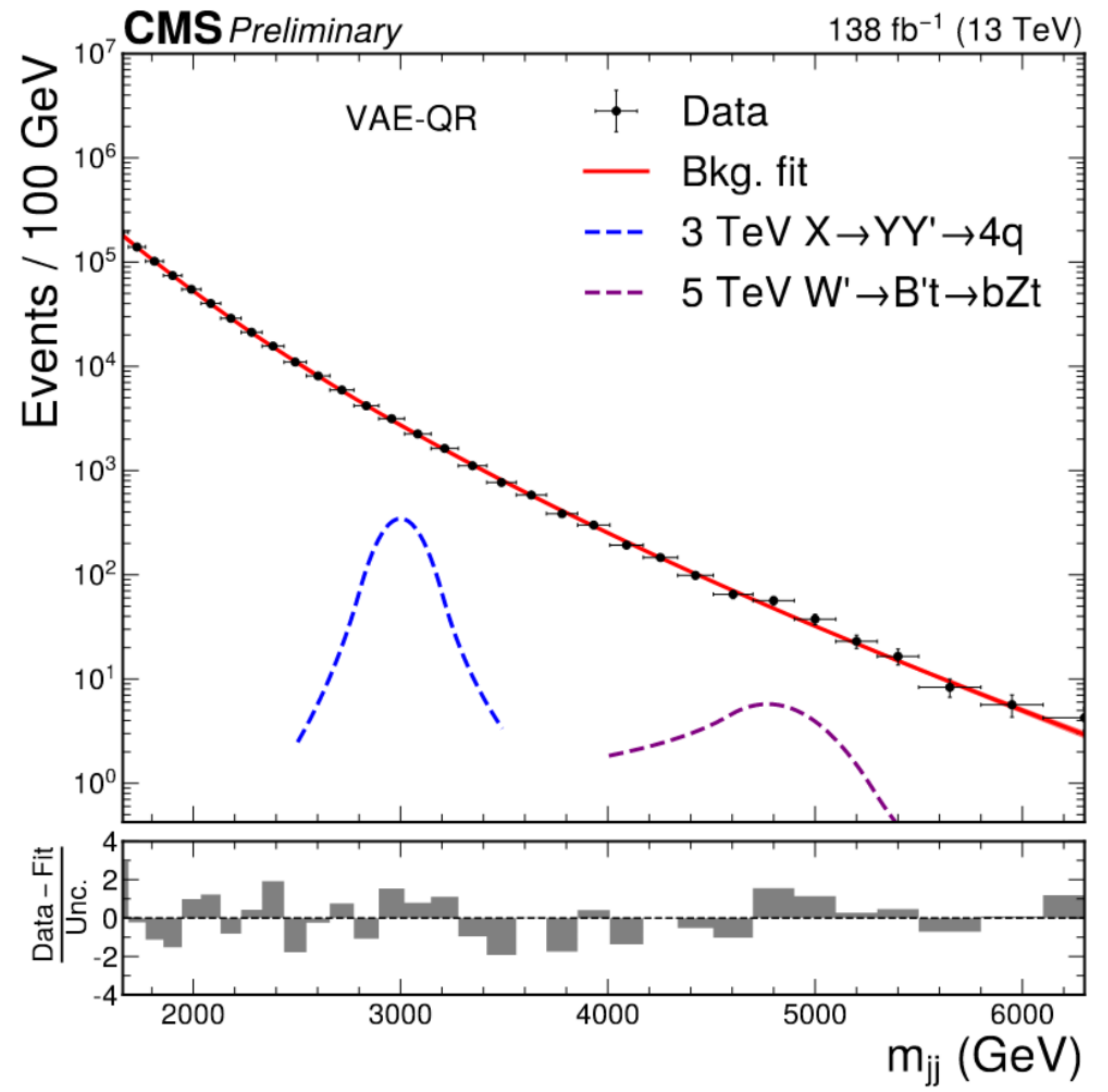
CWoLa Hunting / TNT / CATHODE(-b) / VAE / QUAK

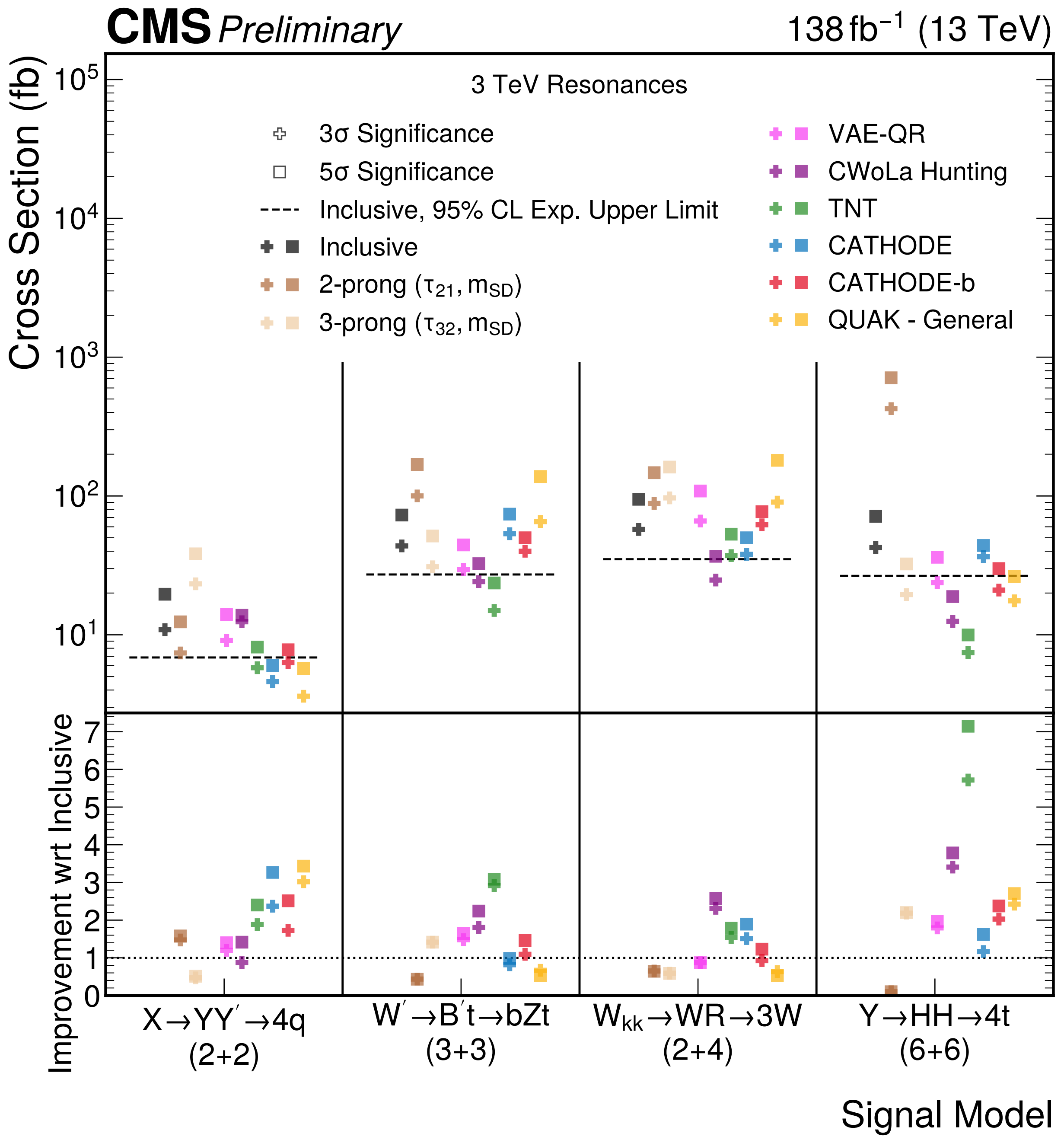


Resonance?

