The Application of Neural Networks for the Calibration of ATLAS Calorimeter Signals

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ATLAS EXPERIMENT

This talk

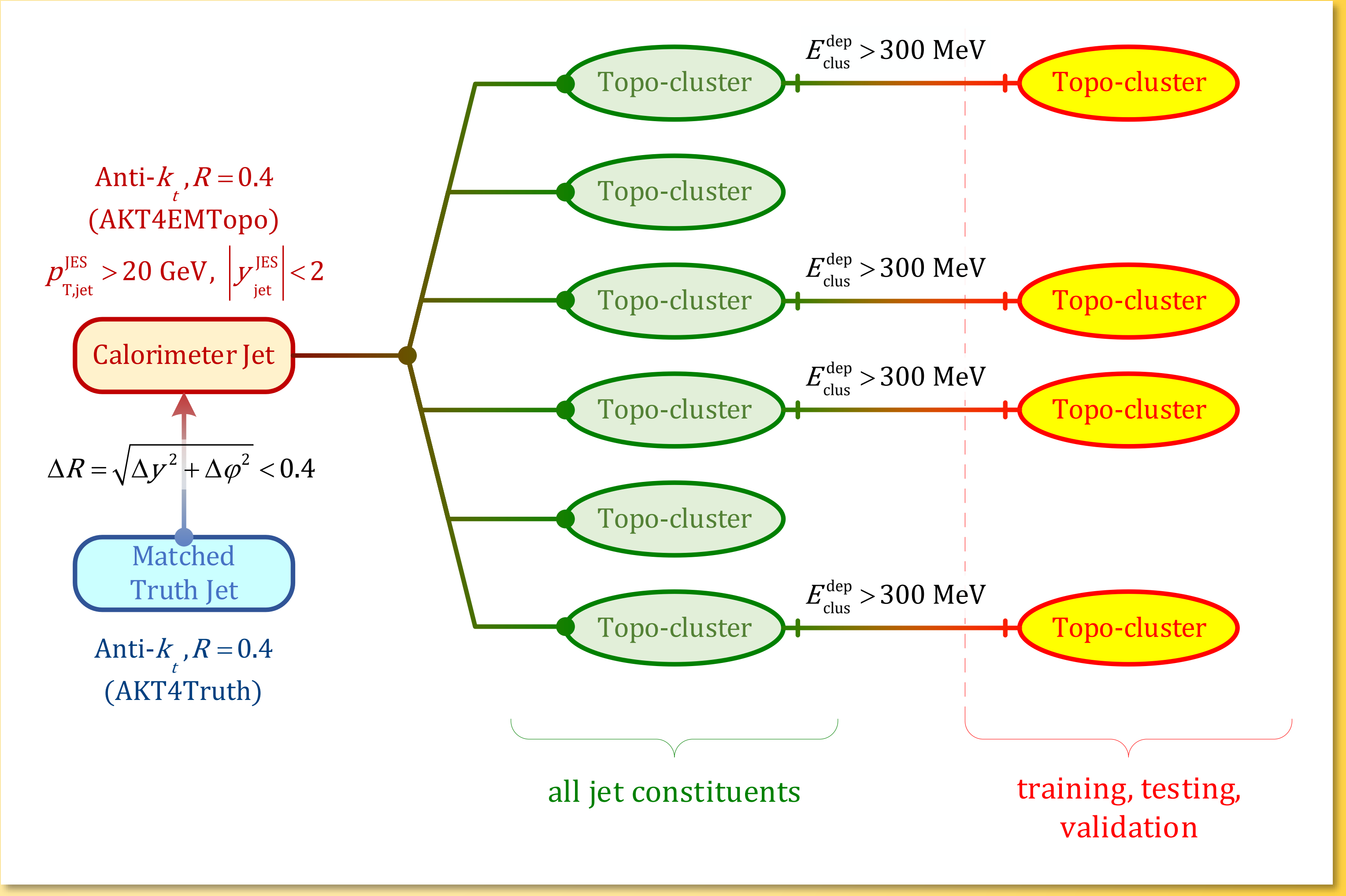
- Motivation
  - Local calibration
  - This project
- Signal feature selection and network designs
  - Sample collection
  - Signal features useful for calibration
  - DNN & BNN networks
- Performance evaluations
  - Prediction power
  - Signa linearity and (local) resolution
- Conclusion
  - Future plans
- Reference
  - All plots (and many more) can be found in ATLAS public note ATL-PHYS-PUB-2023-019

ML-based Local Calibration

- Local calorimeter response and resolution
  - Improved constituent inter-calibration in combined tracking/calorimeter final state reconstruction
    - Better calibrated neutral response in jets – improvement in scale and resolution for all jets, sub-structure variable measurements, measurement of full hadronic recoil (non-jet context), measurement of hadronic event shapes …
  - Replacement for present-day LCW with ML-based approach as a local calibration for topo-clusters
    - LCW: multi-dimensional binned look-up tables → ML: smooth multidimensional calibration functions, no steep steps at bin edges, …
    - LCW: loss of correlations due to average scale factors in bins → ML: exploitation and preservation of correlations, better resolution
- Intentional limitations of approach
  - Looking for practical application to be applied to collision data
    - Extract topo-clusters for training and testing from calorimeter jets in fully simulated events with Run 2 level pile-up
    - Use of cluster moments (constructed features) allows recalibrating at derivation level – all needed data is in the AOD
    - Quick adaptation to changing collision environments (e.g., pile-up) and reconstruction cuts – newly trained networks can be applied at derivation level (data preparation/extraction for physics)
    - No need to go back to full (Tier0) reconstruction, no detailed information (calorimeter cells) needed
  - Single-step approach
    - No dedicated (learned) classification prior to regression on topo-cluster response

Signal Source from MC Simulations

- Full simulation of detector signals in pp collision jet production final states with LHC Run 2 pile-up
  - Jets in central detector region only
  - Need to match generated truth particle jet
- Topo-cluster extracted from jets
  - $E_{\text{clus}}^{\text{dep}} > 300$ MeV
  - Randomly selected for independent training, validation, and test samples
  - No jet-specific information/features used (jet context is fully removed)



Local Hadronic Calibration in ATLAS

Local topo-cluster calibration with Monte Carlo simulations

Standard (LCW) local hadronic calibration

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EM-likelihood | hadronic calibration | outside energy losses

$$E_{\text{clus}}^{\text{had}} = \sum_{\text{cells } i \text{ in cluster}} w_{\text{cell},i}^{\text{geo}} \cdot \left(\mathcal{P}_{\text{clus}}^{\text{EM}} + (1 - \mathcal{P}_{\text{clus}}^{\text{EM}}) \cdot w_{\text{cell},i}^{\text{cal}}\right) \times E_{\text{cell},i} \xrightarrow{\text{measures}} \underbrace{E_{\text{clus}}^{\text{dep}}}_{}$$

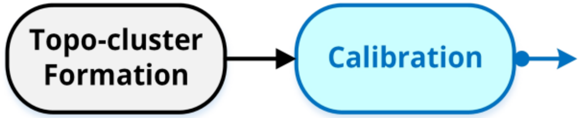
energy deposited in cluster (from MC)

$\mathcal{P}_{\text{clus}}^{\text{EM}}$ & $w_{\text{cell}}^{\text{cal}}$ from *look-up tables* employing cluster moments & cell signal features

1. **Classification** – look up likelihood for cluster being of EM nature $0 \leq \mathcal{P}_{\text{clus}}^{\text{EM}} \leq 1$
2. **Hadronic calibration** – apply cell signal weights to correct hadronic signals to EM scale ($e/h > 1 \xrightarrow{\text{calibrate to}} e/h = 1$)
3. **Out-of-cluster corrections** – correct for energy lost due to cells missed in cluster formation
4. **Dead material corrections** – correct for energy losses in inactive material in the proximity of the topo-cluster

Machine-learning-based (ML-based) local calibration

(proof of concept study)



learned calibration

$$E_{\text{clus}}^{\text{ML}} = C_{\text{clus}}^{\text{ML}}\left(\mathfrak{O}_{\text{clus}}^{\text{ML}}\right) \cdot E_{\text{clus}}^{\text{EM}} \xrightarrow{\text{measures}} E_{\text{clus}}^{\text{dep}}$$

energy deposited in cluster (from MC)

$E_{\text{clus}}^{\text{ML}} \mathrel{\hat{=}} E_{\text{clus}}^{\text{had}}$ — $E_{\text{clus}}^{\text{EM}}$: *basic cluster signal (EM scale)*

$$\mathcal{R}_{\text{clus}}^{\text{ML}}\left(\mathfrak{O}_{\text{clus}}^{\text{ML}}\right) \xrightarrow{\text{predicts}} \mathcal{R}_{\text{clus}}^{\text{EM}} = \frac{E_{\text{clus}}^{\text{EM}}}{E_{\text{clus}}^{\text{dep}}} \xrightarrow{\text{yields}} C_{\text{clus}}^{\text{ML}}\left(\mathfrak{O}_{\text{clus}}^{\text{ML}}\right) = \frac{1}{\mathcal{R}_{\text{clus}}^{\text{ML}}\left(\mathfrak{O}_{\text{clus}}^{\text{ML}}\right)}$$

1. **No explicit classification** – variables used to determine $\mathcal{P}_{\text{clus}}^{\text{EM}}$ added to feature set $\mathfrak{O}_{\text{clus}}^{\text{ML}}$
2. **Hadronic calibration** – apply scale factor to cluster signal $E_{\text{clus}}^{\text{EM}}$ to measure $E_{\text{clus}}^{\text{dep}}$

Calibration from response predictions $\mathcal{R}_{\text{clus}}^{\text{ML}}\left(\mathfrak{O}_{\text{clus}}^{\text{ML}}\right)$ obtained by regression fits $\mathcal{R}_{\text{clus}}^{\text{ML}}\left(\mathfrak{O}_{\text{clus}}^{\text{ML}}\right) \mapsto \mathcal{R}_{\text{clus}}^{\text{EM}}$ employing feature set $\mathfrak{O}_{\text{clus}}^{\text{ML}}$

Feature Set Composition

❖ Focus on observables contributing to response

A. Deposited energy represented by signal (in a complex way)

B. Detector geometry – signal characteristics of calorimeter sub-systems: variations in level of signal non-compensation ($e/h > 1$), absorption power/leakage, energy sharing around inactive regions …

C. Shower development – differences between EM and HAD showers: starting point, size, spread and compactness …

D. Intrinsic shower fluctuations – variations in the shower development of (hadronic) showers

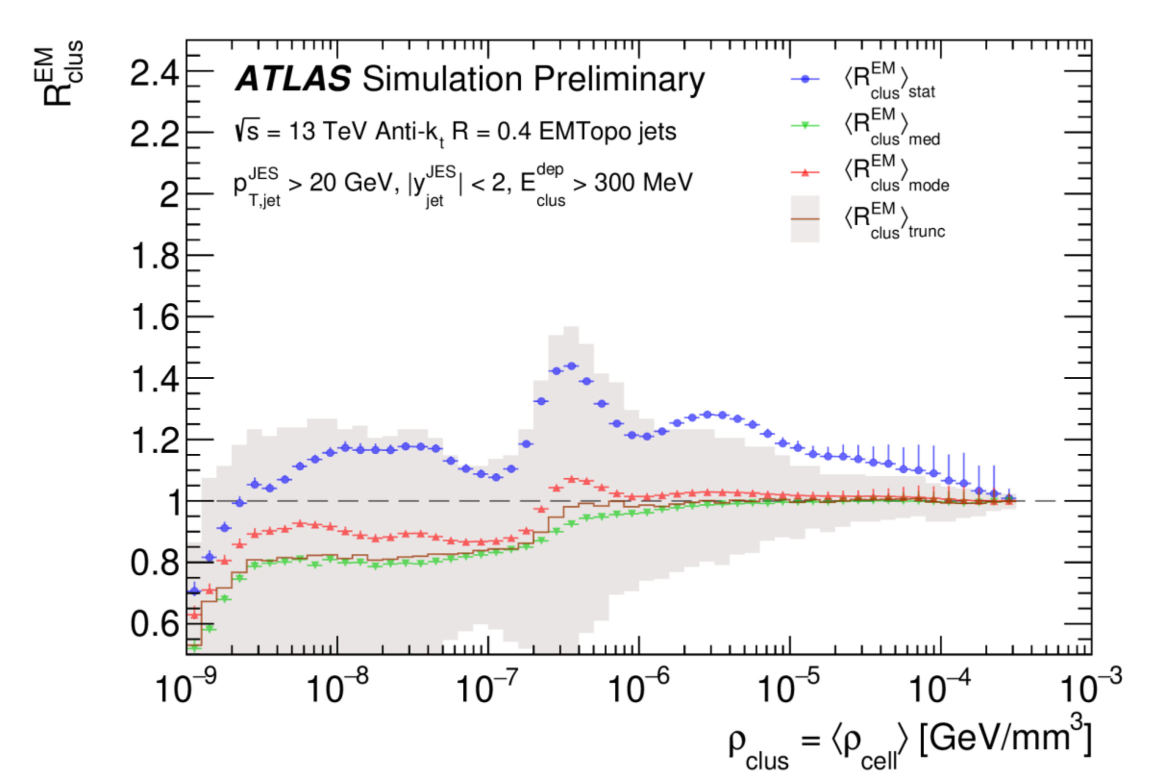
E. Signal strength and relevance – signal significance measured by signal-over-noise

