

# ATLAS FAST SIMULATION – From Classical to Deep Learning

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On behalf of ATLAS Collaboration

*ATLAS, one of the largest experiments at the Large Hadron Collider, has a broad physics program, ranging from precision measurements to the discovery of new interactions. Completing that program requires gargantuan amounts of simulated Monte Carlo events. Detailed detector simulation with Geant4 provides good agreement to data, but, due to the complexity of the detector, the CPU resources required are extraordinary. For more than 10 years, ATLAS has developed and utilized tools that replace the slowest part of the simulation - the calorimeter shower simulation - by faster alternatives. AtFast3, or AF3, is the latest generation of high precision fast simulation in ATLAS. AF3 combines Geant4 with a parametrization-based Fast Calorimeter Simulation and a new deep learning-based Fast Calorimeter Simulation. AF3 has achieved the speed up required to meet the computing challenges and Monte Carlo needs for Run 3. With unprecedented precision and the ability to model jet substructure, AF3 can be used to simulate almost all physics processes. For high luminosity LHC, further improvement in physics modeling along with a fast simulation for the inner detector is expected.*

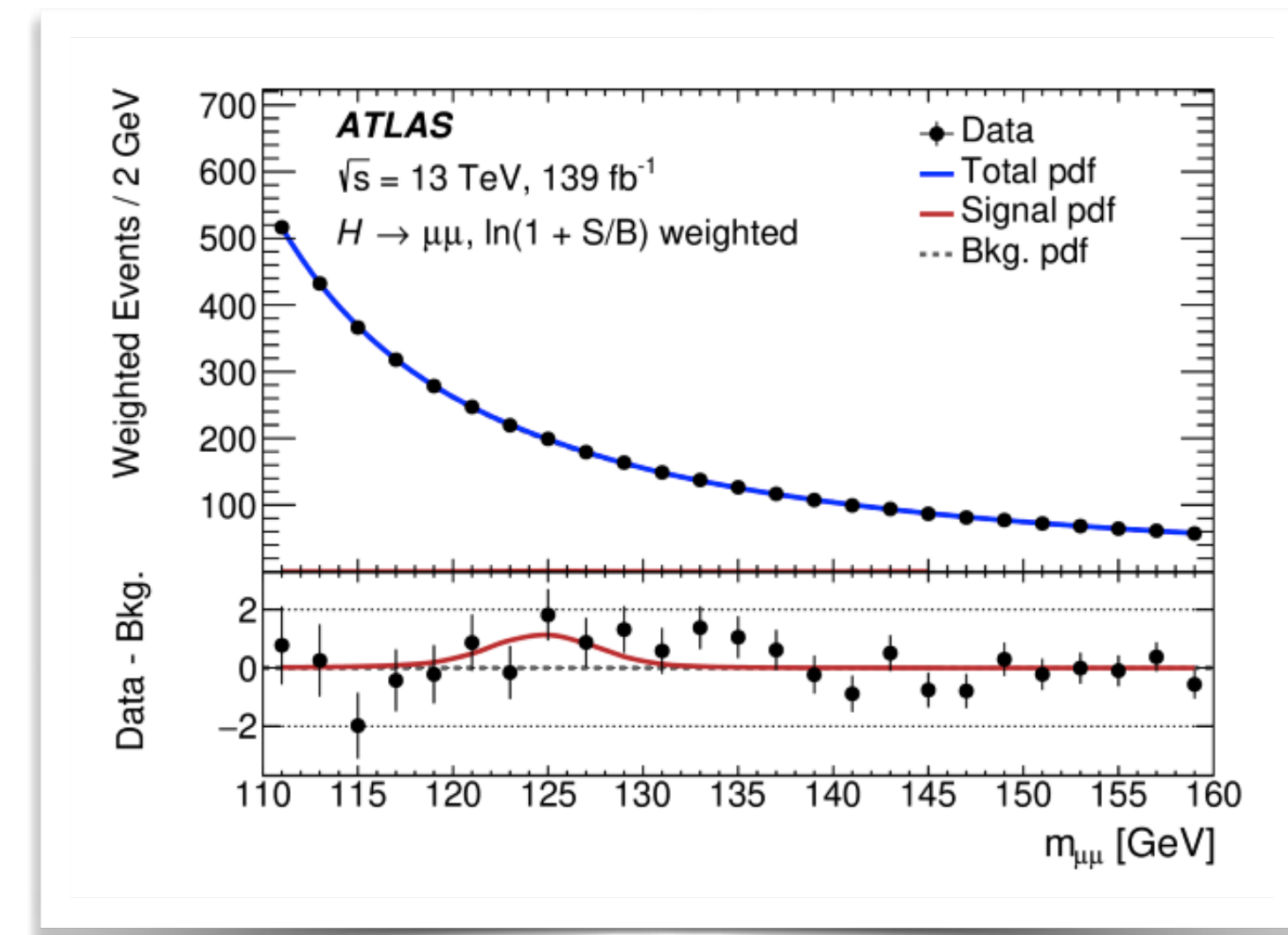
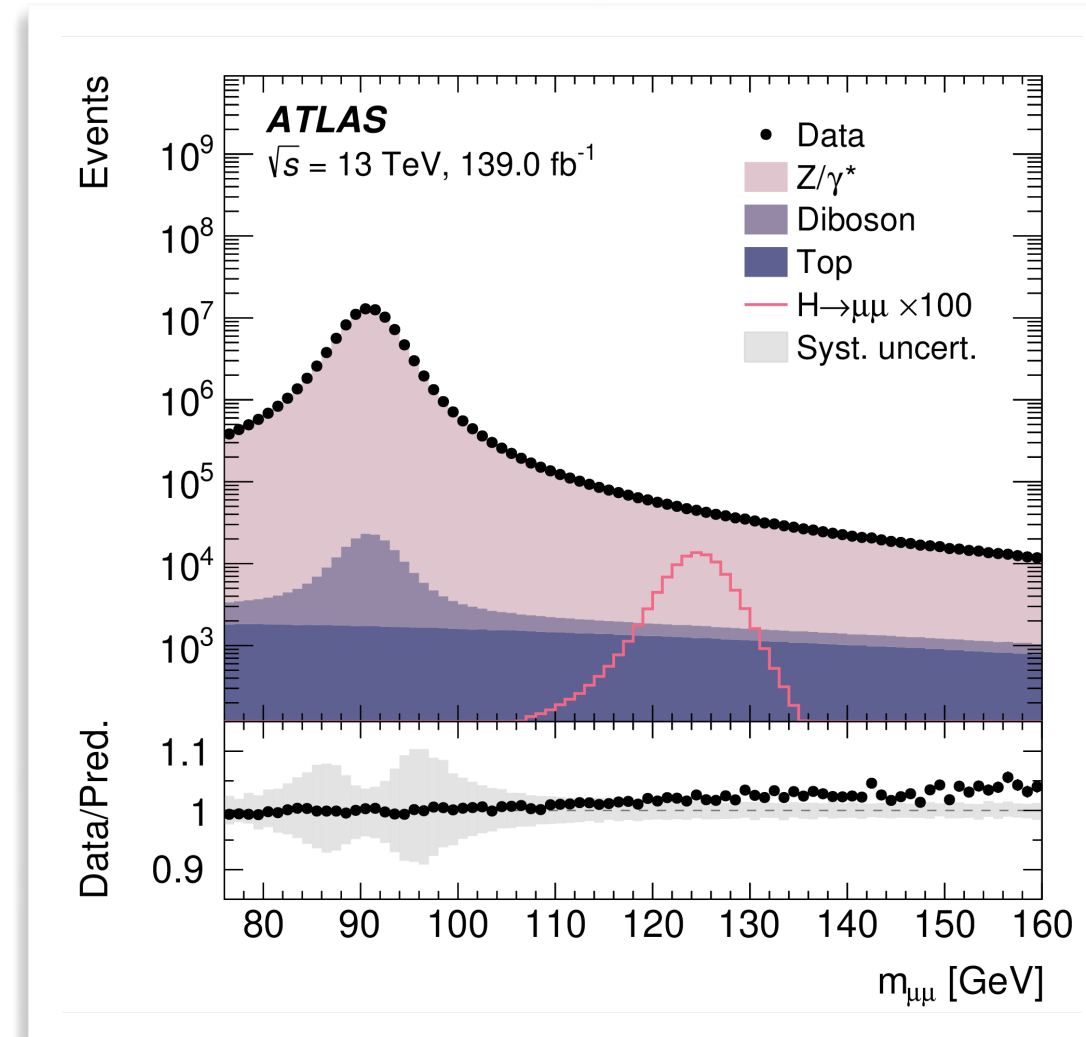
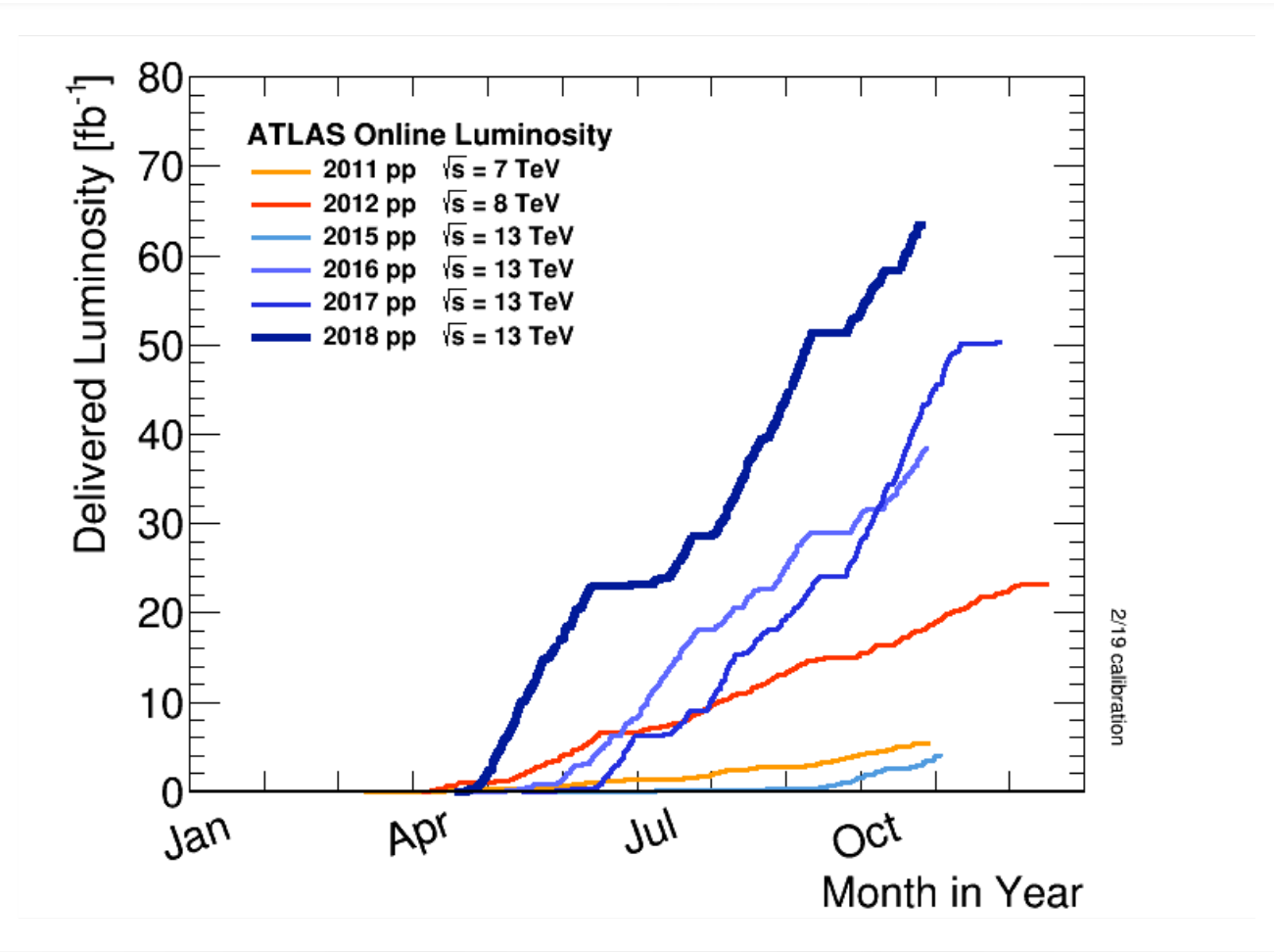


# ATLAS physics program - Importance of simulated events

- ◆ ATLAS collaboration covers a **wide ranging physics program** - from precision measurements to searches for new physics interaction.
- ◆ **Monte Carlo simulated events (both hard scatter and pile up)** are integral to this process - requiring a statistics equivalent to several times of the data luminosity.
- ◆ At 13 TeV center of mass energy, ATLAS recorded  $147 \text{ fb}^{-1}$  of data which will **increase significantly** in Run 3 and during High Luminosity(HL-) LHC.

*Dimuon invariant mass in the range 76–160 GeV. Data in points are compared to a full set of fully simulated background processes and the total background prediction is scaled to the integrated data yield. The  $H \rightarrow \mu\mu$  signal shown is the sum of the ggF, VBF, VH and ttH as open line, normalized to one hundred times the SM prediction for visibility.*

*The invariant-mass spectrum of the reconstructed muon-pairs in ATLAS data. Events are weighted according to the expected signal-to-background ratio of their category. In the top panel, the signal-plus-background fit is visible in blue, while in the lower panel the fitted signal (in red) is compared to the difference between the data and the background model.*

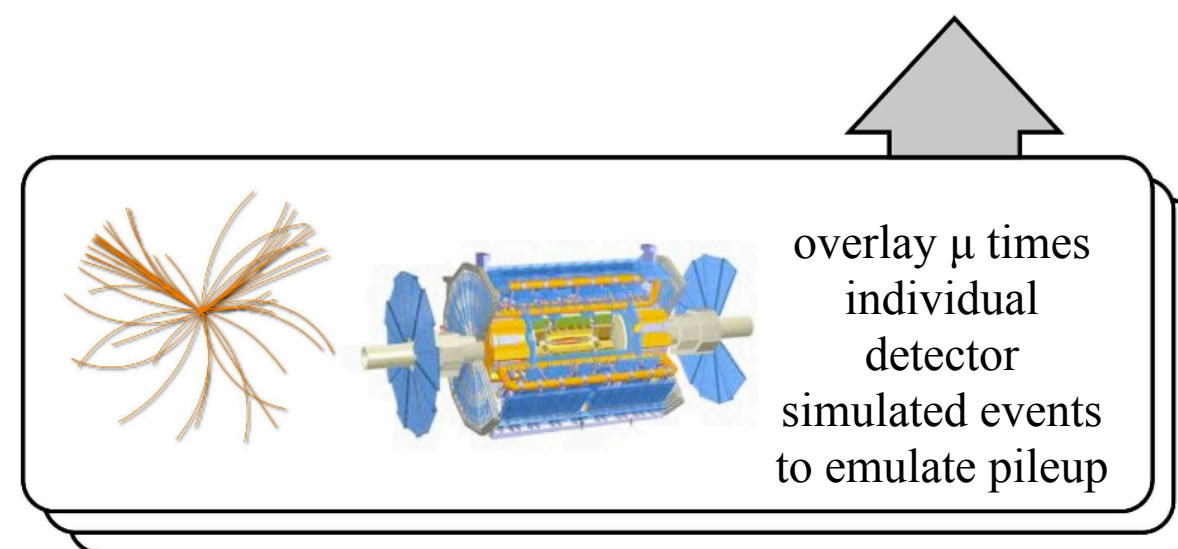
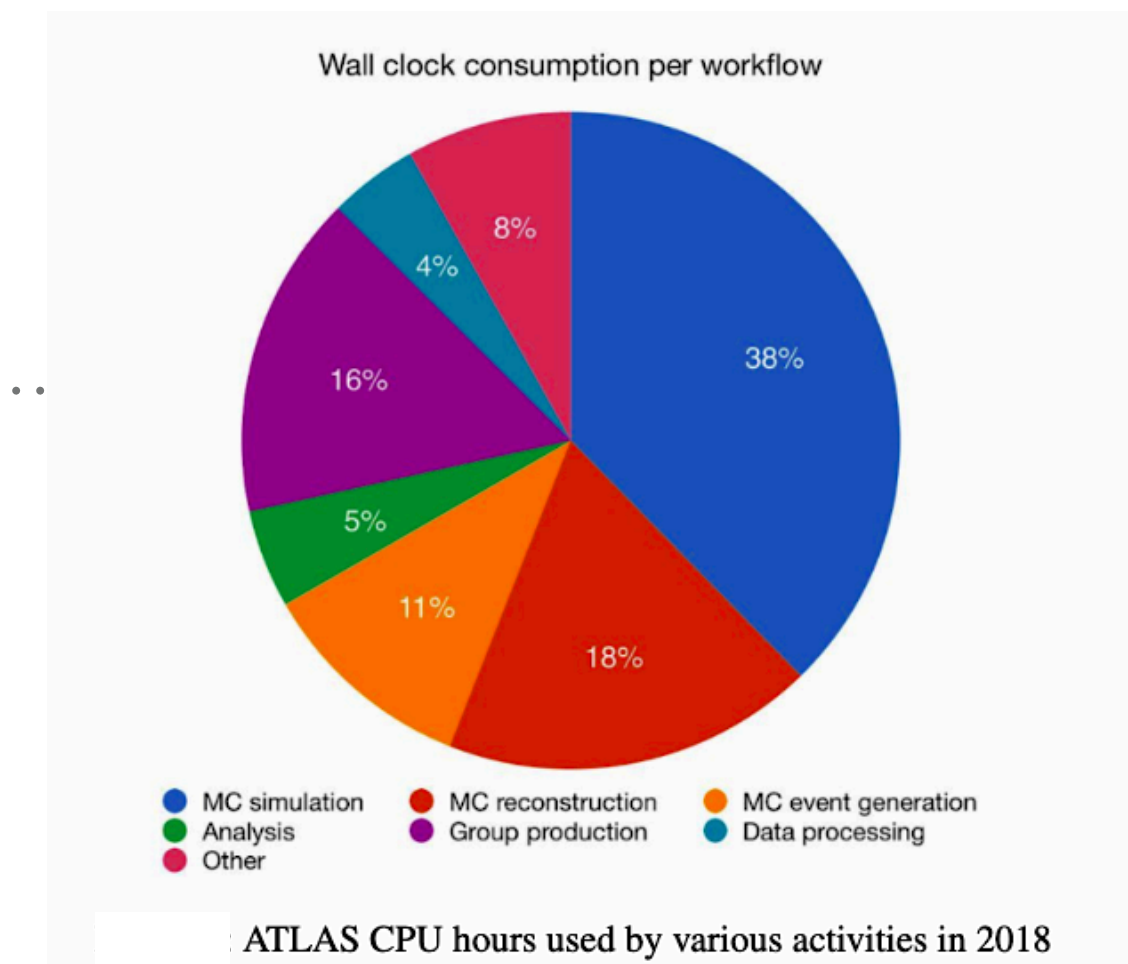
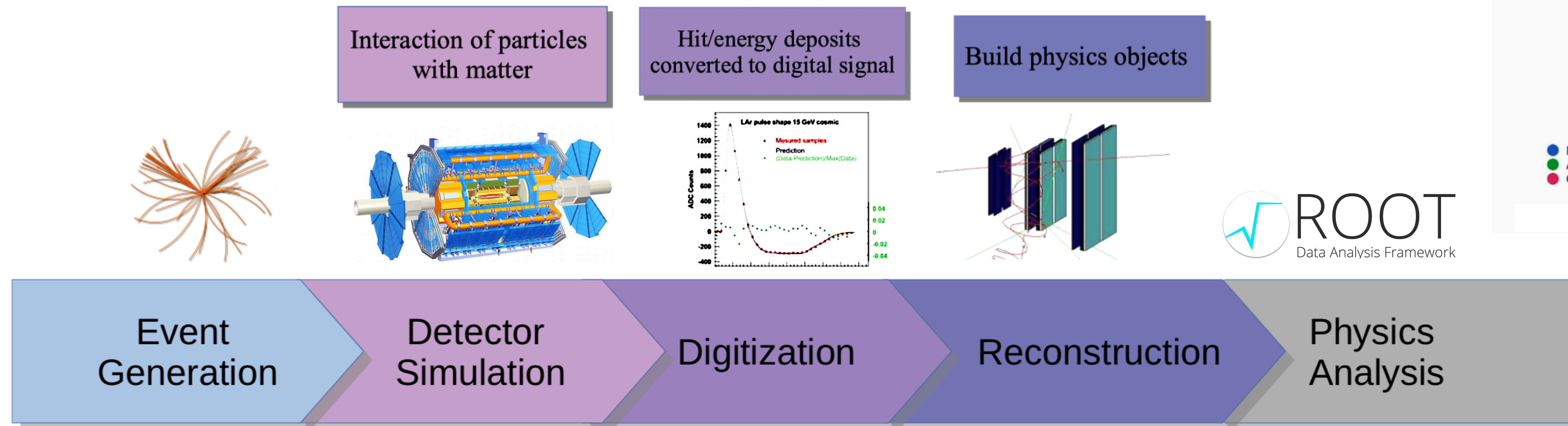


*First hint of the Higgs boson decaying to a muon pair! with significance of 2.0 standard deviations.*

*More data to be collected in Run 3 and during the operation of the High-Luminosity LHC will help close in on this first hint!.*



# ATLAS Monte Carlo production steps



Subdetector	Simulation window [ns]
BCM	-50, +25
Pixel trackers	-50, +25
SCT	-50, +25
TRT	-50, +50
LAr calorimeter	-801, +126
Tile calorimeter	-200, +200
Muon chambers	-1000, +700

## Detector Simulation:

- ◆ Dense hit content in inner trackers
- ◆ Complex geometry with lots of volumes and complicated boundaries

## Digitization:

- ◆ Large number of inner tracker readout channels
- ◆ Complex modeling of readout emulation

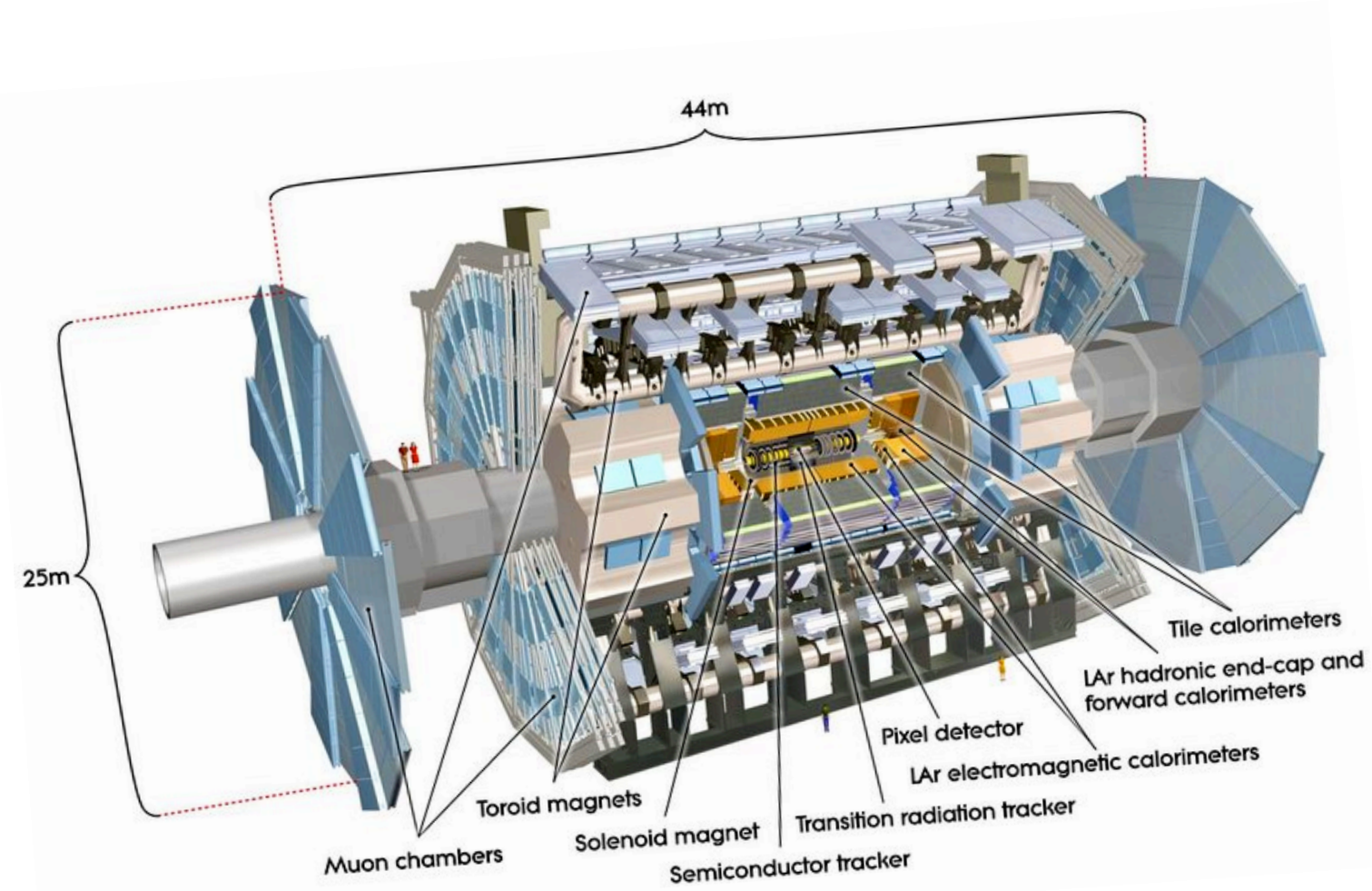
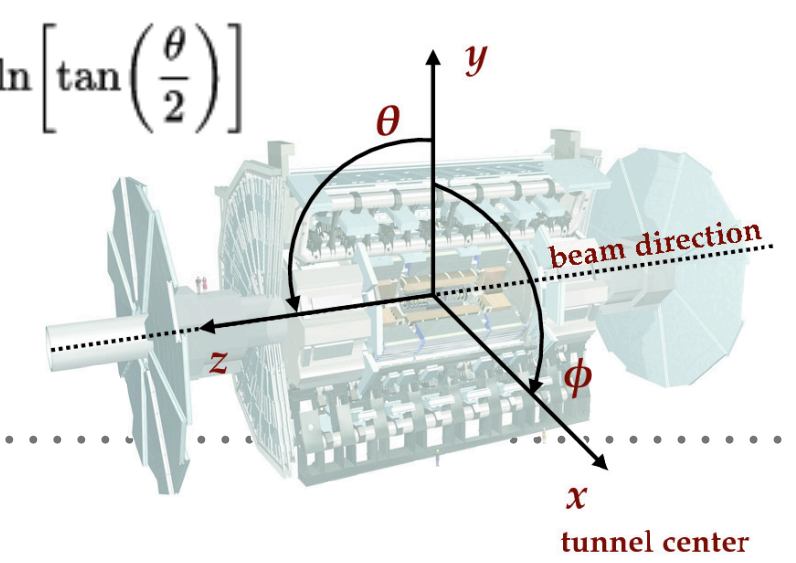
## Reconstruction:

- ◆ Pattern recognition (combinatorics) function of average pileup - tracking

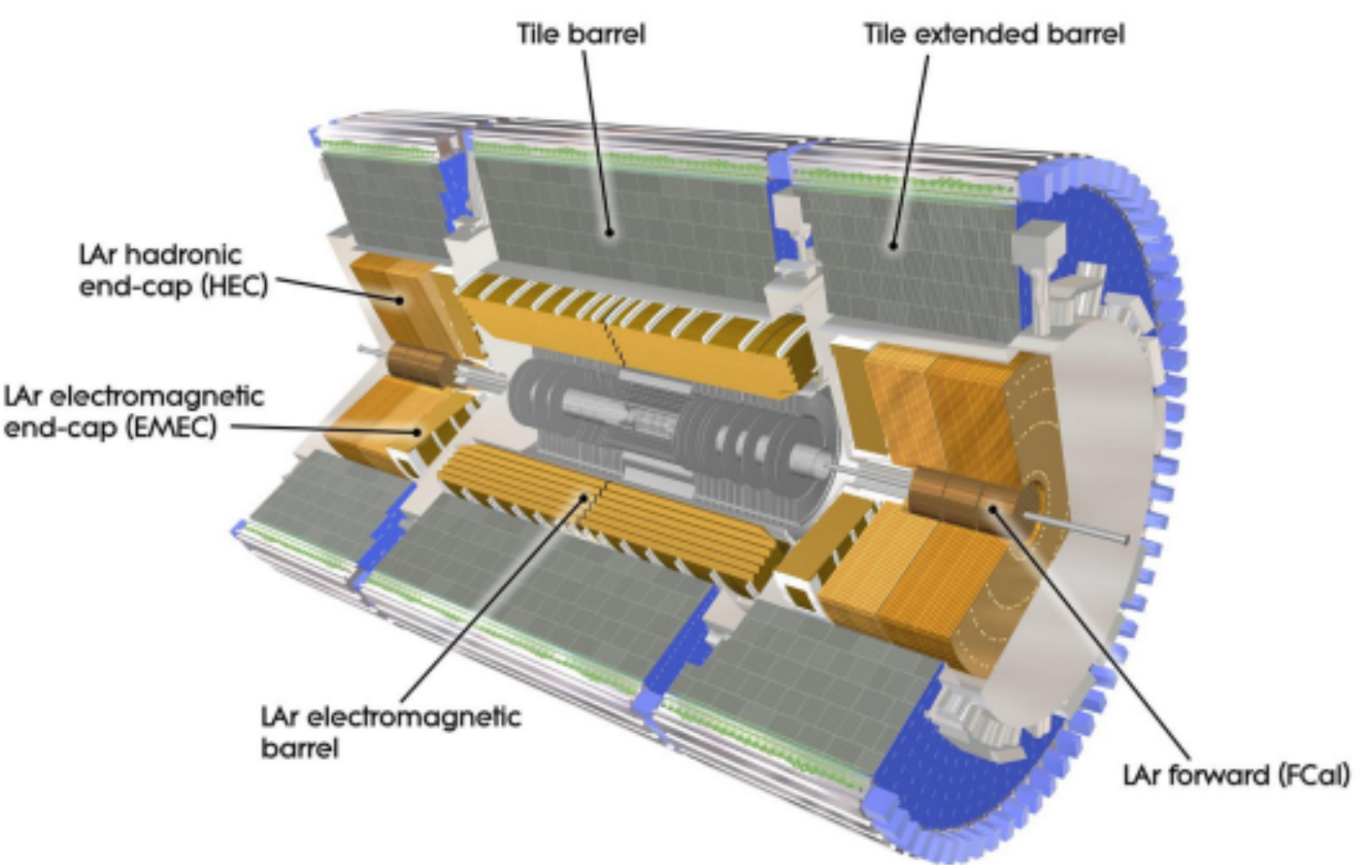


# ATLAS Calorimeter

$$\eta \equiv -\ln \left[ \tan \left( \frac{\theta}{2} \right) \right]$$

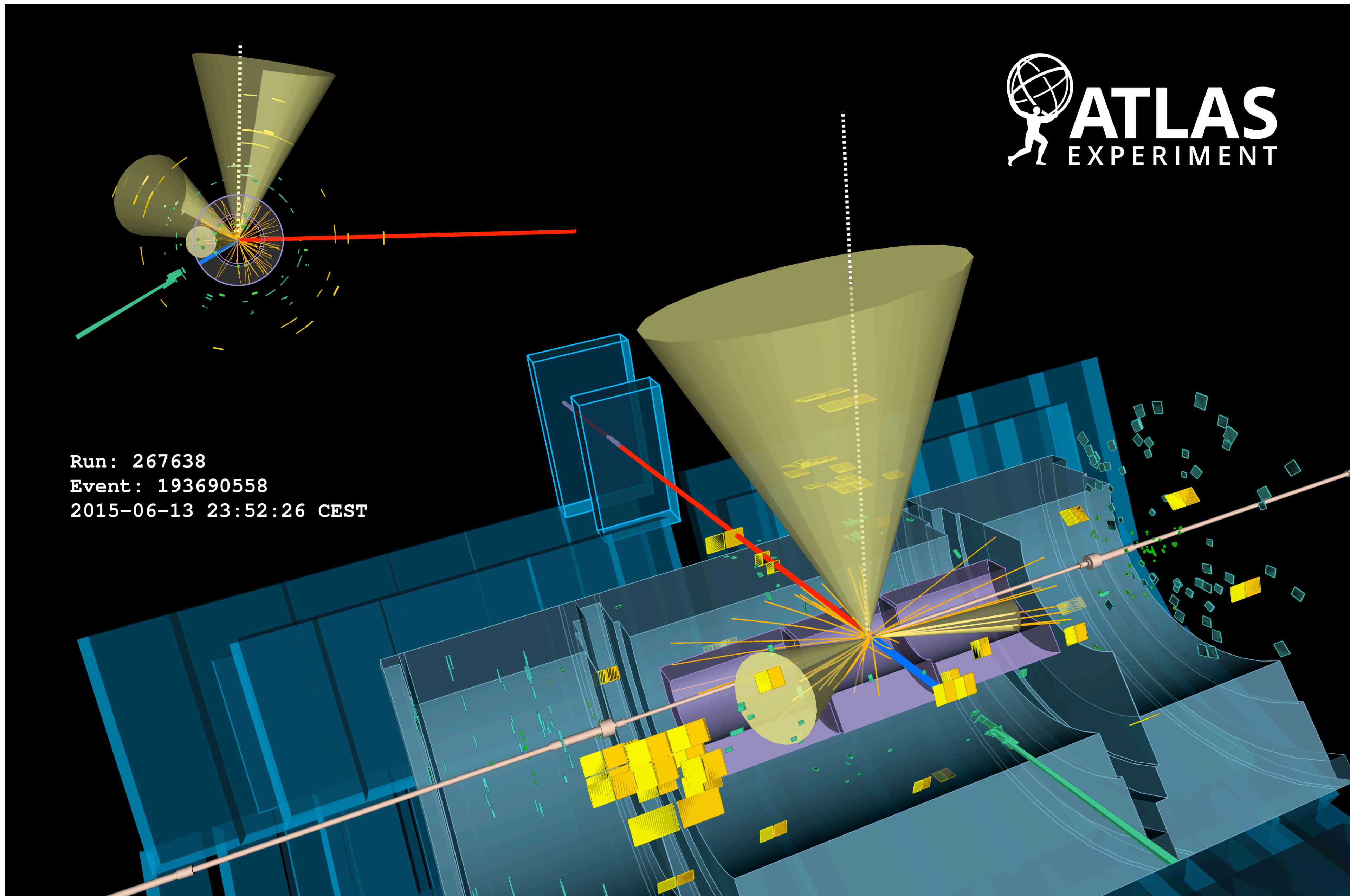


- ◆ ATLAS detector covers nearly the **entire solid angle** around the collision point.
- ◆ **Inner tracking Detector (ID)** - Provide good charged-particle momentum resolution and reconstruction efficiency in the inner tracker for offline tagging of  $\tau$ -leptons and b-jets.
- ◆ **Electromagnetic and Hadronic calorimeters** - Sampling calorimeter with complex geometries and boundaries. Provide electron and photon identification and accurate jet and missing transverse energy measurements.
- ◆ **Muon Spectrometer (MS)** - Good muon identification and momentum resolution over a wide range of momenta.



Calorimeter	Layers	Module Name	$\eta$ -coverage	Sampling Layer
Electromagnetic calorimeters	4	Electromagnetic Barrel (EMB)	$ \eta  < 1.5$	PreSamplerB, EMB1, EMB2, EMB3
	4	Electromagnetic Endcap (EMEC)	$1.5 <  \eta  < 1.8$	PreSamplerE
			$1.5 <  \eta  < 3.2$	EME1, EME2
Hadronic calorimeters			$1.5 <  \eta  < 2.5$	EME3
	4	Hadronic Endcap (HEC)	$1.5 <  \eta  < 3.2$	HEC0, HEC1, HEC2, HEC3
	3	Tile Barrel (TileBar)	$ \eta  < 1.0$	TileBar0, TileBar1, TileBar2
	3	Tile Extended Barrel (TileExt)	$0.8 <  \eta  < 1.7$	TileExt0, TileExt1, TileExt2
Forward calorimeter	3	Tile Gap (TileGap)	$1.0 <  \eta  < 1.6$	TileGap1, TileGap2, TileGap3
	3	FCal	$3.1 <  \eta  < 4.9$	FCal0, FCal1, FCal2
Transition regions	-	between barrel and endcap	$ \eta  \approx 1.45$	-
	-	between outer and inner wheel of endcap	$ \eta  = 2.5$	-
	-	between endcap and FCal	$ \eta  \approx 3.2$	-





Run: 267638  
 Event: 193690558  
 2015-06-13 23:52:26 CEST

*Display of a top anti-top quark pair candidate event from proton-proton collisions recorded by ATLAS with LHC stable beams at a collision energy of 13 TeV.*

*The red line shows the path of a muon with transverse momentum around 140 GeV through the detector.*

*The blue line shows the path of an electron with transverse momentum around 170 GeV through the detector.*

*The green and yellow bars indicate energy deposits in the liquid argon and scintillating-tile calorimeters, from these deposits 3 jets are identified with transverse momenta between 30 and 80 GeV.*

*Two of the jets are identified as having originated from b-quarks.*

*Tracks reconstructed from hits in the inner tracking detector are shown as arcs curving in the solenoidal magnetic field*



# Shower generation

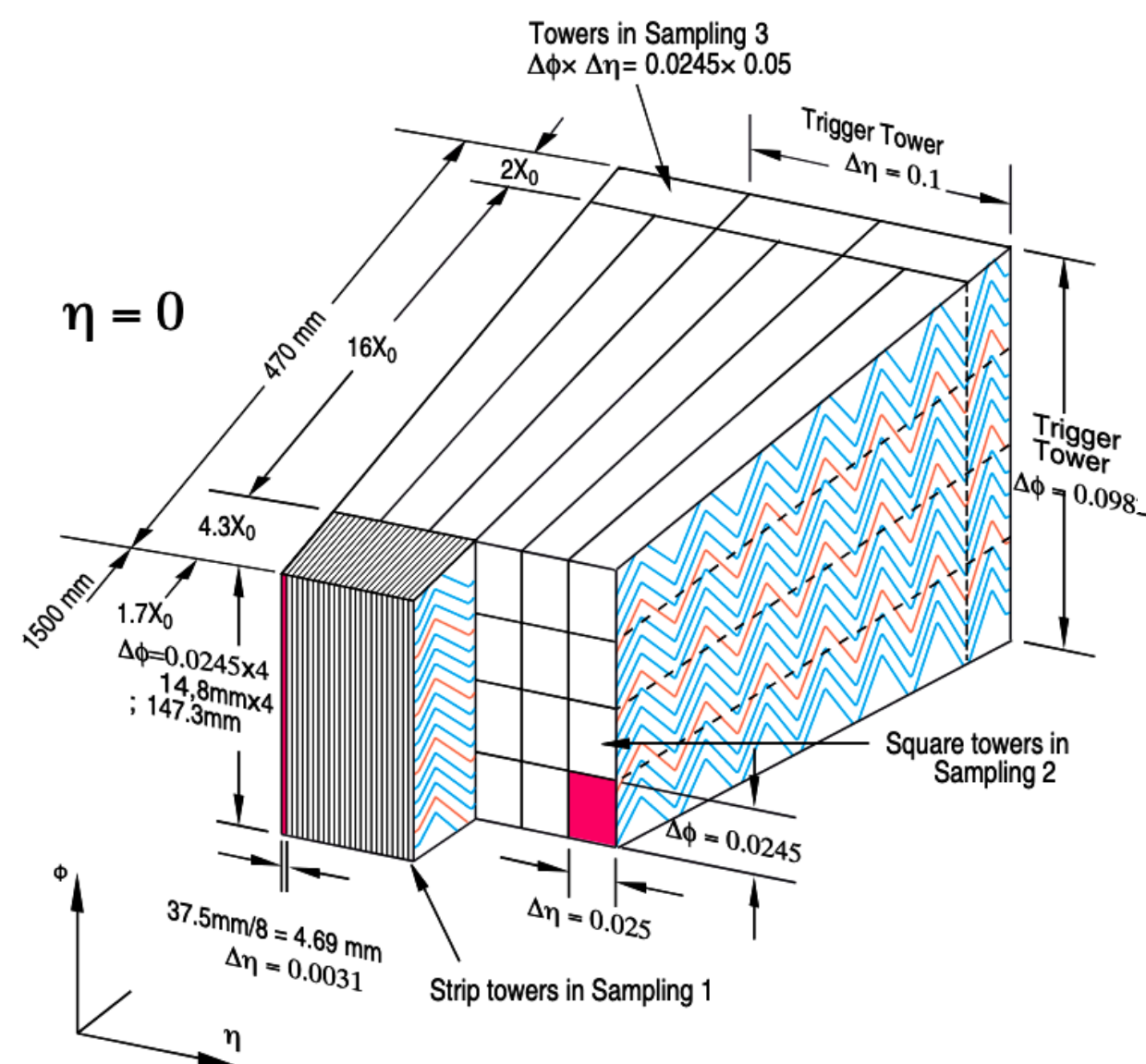
## Electromagnetic (EM) Cal:

- Liquid Argon (active)
- Pb/Cu/Tungsten (absorber)

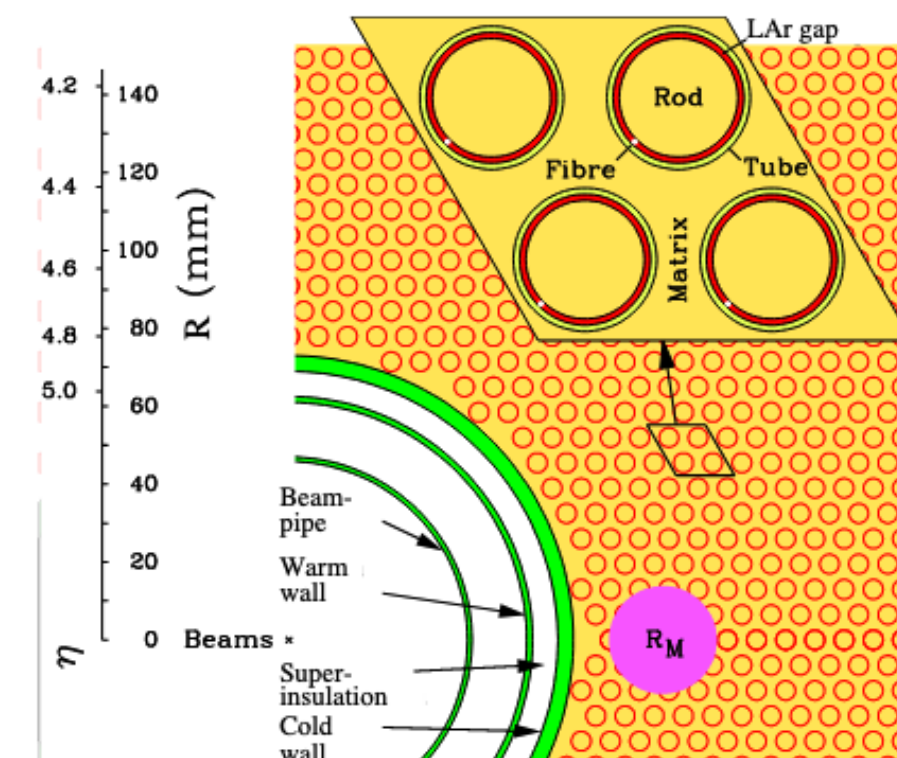
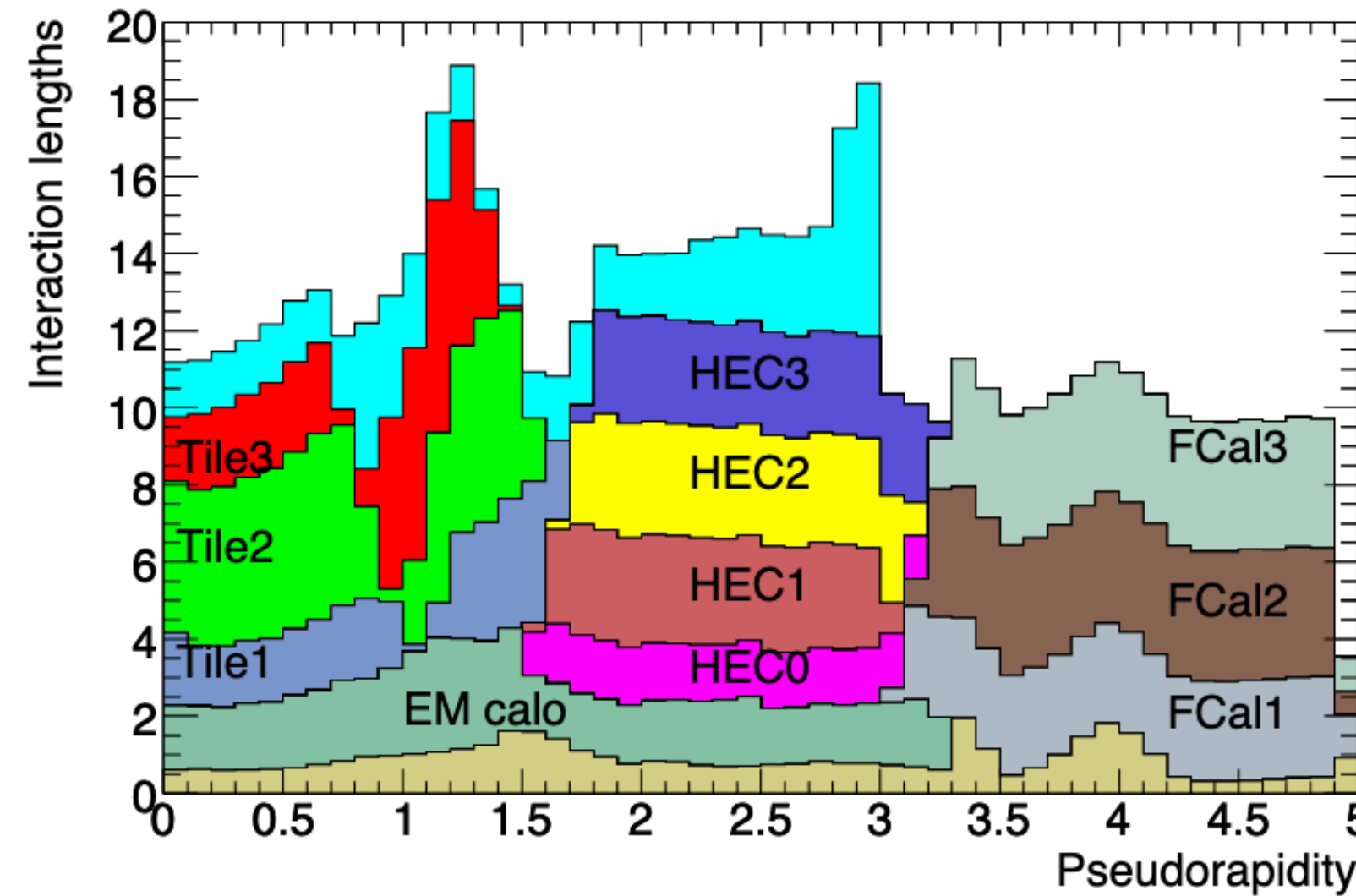
## Hadronic/Tile Cal:

- Scintillating tiles (active)
- Steel (absorber)

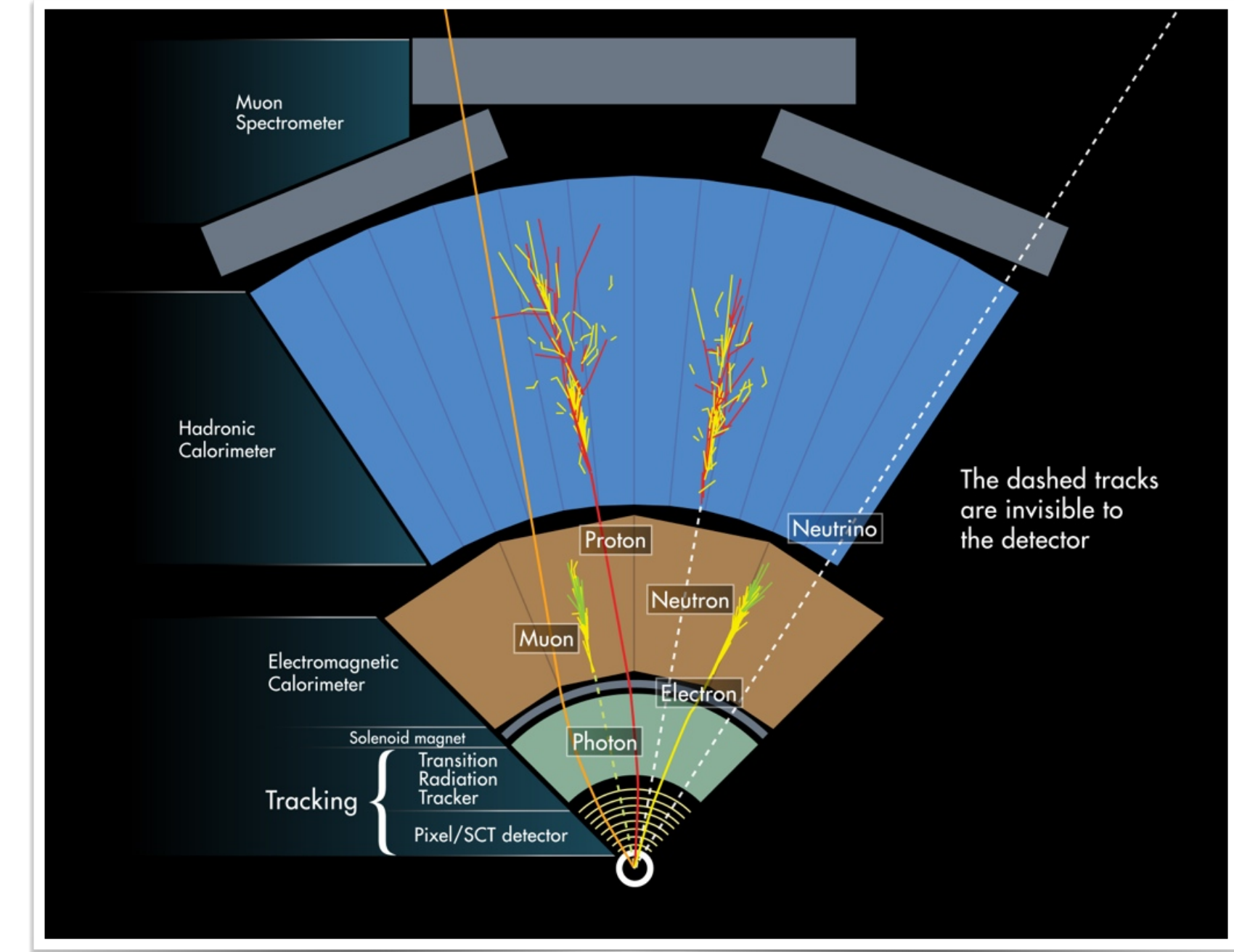
◆ 80% of the total simulation time is required for shower simulation (based on a typical  $t\bar{t}$  event) - dense materials, unusual geometry e.g. accordion shape



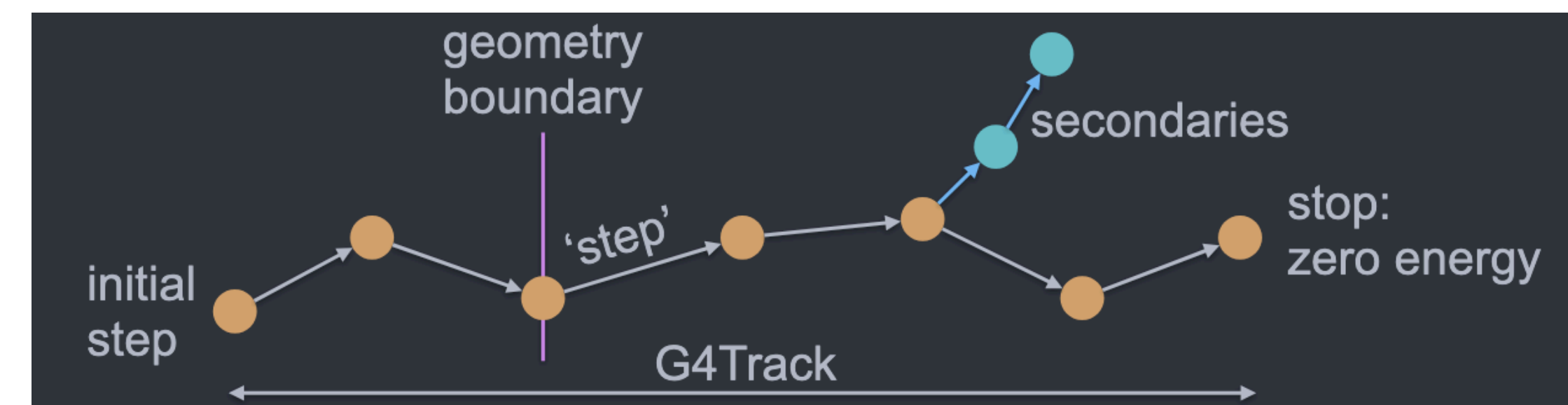
EM barrel



FCal



Simulation in Geant4 with each Geant4 process responsible for the smallest unit called 'step'

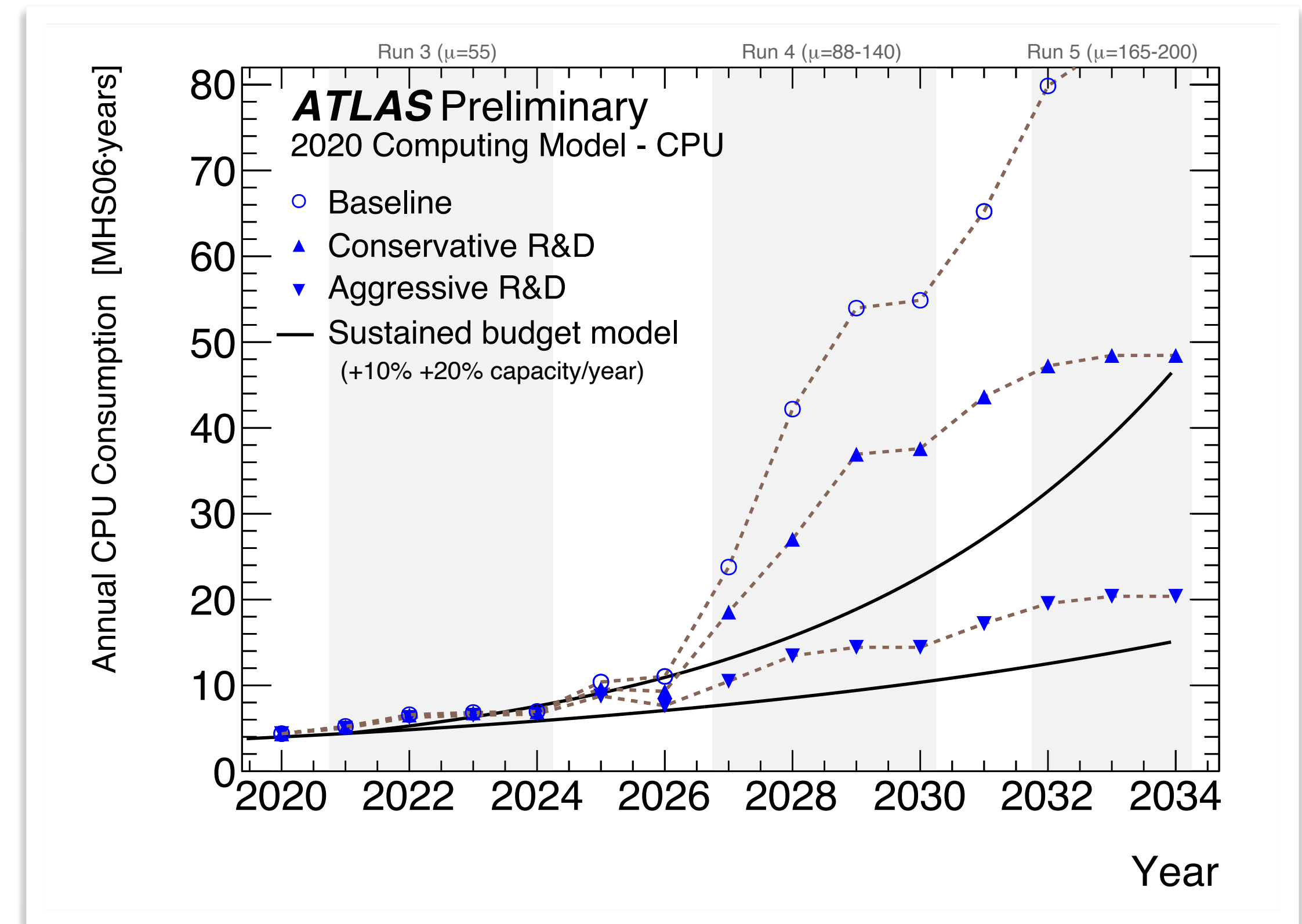


No. of steps  $\propto$  simulation time



# Challenges in Simulation: Run 3 & beyond

- Simulation of the ATLAS detector with Geant4 is CPU intensive.
- The CPU requirements will increase due to the increased luminosity and pileup in Run 3 & HL-LHC.
- In Run 3, > 50% of all events will be simulated with fast simulation increasing to > 75% in Run 4 to mitigate this.
- Beyond Run 3 **fast Inner Detector (ID) simulation** along with **fast digitization** can be used. [2]
- We can also utilize the inherent parallelism of fast calorimeter simulation with GPUs. [3]



[1] [HS06 benchmark](#)