Fit m_{jj} spectrum and obtain significance

- Improvement in cross section needed for 5 σ discovery compared to inclusive dijet search by up to factor of 7

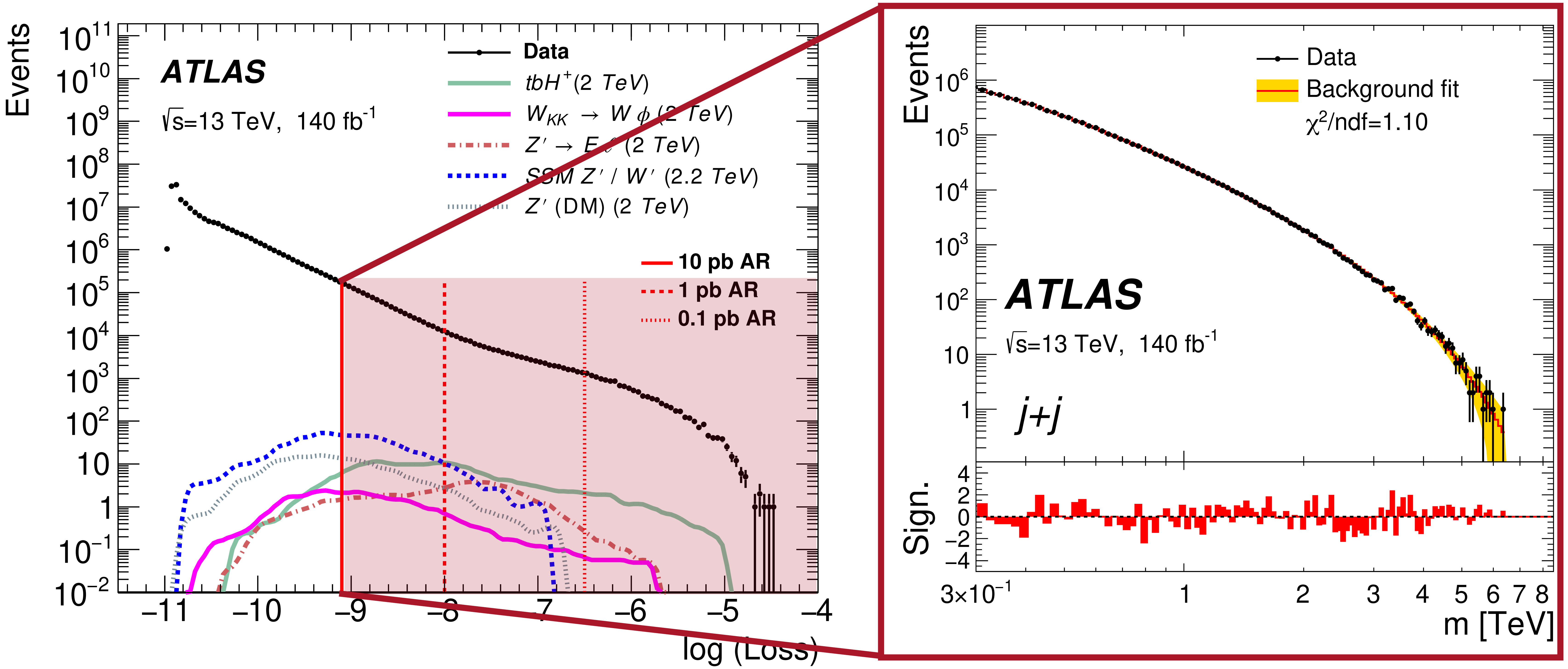


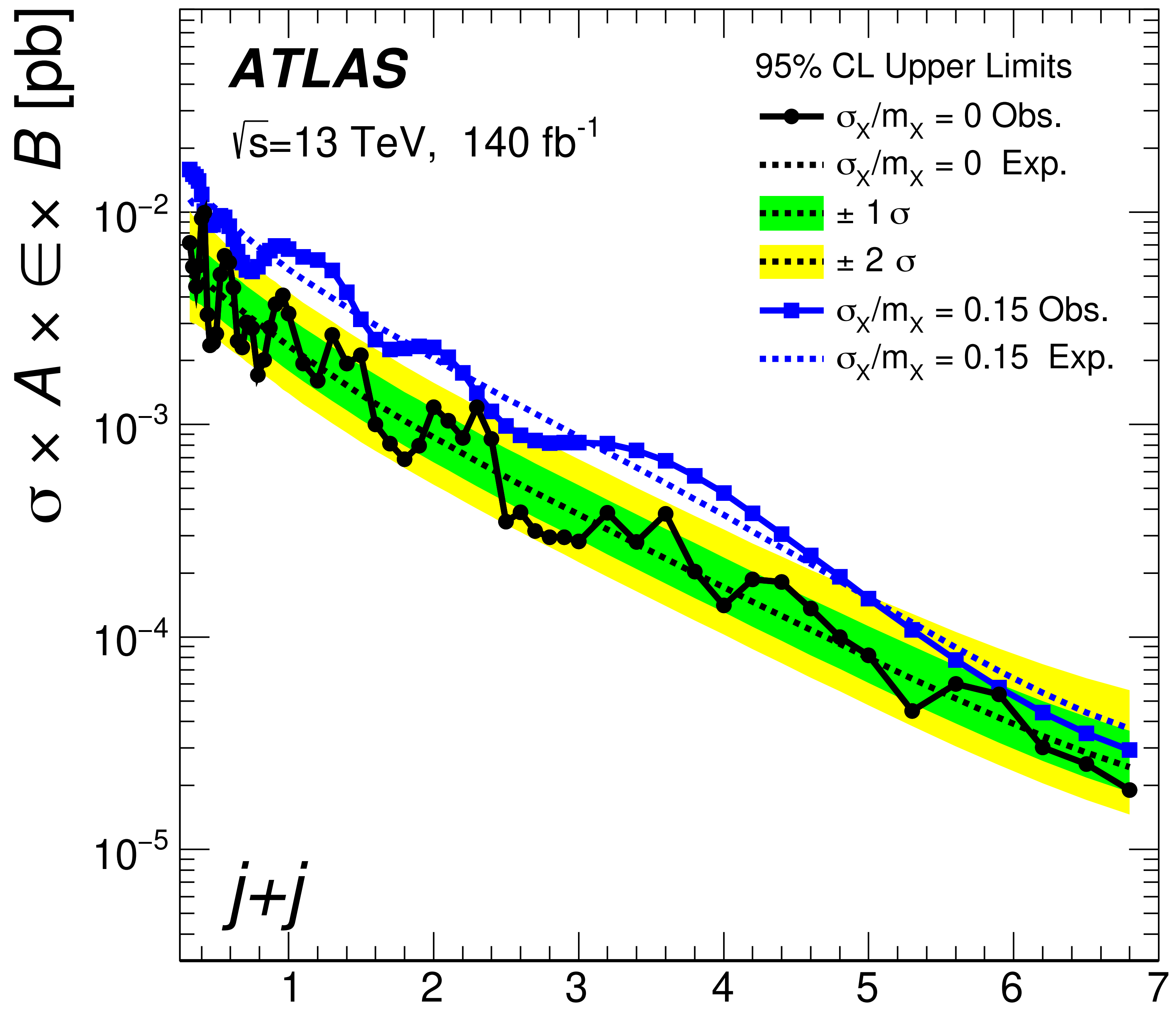


ANOMALY DETECTION: OBJECT PAIRS

- Autoencoder applied to physics-informed representation (rapidity-mass matrix)
- Anomaly score selection corresponding to 10 pb
- Model-independent limits placed in 9 final states: **j+j**, j+b, b+b, j+e, b+e, j+γ, j+μ, b+μ, and b+γ

$$
\begin{pmatrix}
e_T^{miss} & m_T(j_1) & m_T(j_2) & \dots m_T(j_N) & m_T(\mu_1) & m_T(\mu_2) & \dots m_T(\mu_N) \\
h_L(j_1) & e_T(j_1) & m(j_1,j_2) & \dots m(j_1,j_N) & m(j_1,\mu_1) & m(j_1,\mu_2) & \dots m(j_1,\mu_N) \\
h_L(j_2) & h(j_1,j_2) & \delta e_T(j_2) & \dots m(j_2,j_N) & m(j_2,\mu_1) & m(j_2,\mu_2) & \dots m(j_2,\mu_N) \\
\dots & \dots & \dots & \dots, & \dots & \dots & \dots \\
h_L(j_N) & h(j_1,j_N) & \dots & \dots \delta e_T(j_N) & m(j_N,\mu_1) & m(j_N,\mu_2) & \dots m(j_N,\mu_N) \\
h_L(\mu_1) & h(\mu_1,j_1) & h(\mu_1,j_2) & \dots h(\mu_1,j_N) & e_T(\mu_1) & m(\mu_1,\mu_2) & m(\mu_1,\mu_N) \\
h_L(\mu_2) & h(\mu_2,j_1) & h(\mu_1,j_2) & \dots h(\mu_2,j_N) & h(\mu_1,\mu_2) & \delta e_T(\mu_2) & m(\mu_2,\mu_N) \\
\dots & \dots & \dots & \dots & \dots & \dots & \\
h_L(\mu_N) & h(\mu_N,j_1) & h(\mu_N,j_2) & \dots h(\mu_N,j_N) & h(\mu_N,\mu_1) & h(\mu_N,\mu_2) & \delta e_T(\mu_N)
\end{pmatrix}
$$