F. Collision environment – effects of event topology/nearby signals (isolation) and pile-up on the topo-cluster signal

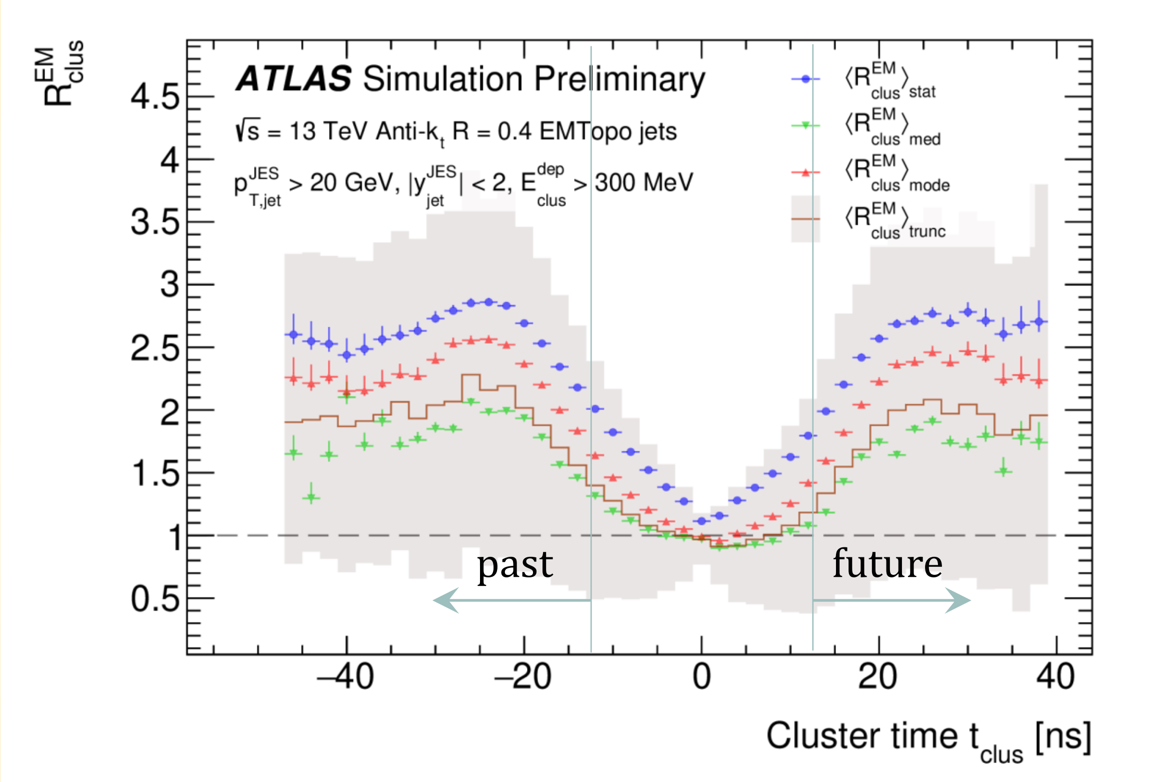
Category	Symbol	LCW	Comment
kinematics	$E^{\mathrm{EM}}_{\mathrm{clus}}$	yes	signal at the electromagnetic energy scale (A)
	$y^{\mathrm{EM}}_{\mathrm{clus}}$	yes	rapidity at the electromagnetic energy scale (B)
signal strength timing	$\zeta^{\mathrm{EM}}_{\mathrm{clus}}$	no	signal significance (E)
	t_{clus}	no	signal timing (C,D,F)
	$\mathrm{Var}_{\mathrm{clus}}(t_{\mathrm{cell}})$	no	variance of t_{cell} distribution (D,F)
shower depth shower shape compactness	λ_{clus}	yes	distance of centre-of-gravity from calorimeter front face (C,D)
	$\lvert\vec{c}_{\mathrm{clus}}\rvert$	no	distance of centre-of-gravity from nominal vertex (C,D)
	f_{emc}	no	fraction of energy in electromagnetic calorimeter (C)
	$\langle\rho_{\mathrm{cell}}\rangle$	yes	cluster signal density measure (C,D)
	$\langle\mathfrak{m}^2_{\mathrm{long}}\rangle$	no	energy dispersion along main cluster axis (C)
	$\langle\mathfrak{m}^2_{\mathrm{lat}}\rangle$	no	energy dispersion perpendicular to main cluster axis (C)
	$p_{\mathrm{T}}D$	no	signal compactness measure (C,D)
topology	f_{iso}	no	cluster isolation measure (F)
pile-up	N_{PV}	no	number of reconstructed primary vertices (F)
	μ	no	number of interactions per bunch crossing (F)

$$\mathfrak{O}^{\mathrm{ml}}_{\mathrm{clus}} = \{\underbrace{E^{\mathrm{EM}}_{\mathrm{clus}}, y^{\mathrm{EM}}_{\mathrm{clus}}}_{\text{kinematics}}, \overbrace{\zeta^{\mathrm{EM}}_{\mathrm{clus}}, t_{\mathrm{clus}}, \mathrm{Var}_{\mathrm{clus}}(t_{\mathrm{cell}})}^{\text{signal strength and timing}}, \underbrace{\lambda_{\mathrm{clus}}, \lvert\vec{c}_{\mathrm{clus}}\rvert, \langle\rho_{\mathrm{cell}}\rangle, \langle\mathfrak{m}^2_{\mathrm{long}}\rangle, \langle\mathfrak{m}^2_{\mathrm{lat}}\rangle, p_{\mathrm{T}}D, f_{\mathrm{emc}}}_{\text{shower location (depth), shapes and compactness}}, \overbrace{f_{\mathrm{iso}}}^{\text{topology (isolation)}}, \underbrace{N_{\mathrm{PV}}, \mu}_{\text{event/pile-up}}\}$$

Response Dependence on Features



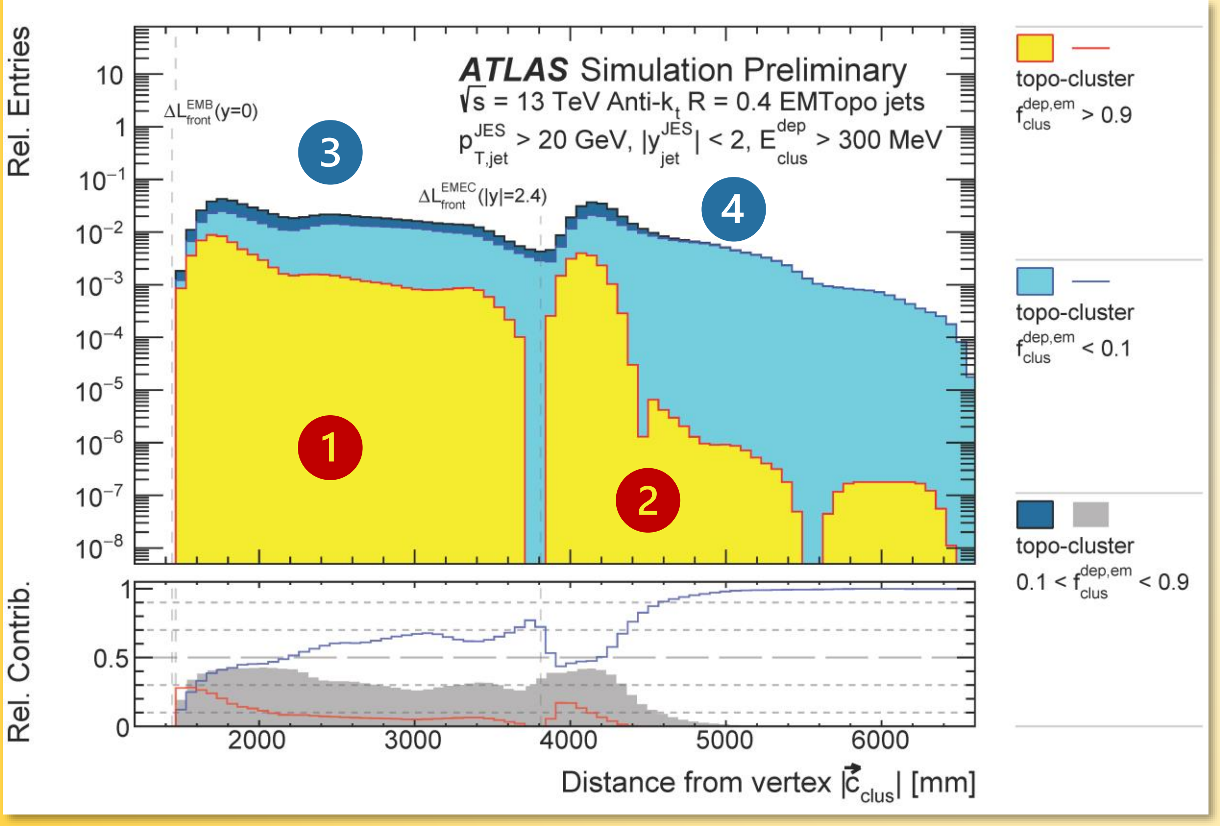
Measure for tendency of centrality influences ML setup → loss function definition

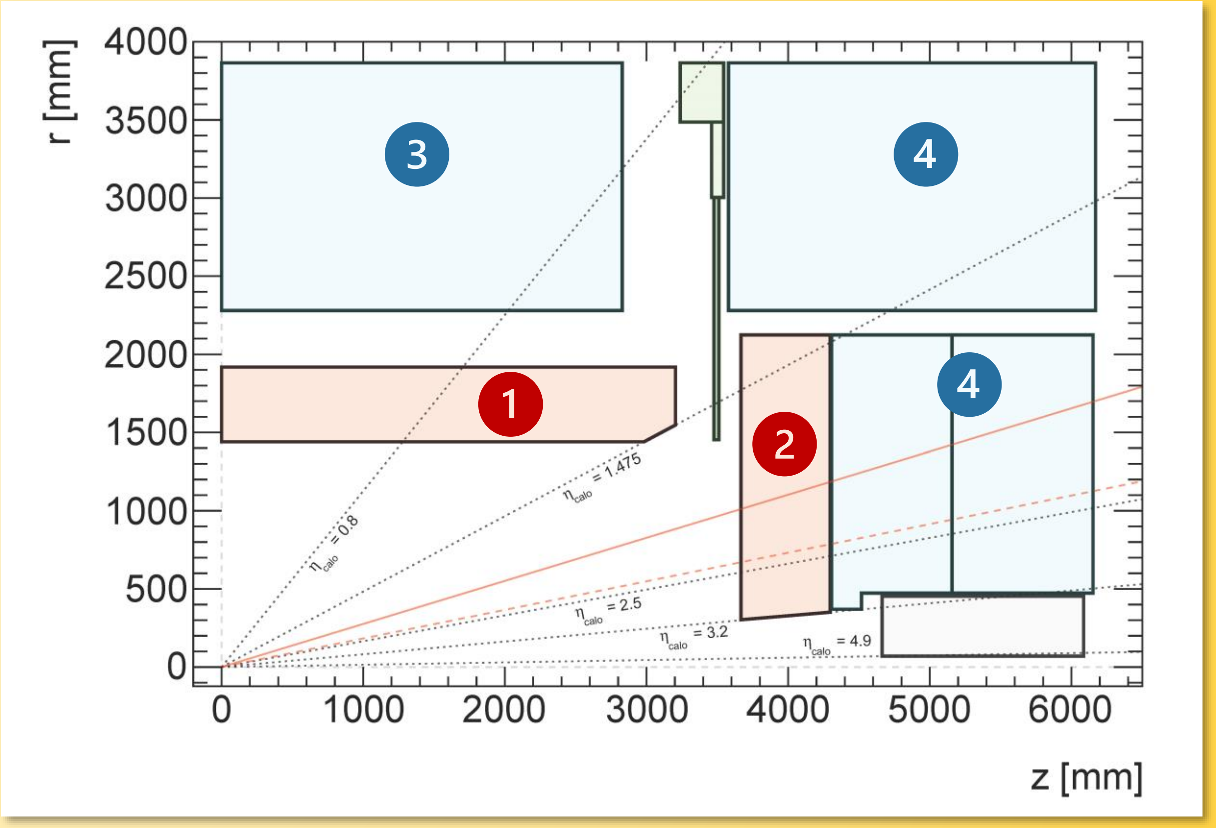


Cluster timing is affected by (out-of-time) pile-up → response increased by additional signals from nearby past bunch crossing and the following one