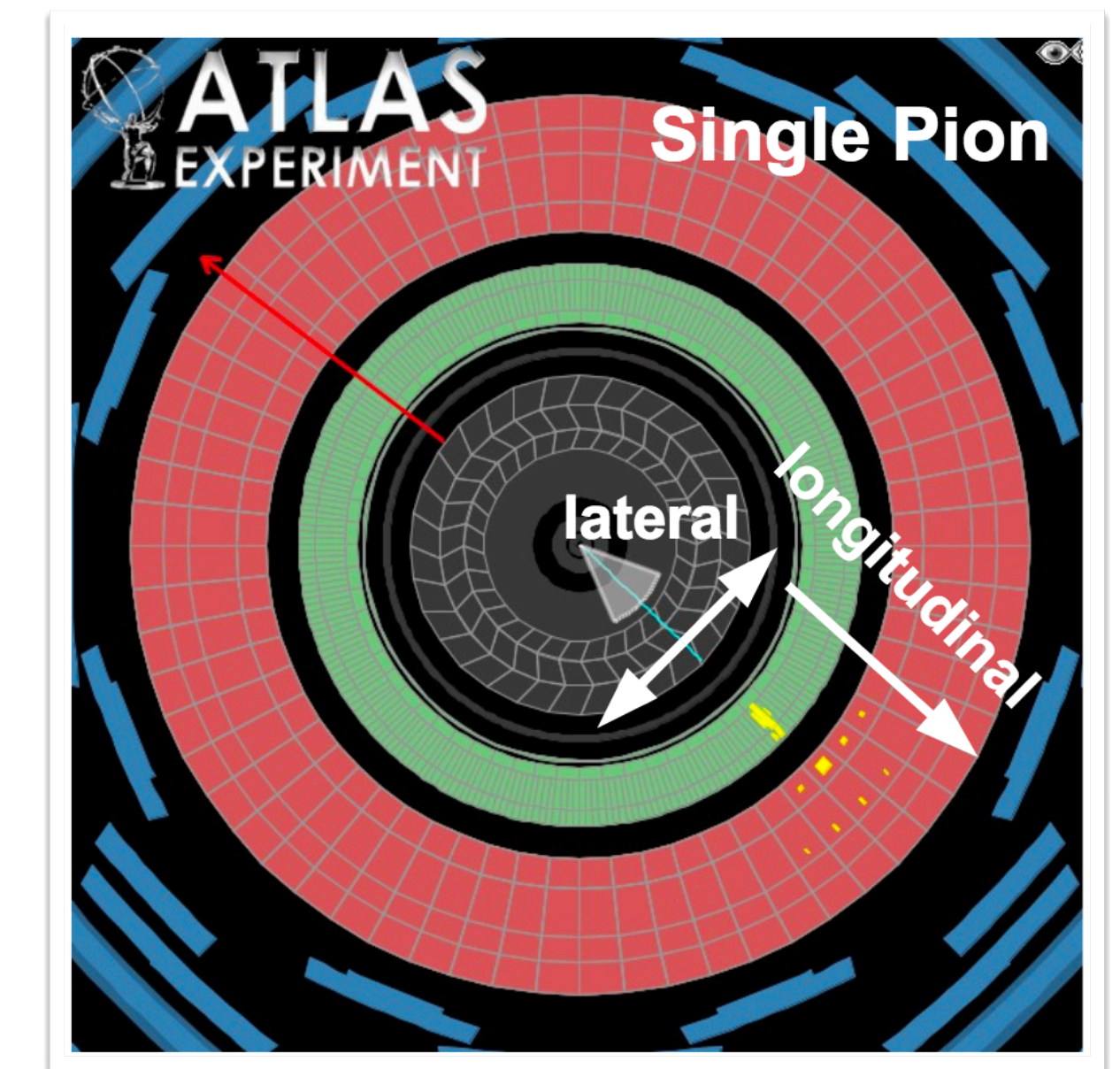
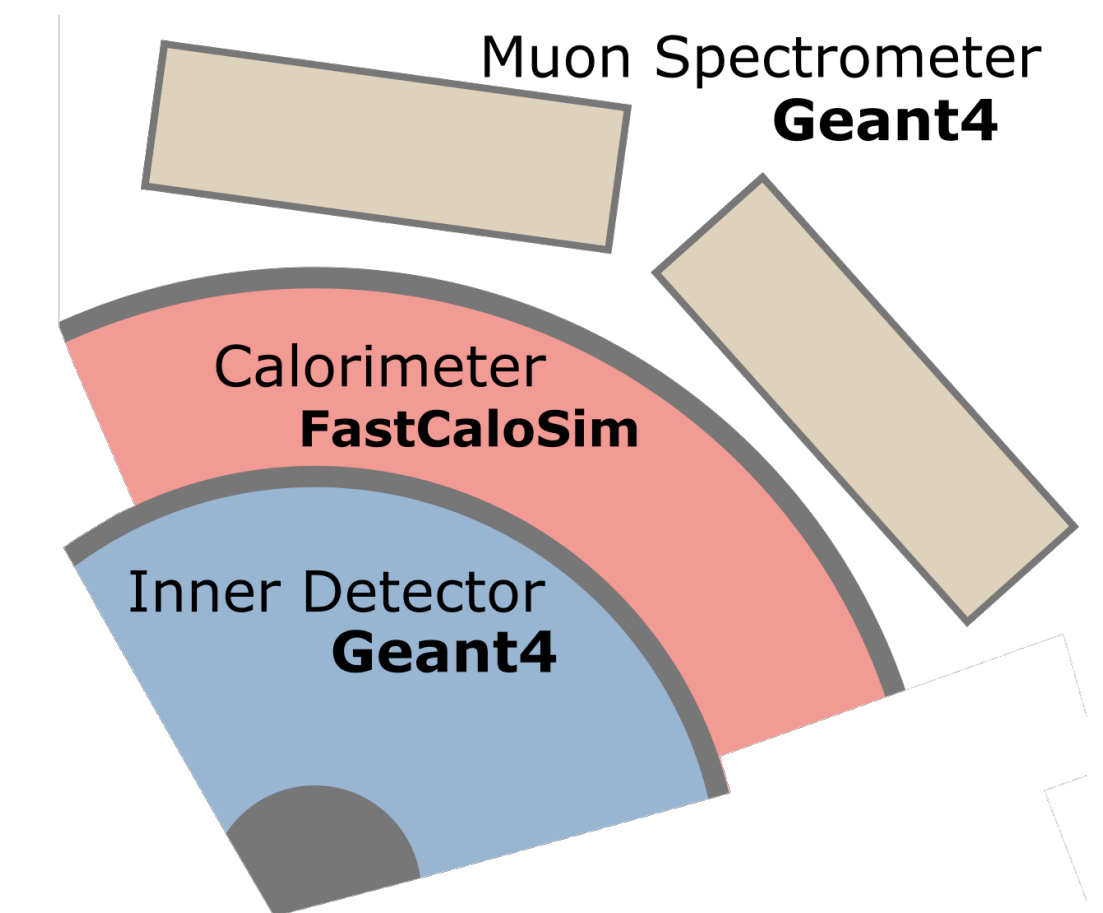
[2] [See talk on Fast Simulation Chain](#)

[3] [See talk on Porting Parametrized Calorimeter Simulation to GPU](#)



# Parametrized Fast simulation in Run 1 & Run 2: ATLFastII (AF2)

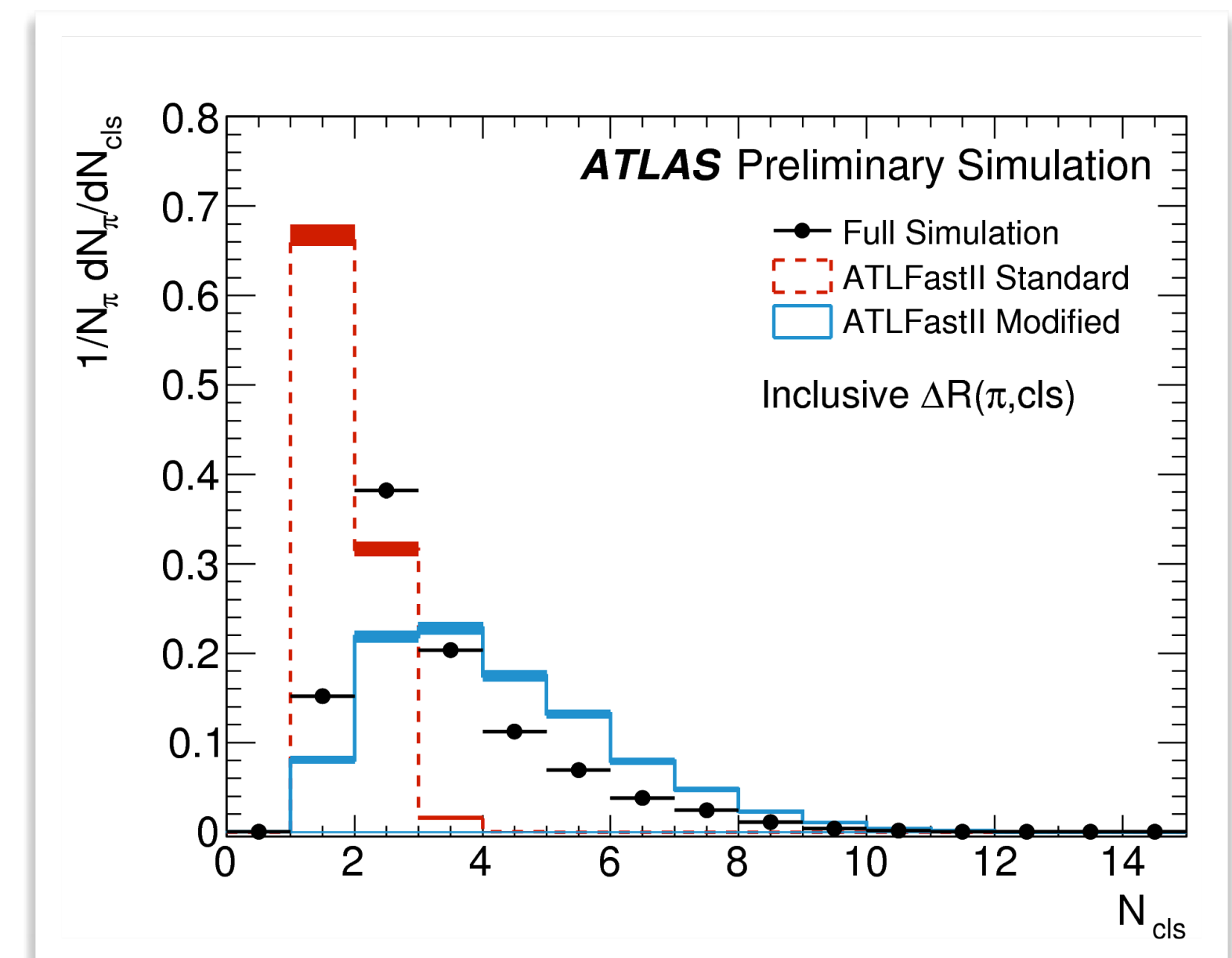
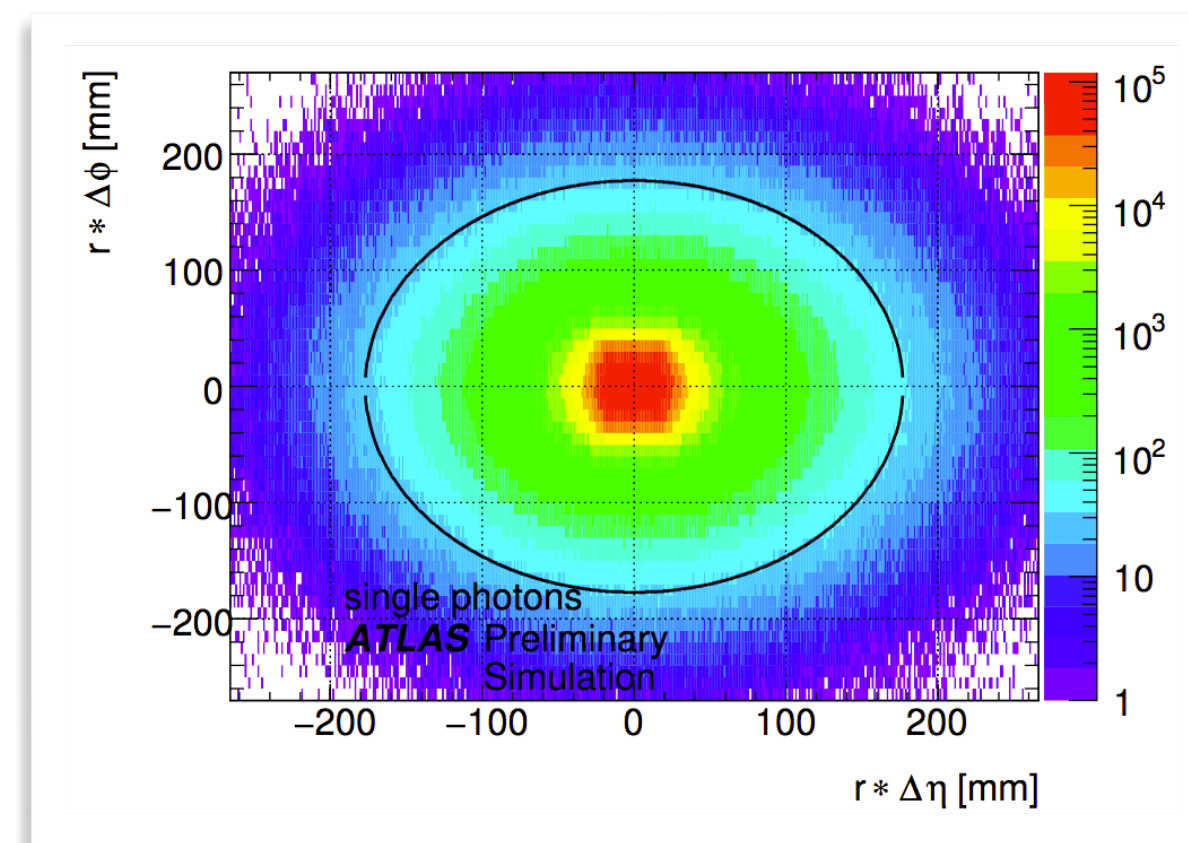
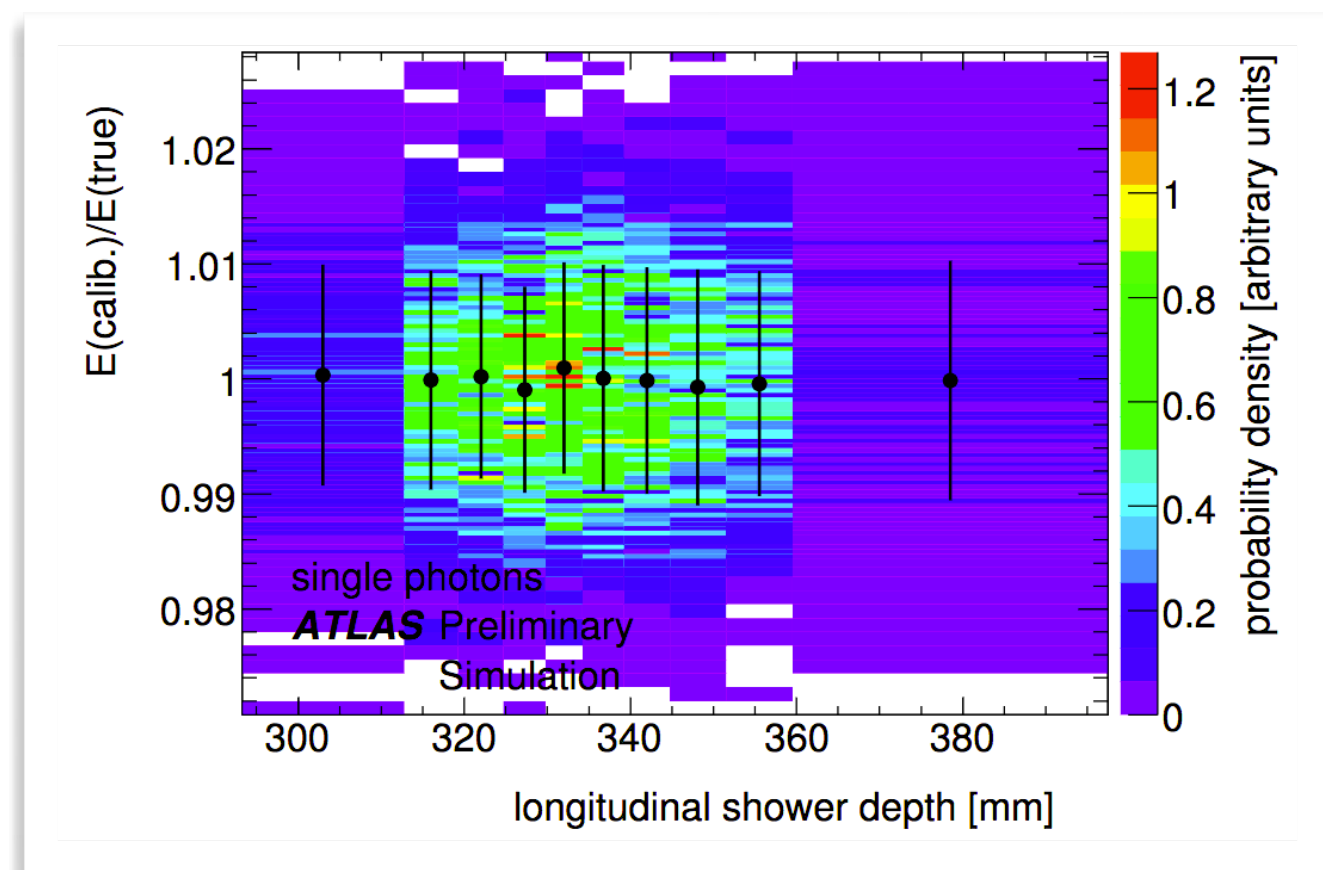
- ◆ AtIFast2 (AF2) - a combination of Geant4 for ID, MS and a parametrized calorimeter simulation (**FastCaloSimV1**) is used in ATLAS during Run 1 and Run 2.
- ◆ Instead of simulating particle interactions, directly parametrize the **detector response** of single particles entering the calorimeter system.
- ◆ Parametrize the single particle shower development in **longitudinal** (energy) and **lateral** (shape) directions.
- ◆ Use the parametrization at simulation step to deposit energy in calorimeter cells using **simplified (cuboid) geometry**.





# AF2 parametrization and performance

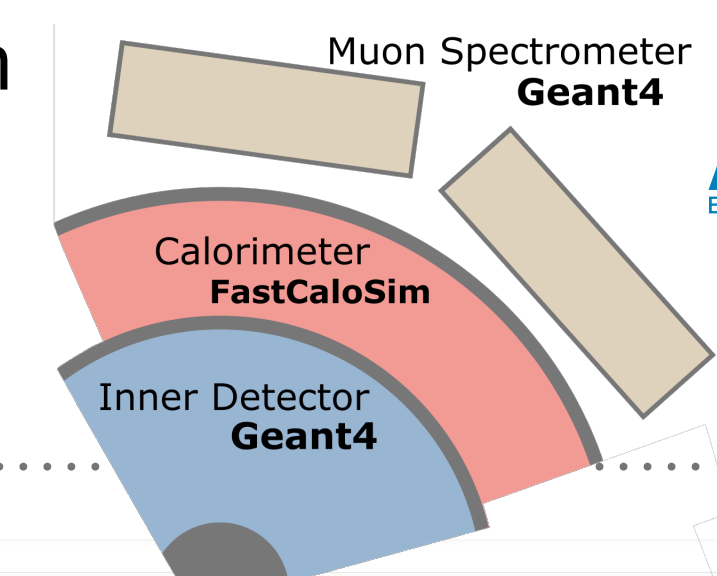
- ◆  $e/\gamma$  and  $\pi$  are used for electromagnetic and hadronic shower parametrization respectively.
- ◆ Longitudinal shower: **energy vs shower depth** and **correlation between layers**
- ◆ Lateral shower: **Average shower profile** from a fitted radial symmetric function for each layer.
- ◆ Good average shower description but complex variables e.g. **jet substructure** is not well modeled.
- ◆ No lateral parametrization for Forward Calorimeter (FCal), particles escaping calorimeter volume (*punch through*)
- ◆ In Run 2, ~50% of all simulation was done using AF2.



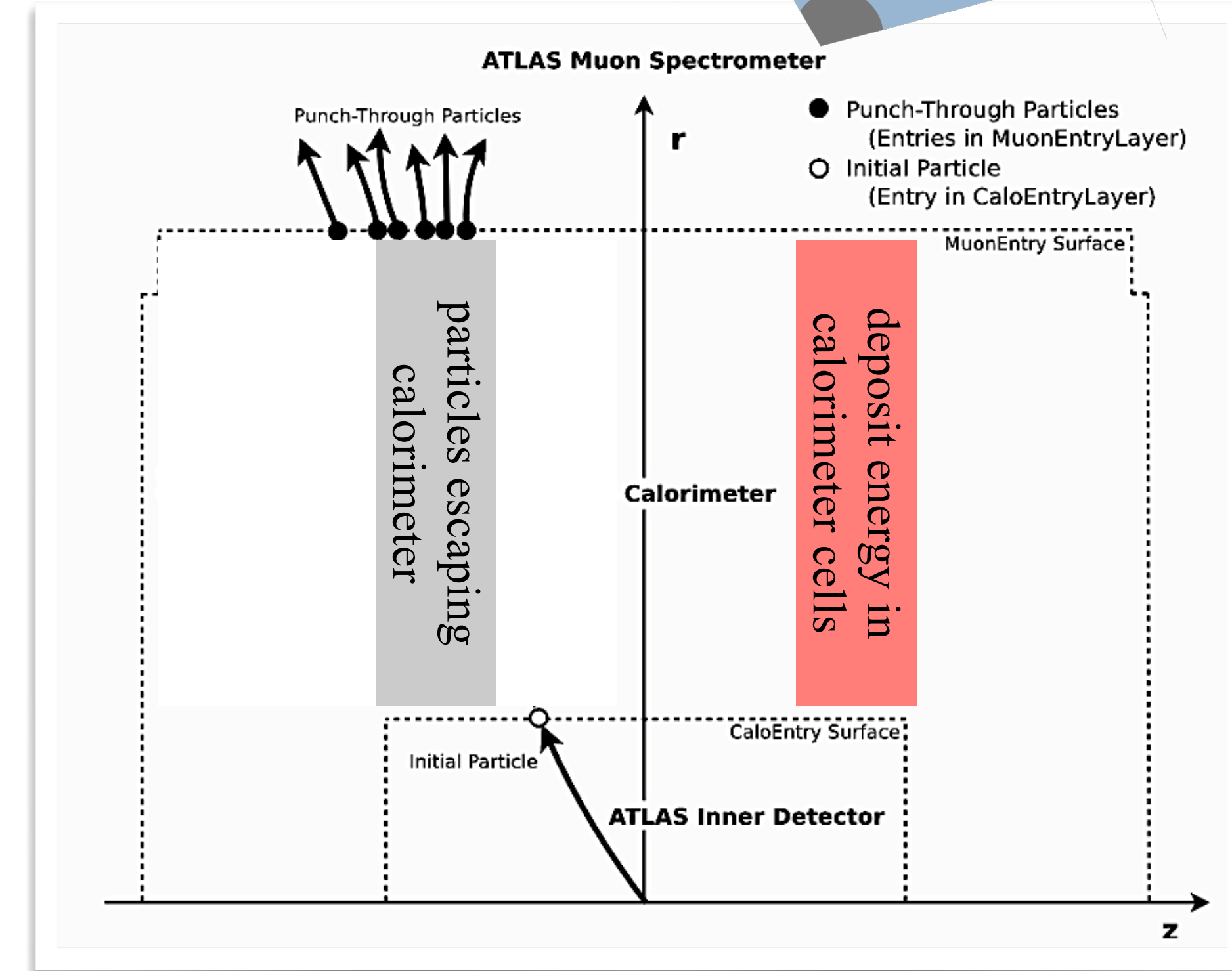
AF2 is **tuned to data** instead of Geant4 - requires a **separate set of calibrations** for reconstructed objects



# Fast simulation in Run 3 & beyond: ATLFast 3 (AF3)



- AF3 improves physics performance significantly over AF2 and will meet the fast simulation needs of ATLAS for Run 3.
- AF3 uses two distinct approach of shower generation (includes FCal):
  - Parametrization based modeling - **FastCaloSim V2 (FCSV2)**
  - Generative Adversarial Network (GAN) based modeling - **FastCaloGAN (FCSGAN)**
- Dedicated parametrization for **punch through particles** - particles escaping calorimeter volume.



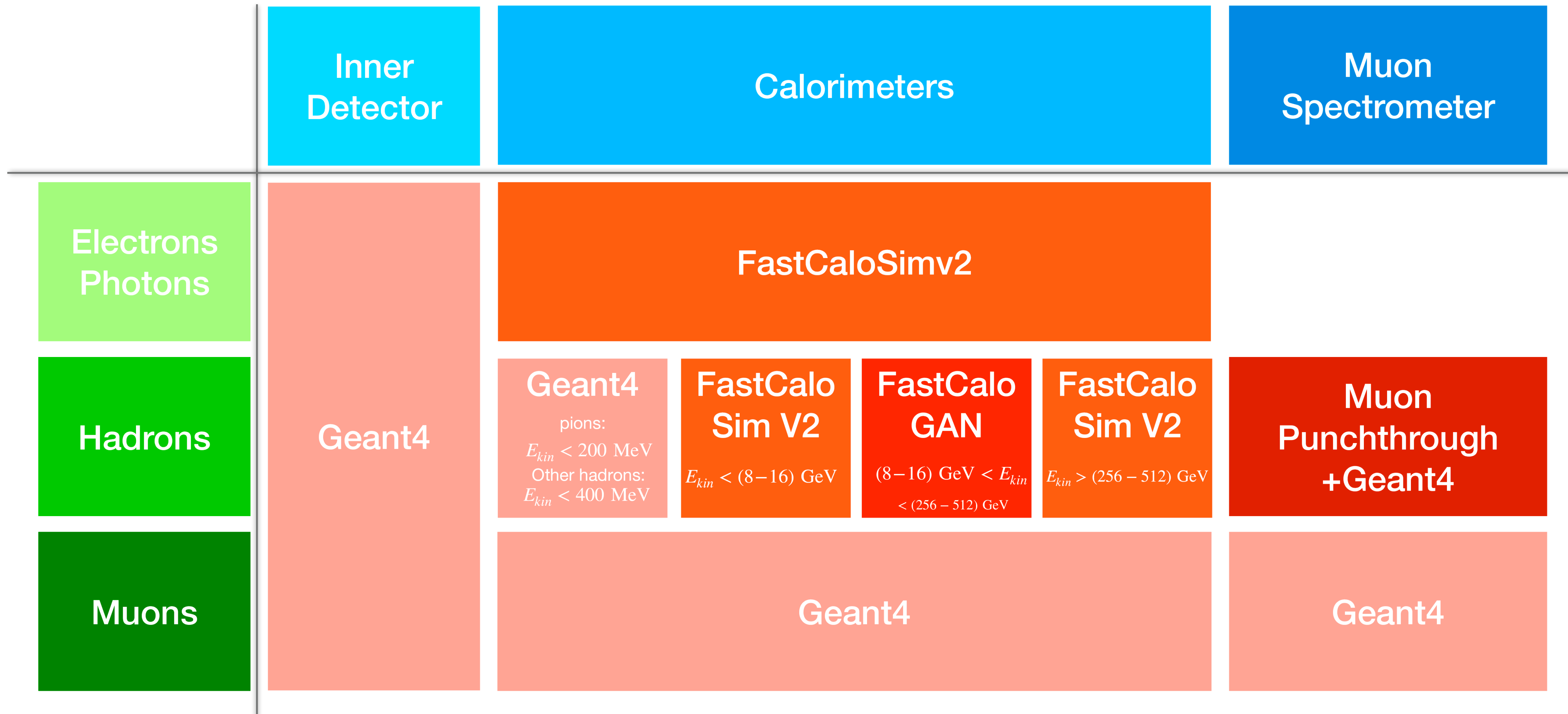
<b>FastCaloSim V2</b>	Used for electron, photon and low or high energy hadrons
<b>FastCaloGAN</b>	Used for medium energy hadrons
<b>Punch Through</b>	Used for simulating particles that exit the calorimeter and enters Muon Systems (MS)
<b>Geant4</b>	Used for simulating very low energy hadrons in the Calorimeter, all particles in the MS and ID.