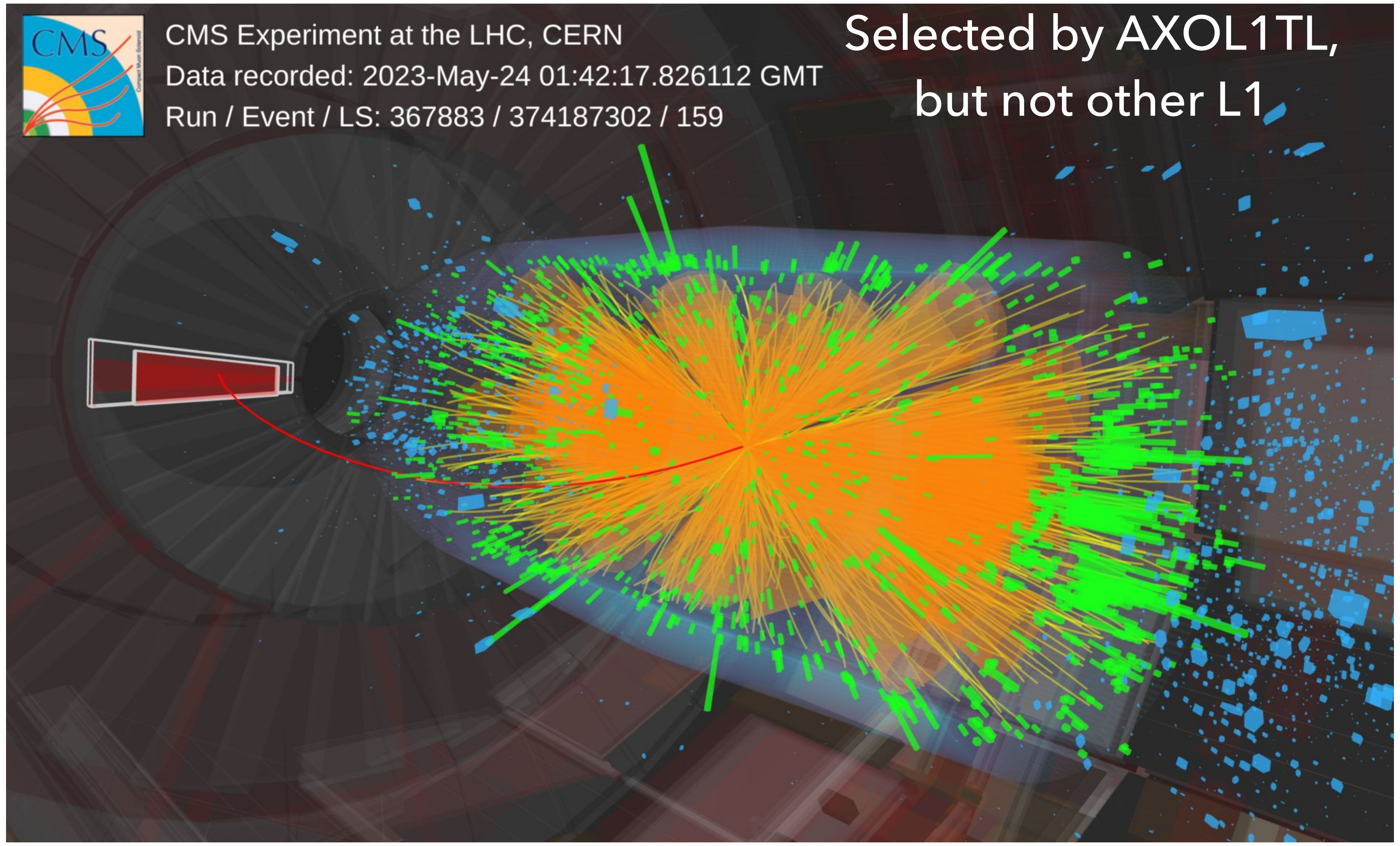


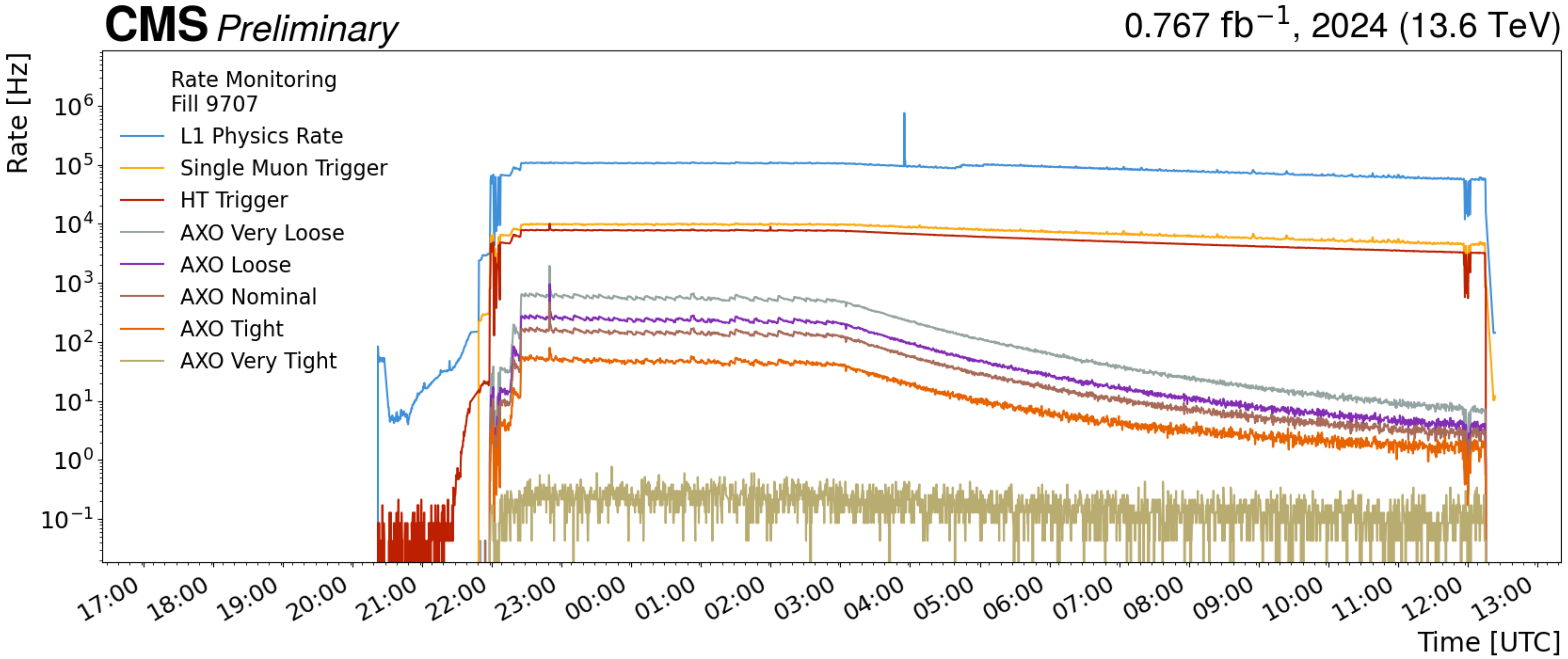


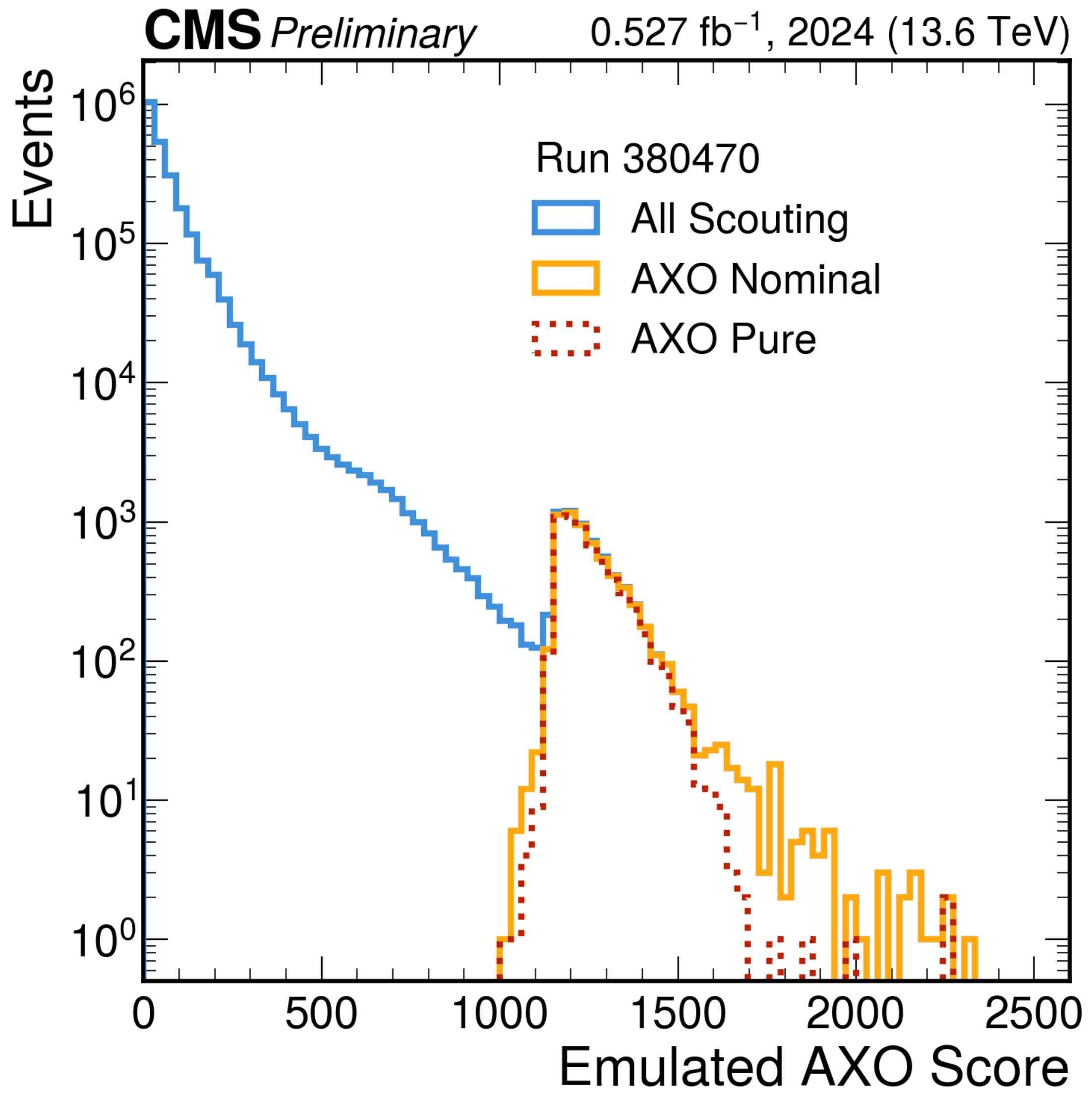
ANOMALY DETECTION @ LEVEL-1 TRIGGER

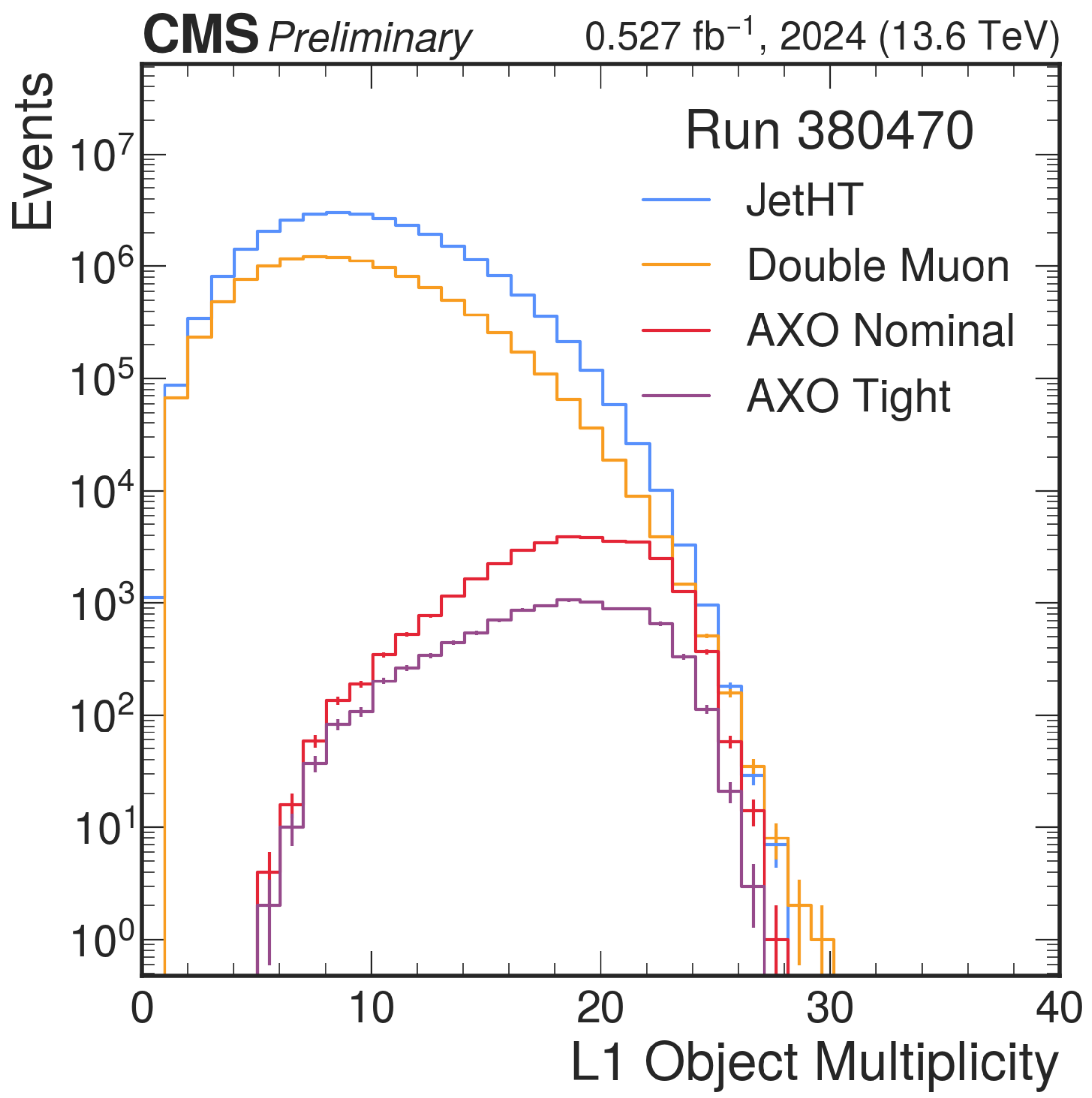
CMS-DP-2023-079
CMS-DP-2024-XXX

- AXOL1TL anomaly detection algorithms for the level-1 trigger based on a variational autoencoder
- AXOL1TL rates and score distributions for 2024 data taking
- Pure contribution shows AXOLT1TL selects unique events relative to existing level-1 trigger
- Preference for high multiplicity events