Challenge: Feature Distributions

- Example: complex distribution of topo-cluster distance from nominal vertex



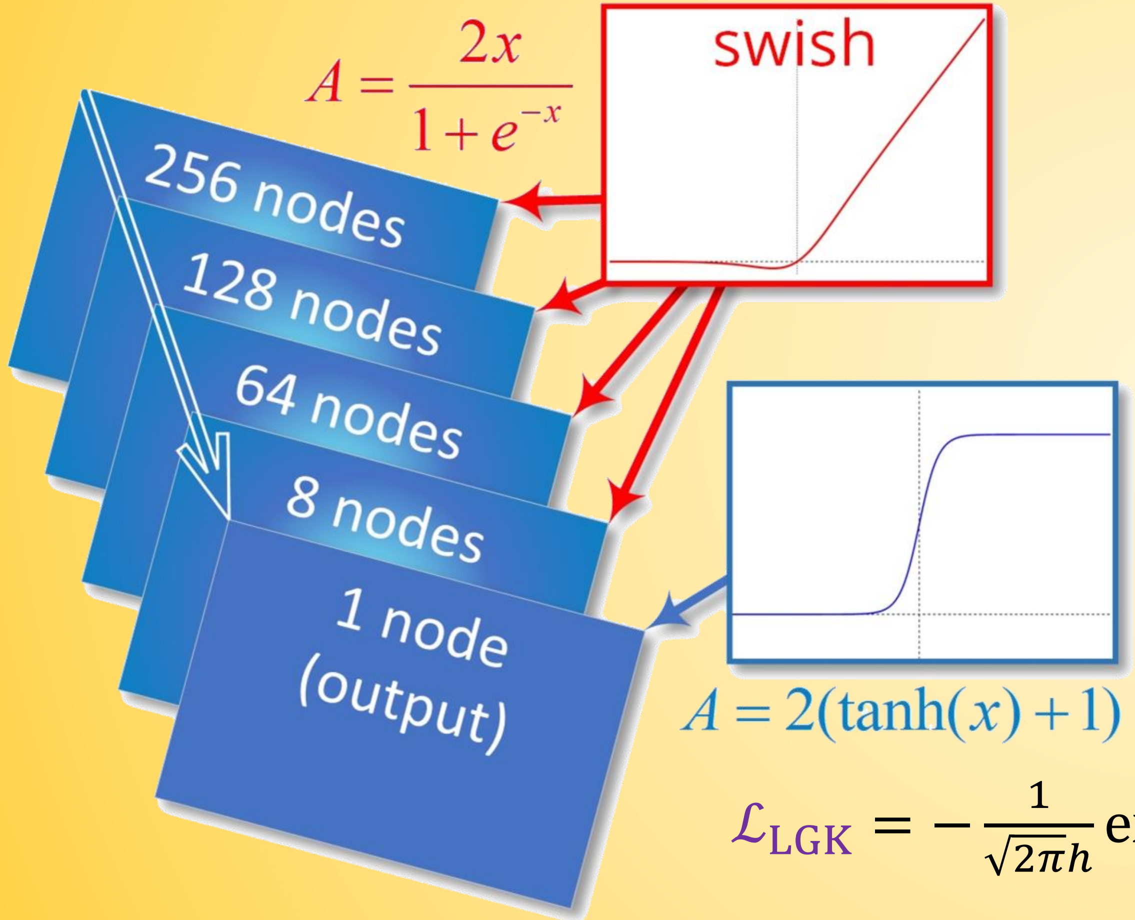


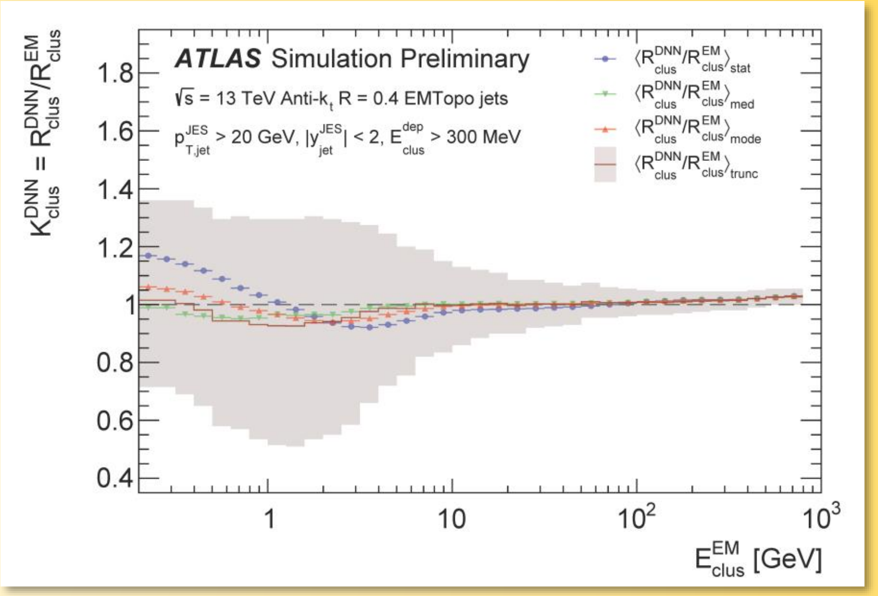
predominantly $e^{\pm}/\gamma$ | mixed | predominantly hadronic

contribution to deposited energy

Neural Network Designs: DNN

- ❖ Highly tuned configuration





Loss function trains the mode:

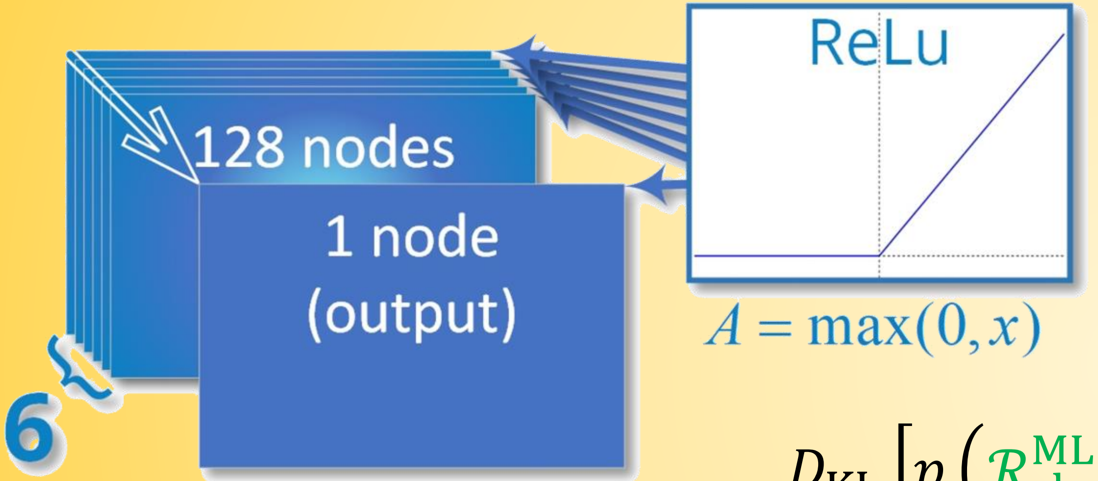
1st pass: $h = 0.1, \alpha = 0.05$

2nd pass (seeded with 1st pass model)**:** $\alpha = 0$

$$\mathcal{L}_{\mathrm{LGK}} = -\frac{1}{\sqrt{2\pi h}} \exp\left[\frac{1}{2h}\left(\frac{\mathcal{R}^{\mathrm{ML}}_{\mathrm{clus}}(\mathfrak{O}^{\mathrm{ML}}_{\mathrm{clus}})}{\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}} - 1\right)^2\right] + \alpha \left|\frac{\mathcal{R}^{\mathrm{ML}}_{\mathrm{clus}}(\mathfrak{O}^{\mathrm{ML}}_{\mathrm{clus}})}{\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}} - 1\right|$$

Neural Network Designs: BNN

❖ First attempt*



Negative log-likelihood loss function with regularization by (reverse) Kullback-Leibler (KL) divergence D_{KL} *models* $\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}$ *distribution*

$$D_{\mathrm{KL}}\left[p\left(\mathcal{R}^{\mathrm{ML}}_{\mathrm{clus}}\left(\mathfrak{D}^{\mathrm{ML}}_{\mathrm{clus}}\right)\right), q\left(\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}\right)\right] = \left\langle \log \frac{p\left(\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}\right)}{q\left(\mathcal{R}^{\mathrm{ML}}_{\mathrm{clus}}\left(\mathfrak{D}^{\mathrm{ML}}_{\mathrm{clus}}\right)\right)} \right\rangle_{q\left(\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}\right)}$$

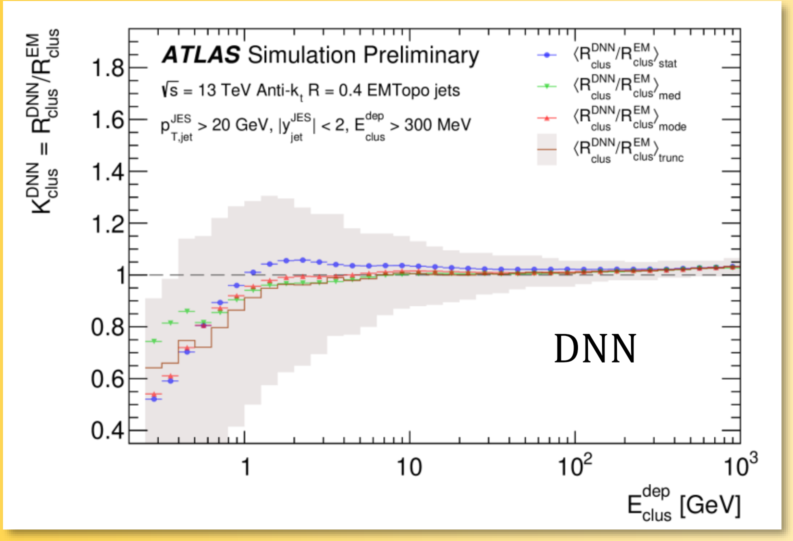
$$\mathcal{L}_{\mathrm{BNN}} \sim -\log\left(p_{\mathrm{train}} = \sum_{i=1}^{6} \mathcal{G}_i\left(\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}, \mathfrak{D}^{\mathrm{ML}}_{\mathrm{clus}}; \mu_i, \sigma_i\right)\right) + D_{\mathrm{KL}}\left[p\left(\mathcal{R}^{\mathrm{ML}}_{\mathrm{clus}}\left(\mathfrak{D}^{\mathrm{ML}}_{\mathrm{clus}}\right)\right), q\left(\mathcal{R}^{\mathrm{EM}}_{\mathrm{clus}}\right)\right]$$

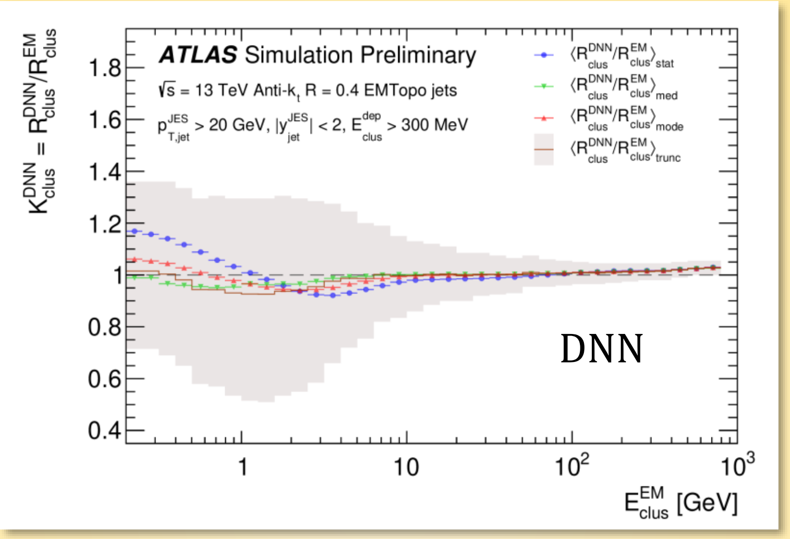
↪ uncertainties (1) for model and (2) from training statistics → under further investigation

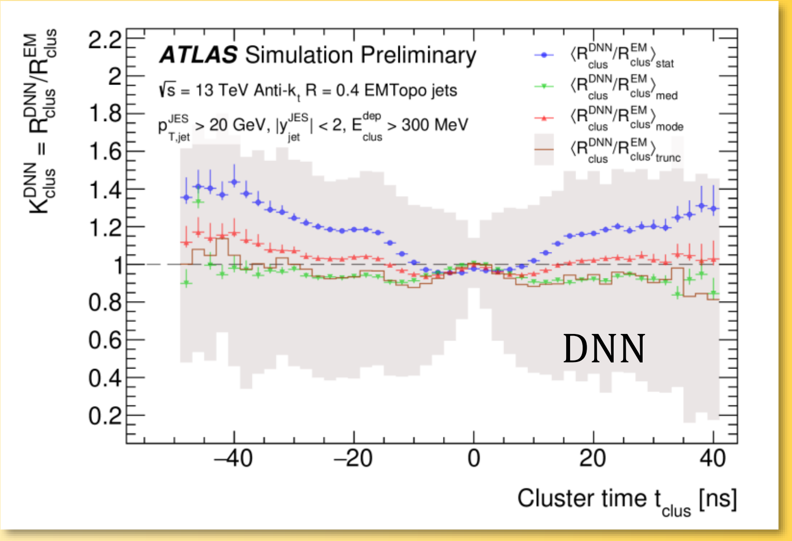
*with many thanks to Tilman Plehn & Michel Luchmann for providing the code and lots of advice