- AF3 provides a speed gain by a factor of -
  - O(500) for calorimeter only simulation
  - O(10) for full detector simulation

*AF3 targets achieving identical modeling to Geant4 requiring only one set of calibrations*

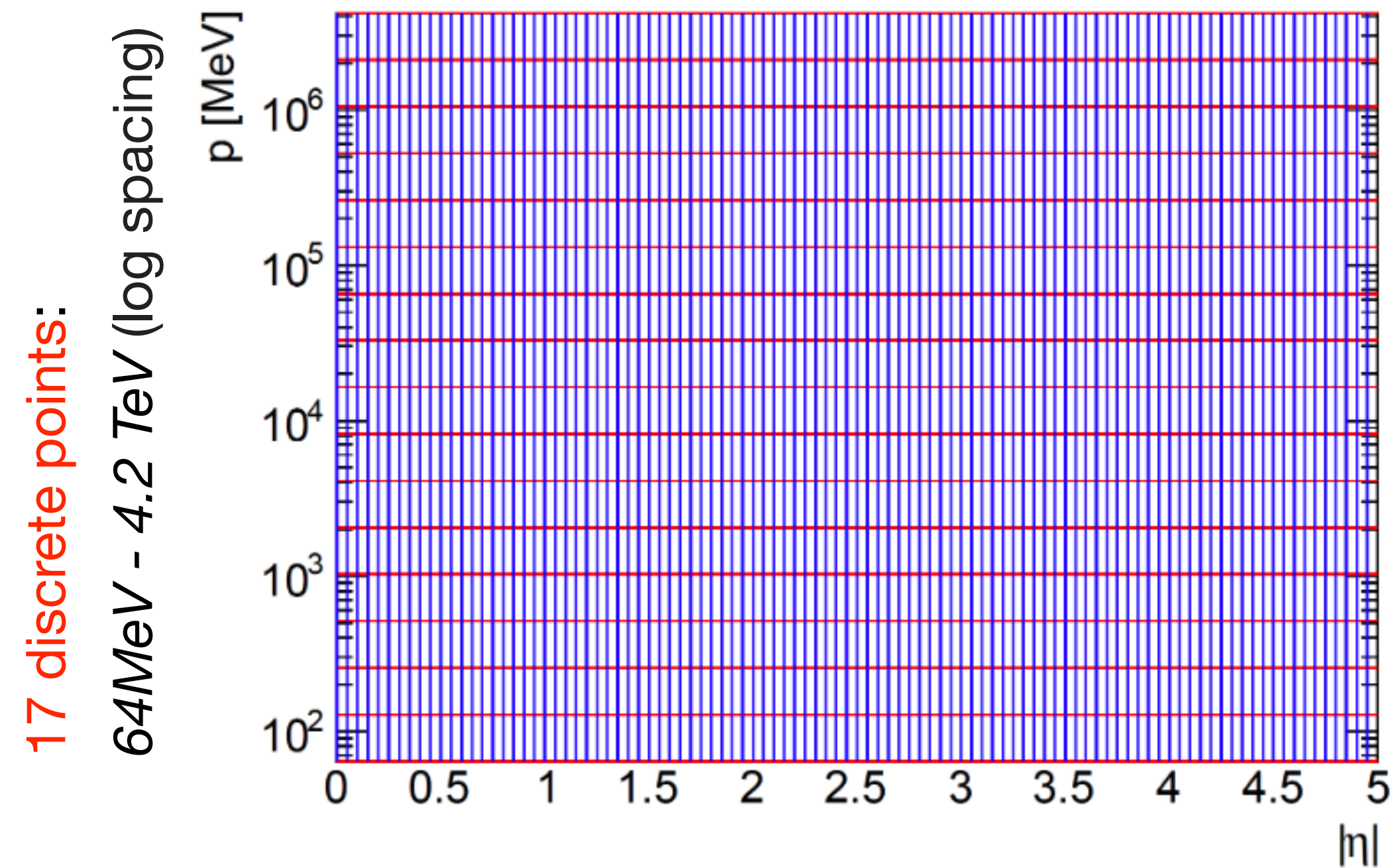


# AF3 Configuration



# Input datasets for AF3 modeling

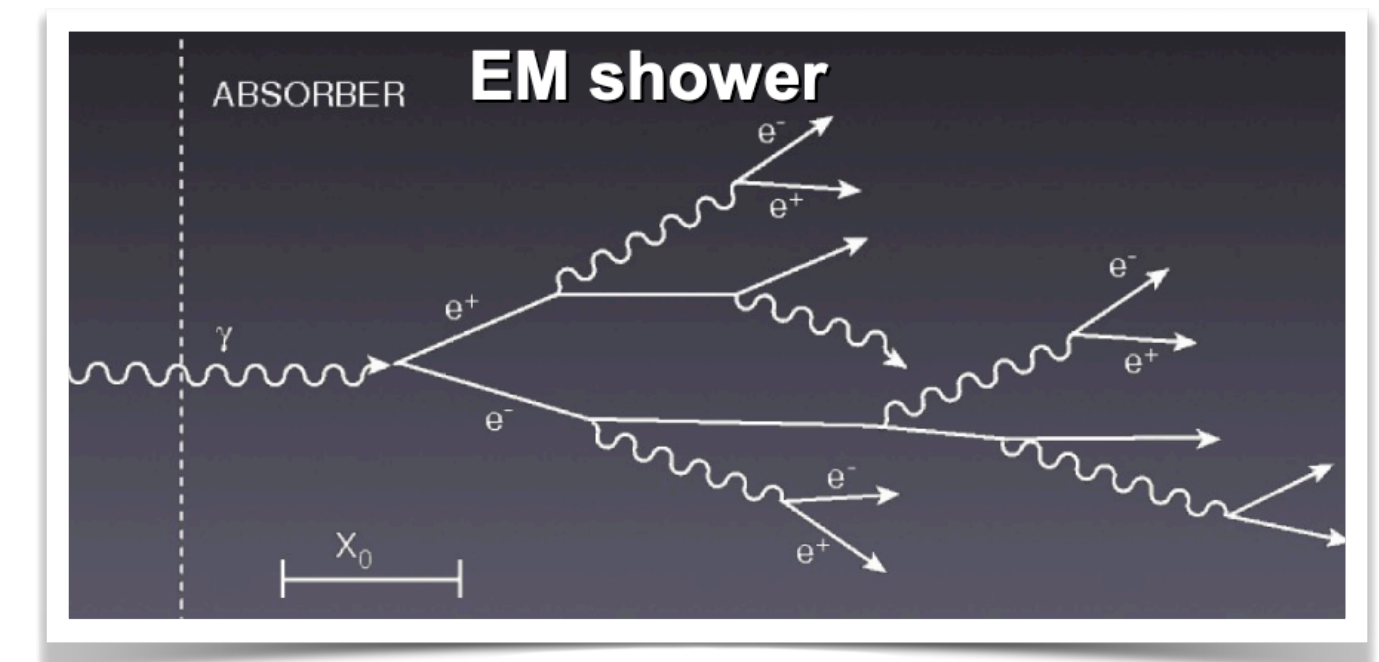
Geant4 simulated **single particles** generated at **the calorimeter surface** is used for modeling AF3



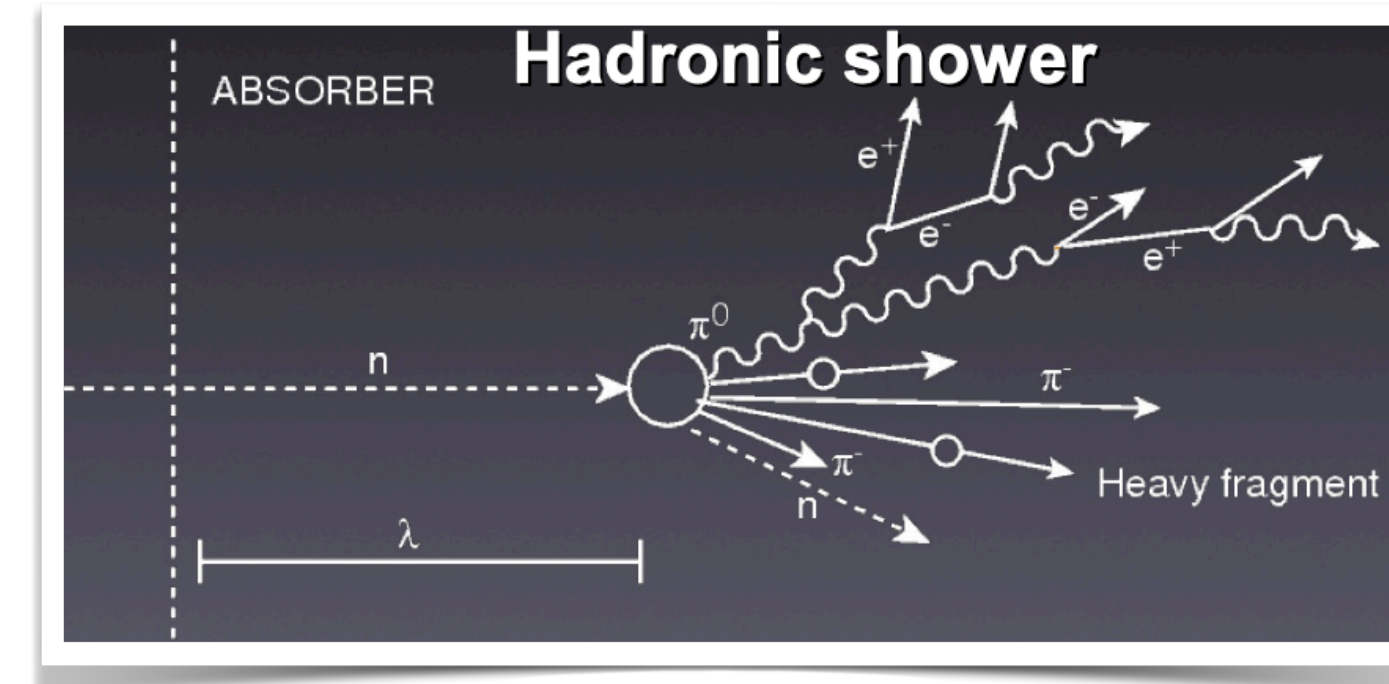
100 bins of **size 0.05** covering  $0 \leq |\eta| \leq 5$

Detail G4 steps (granular energy deposit)  
 No primary vertex smearing in simulation  
 Noise, cross-talk between neighboring cells and bad cells turned off in digitization.

**Photons:** for photon shower  
**Electrons ( $e^\pm$ ):** for electron shower



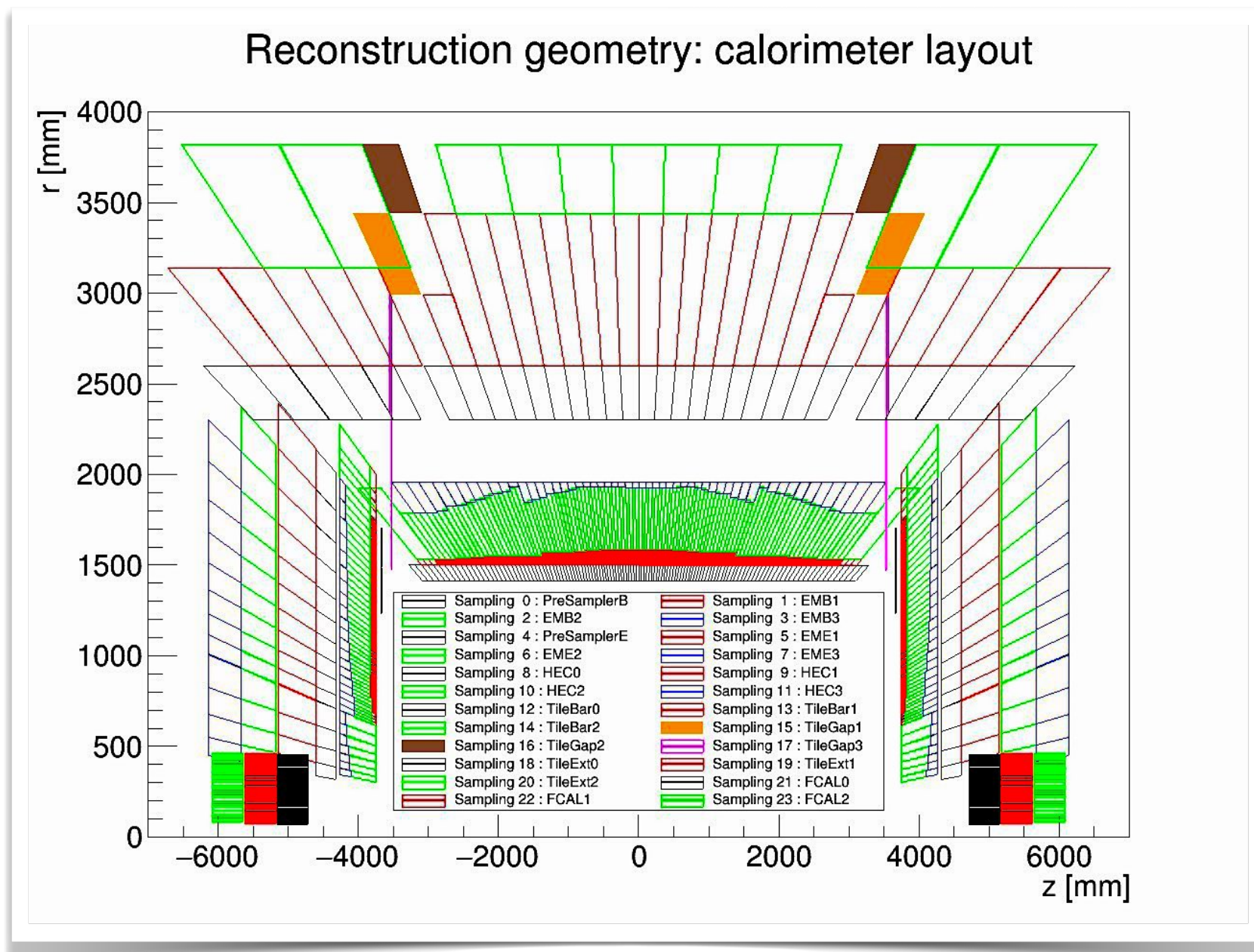
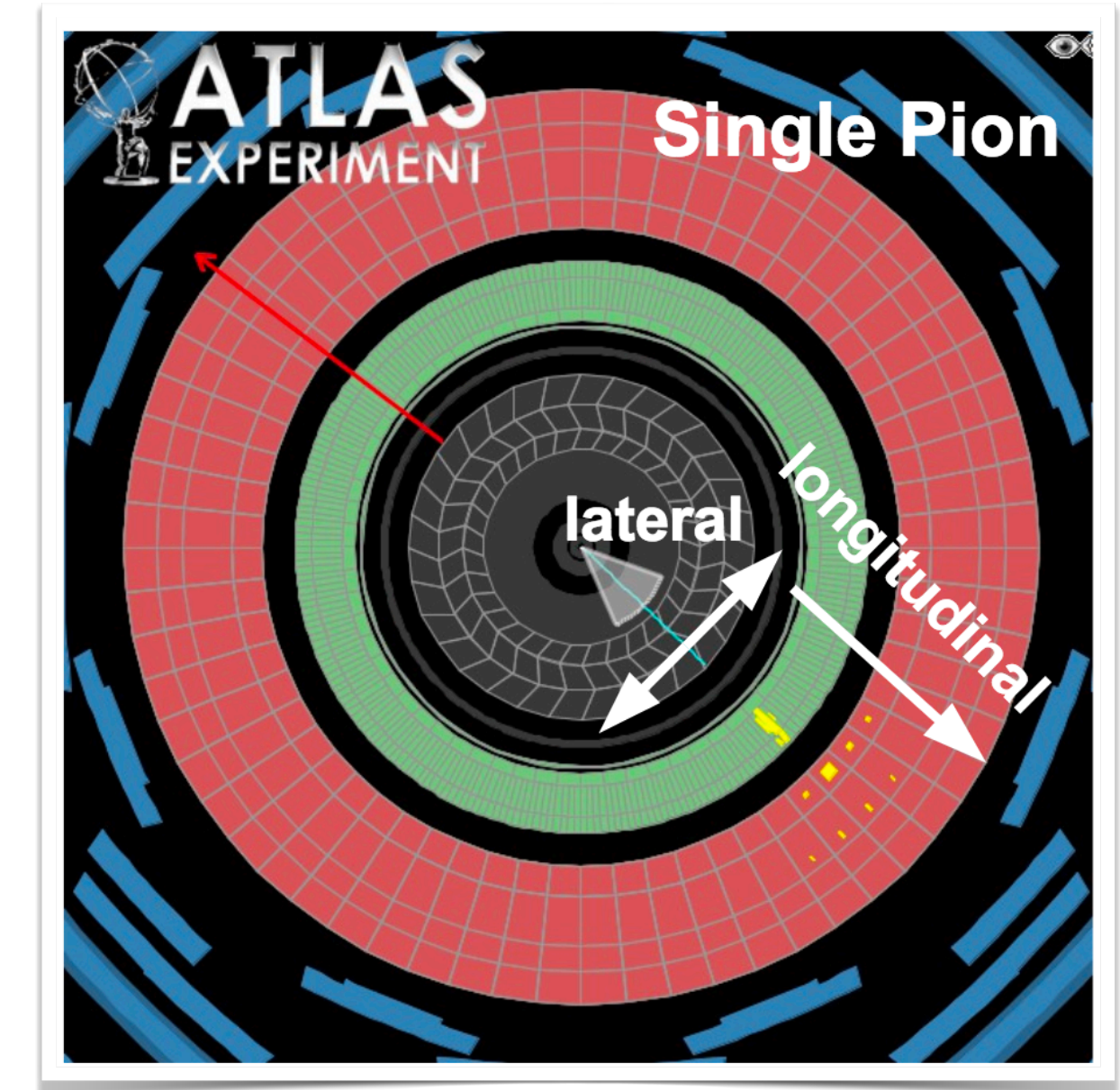
**Pions ( $\pi^\pm$ ):** for hadronic shower





# Parametrization based - FastCaloSim V2

- ◆ FastCaloSim V2 follows the same principle of shower parametrization (longitudinal and lateral) as in FastCaloSim V1
- ◆ However targets to achieve the following:
  - ◆ better modeling of the physics processes
  - ◆ keep the memory footprint of the parametrization small

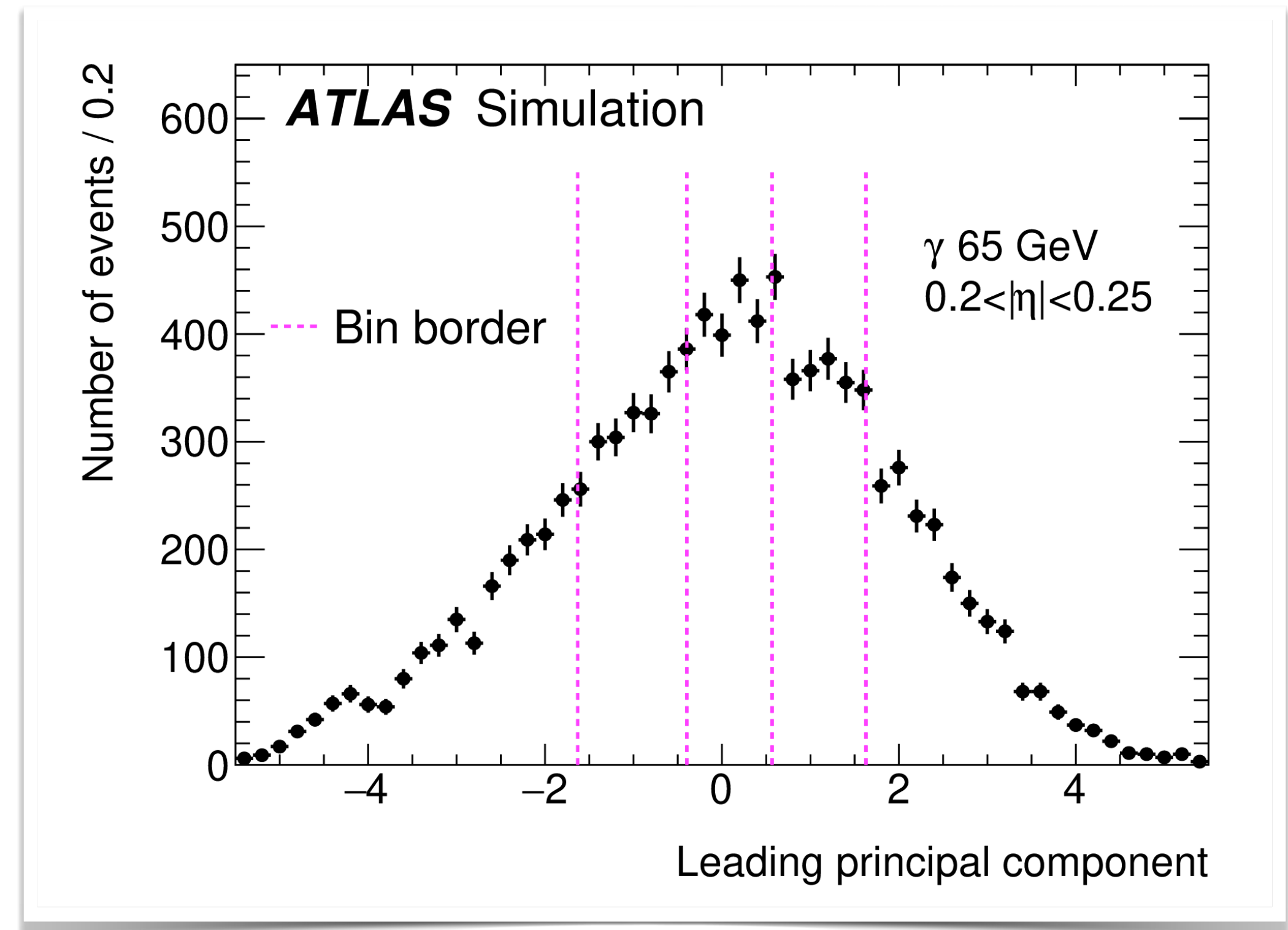
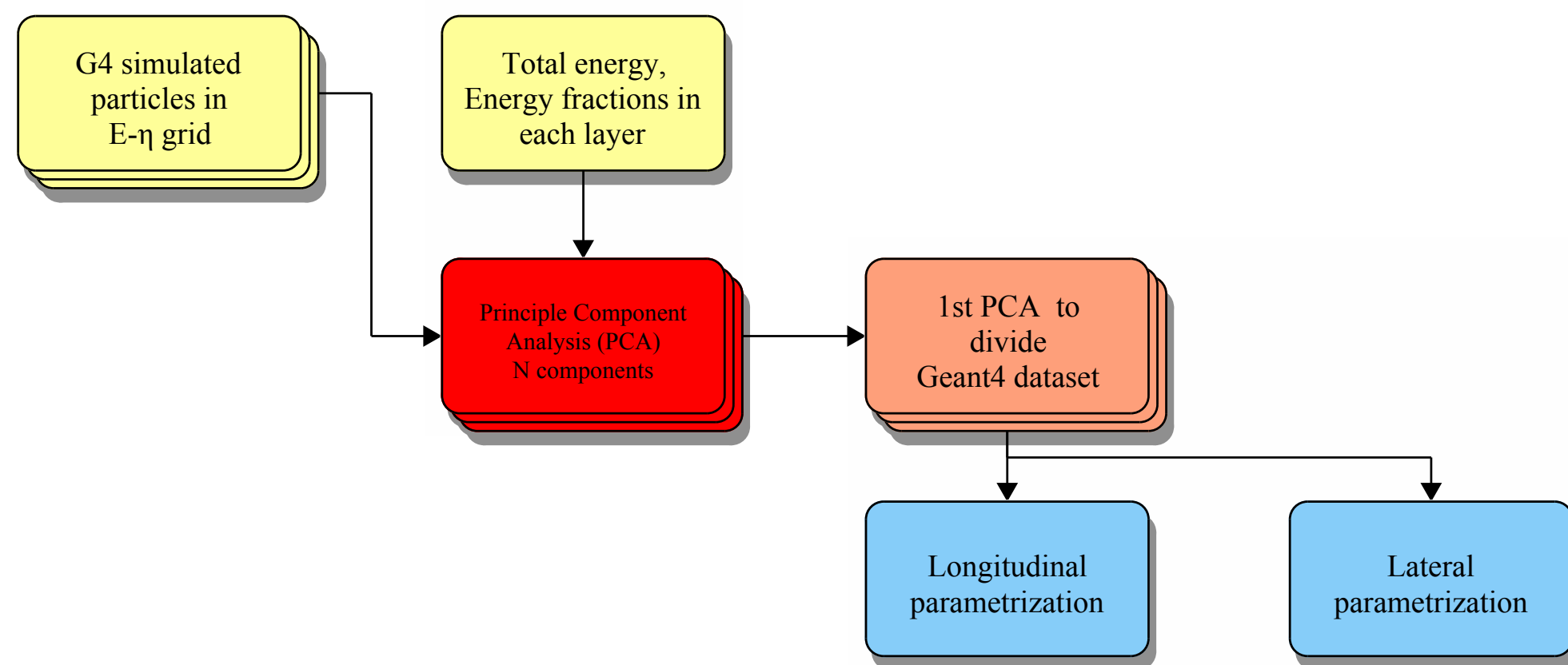
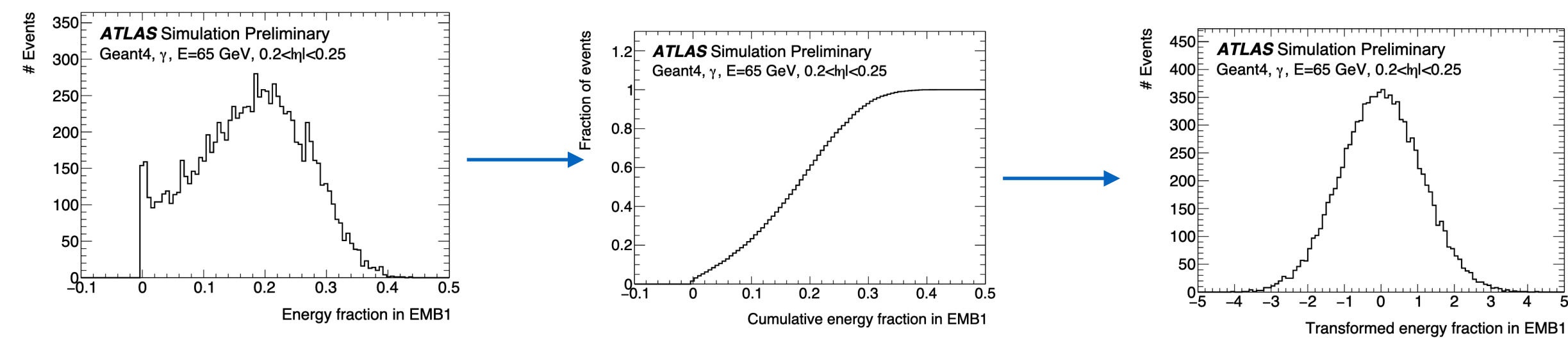


- ◆ The energy in each sampling layer is highly correlated.
- ◆ Classify showers based on the depth on the interaction point (i.e. depth at where a particle initiates the shower)
- ◆ The longitudinal and lateral parametrization is done for each for the shower type, for each calorimeter layers.



# Shower Classification

- ◆ To **remove the energy correlation** between layers - single particles are classified based on its depth on interaction point.
- ◆ The energy fraction of each layer, total energy for all particles are used to perform a Principal Component Analysis (PCA).