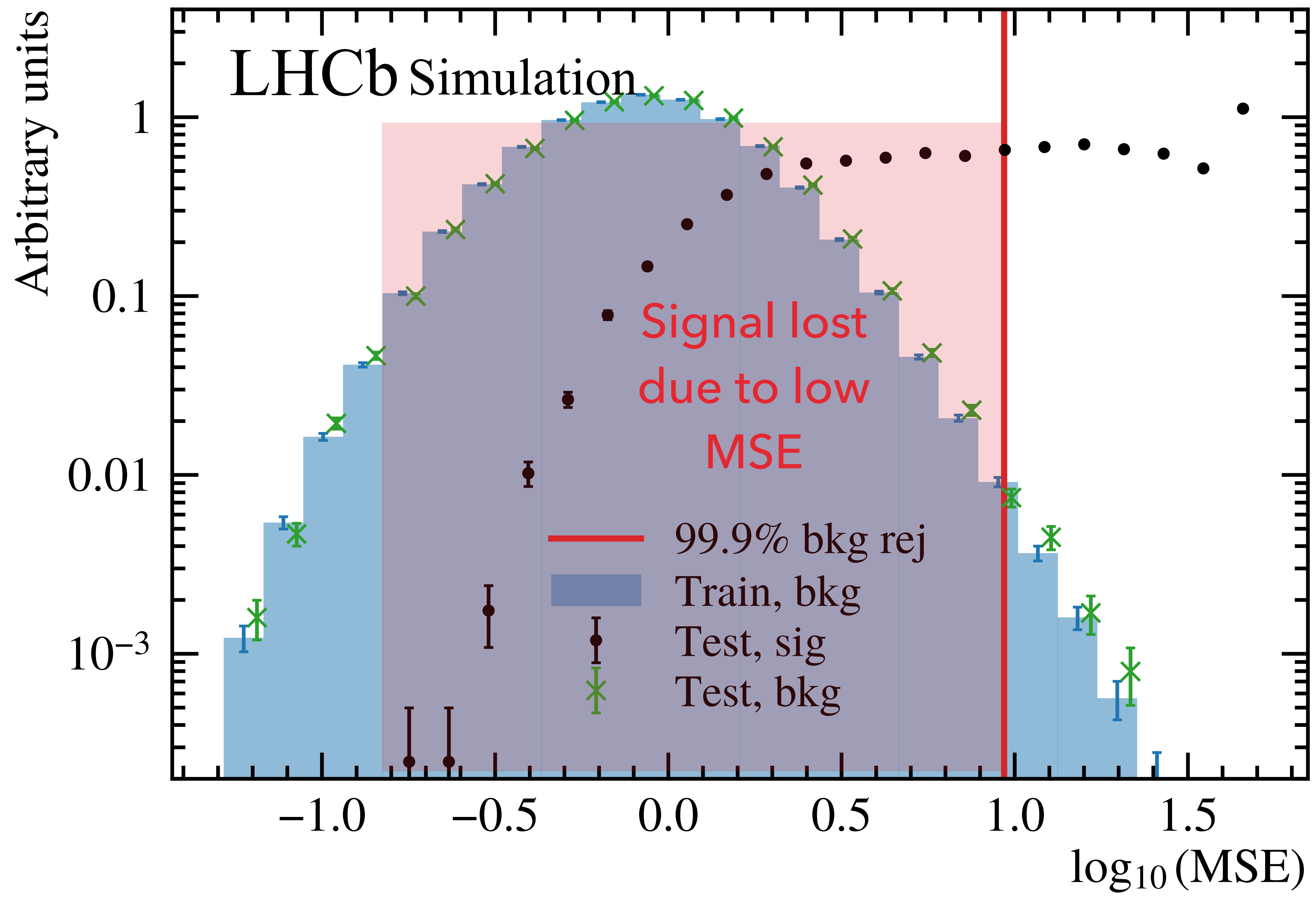






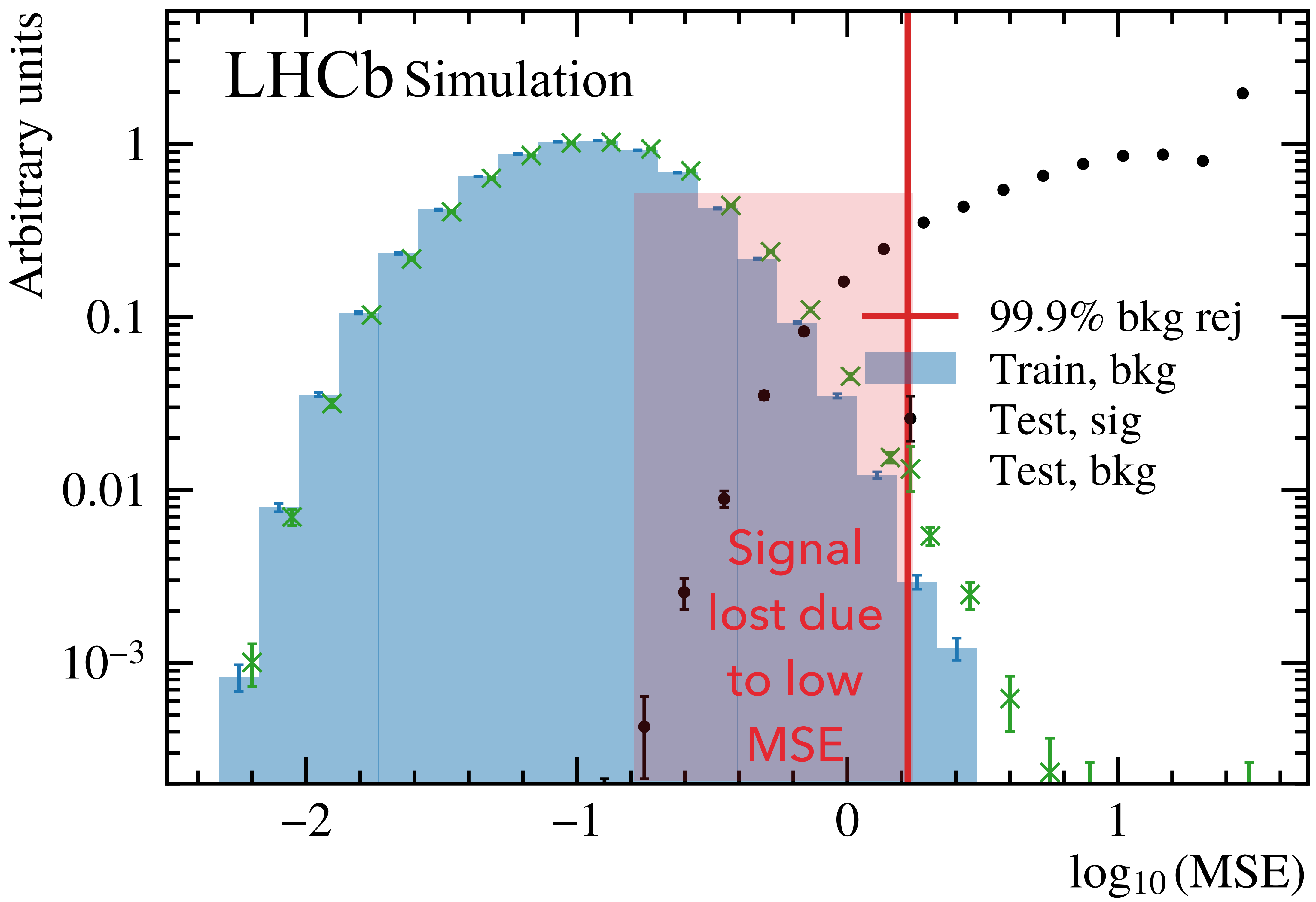
NORMALIZED AUTOENCODER

- Autoencoders can be too good at reconstructing signal, meaning signal is not flagged as anomalous (high reconstruction error)
- Normalized autoencoder approach designed to mitigate this issue—align low reconstruction error phase space with background phase space