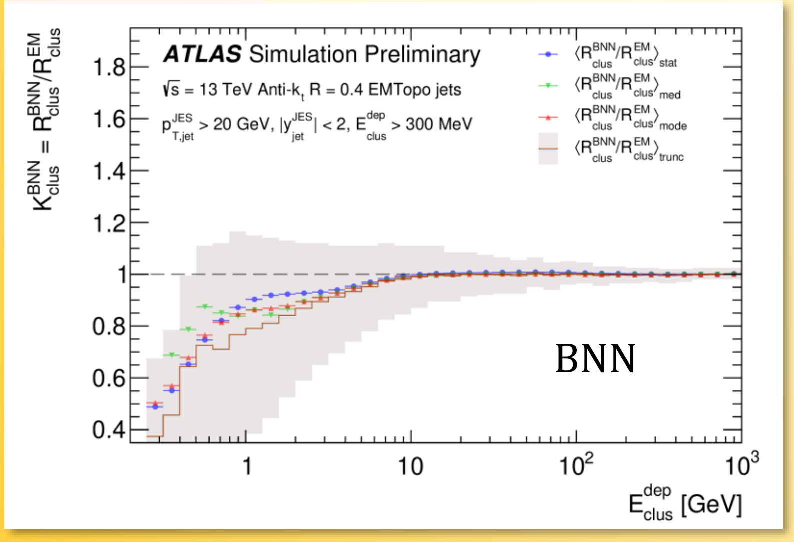
Prediction Power

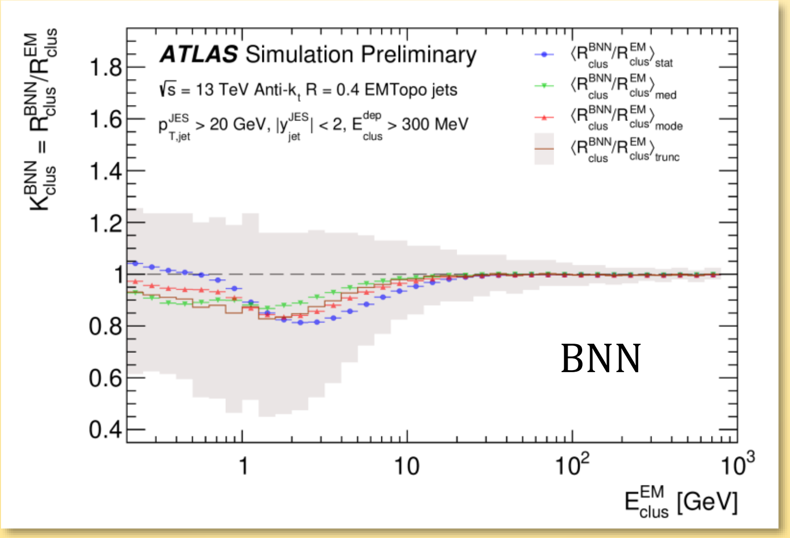
$$K_{\mathrm{clus}}^{\mathrm{DNN(BNN)}} = R_{\mathrm{clus}}^{\mathrm{DNN(BNN)}} / R_{\mathrm{clus}}^{\mathrm{EM}}$$

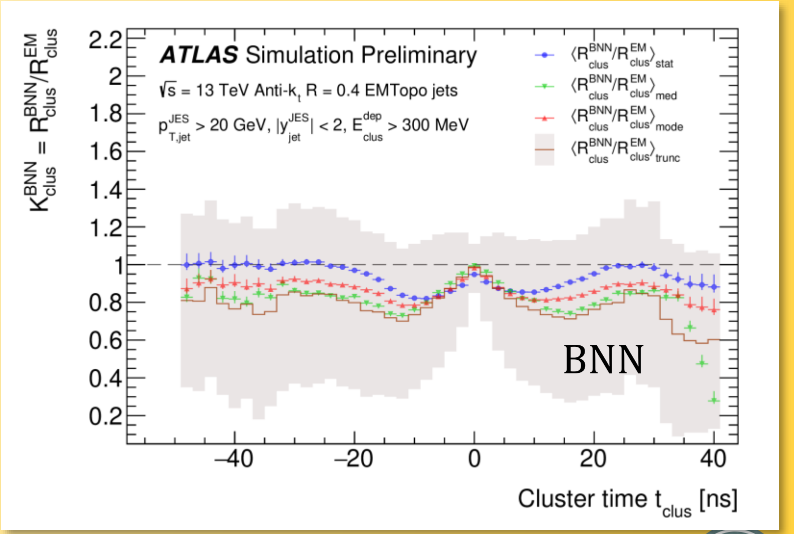






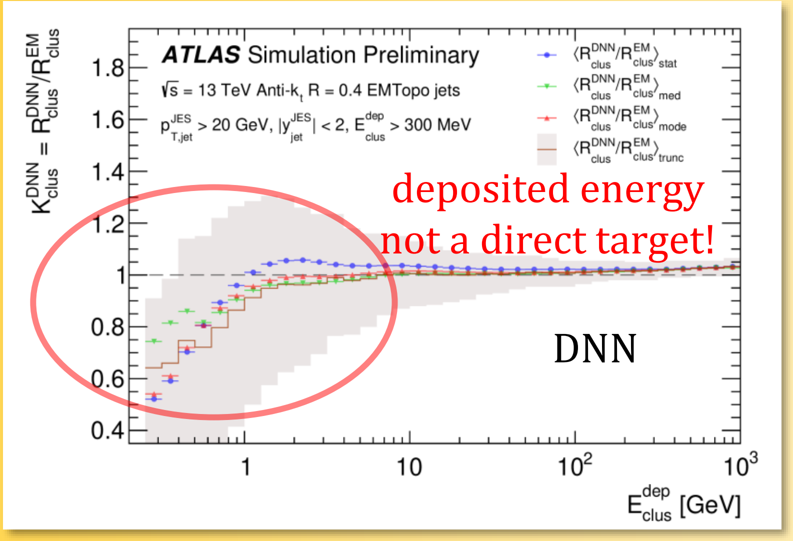


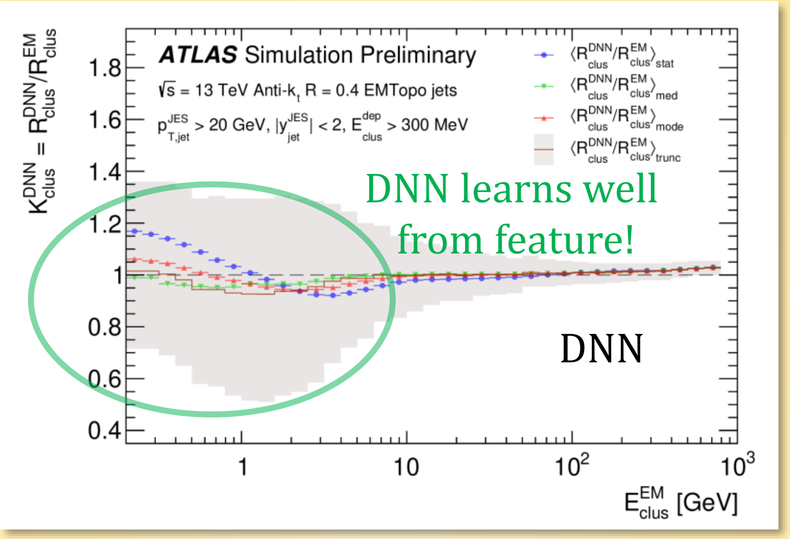


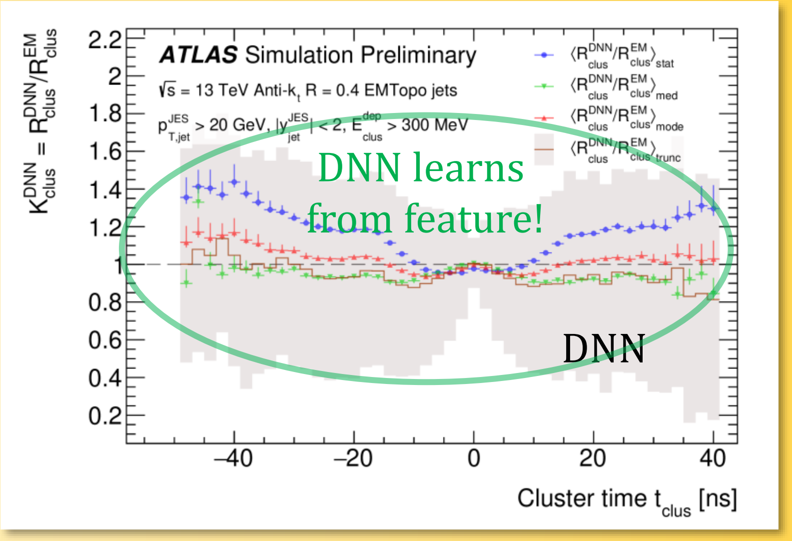


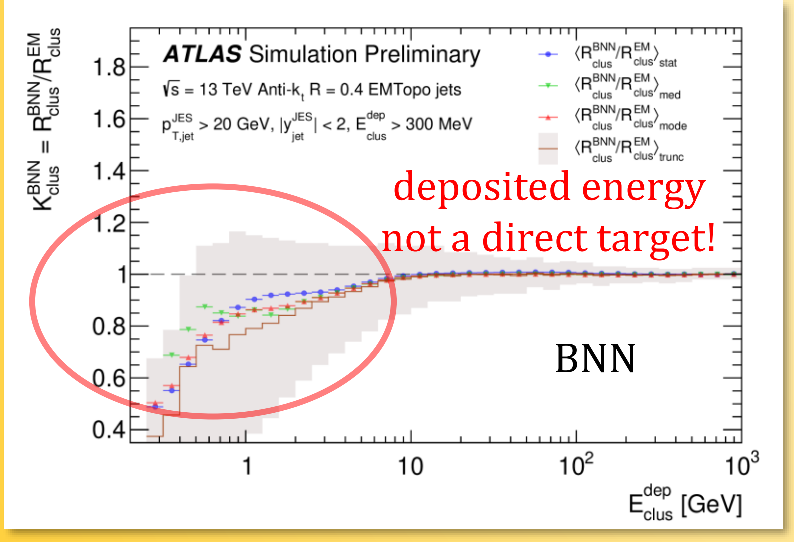
Prediction Power

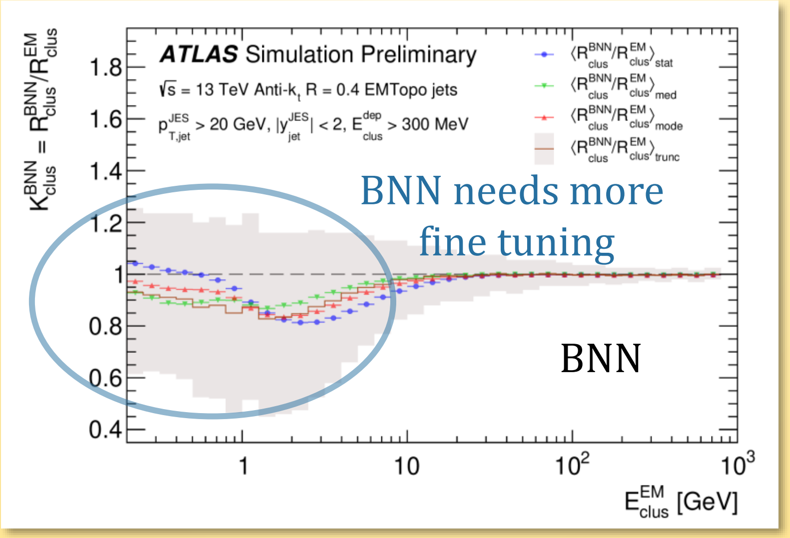
$$K_{\text{clus}}^{\text{DNN(BNN)}} = R_{\text{clus}}^{\text{DNN(BNN)}} / R_{\text{clus}}^{\text{EM}}$$