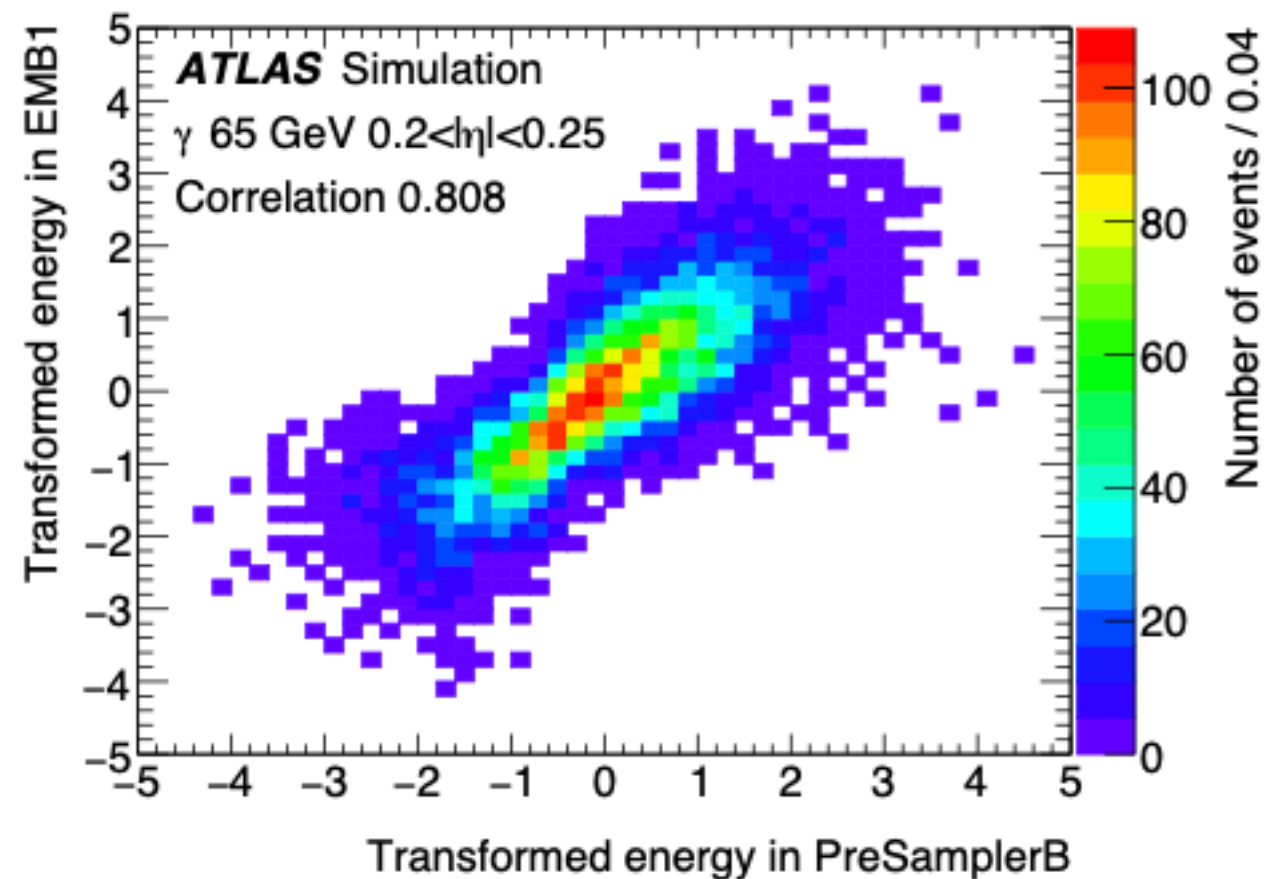


Leading principal component is used to divide the particles in **quantiles**

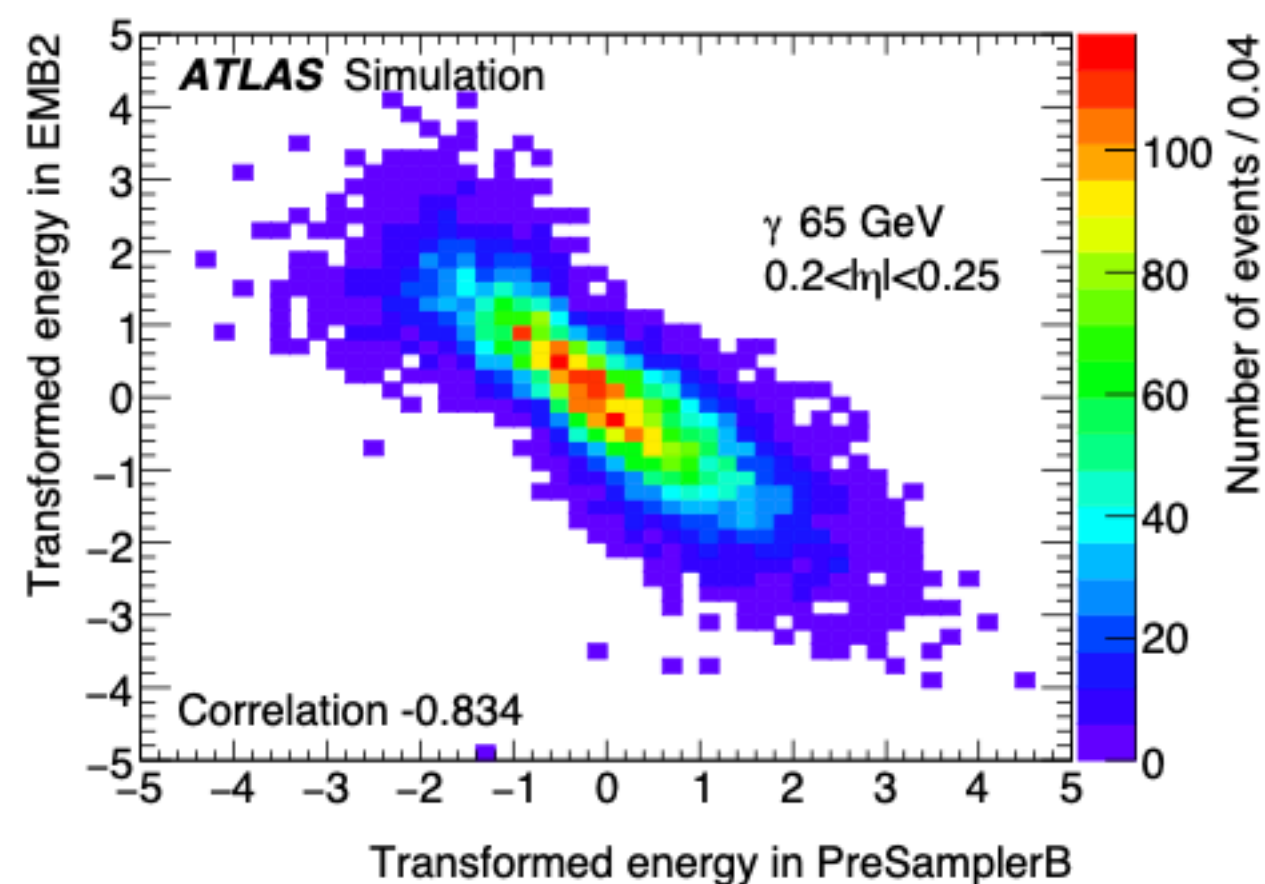


# Validation of shower classification - energy decorrelation

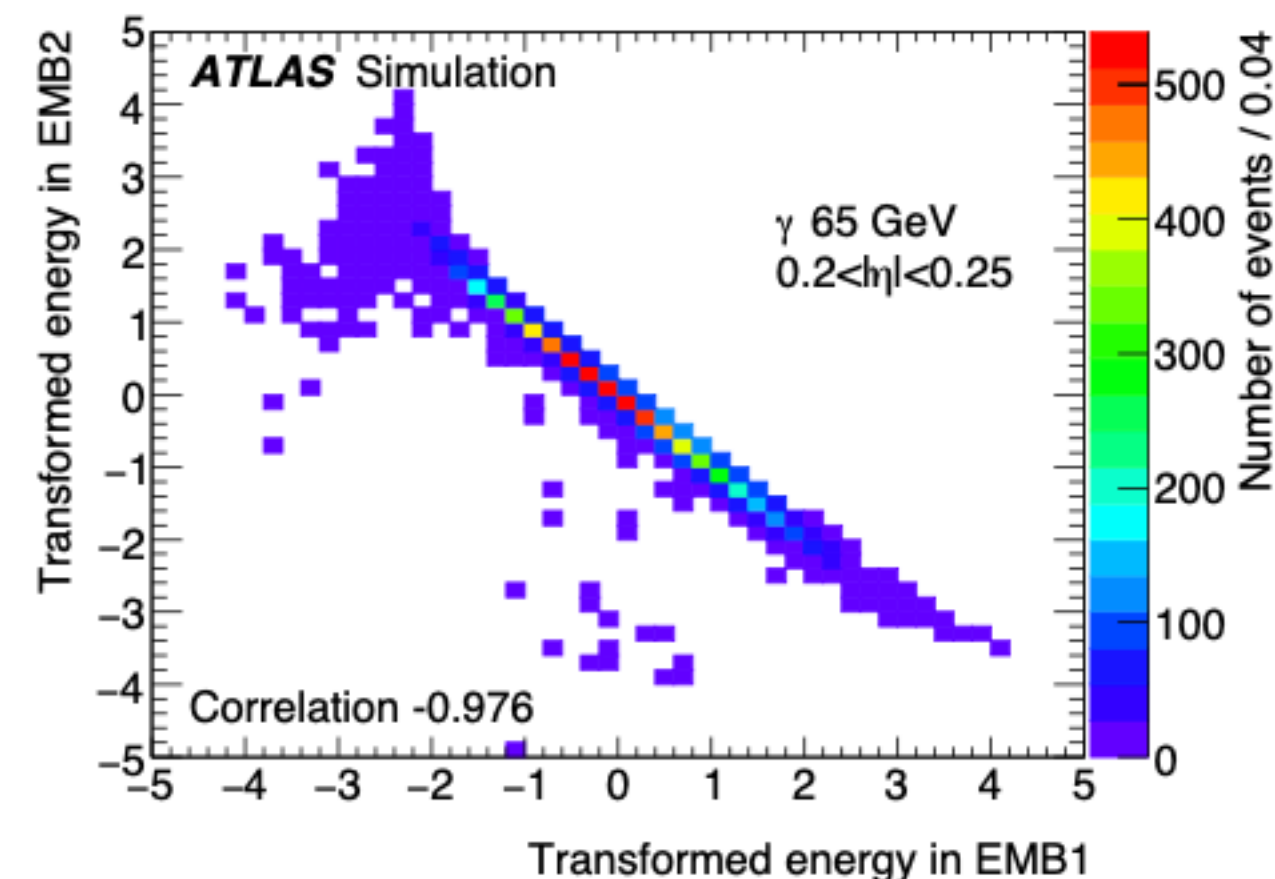
Before PCA:



(a)

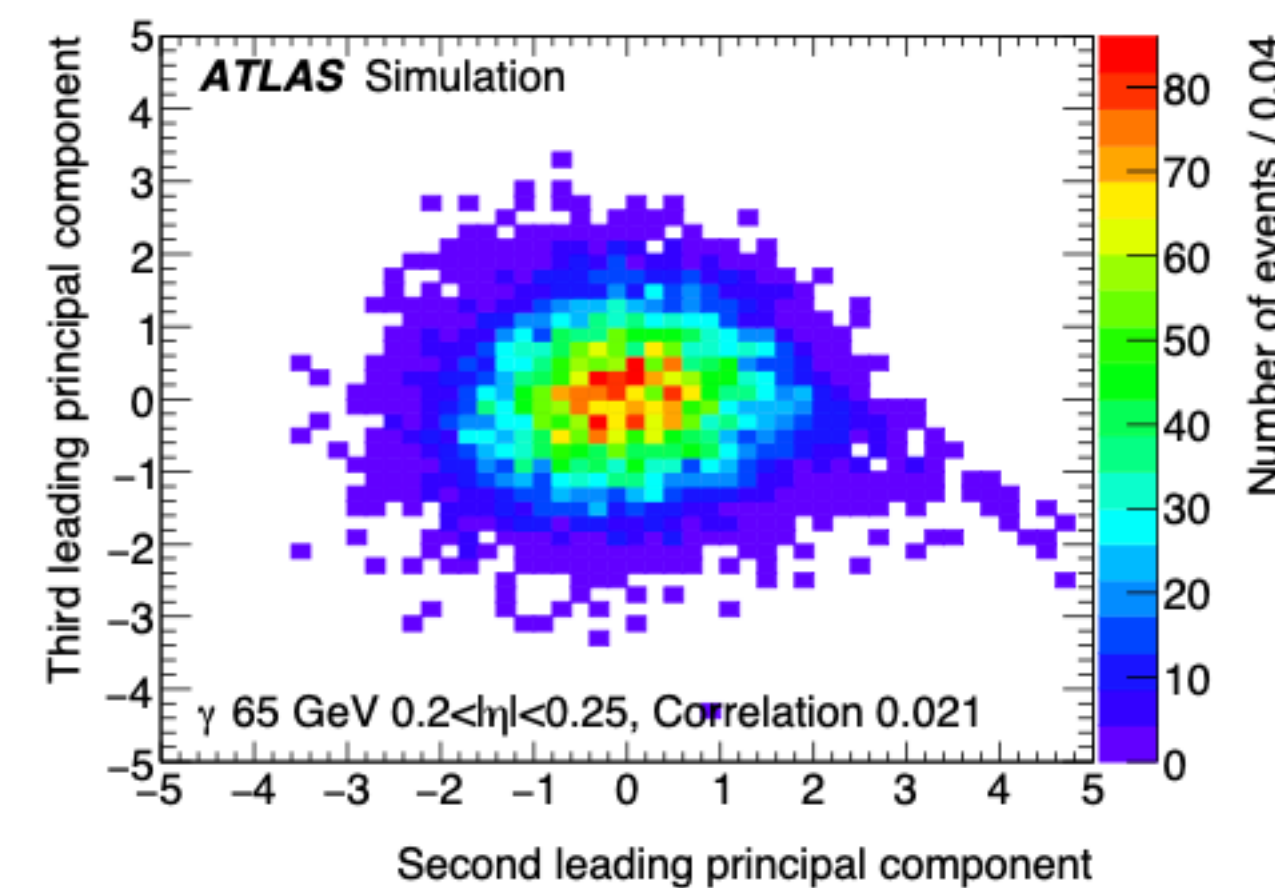
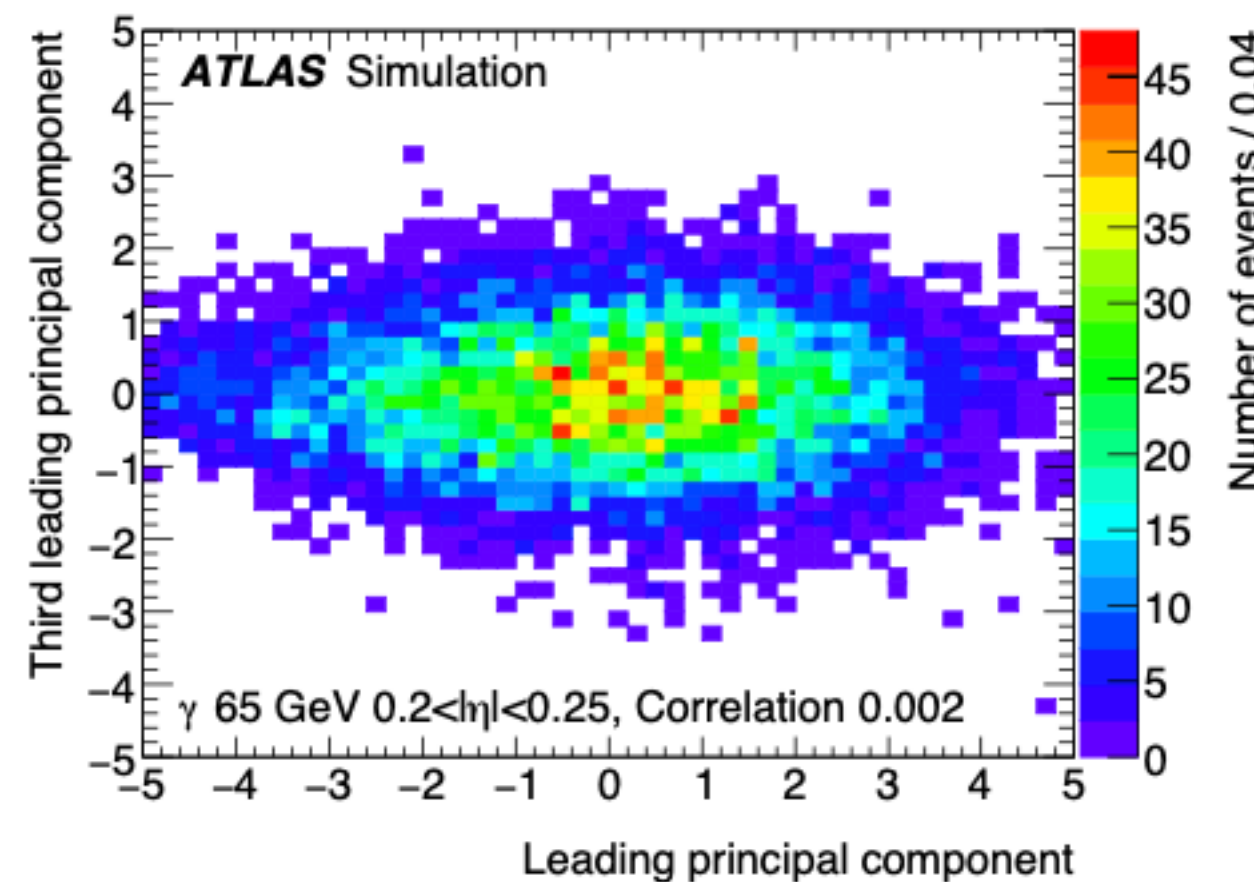
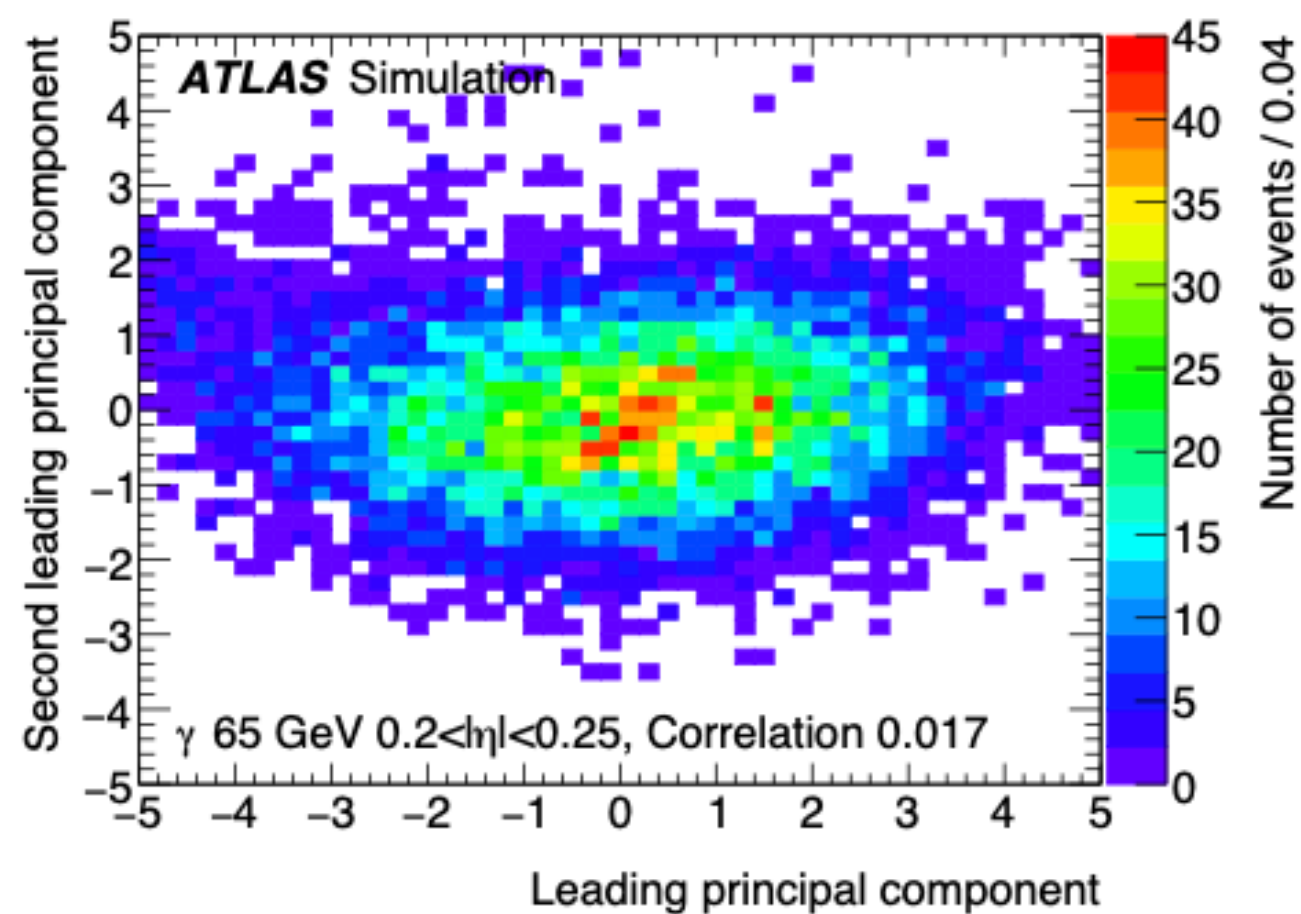


(b)



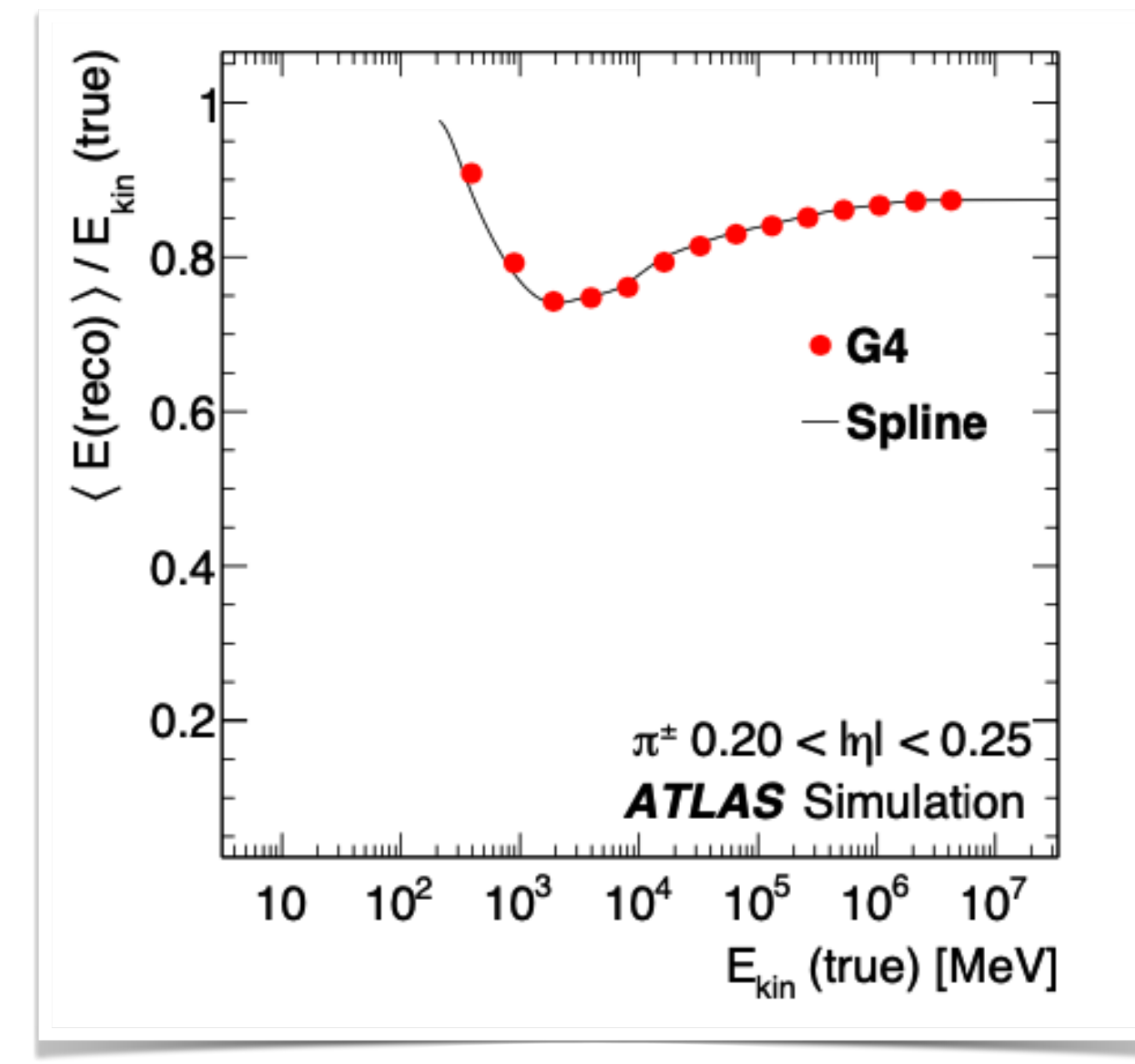
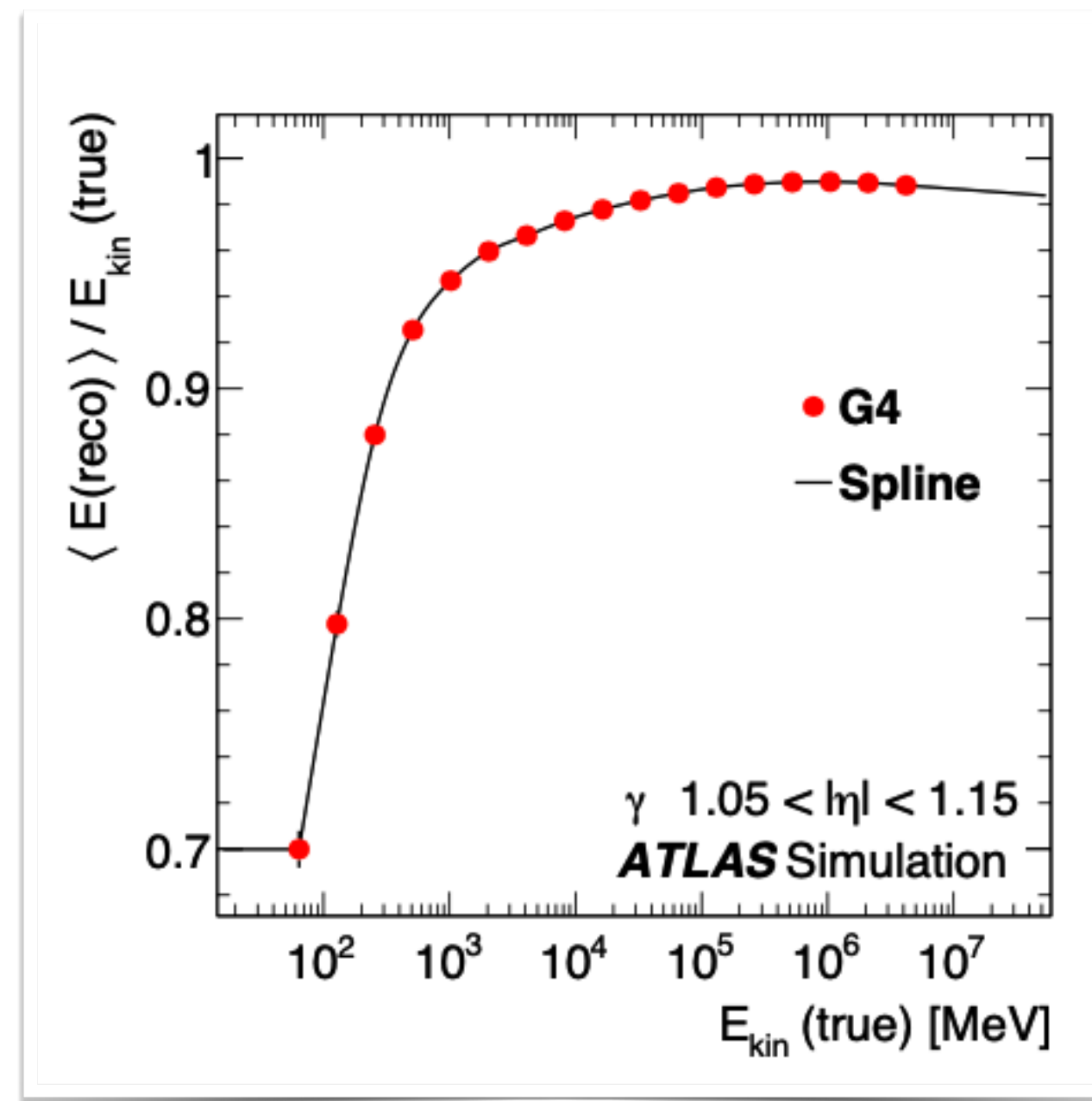
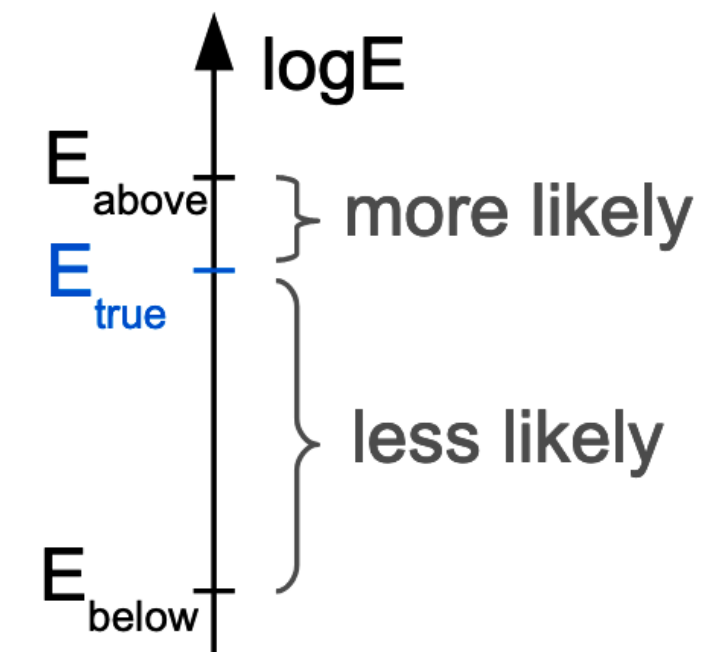
(c)

After PCA:



# Energy Parametrization & Interpolation

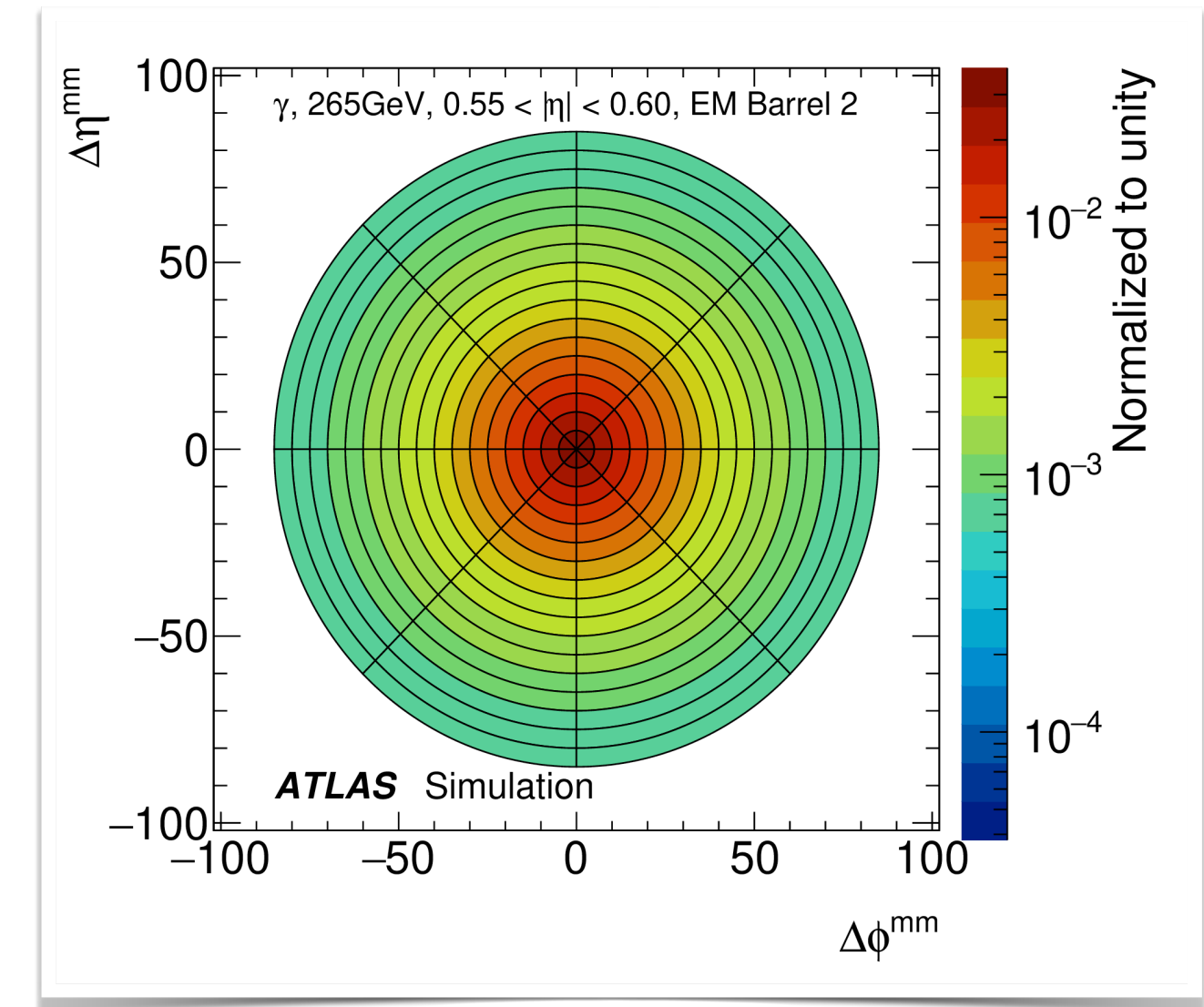
- ◆ **Additional PCA on each bins** of 1<sup>st</sup> Principal Component and the cumulative distributions, mean & RMS of the gaussians along with the PCA matrix is saved for energy parametrization - for the 17 discrete points.
- ◆ A piece-wise polynomial (spline) is used to fit the 17 energy points for **interpolation**.
- ◆ During simulation the parametrization is **randomly selected based** on the logarithm distance of  $E_{\text{true}}$  from parametrization grid.