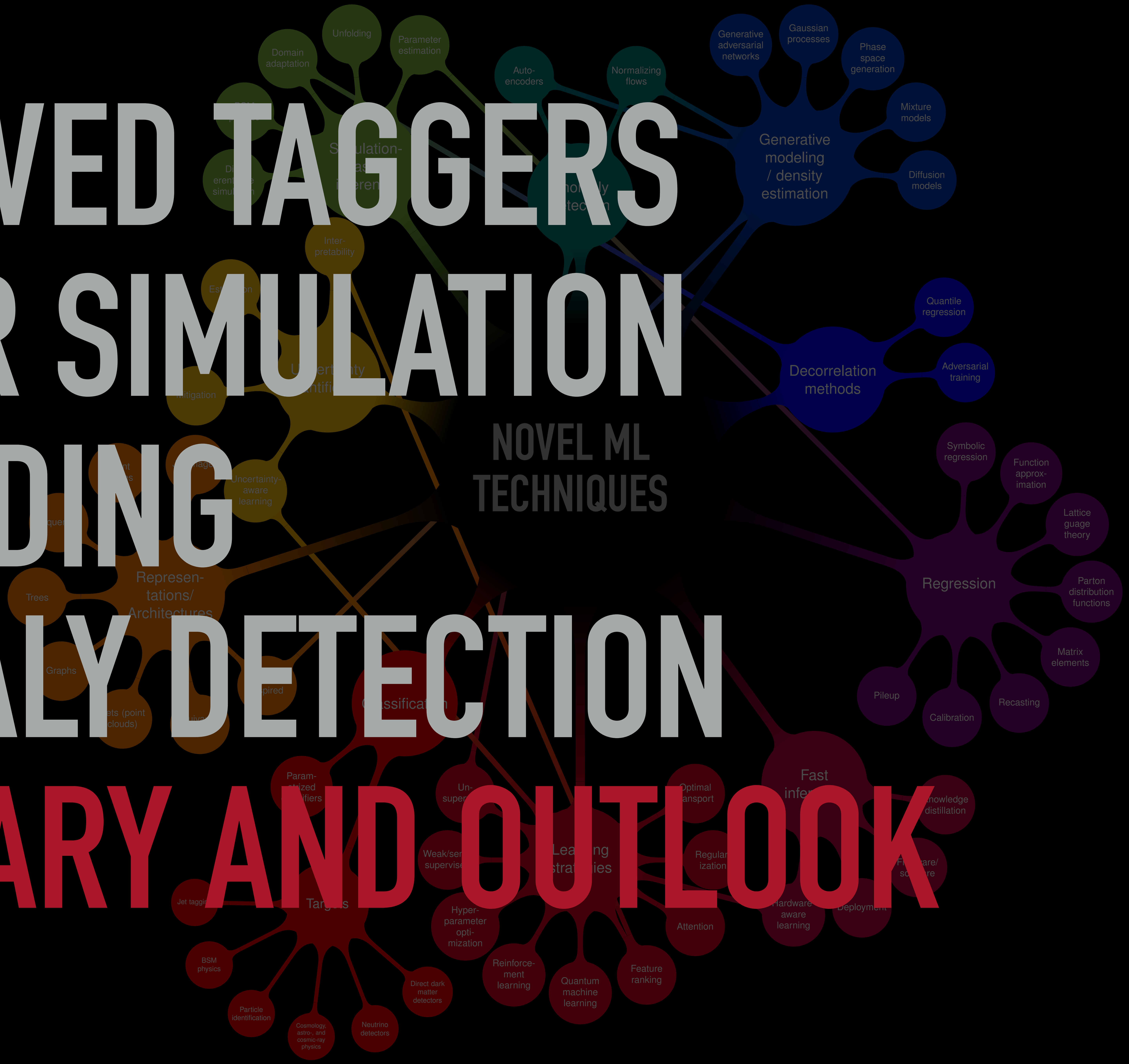


NORMALIZED AUTOENCODER

- Model data as $p_\theta(x) \propto \exp\left[-\mathrm{MSE}\left(x, \mathrm{AE}_\theta(x)\right)\right]$ and minimize $-\ln p_\theta(x)$
- In practice, approximately minimize this through clever reframing
  - Sample "negative" samples from $p_\theta(x)$ using MCMC
  - Sample "positive" samples from $p_{\mathrm{data}}(x)$
  - Minimize difference in expected MSE between negative and positive samples
- With this change in training, can capture more signal as anomalous!

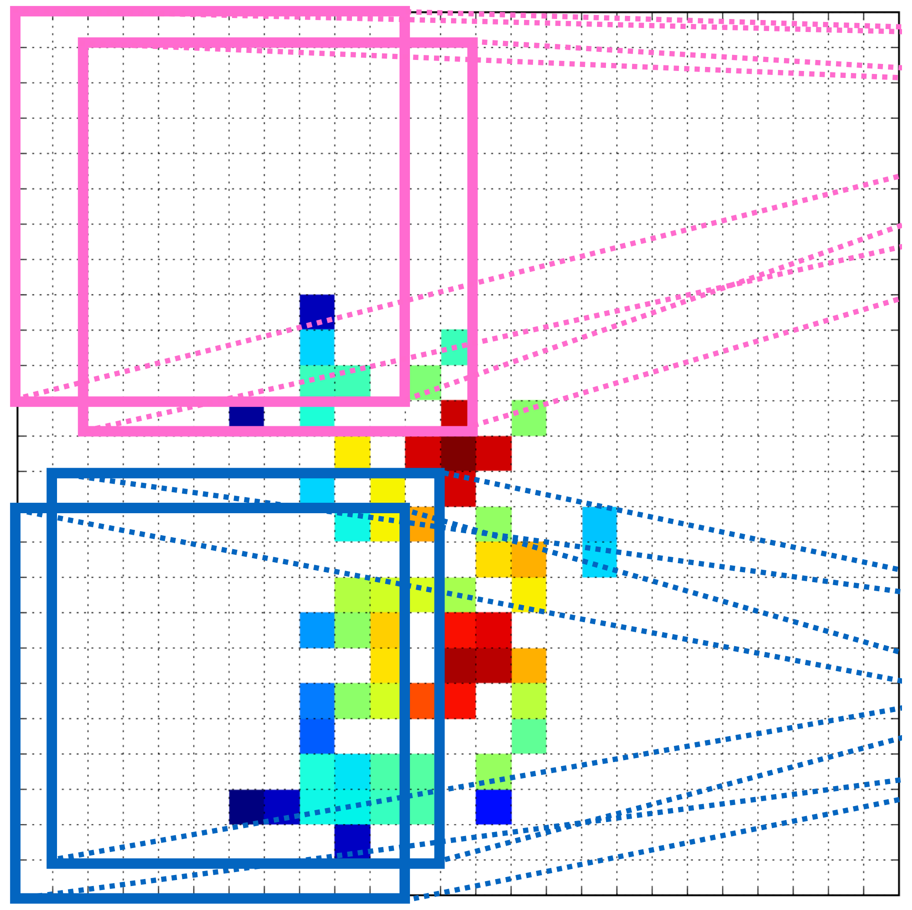


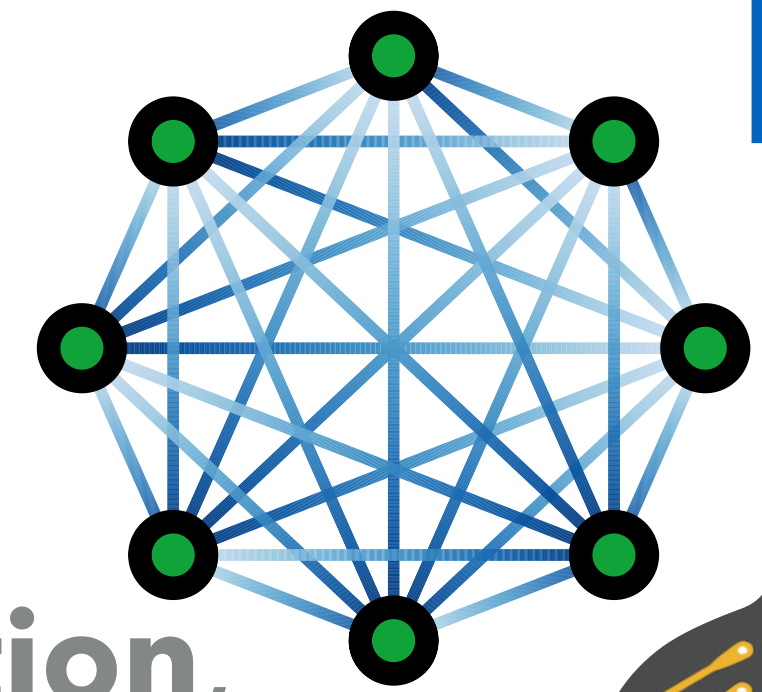
IMPROVED TAGGERS
FASTER SIMULATION
UNFOLDING
ANOMALY DETECTION
SUMMARY AND OUTLOOK