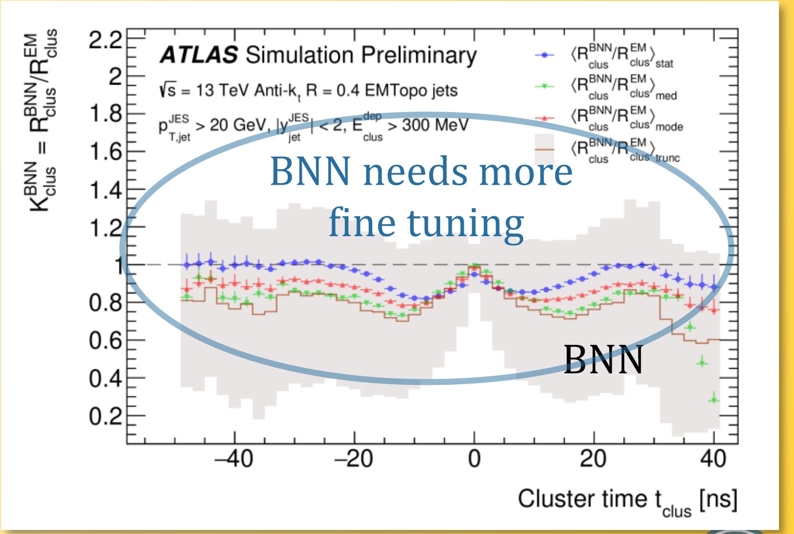




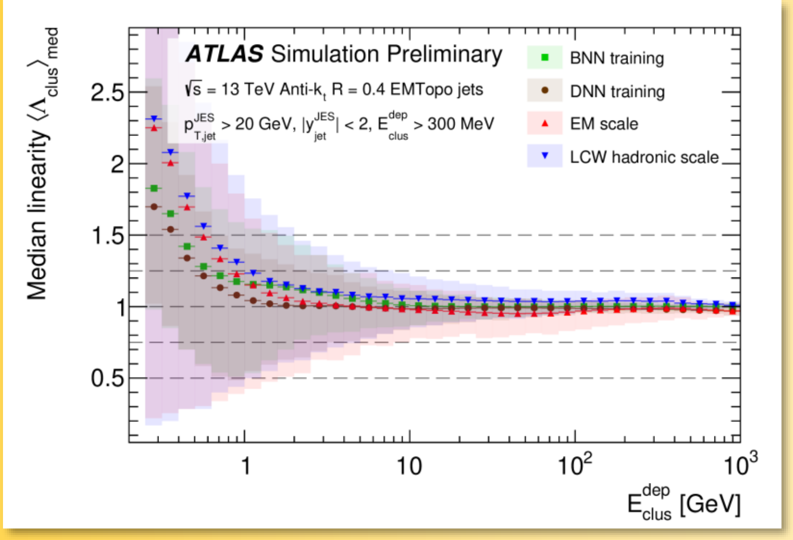


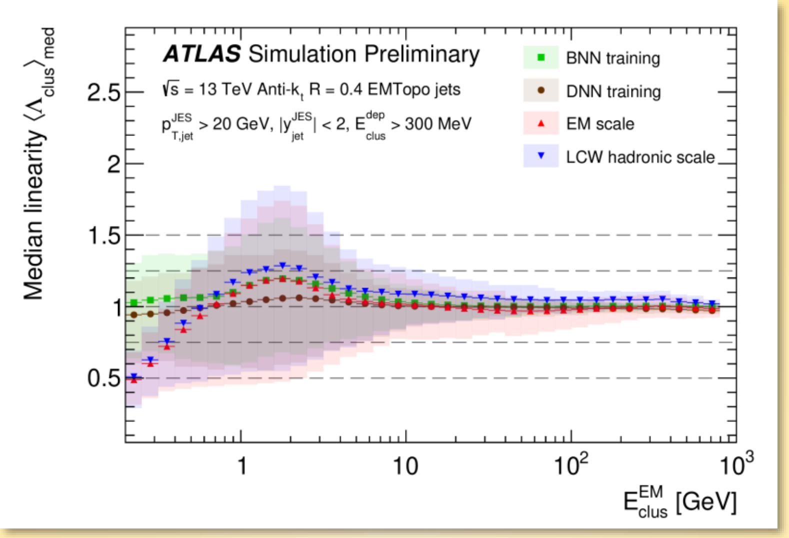


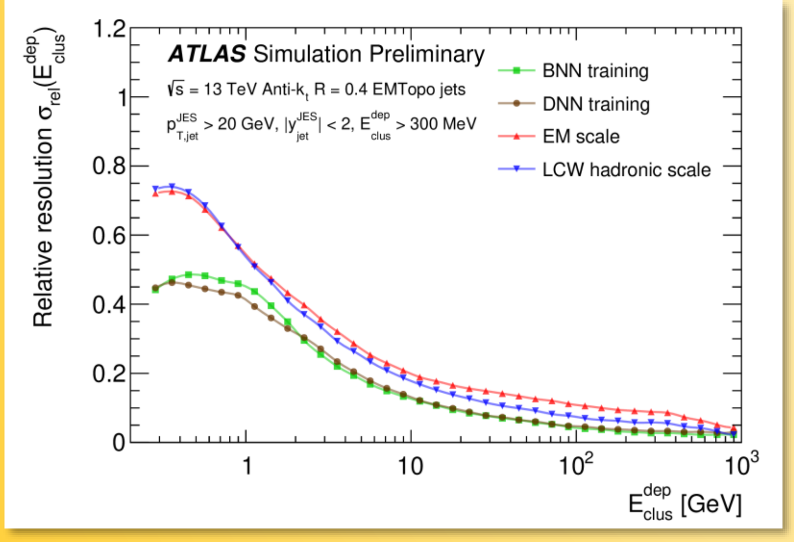


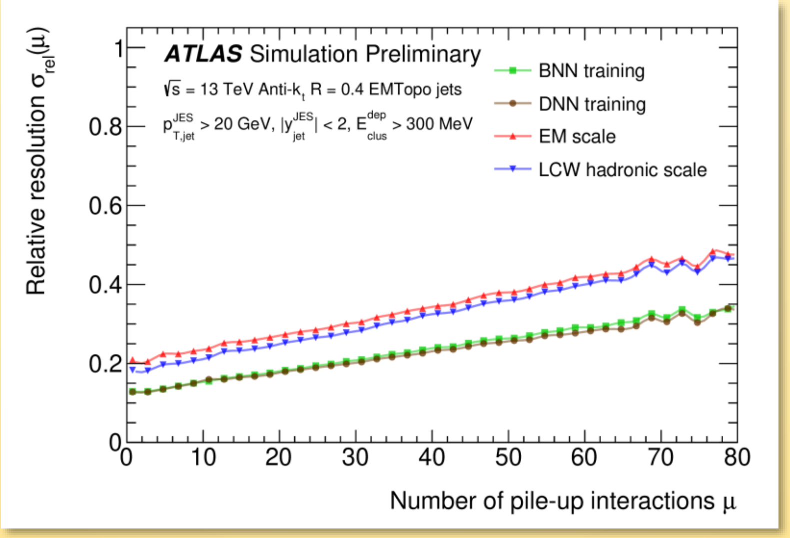


Signal Linearity & Resolution







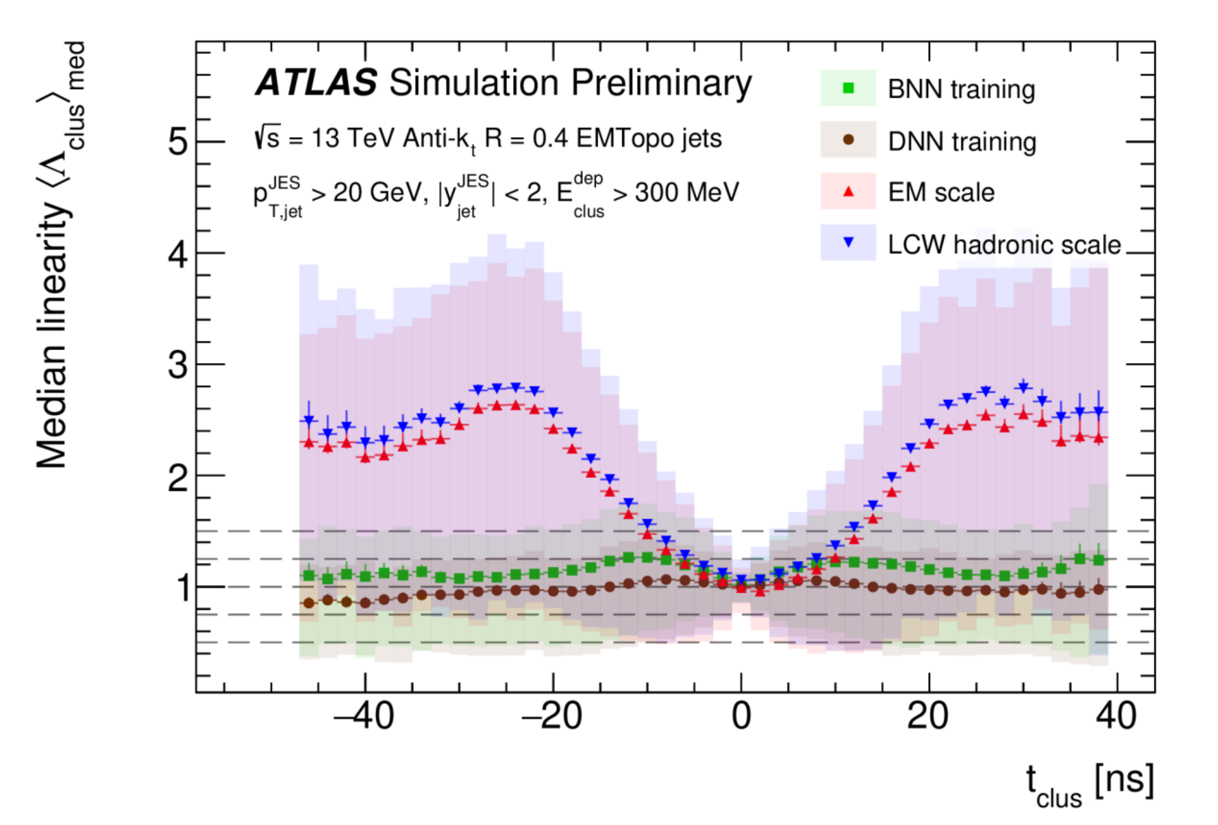


- **Linearity**
  - $\langle \Lambda_{\mathrm{clus}} \rangle_{\mathrm{med}} = \left\langle E_{\mathrm{clus}}^{\mathrm{reco}} / E_{\mathrm{clus}}^{\mathrm{dep}} \right\rangle_{\mathrm{med}}$
  - $E_{\mathrm{clus}}^{\mathrm{reco}} \in \{E_{\mathrm{clus}}^{\mathrm{EM}}, E_{\mathrm{clus}}^{\mathrm{LCW}}, E_{\mathrm{clus}}^{\mathrm{DNN}}, E_{\mathrm{clus}}^{\mathrm{BNN}}\}$
- **Resolution**
  - $\sigma_{\mathrm{rel}} = \mathrm{IQR}_{\mathrm{clus}}^{\Lambda_{\mathrm{clus}}} / (2 \cdot \langle \Lambda_{\mathrm{clus}} \rangle_{\mathrm{med}})$
- **Findings**
  - Improved linearity as a function of features for DNN and BNN
  - Present day LCW calibration agnostic to some features (not $E_{\mathrm{clus}}^{\mathrm{EM}}$!)
  - Local energy resolution significantly improved
  - Pile-up effects on resolution generally reduced – slight improvement in slope as well

Maybe there is more?

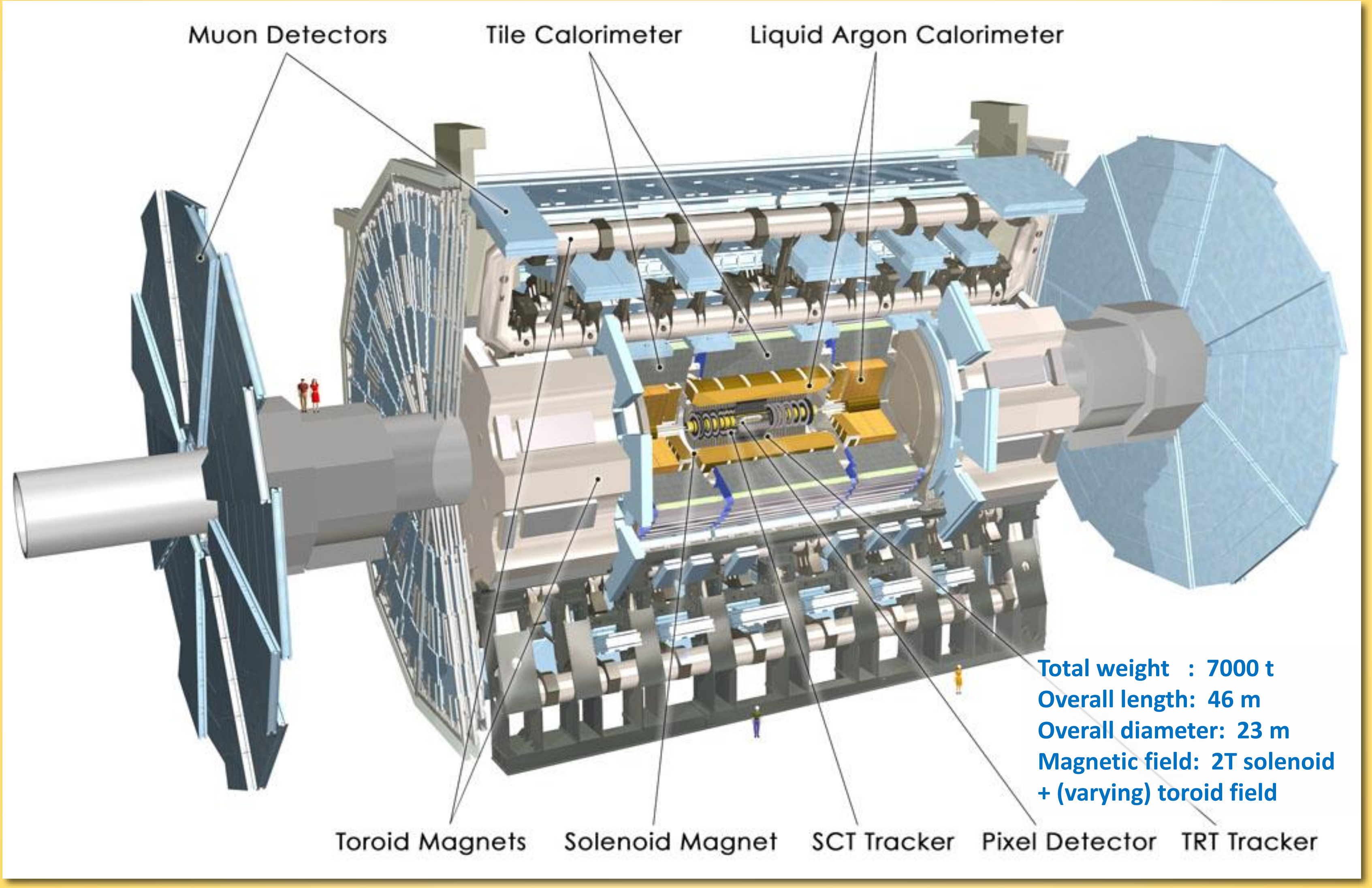
- Out-of-time pile-up mitigation
  - DNN/BNN learn time dependence of response very well – significantly improved signal linearity
  - Yields “built-in” correction for pile-up
  - Can provide basis for classification as well (?)
- Other expectations for performance improvements
  - Tests in full jet context still outstanding – what happens to pure ($E_{\text{clus}}^{\text{dep}} = 0$) and pile-up dominated topo-clusters ($E_{\text{clus}}^{\text{dep}} < 300$ MeV)
  - Local resolution improvement promising for (softer) hadronic recoil reconstructions
- Exploration of BNN
  - Understanding of uncertainty predictions – contribution to “bottoms-up” systematics
  - Now an ATLAS project with help from theorists