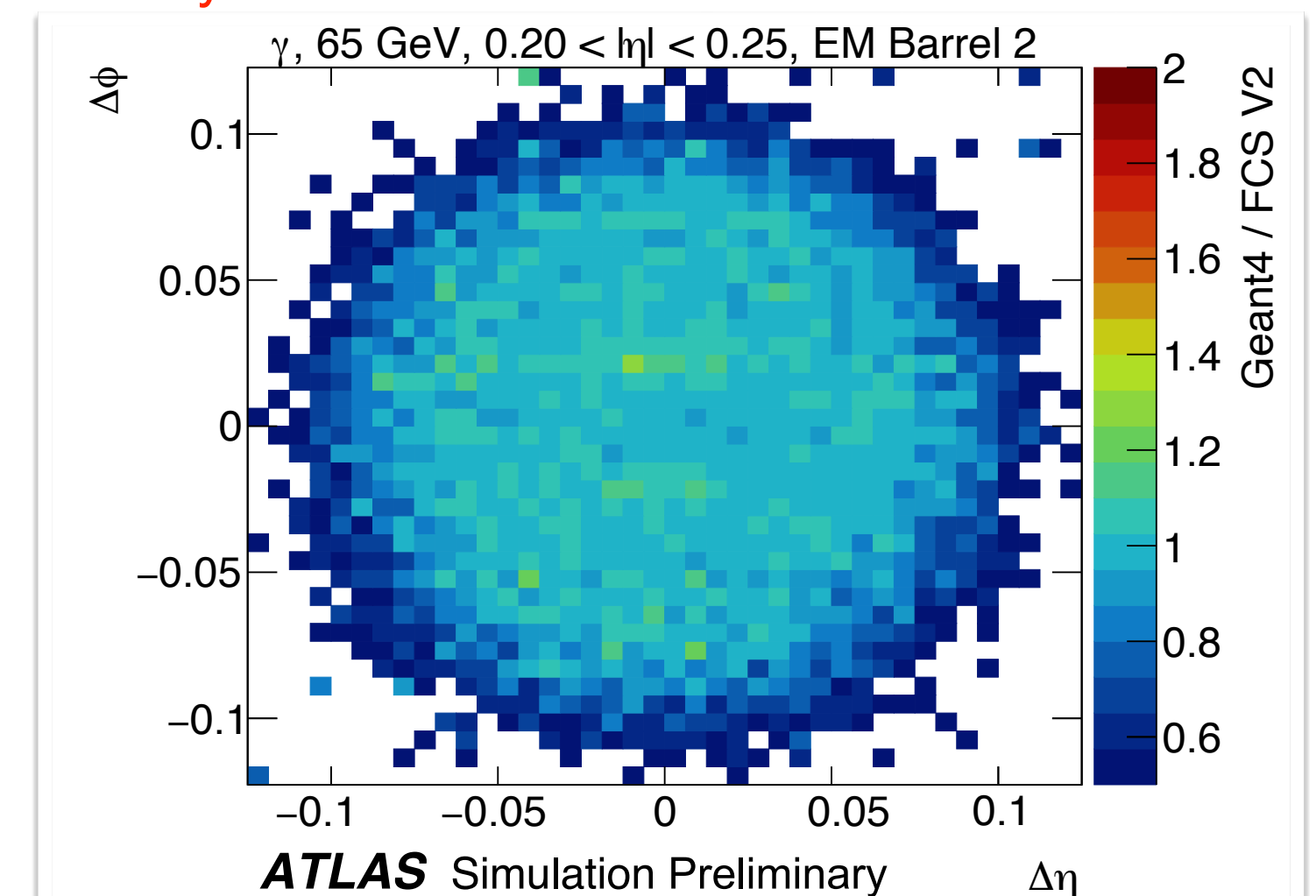


# Lateral shower shape parametrization

- ◆ The distribution of energy in lateral direction **averaged over many showers** is parametrized over a certain **radial distance** ( $r$ ) containing 99.5% of the total energy and 8-bins in the **angular direction** ( $\alpha$ ).
- ◆ The **bin size (1 or 5mm)** in the radial direction is coarser compared to G4 steps but **finer compared calorimeter cell size** in each layer.
- ◆ Shower centers are **corrected by average longitudinal depth** of energy deposits in each PCA bin.
- ◆ This parametrization is done for **each layer and PCA** bin for each parametrization grid point.
- ◆ These 2D histograms are used as PDF during simulation to randomly generate quantized energy deposits (hits)

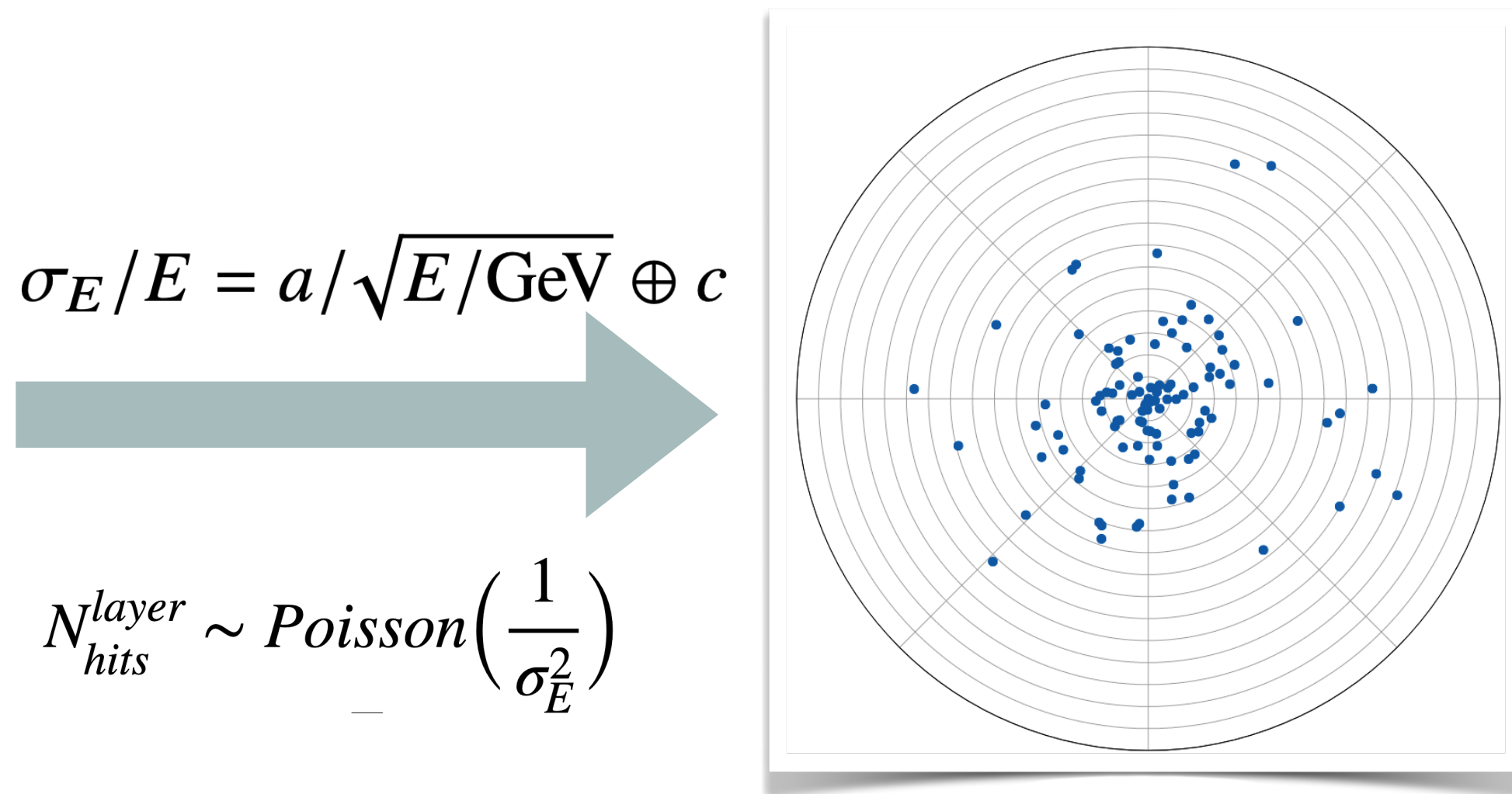
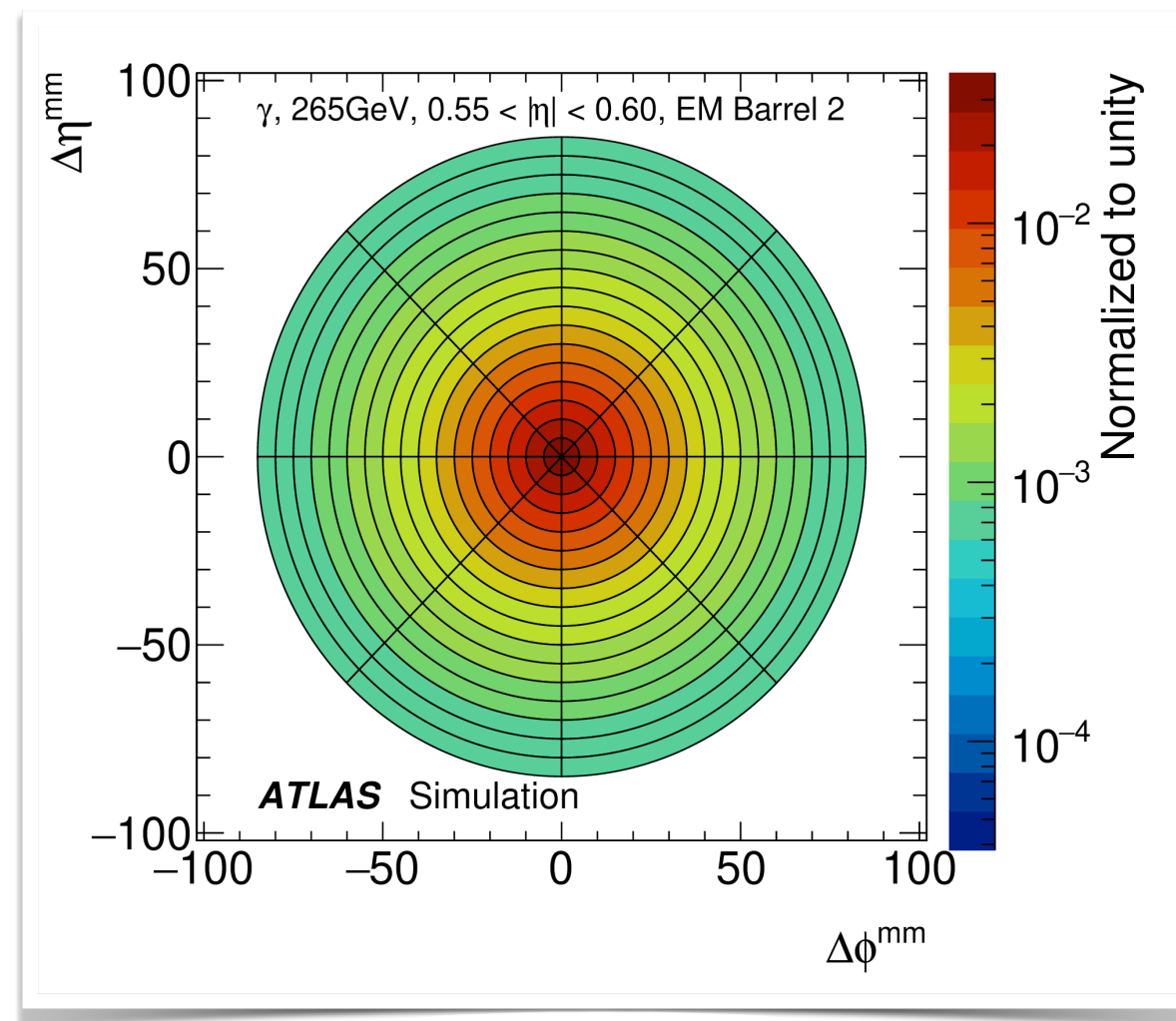


toy simulation



# Simulation of lateral shower

- ◆ Generation of shower is a **stochastic process** with the average shower gives the PDF.
- ◆ Energy is deposited using  $N_{hits}$  of **equal energy**.
- ◆  $N_{hits}$  is calculated such that it gives the **same Poisson RMS as the resolution of the calorimeter layer**.



$E_{hit} = E_{layer} / N_{hits}$

Calorimeter technology	Constant term $c$	Stochastic term $a$
LAr EM barrel and endcap	0.2%	10.1%
Tile	5.5%	56.4%
LAr hadronic endcap	0	76.2%
FCal	3.5%	28.5%

*Hadronic showers have larger intrinsic fluctuations and the stochastic terms are calculated for each layer and  $\eta$  region*

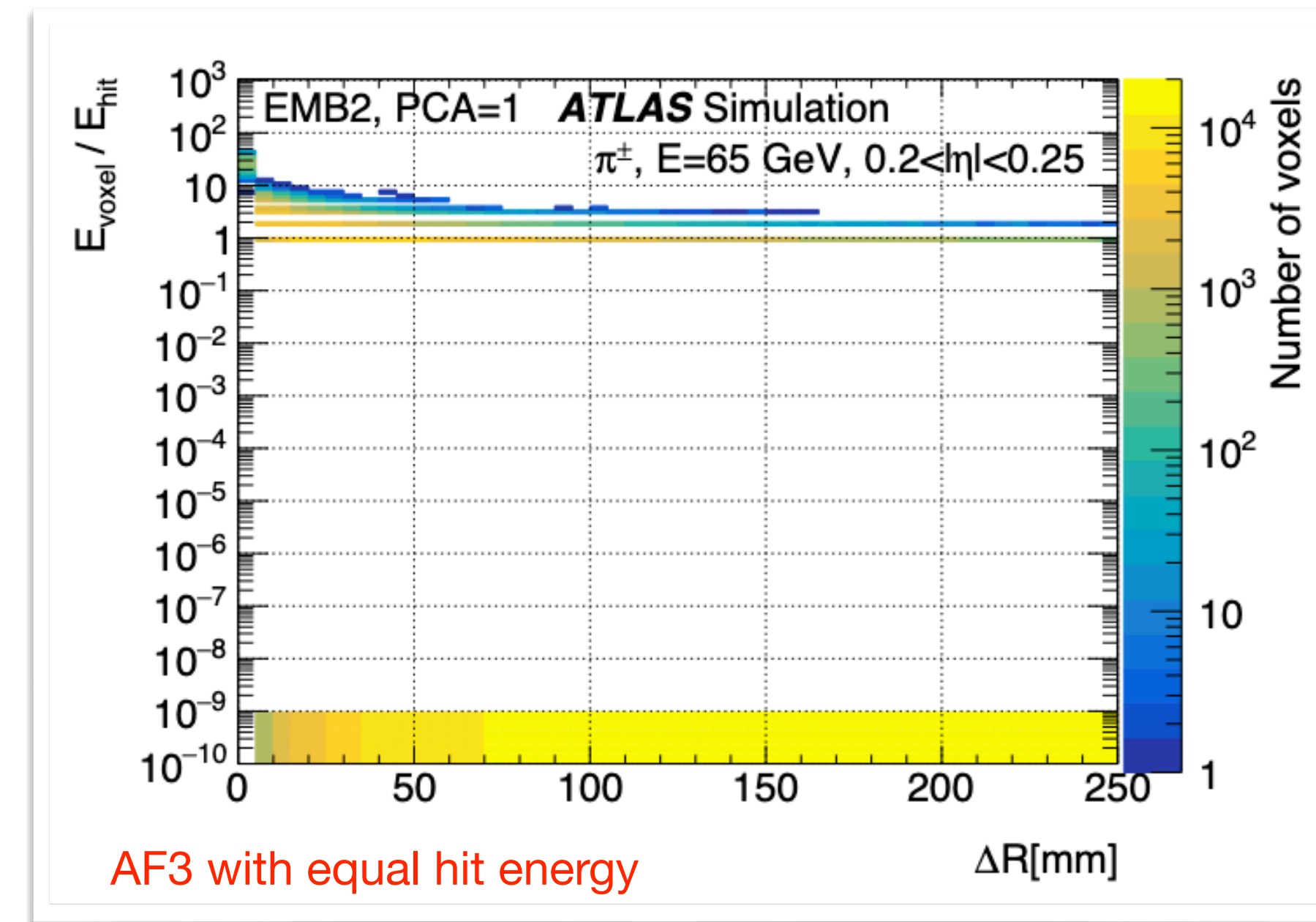
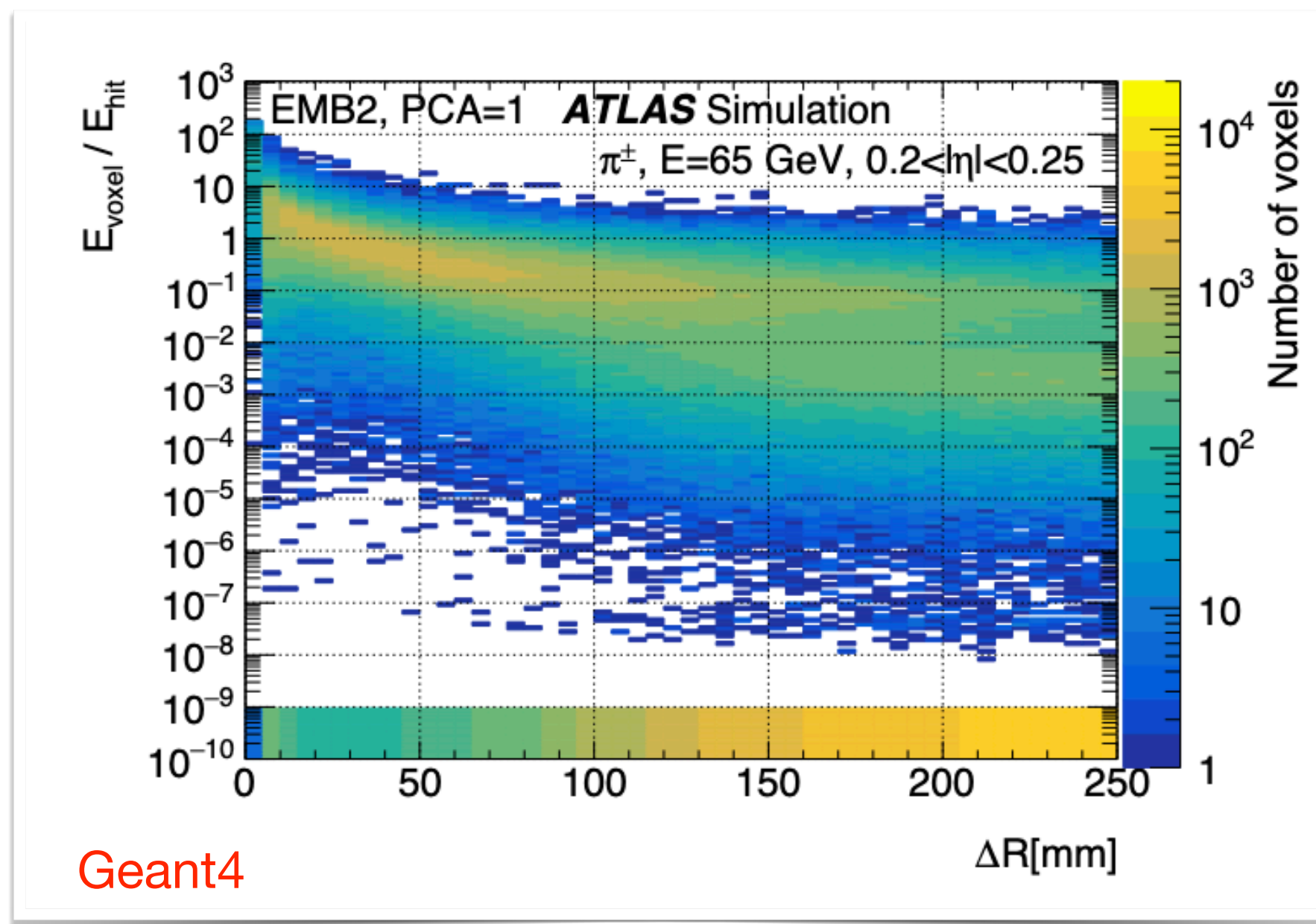
Calorimeter	Stochastic term $a$
EM	30 - 40%
Tile	50 - 60%
Hadronic endcap	60 - 80%
FCal	80 - 100%

This model with **equal energy** hits works well for **EM showers** but require hit **reweighting** for **Hadronic showers**.



# Weighted hit simulation for hadrons (1)

- ◆ Hadronic calorimeter layers have **large stochastic terms** (> 30%) leading to **large energy deposits** (100 - 300 MeV) for hits with equal energy.
- ◆ Even only few hits far away from the shower center have **large probability** to create clusters.
- ◆ These low energy clusters introduce mismodeling in the total number of clusters.



$E_{\text{voxel}}$  - bins in average shower histogram

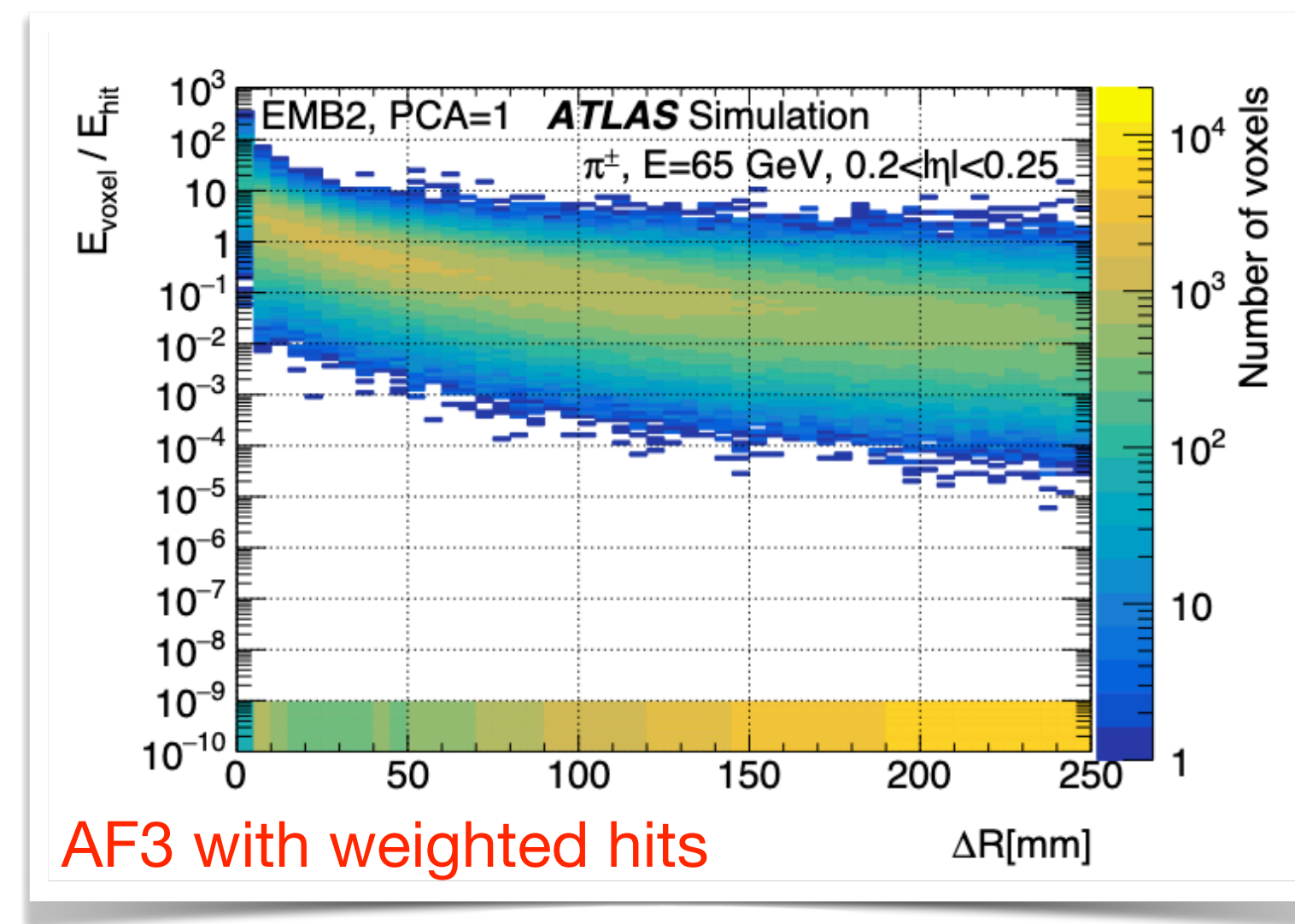
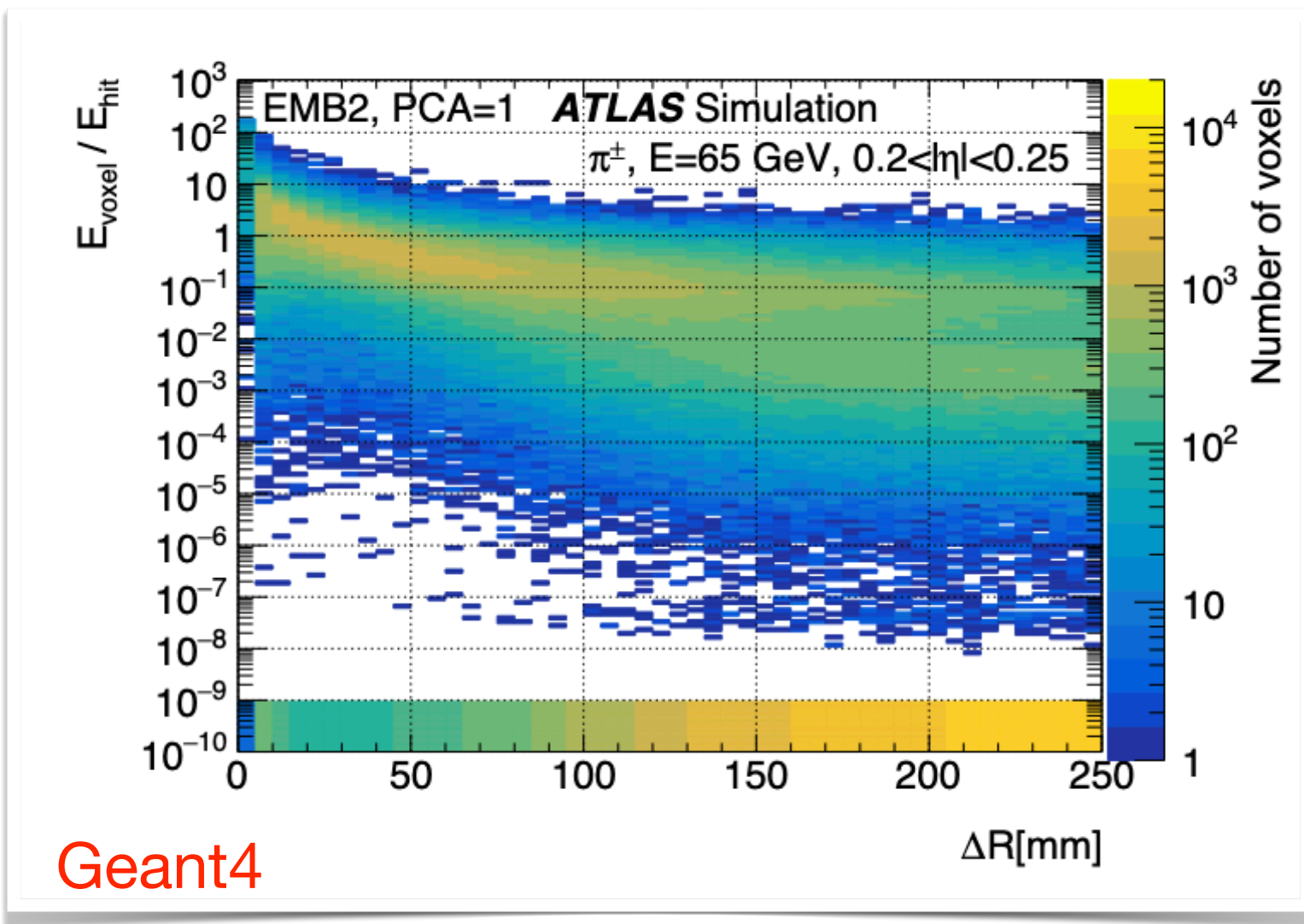
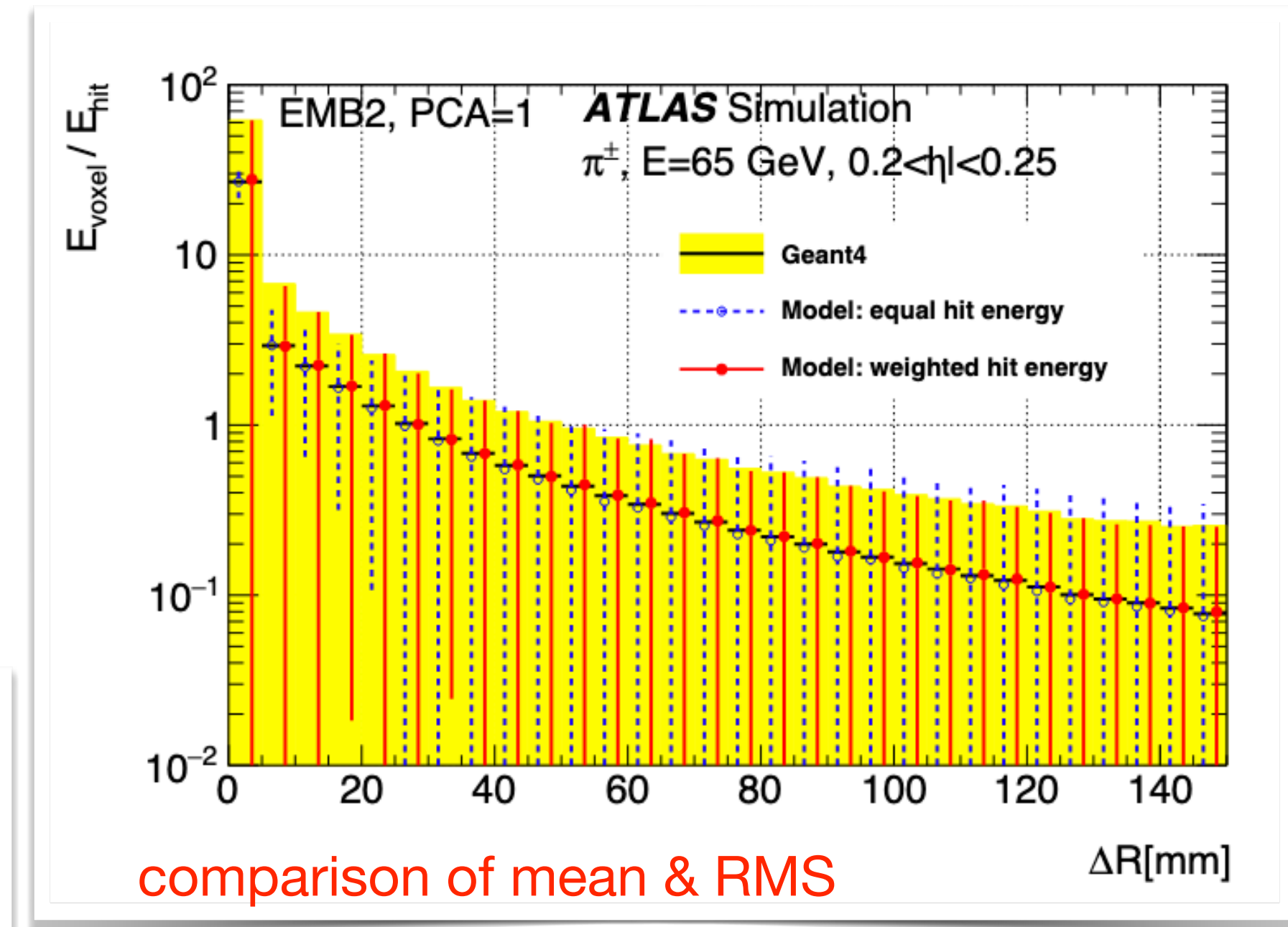
$E_{\text{voxel}} / E_{\text{hit}}$  - **energy fraction in each bin** of avg. shower

$\Delta R$  [mm] - radial distance from shower center in mm unit

Equal hit energy deposition creates **large number of clusters** away from the center of the shower not observed in Geant4!