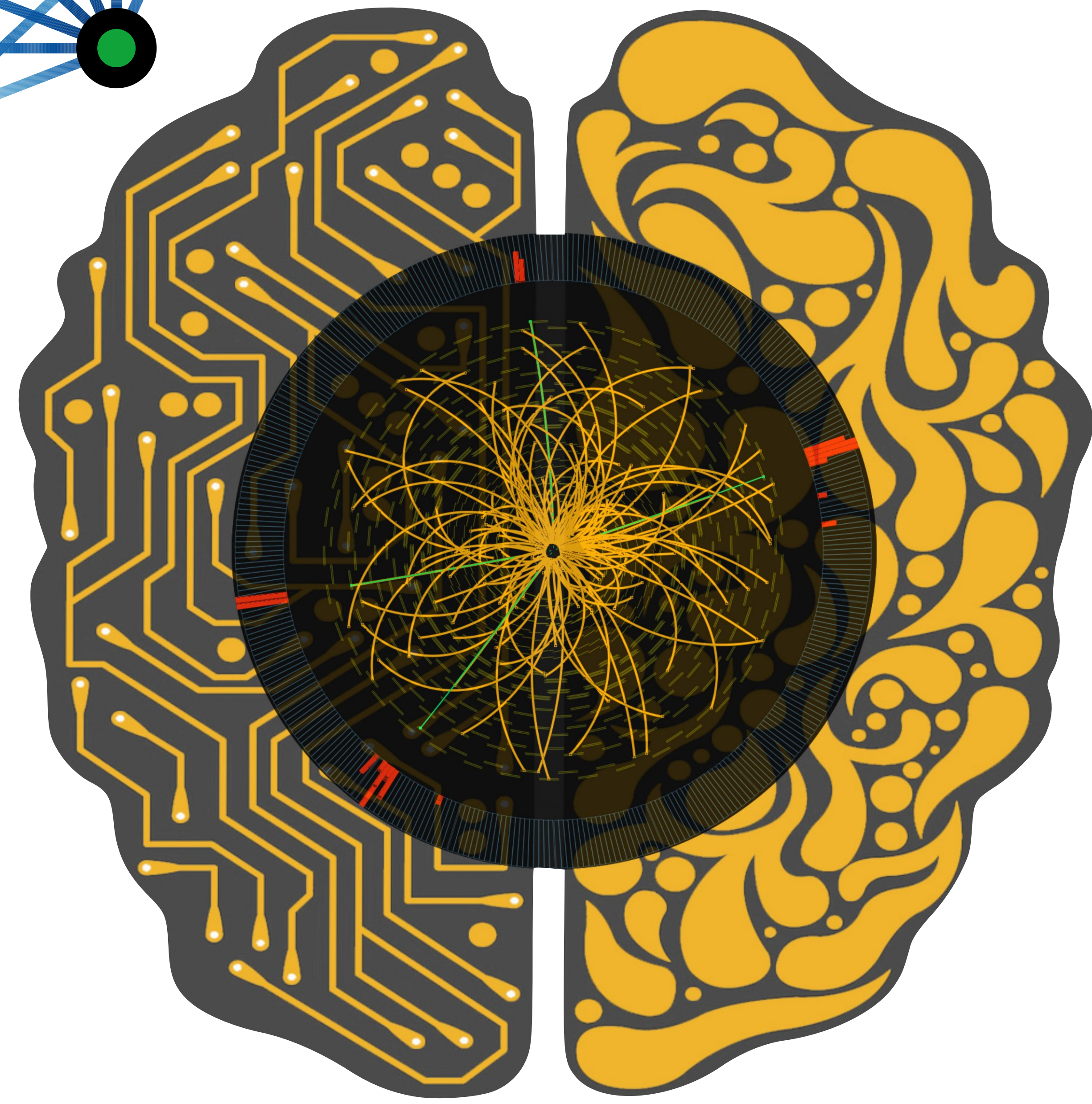


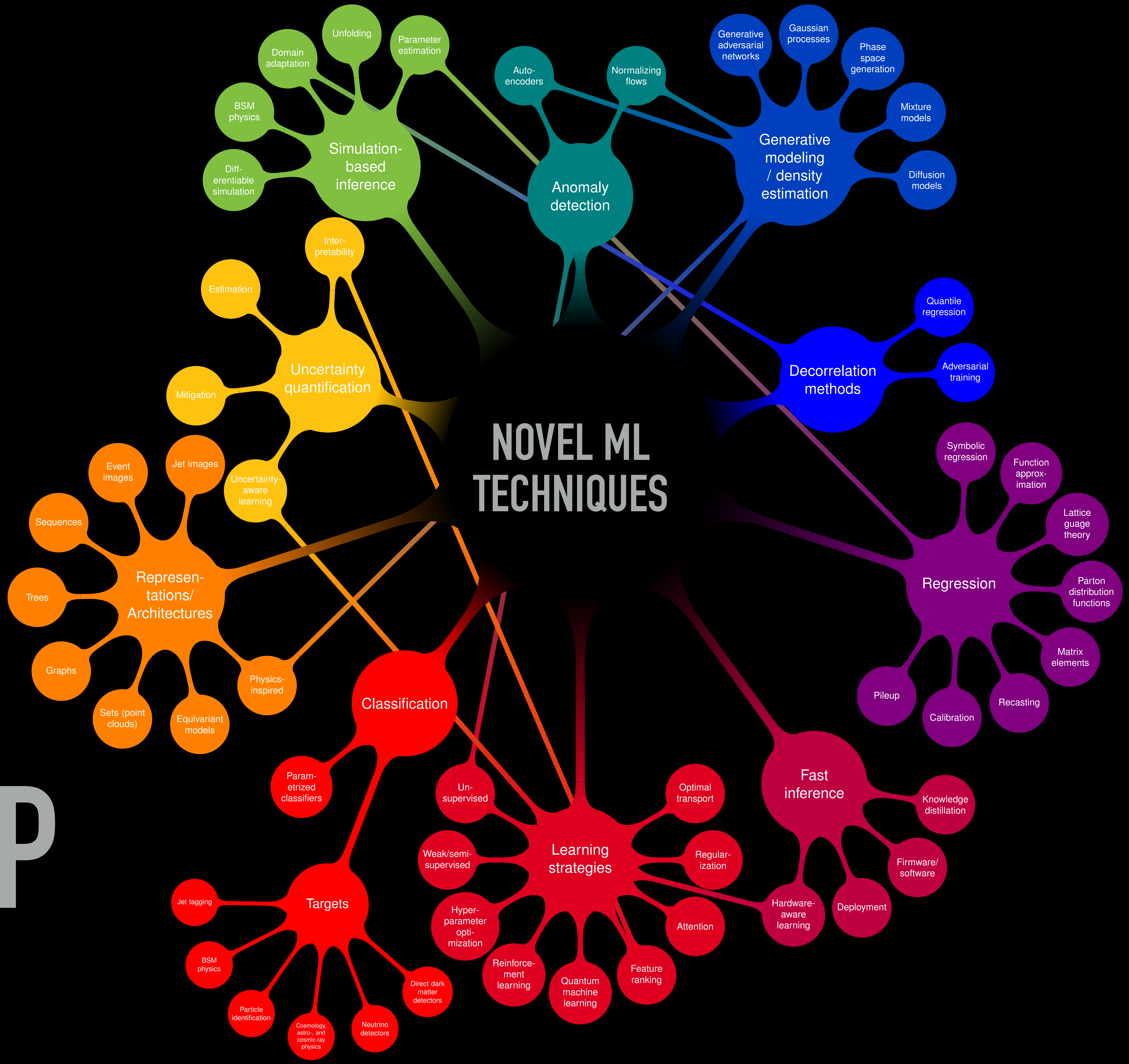
SUMMARY AND OUTLOOK

- Dizzying array of ***ML opportunities, innovations, and applications*** in ***LHC experiments***, which directly ***impact physics results***
- New ideas re-thinking what is the best way to apply ML
  - Not only concerned with performance but also **robustness**, **interpretability**, and insensitivity to modeling uncertainties…
  - Use cases **beyond classification** including **simulation**, **unfolding**, **anomaly detection**, and more…
- ML enables **new searches and measurements** that were impossible before