Very promising first results for (specific) topo-clusters found in realistic *pp* collision environment!



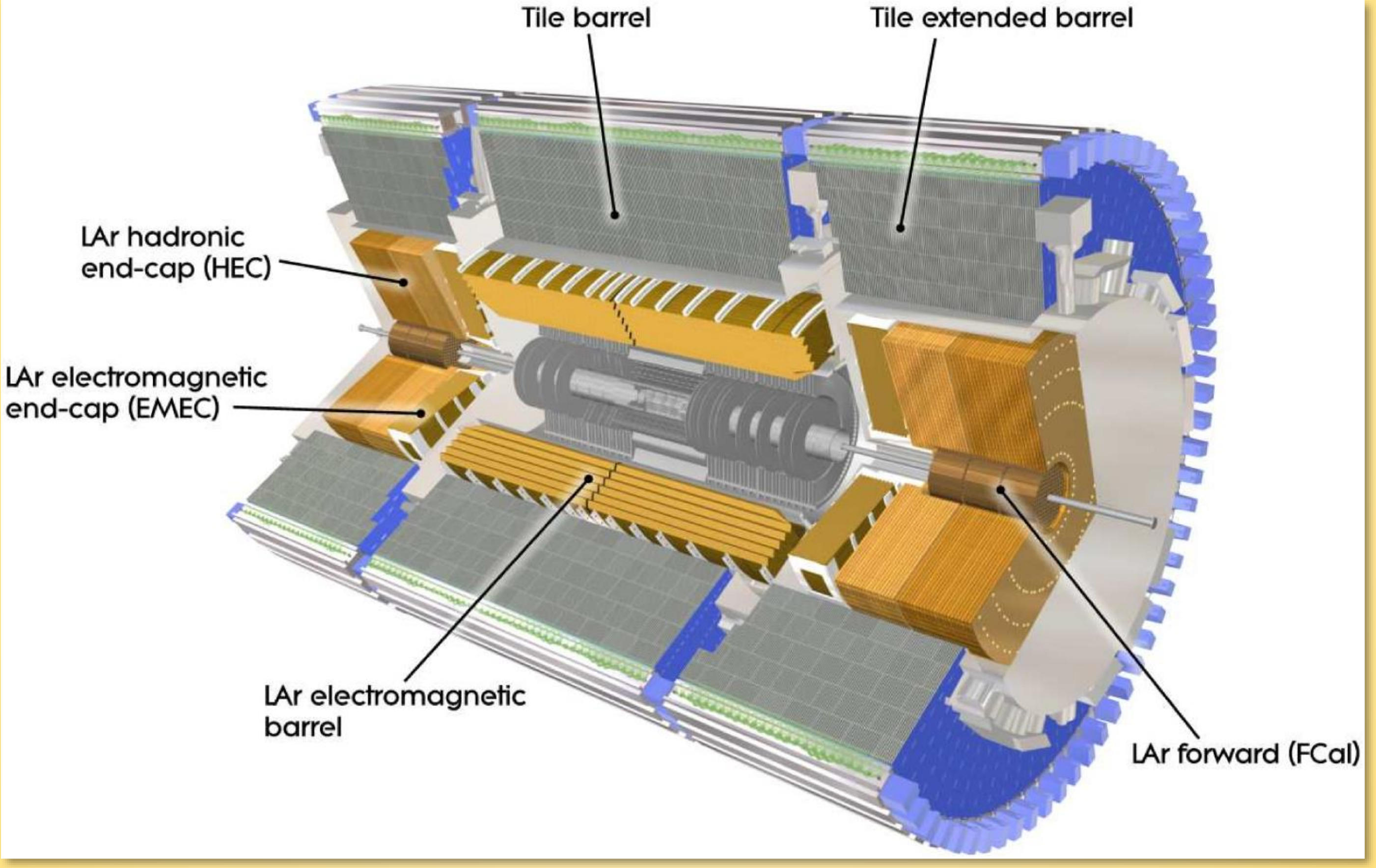
Backup & Extra Slides

Moving on to the Experiment…

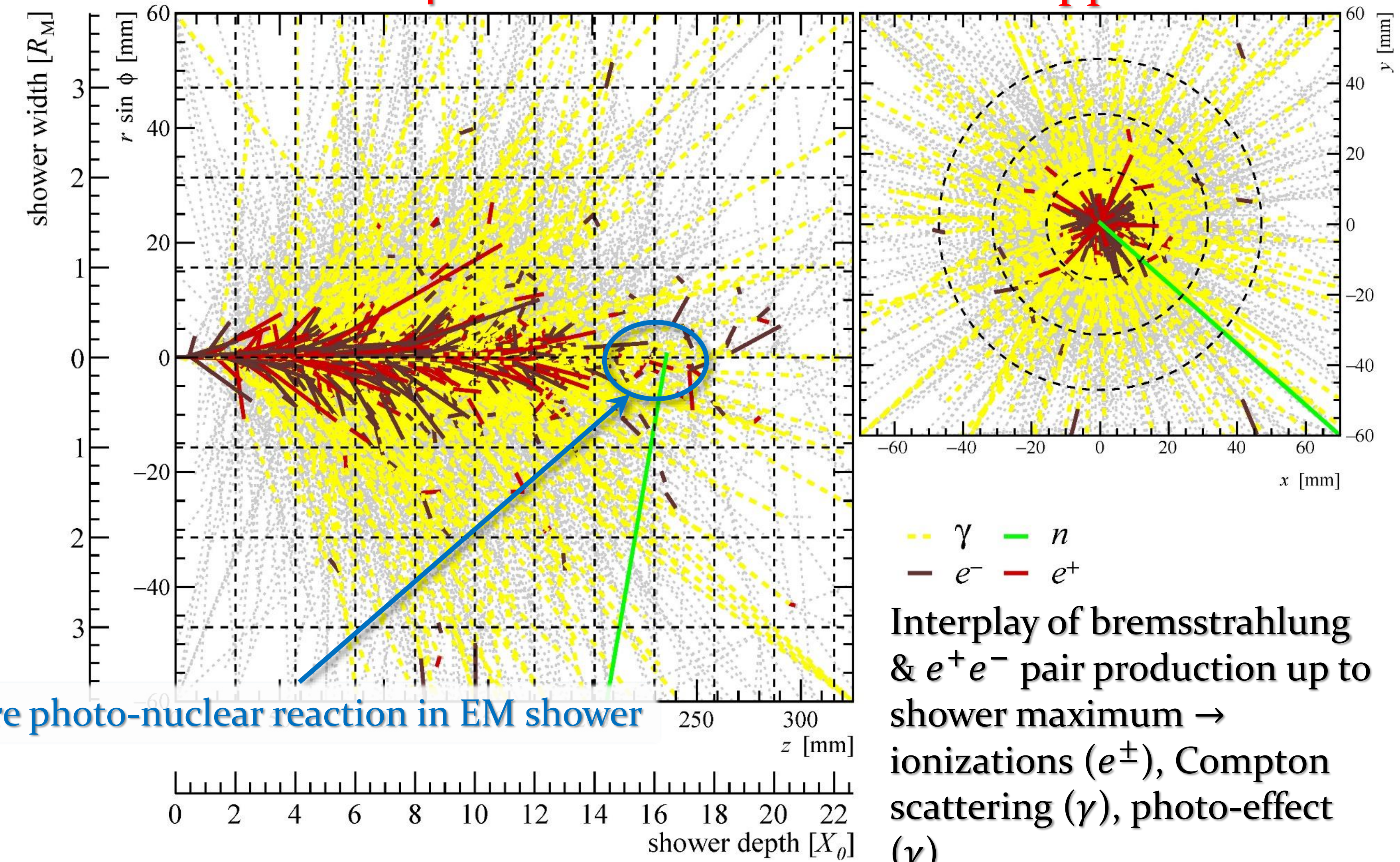


Detector Component of Interest

- ❖ ATLAS calorimeter system (similar for CMS)