# Weighted hit simulation for hadrons (2)

- ◆ The equal hit energy model can reproduce the mean well but not the RMS.
- ◆ Introduce **weights** to change the RMS of each bin to reproduce the RMS of the Geant4 distribution.
- ◆ Additional smearing is applied to include unaccounted fluctuations.

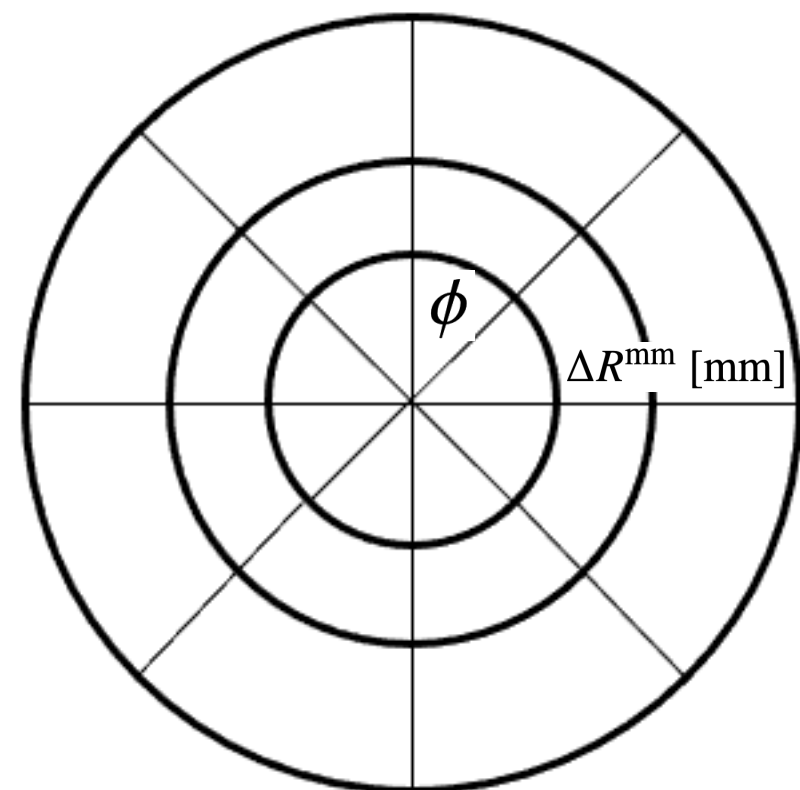


Weighted hit model significantly improves modeling of hadron showers!



# Shower Generation using Deep Learning - FastCaloGAN

- ◆ Use deep generative network to simulate shower generation **in the entire calorimeter** - providing both **longitudinal** (including correlation between layers) and **lateral shower** modeling - **Generative Adversarial Network (GAN)**, Variational Auto Encoders (VAE).
- ◆ **Pre-processing / voxelization** techniques plays an important role in model performance.
- ◆ Previous attempts of GAN and VAE training at the cell level ([ATL-SOFT-PUB-2018-001](#))
- ◆ FastCaloGAN uses hits **voxelized** in the same frame of reference  $(r, \alpha)$  as in FCS V2 shape parametrization - **optimized** for each particle and  $\eta$  bins



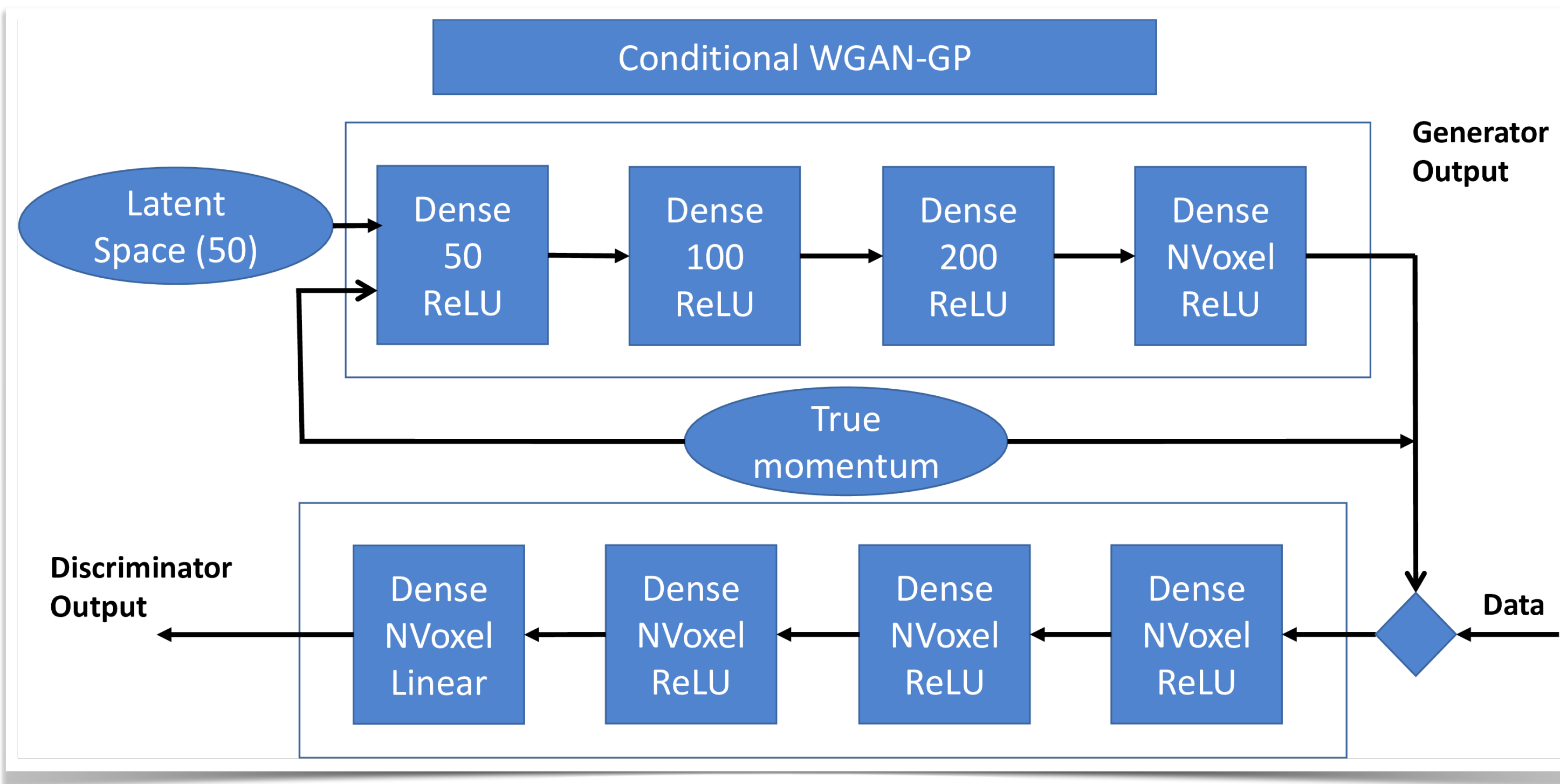
The binning used for the voxelization of pions in the different calorimeter layers for FastCaloGAN in the  $0 < |\eta| < 0.8$  range. Each ellipsis indicates when the same binning continues until the subsequent listed number.

Layer	Bin boundaries in $\Delta R^{\text{mm}}$ [mm]	Number of bins in $\phi$
PreSamplerB	5, 10, 30, 50, 100, 200, 400, 600	1
EMB1	1, 4, 7, 10, 15, 30, 50, 90, 150, 200	10
EMB2	5, 10, 20, 30, 50, 80, 130, 200, 300, 400	10
EMB3	50, 100, 200, 400, 600	1
TileBar0	10, 20, 30, ... 100, 130, 160, 200, 250 ... 400, 1000, 2000	10
TileBar1	10, 20, 30, ... 100, 130, 160, 200, 250, ... 400, 600, 1000, 2000	10
TileBar2	0, 50, 100, ... 300, 400, 600, 1000, 2000	1

# Network architecture

ATL-SOFT-PUB-2020-006

Wasserstein loss with gradient penalty (WGAN-GP) is used, **conditioned on the truth momentum** and trained for each  $\eta$  slice but inclusive in energy - resulting **100 GANs** for pions.



NVoxel	Number of voxels
Generator nodes	50, 50, 100, 200, NVoxel
Discriminator nodes	NVoxel, NVoxel, NVoxel, NVoxel, 1
Activation function	ReLU
Optimizer	Adam [60]
Learning rate	$10^{-4}$
$\beta_1$	0.5
$\beta_2$	0.999
Batch size	128
Training ratio (D/G)	5
Gradient penalty ( $\lambda$ )	10

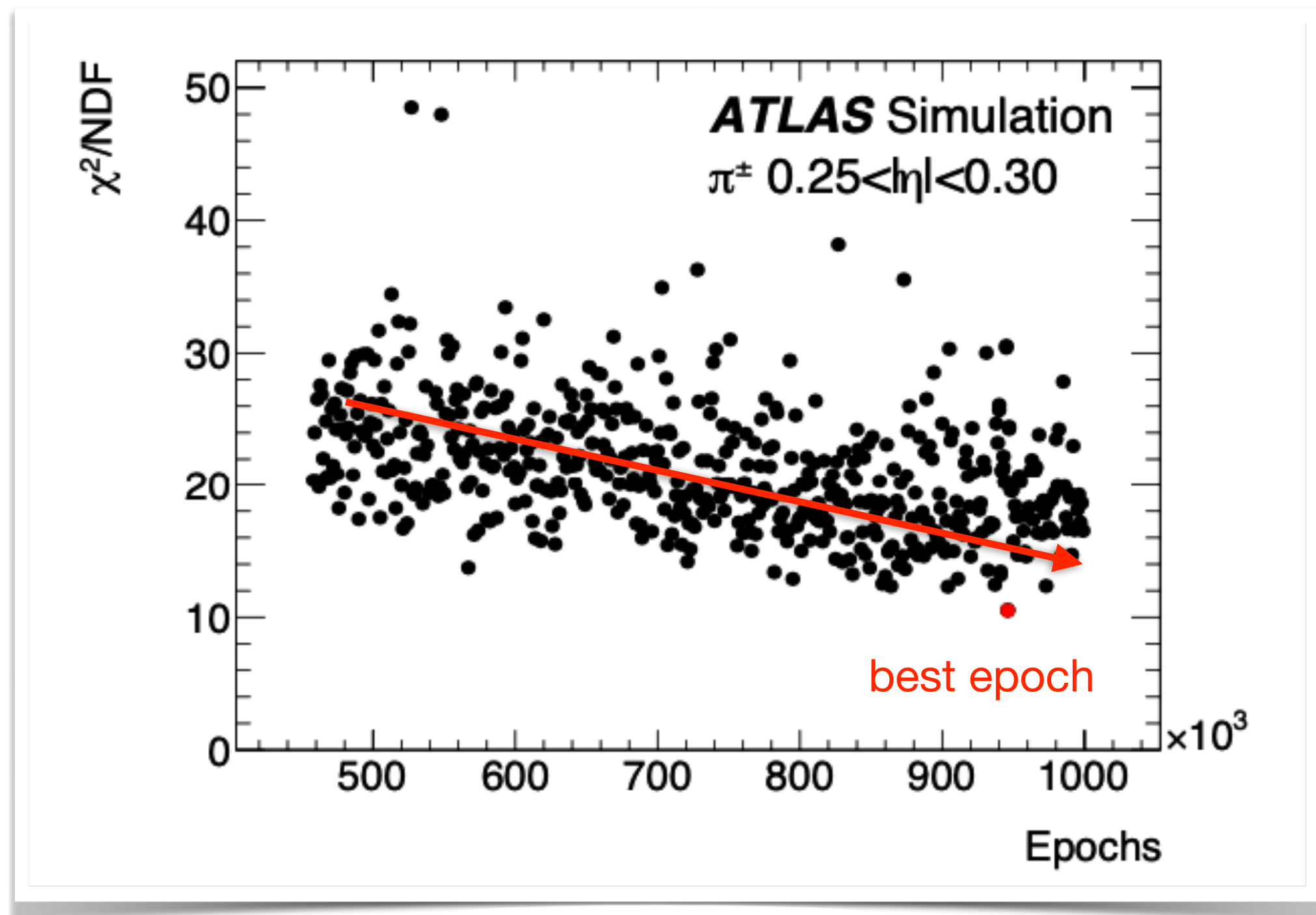
Networks are implemented in **TensorFlow2** - allows training in both CPUs and **GPUs**



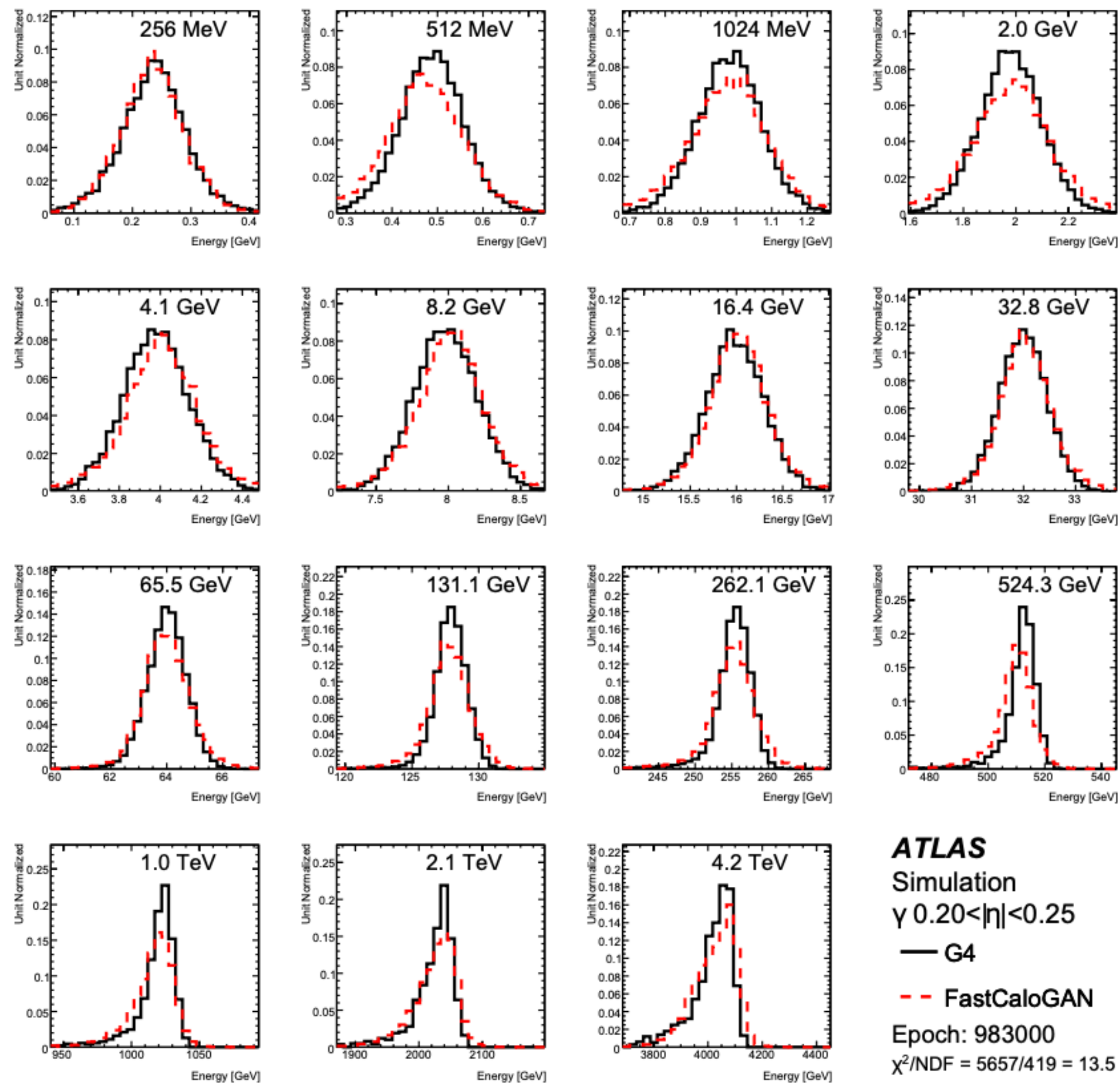
# Training strategy

- ◆ Training a GAN with all energy points (for a fixed  $\eta$ ) does NOT provide good performance.
- ◆ An **incremented** training strategy is used:
  - ◆ start with a single energy point 32 GeV and train for 50K epochs
  - ◆ add new energy points every 20K epoch in the following order: 32 GeV, 64 GeV, 16 GeV, 128 GeV, ...
- ◆ Each GAN is trained for **1M epochs** with a checkpoint saved every 1K epochs.
- ◆ Each GAN requires ~8hrs to train on GPU over HTCondor - **100 days of GPU time** for the entire detector

- ◆ The final epoch is NOT necessarily the best epoch - interplay between the generator and the discriminator.
- ◆  $\chi^2$  between the total energy generated by GAN and Geant4 is used as a metric.
- ◆ At simulation step the GAN with **best epoch** is used to generate hits which are deposited in the corresponding voxels.



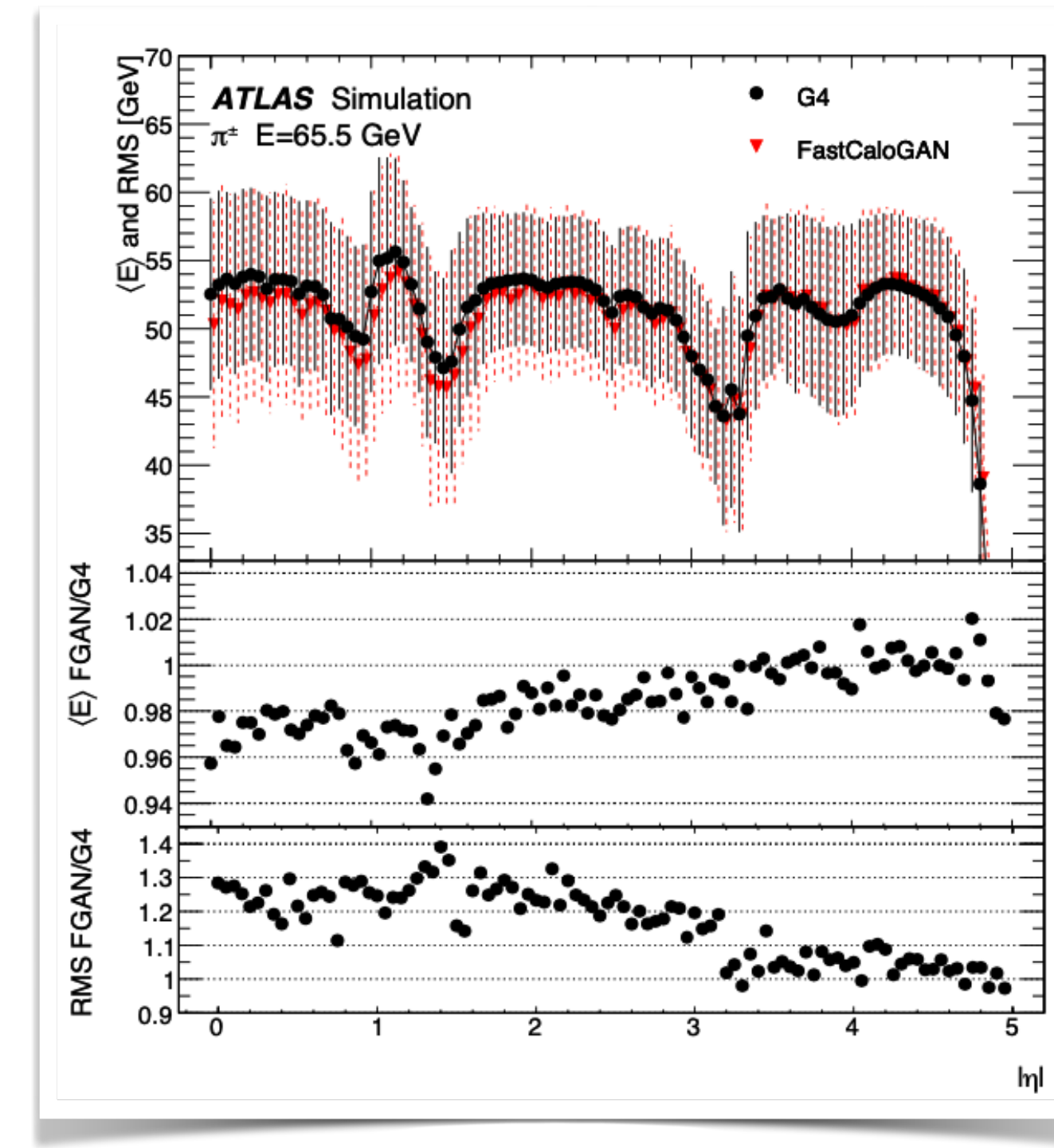
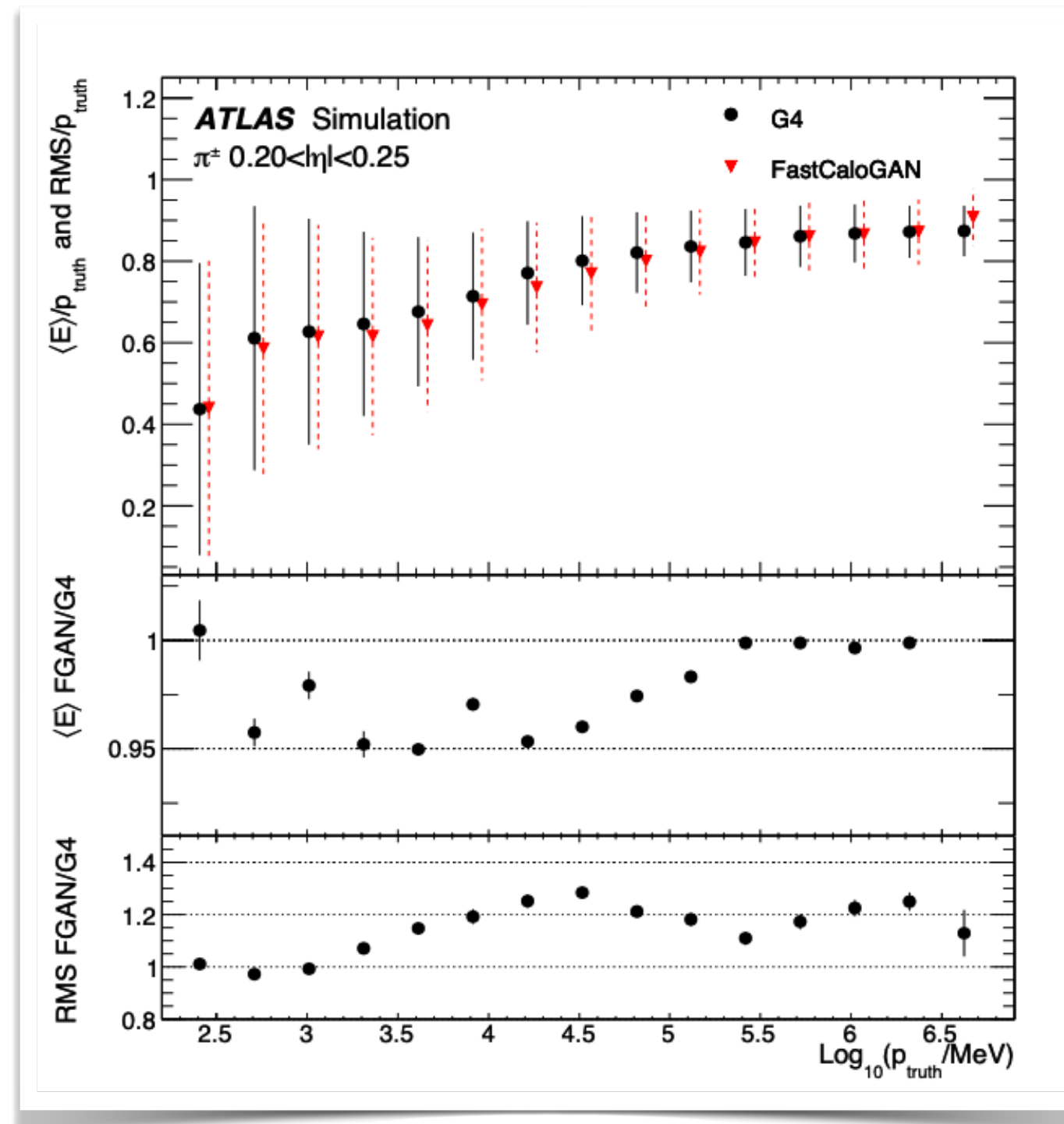
# Performance at best epoch