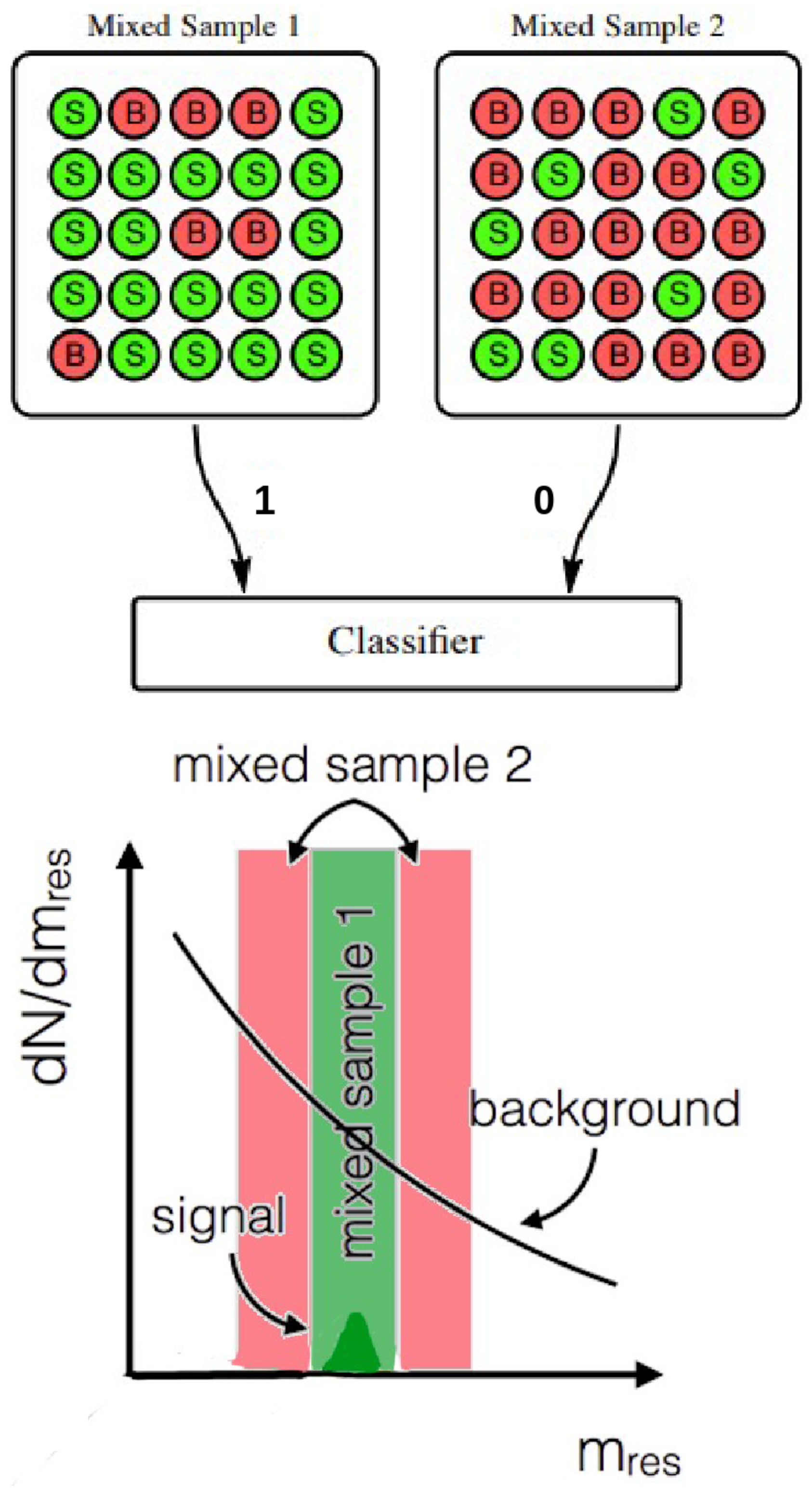


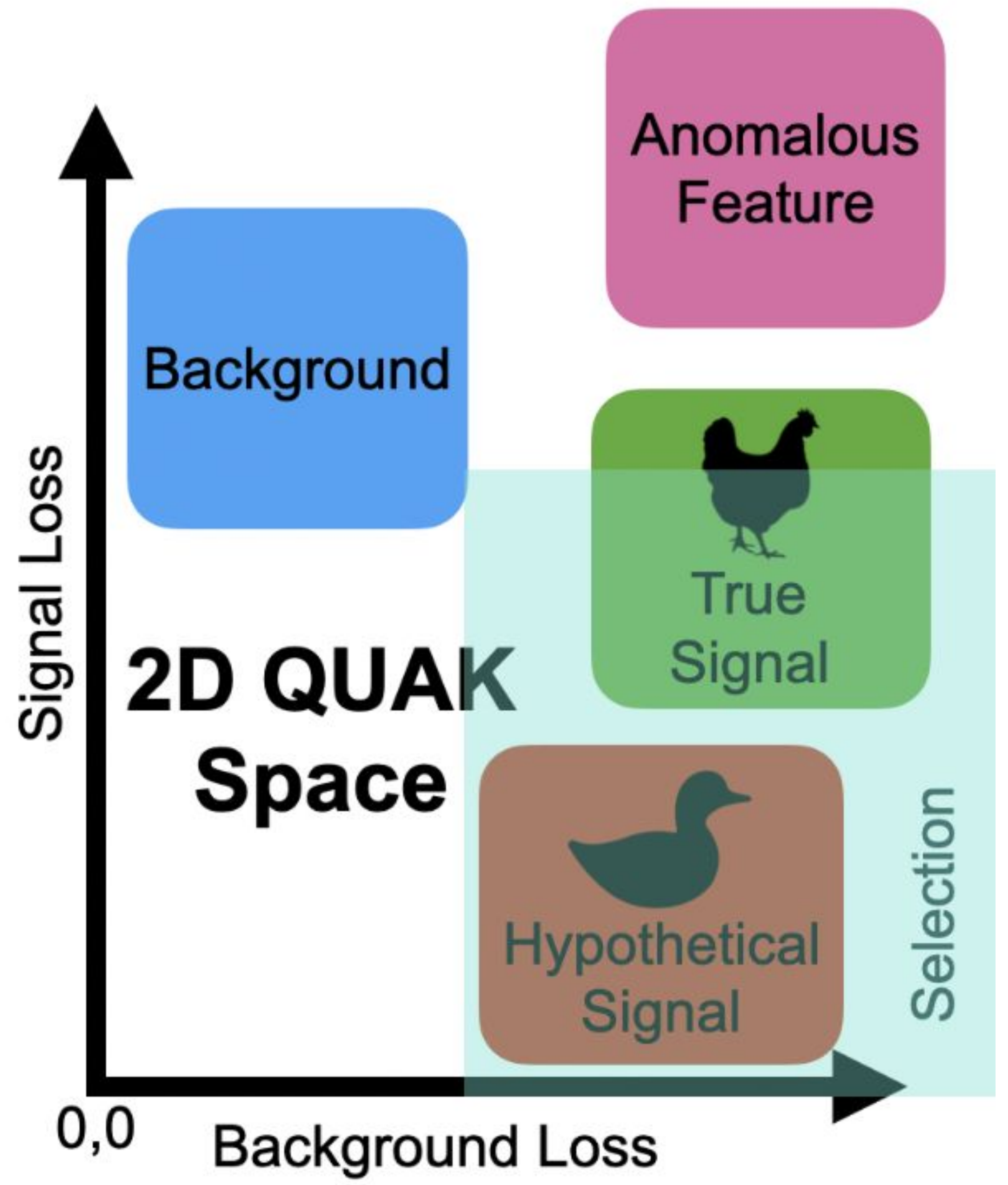

NOVEL ML TECHNIQUES
Simulation-based inference
Unfolding
Domain adaptation
Parameter estimation
BSM physics
Diff-erentiable simulation
Anomaly detection
Auto-encoders
Normalizing flows
Generative modeling / density estimation
Generative adversarial networks
Gaussian processes
Phase space generation
Mixture models
Diffusion models
Decorrelation methods
Quantile regression
Adversarial training
Regression
Symbolic regression
Function approx-imation
Lattice guage theory
Parton distribution functions
Matrix elements
Recasting
Calibration
Pileup
Fast inference
Knowledge distillation
Firmware/ software
Deployment
Hardware-aware learning
Learning strategies
Optimal transport
Regular-ization
Attention
Feature ranking
Quantum machine learning
Reinforce-ment learning
Hyper-parameter opti-mization
Weak/semi-supervised
Un-supervised
Classification
Param-etrized classifiers
Targets
Jet tagging
BSM physics
Particle identification
Cosmology, astro-, and cosmic-ray physics
Neutrino detectors
Direct dark matter detectors
Uncertainty quantification
Inter-pretability
Estimation
Mitigation
Uncertainty-aware learning
Represen-tations/ Architectures
Event images
Jet images
Sequences
Trees
Graphs
Sets (point clouds)
Equivariant models
Physics-inspired

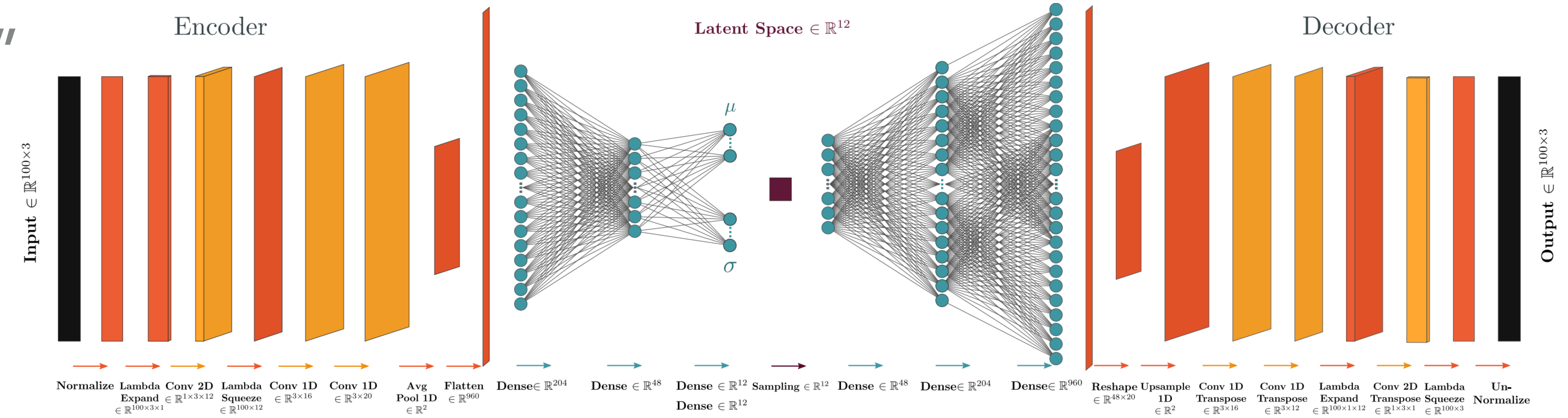
BACKUP

ANOMALY DETECTION: 5 COMPLEMENTARY METHODS

- Weakly supervised
  - **CWoLa Hunting**
  - Tag N' Train (TNT)
  - Classifying anomalies through outer density estimation (CATHODE)
- Unsupervised
  - **Variational autoencoder with quantile regression (VAE-QR)**
- Hybrid: encode "signal prior" based on expected signals
  - Quasianomalous knowledge (QUAK)







- GNN4ITK track reconstruction approaching standard CKF approach