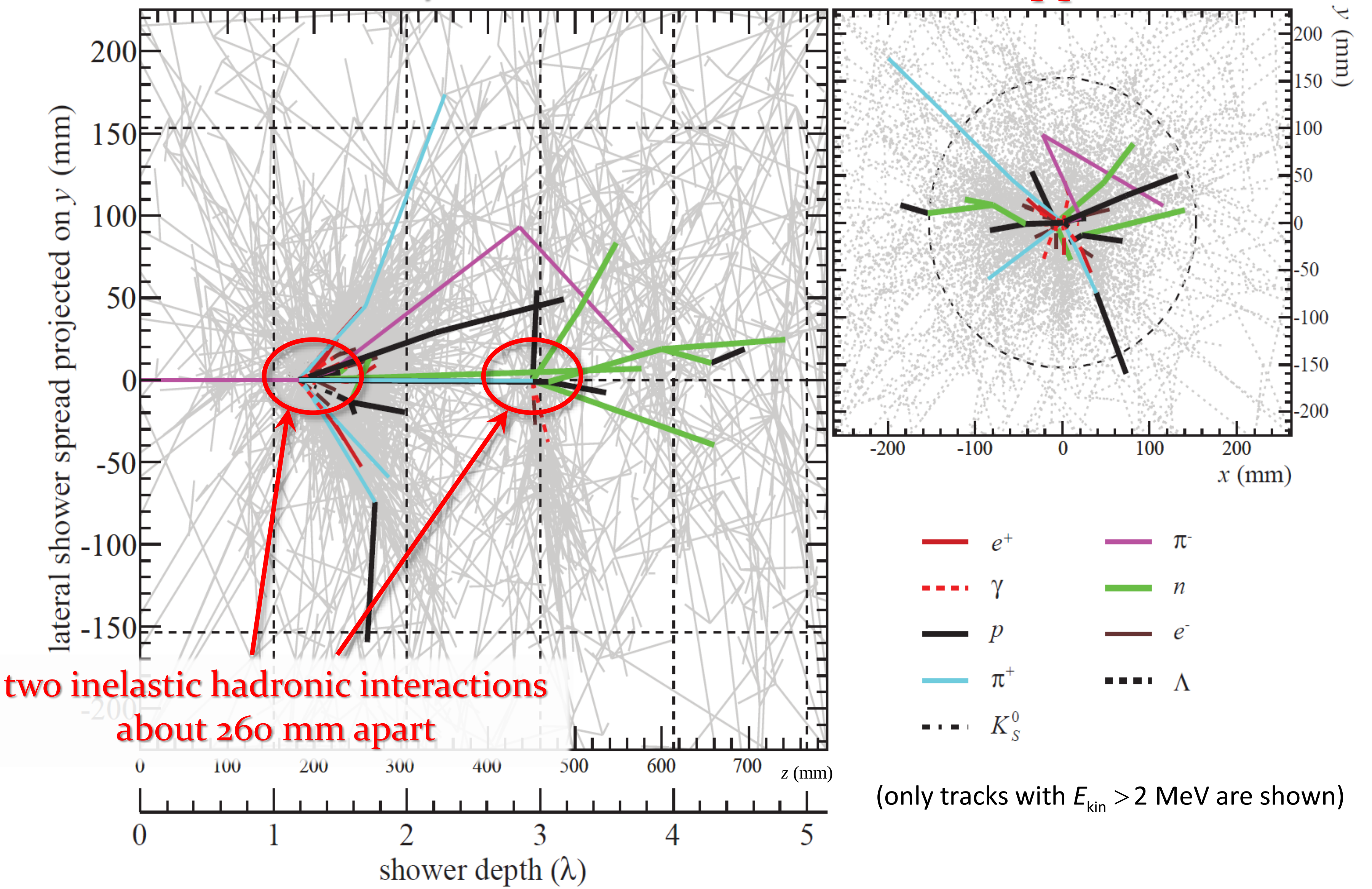


GEANT4 Simulation: 10 GeV e^- in copper



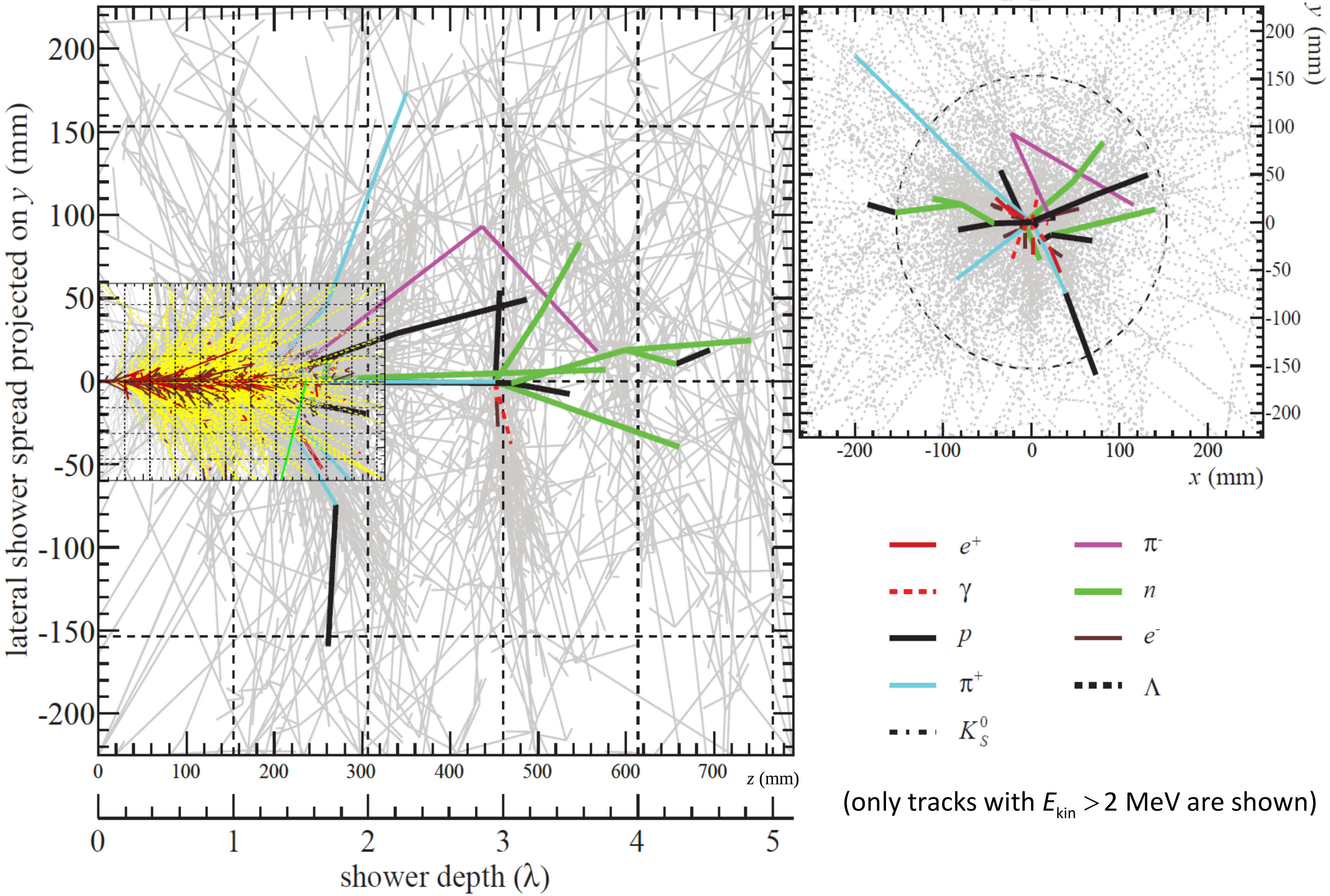
Interplay of bremsstrahlung & e^+e^- pair production up to shower maximum → ionizations ($e^\pm$), Compton scattering (γ), photo-effect (γ)

GEANT4 Simulation: 10 GeV π^+ in copper



(only tracks with $E_{kin} > 2$ MeV are shown)

GEANT4 Simulation: 10 GeV π^+ in copper

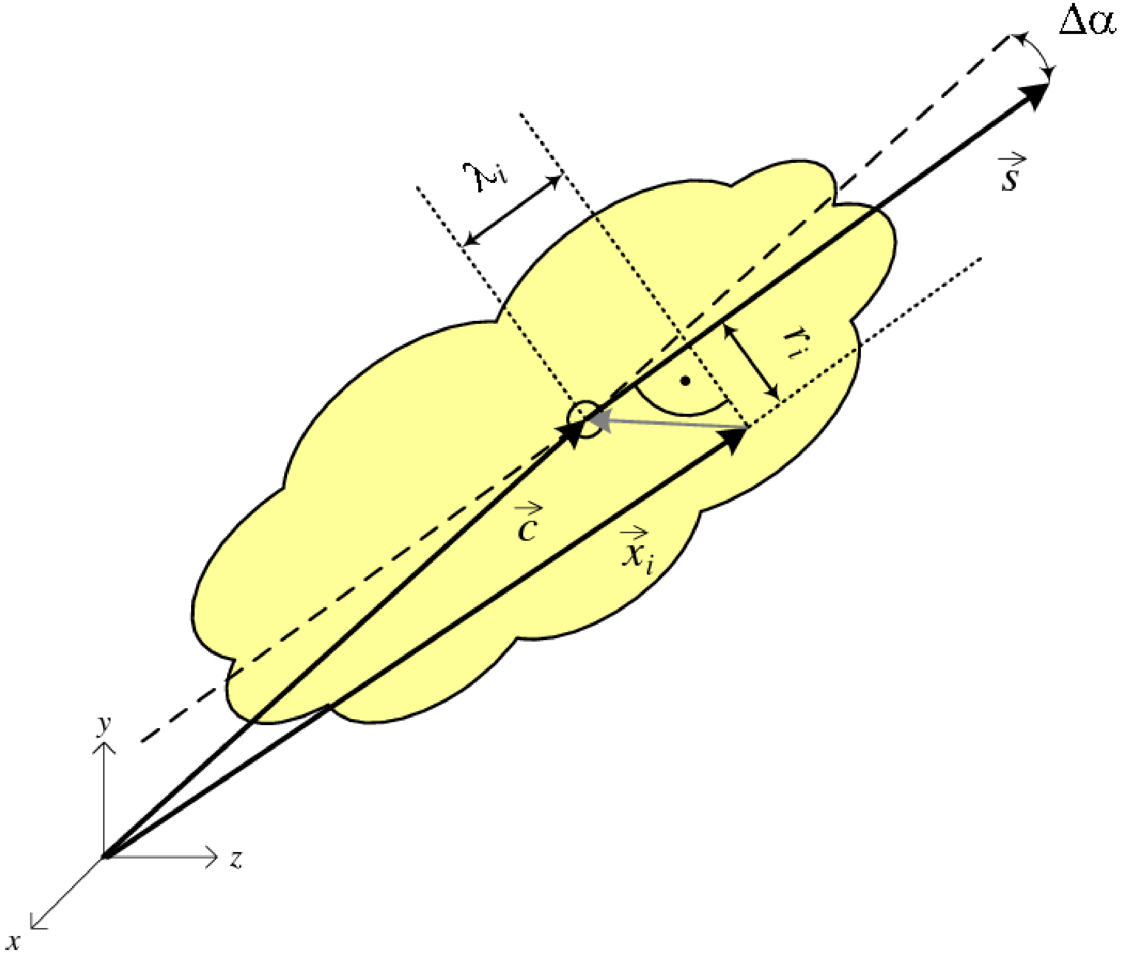


(only tracks with $E_{kin} > 2$ MeV are shown)

ATLAS Calorimeter Features

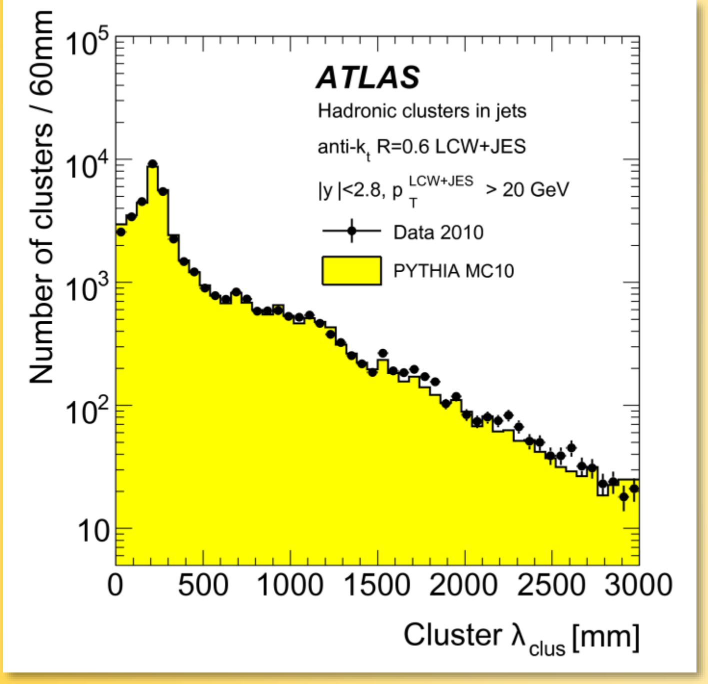
- Hardware
  - Highly granular in central region $|y| < 2.5$, sufficient granularity beyond
  - Non-compensating, hadrons generate less signal than electrons/photons depositing the same energy
- Signal extraction
  - Form three-dimensional clusters of topologically connected cell signals by following signal significance (signal-over-noise) patterns – energy blobs/**topo-cluster**
  - Algorithm features nearest-neighbor growing from a seed – collects neighbors of neighbors if signal significance of neighbor is sufficiently high
  - Applies splitting between local maxima after initial formation
  - Typically reconstructs EM shower into one topo-cluster – hadronic showers can produce > 1 topo-clusters
- Signal calibration
  - Standard LCW algorithm mitigates the non-compensation and corrects for local energy losses introduced by te clustering and losses in inactive material around the topo-cluster
  - LCW uses topo-cluster features representing the signal, the direction, the location and the shape

Geometric Topo-cluster Features



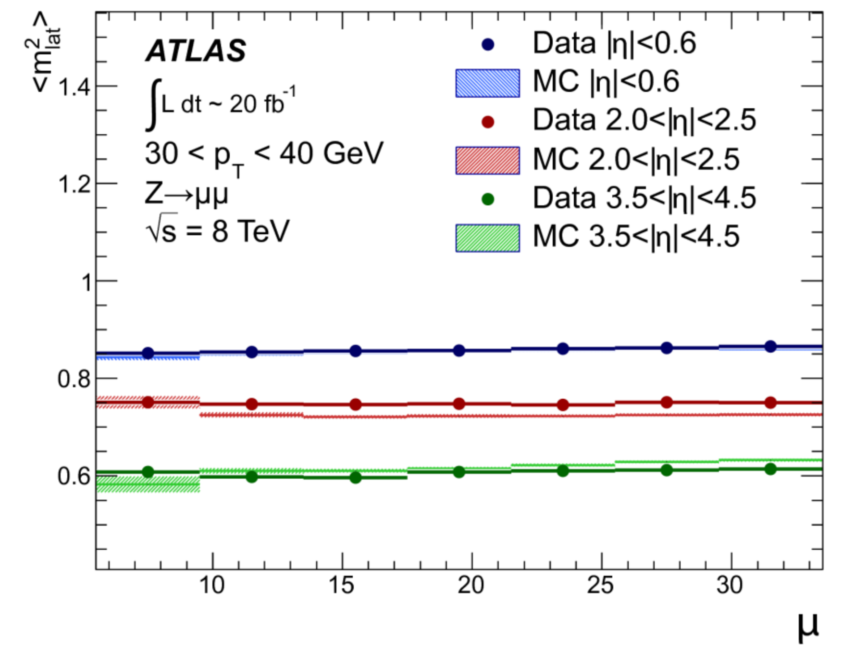
$\vec{c}$	*centre of gravity of cluster, measured from the nominal vertex* $(x = 0, y = 0, z = 0)$ *in ATLAS*
$\vec{x}_i$	*geometrical centre of a calorimeter cell in the cluster, measured from the nominal detector centre of ATLAS*
$\vec{s}$	*particle direction of flight (shower axis)*
$\Delta\alpha$	*angular distance* $\Delta\alpha = \angle(\vec{c}, \vec{s})$ *between cluster centre of gravity and shower axis* $\vec{s}$
λ_i	*distance of cell at* $\vec{x}_i$ *from the cluster centre of gravity measured along shower axis* $\vec{s}$ $(\lambda_i < 0$ *is possible)*
r_i	*radial (shortest) distance of cell at* $\vec{x}_i$ *from shower axis* $\vec{s}$ $(r_i \geq 0)$

Examples of MC Modeling



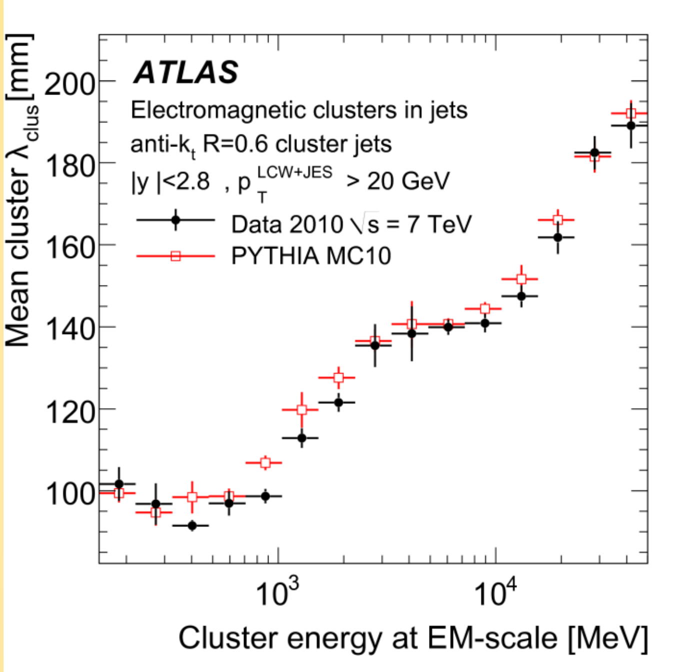
Inclusive spectrum of λ_{clus}

(topo-clusters in jets)



Pile-up dependence of $\langle m_{\text{lat}}^2 \rangle$

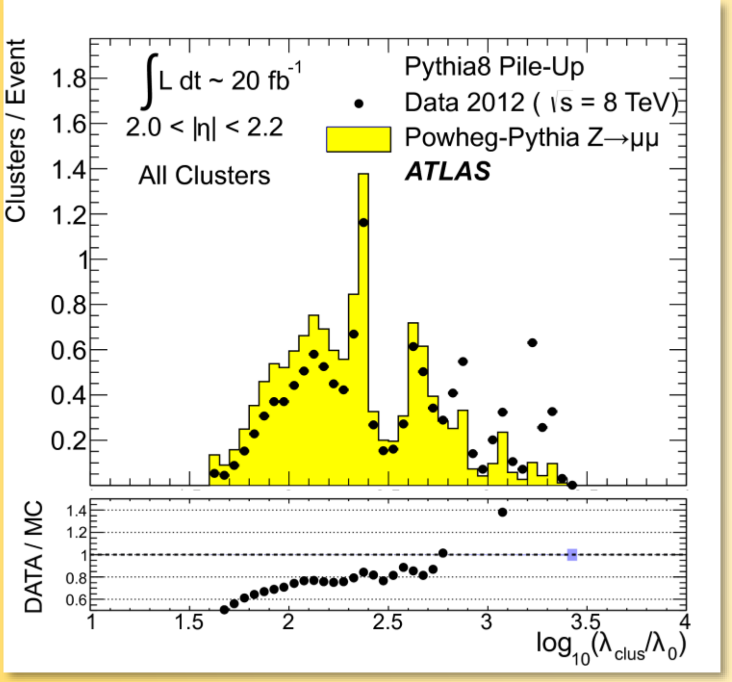
(topo-cluster in jets)



Dependence of $\langle \lambda_{\text{clus}} \rangle$ on $E_{\text{clus}}^{\text{EM}}$

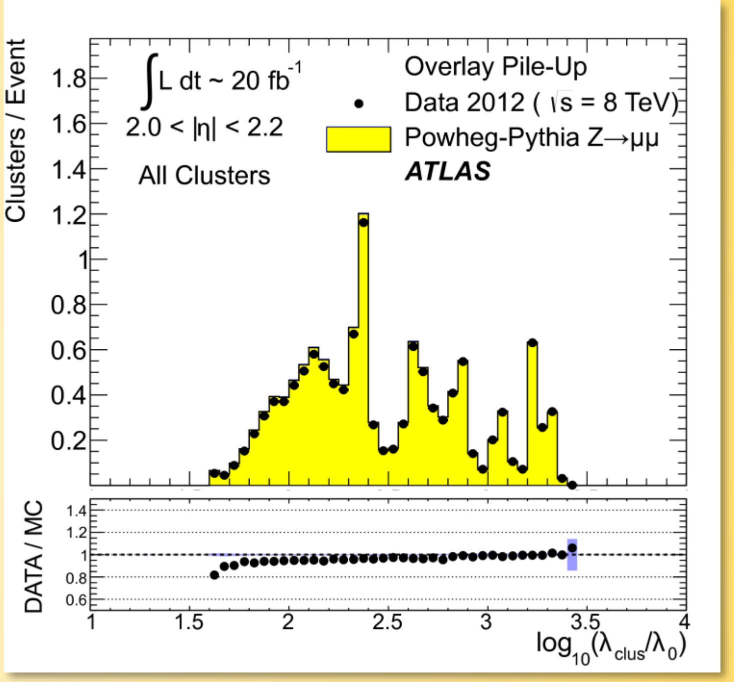
(topo-clusters in jets)

MC Modeling Problems



log(λ_{clus}) distribution of inclusive topo-cluster sample (no jet environment required)

(pile-up insufficiently modeled by MC generator & detector simulation)

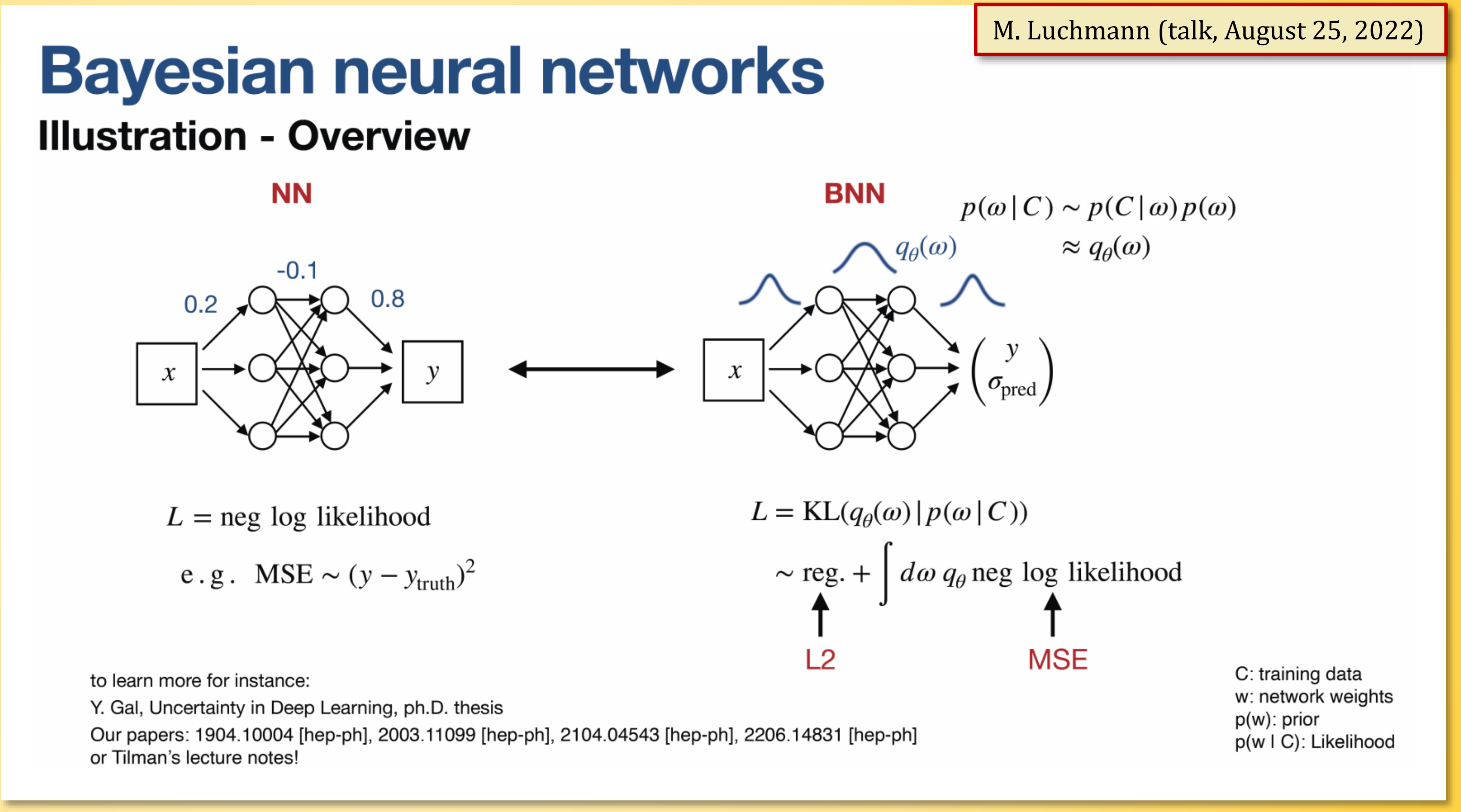


log(λ_{clus}) distribution of inclusive topo-cluster sample (no jet environment required)

(pile-up from data overlaid on hard scatter MC simulation)

Recent Considerations: BNN

- Bayesian networks
  - Principles
    - Sample of networks emulated by sampling weights from trained (Gaussian with mean $\bar{A}(w)$ and width $\sigma_{\mathrm{stoch}}(w)$) weight distributions $q_\theta(w)$ instead of training fixed weights w
    - **Contributes uncertainties** due to sampling ($\sigma_{\mathrm{stoch}}(w)$) from each network and due to training multiple networks simultaneously ($\sigma_{\mathrm{pred}}(w)$) $\Rightarrow$ **calibration model uncertainties**



Inputs from, and discussions with, **P.A. Delsart** & **Ana Peixoto** (both LPSC Grenoble), **Chris Delitzsch** (University of Dortmund) and a lot of advice, technical (implementation) help and code from **T. Plehn** & **M. Luchmann** (both University of Heidelberg)

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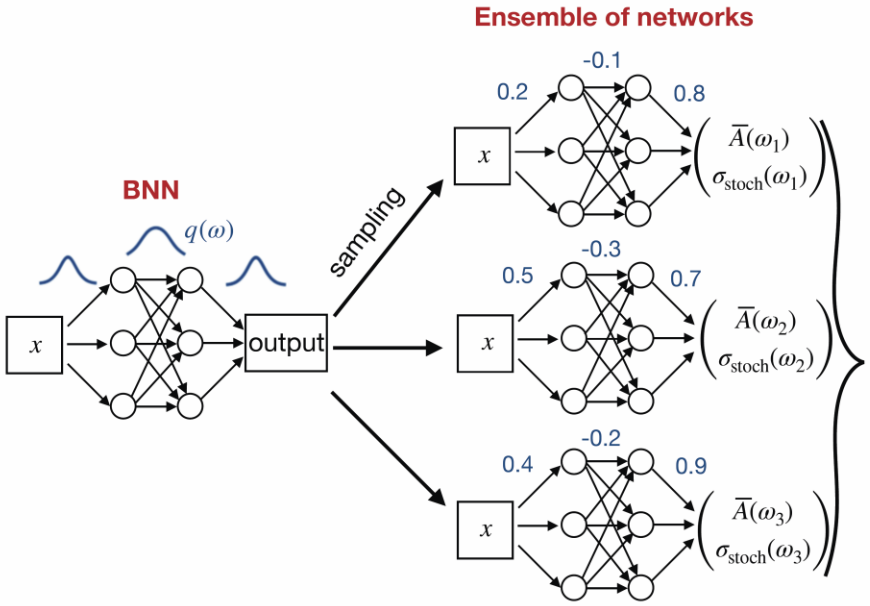
M. Luchmann (talk, August 25, 2022)

Bayesian neural networks

Illustration - BNN as an ensemble of ordinary networks



Output

$$\langle A \rangle = \frac{1}{N} \sum_{i=1}^{N} \bar{A}(w_i)$$

$$\sigma^2_{\text{stoch}} = \frac{1}{N} \sum_{i=1}^{N} \sigma^2_{\text{stoch}}(w_i)$$

$$\sigma^2_{\text{pred}} = \frac{1}{N} \sum_{i=1}^{N} (\langle A \rangle - \bar{A}(w_i))^2$$

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