# FCSGAN Performance in Simulation

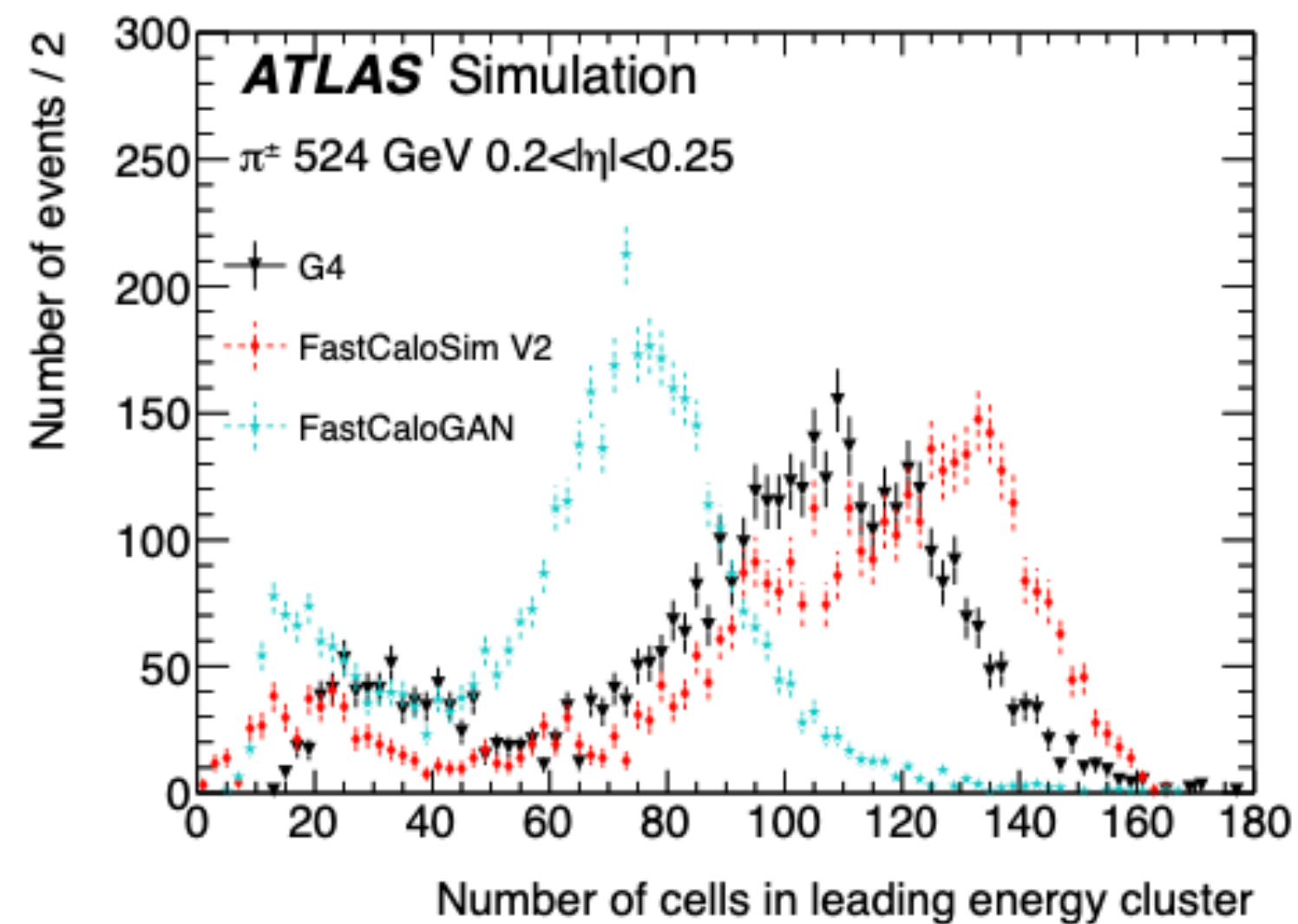
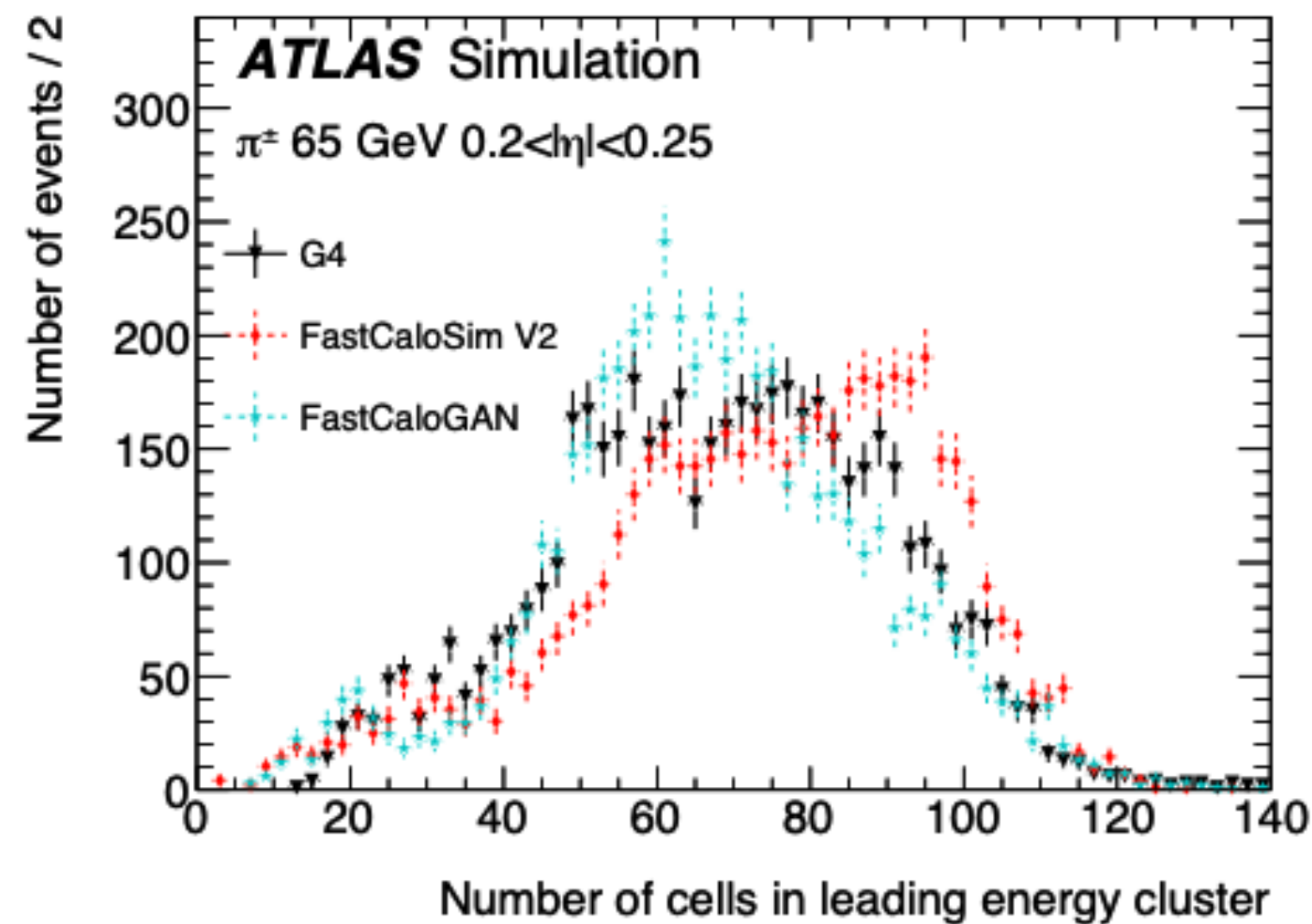
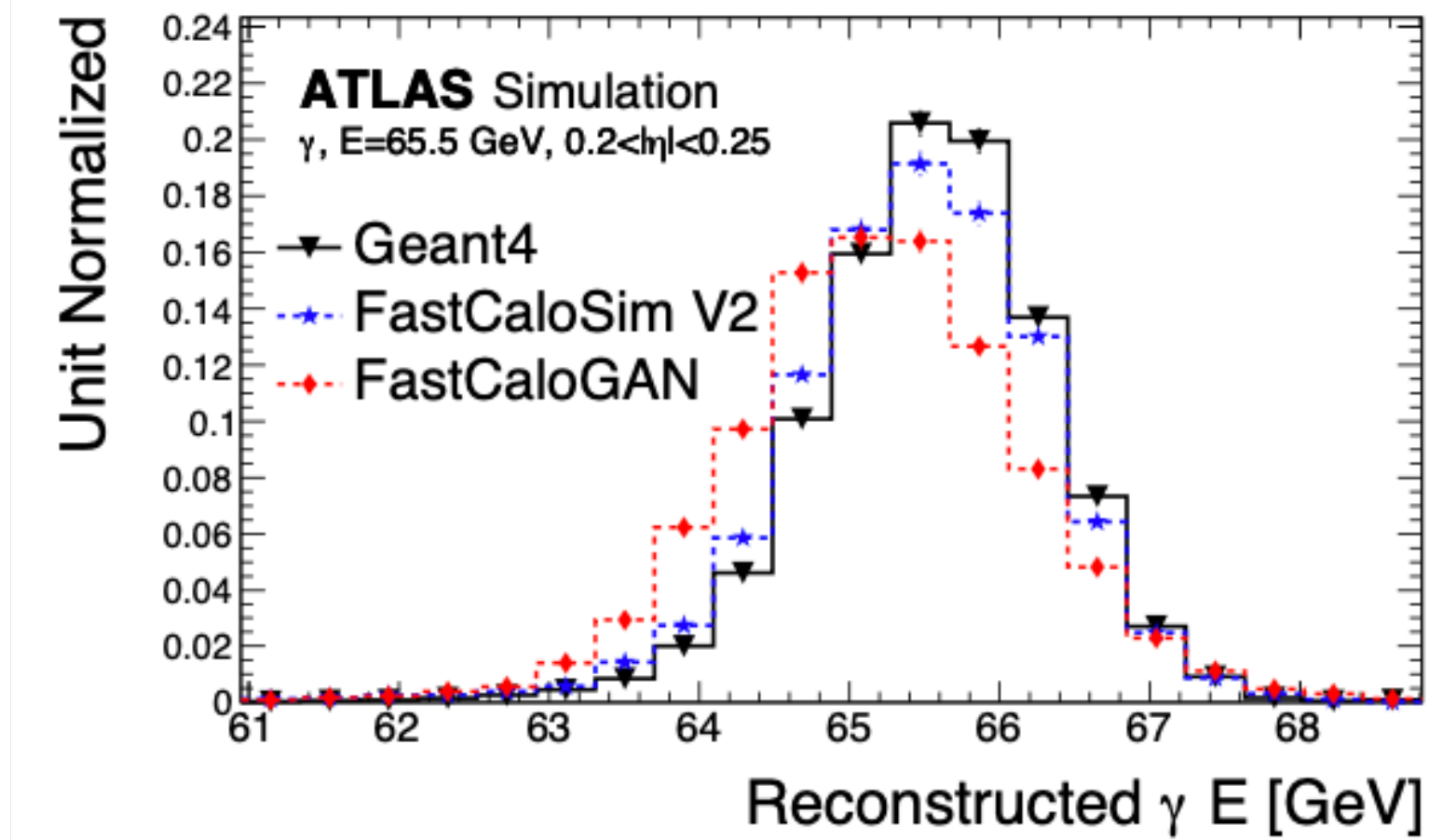
- ◆ FastCaloGAN shows better modeling compared to FCS V2 for hadrons in the **medium energy range**.
- ◆ The exact threshold is determined based on **single cluster** and **jet properties**.
- ◆ AF3 uses FCSGAN for hadron showers in the range:  **$16 \text{ GeV} \leq E_{\text{kin}} \leq 256 \text{ GeV}$**
- ◆ The total energy of the FastCaloGAN is **scaled to the energy of FCS V2** - allows smooth transition between the two simulation flavors.



**Fully implemented** in the ATLAS simulation infrastructure and used as part of AF3 for sample production!

# What about photons and low/high energy pions?

- ◆ For photons, the reconstructed mean energy is shifted
- ◆ For low and high energy pions, too few energy deposits in cells of the leading cluster.
- ◆ Some of the issues are expected to be resolved in the future.



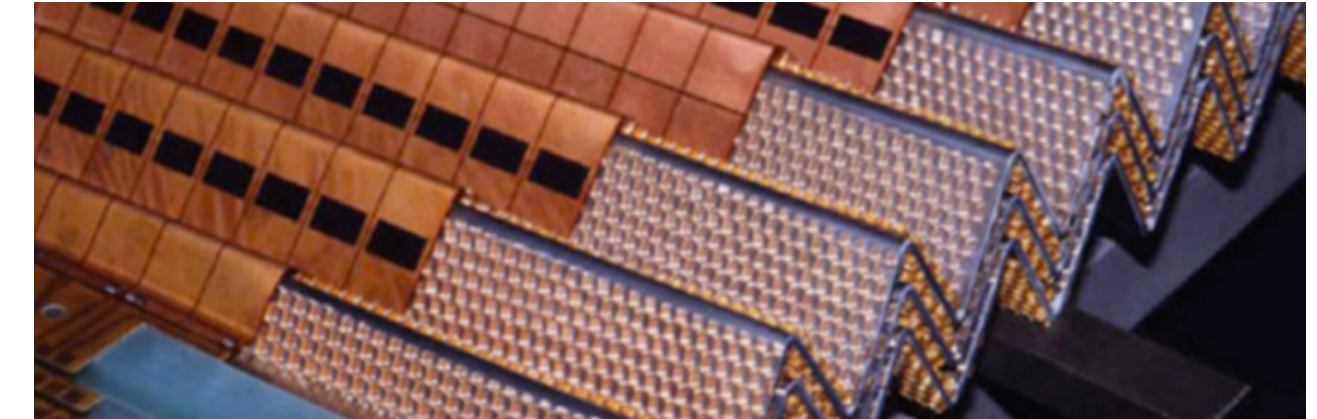
We also released some datasets for training under CERN open data!

<https://opendata-qa.cern.ch/record/15012>



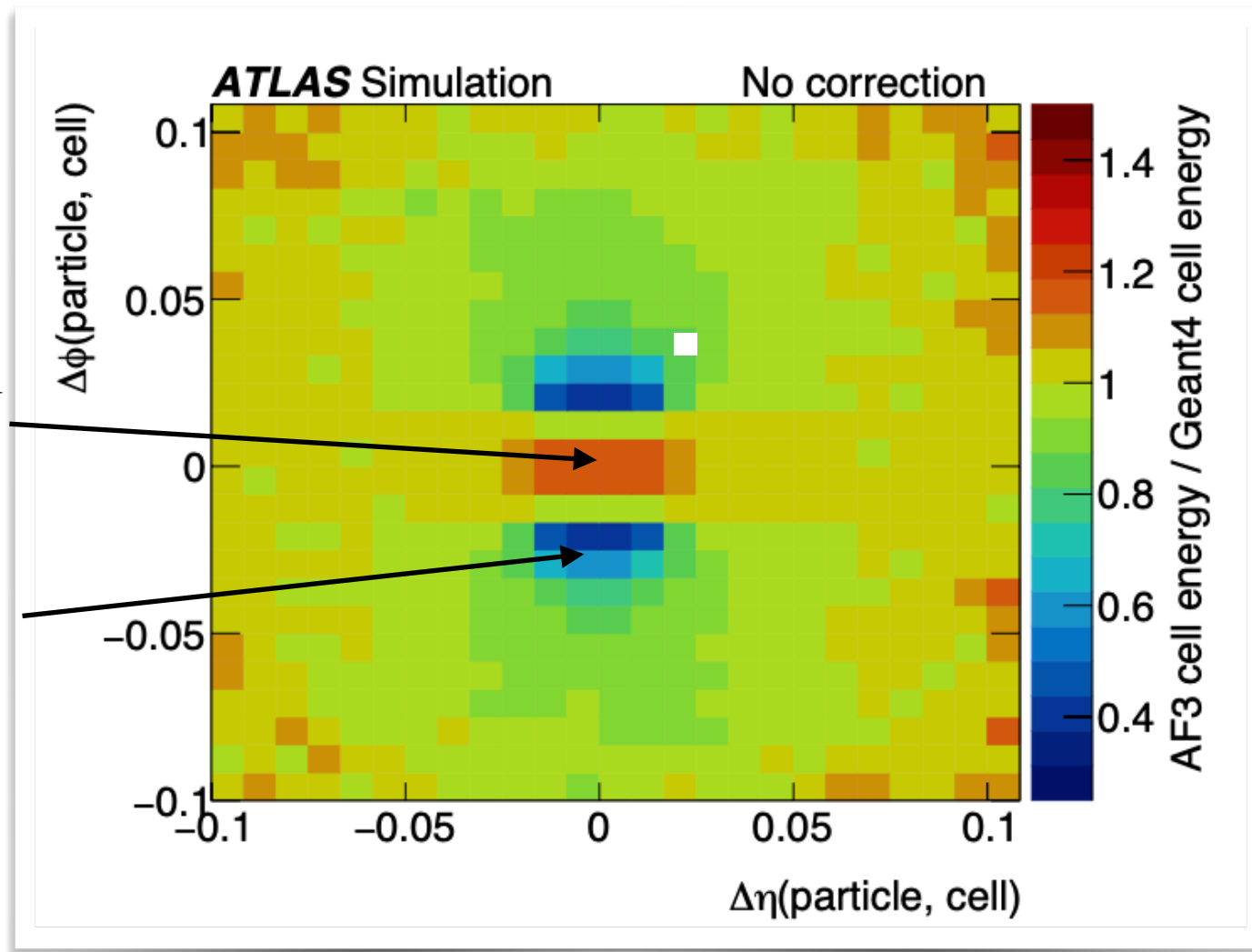
# Assigned quantized energy (hits) to calorimeter cells

- ◆ Simulated hits (from FCS V2 or FCSGAN) are assigned to cells assuming **simplified cuboid geometry**.
- ◆ Derive a **probability density function** (PDF) from the difference of cell assignment efficiency calculated in Geant4 and AF3.
- ◆ Use the PDF to randomly **assign a displacement to a hit** before assigning to a cell.

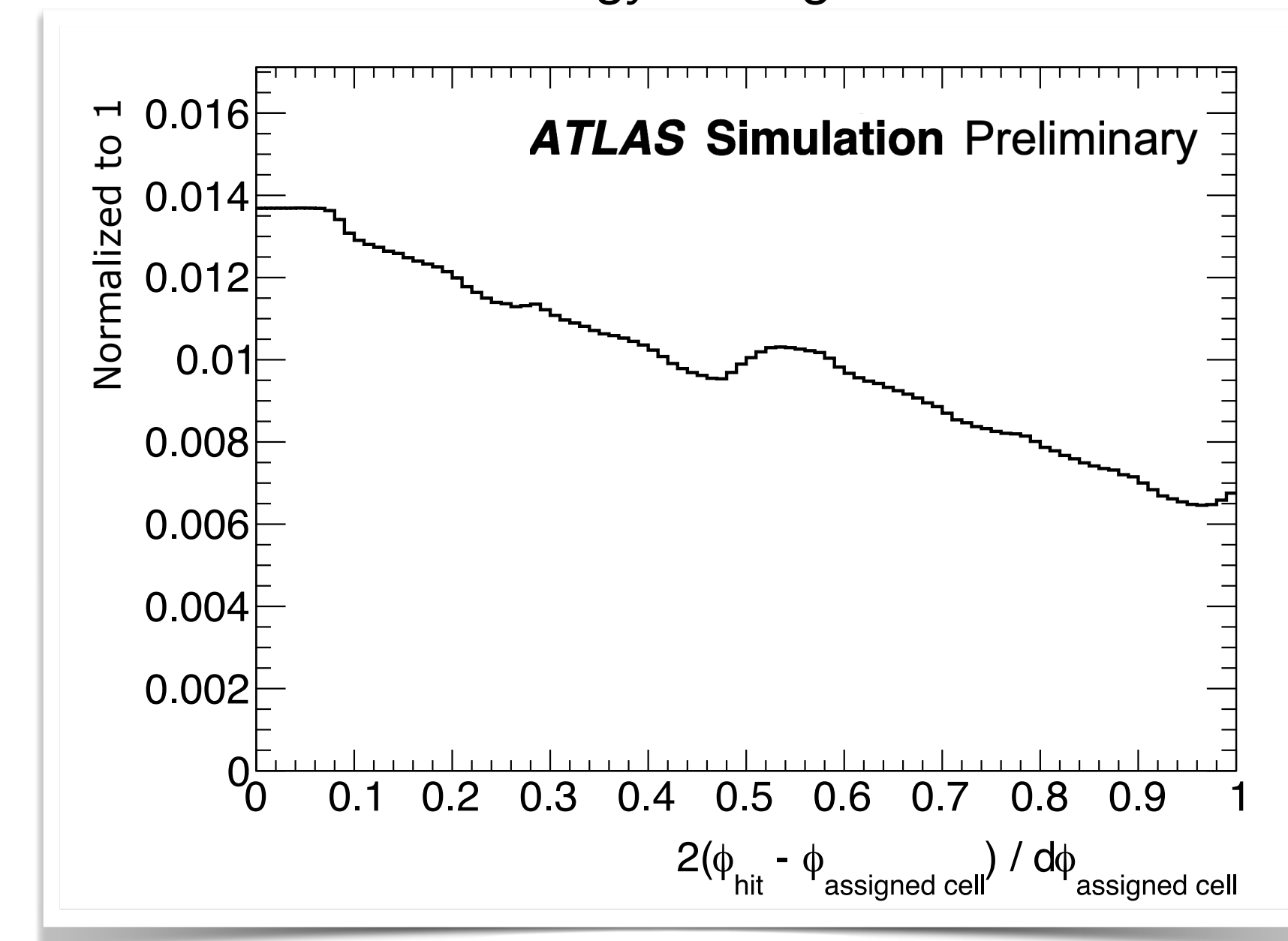
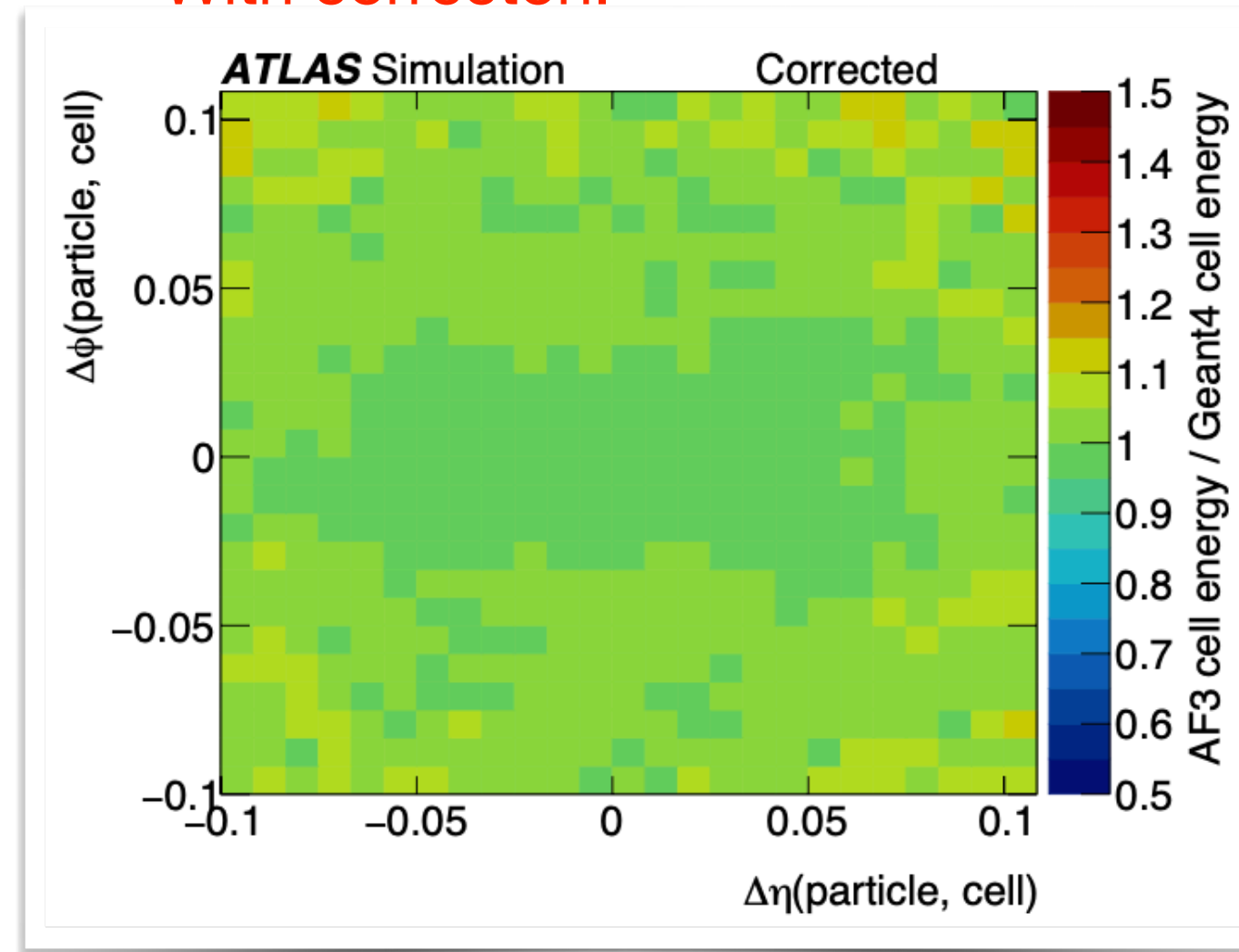


*Probability function describing the chance that the energy belongs to this cell*

Without correction:



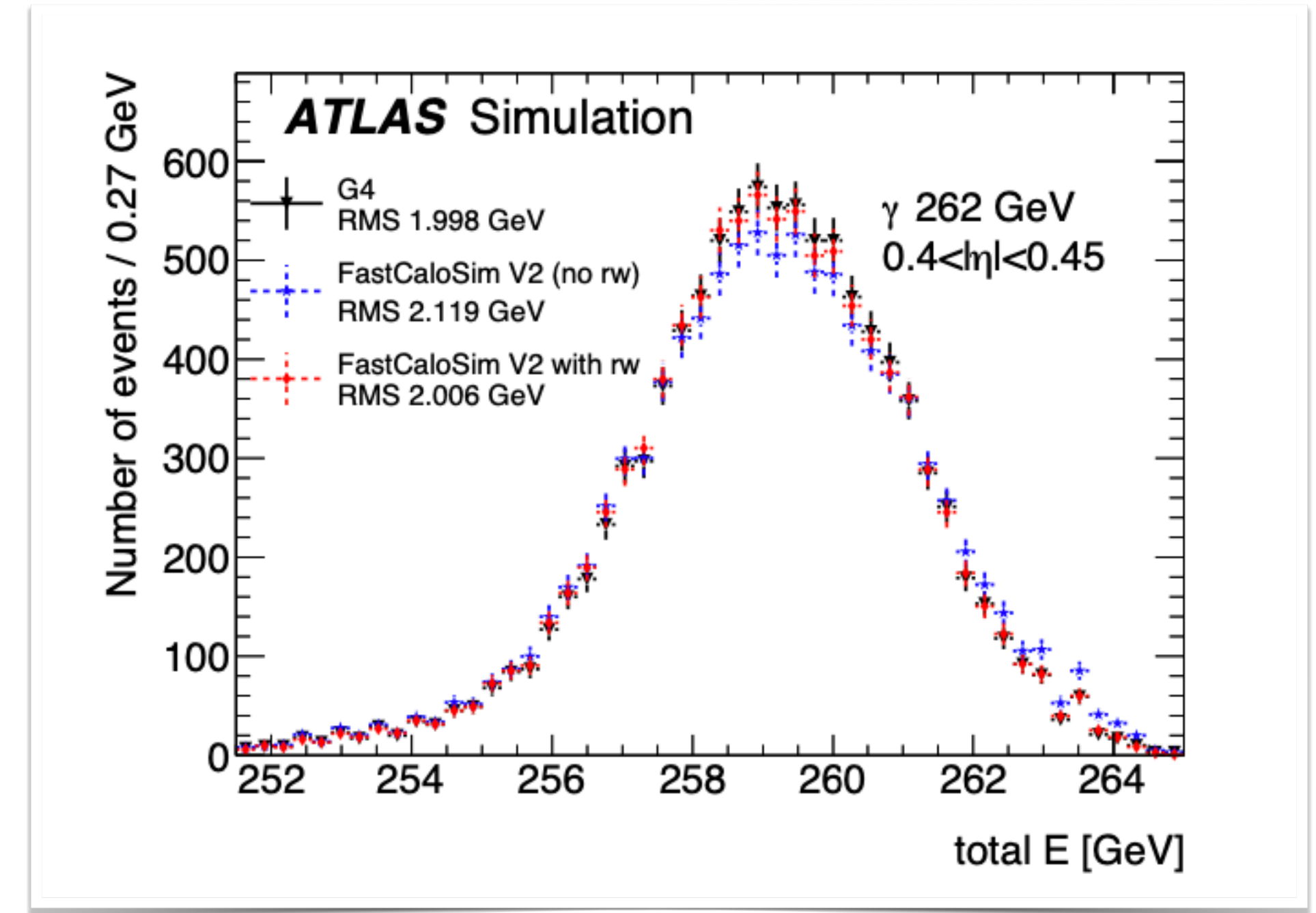
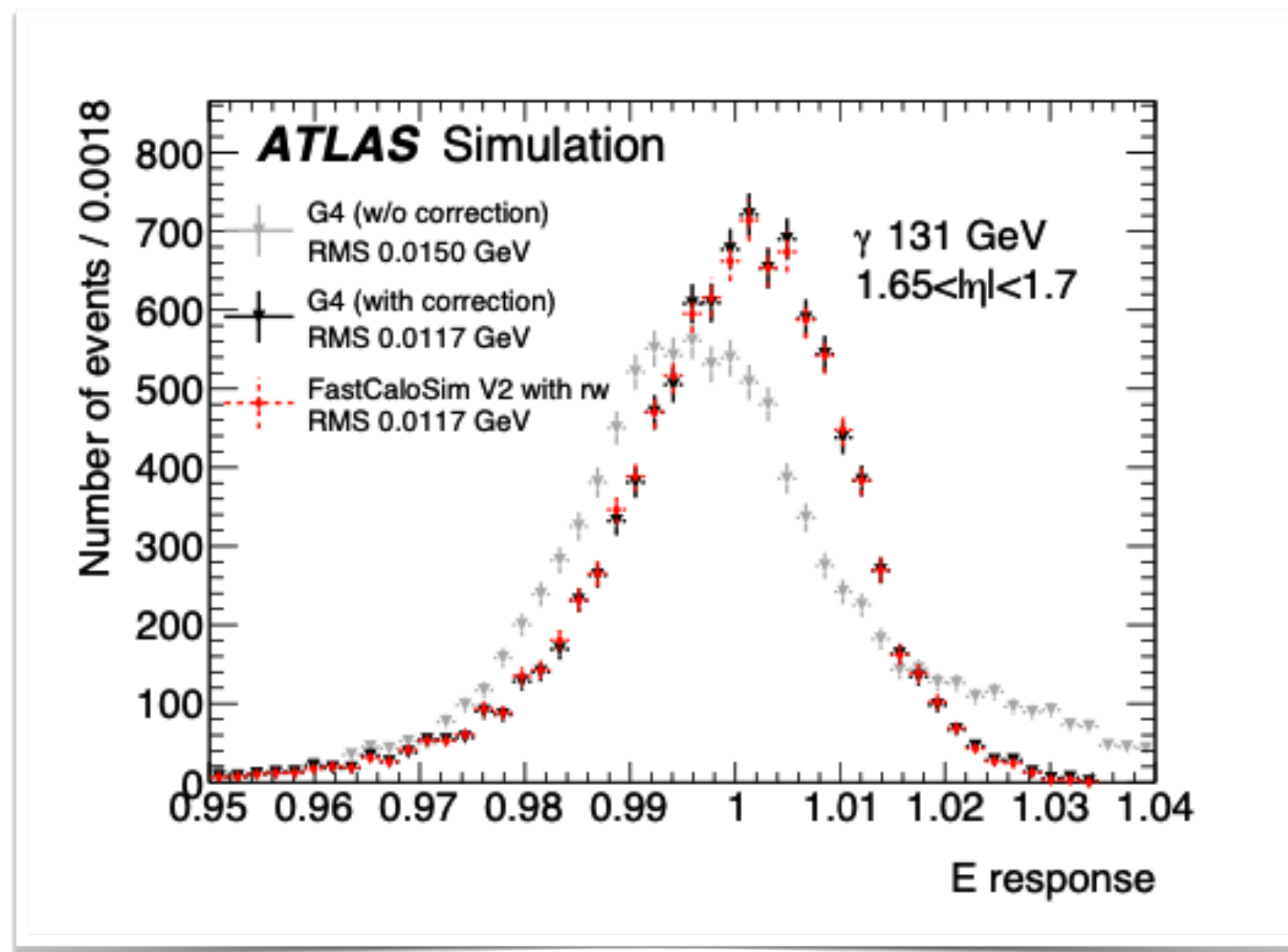
With correction:



Closure with Geant4 with the correction applied!

# Corrections to improve energy resolution

- ◆ **Probabilistic reweighting** to reject simulated energy far off from the G4 distribution - using a PDF derived from simulated over expected energy.

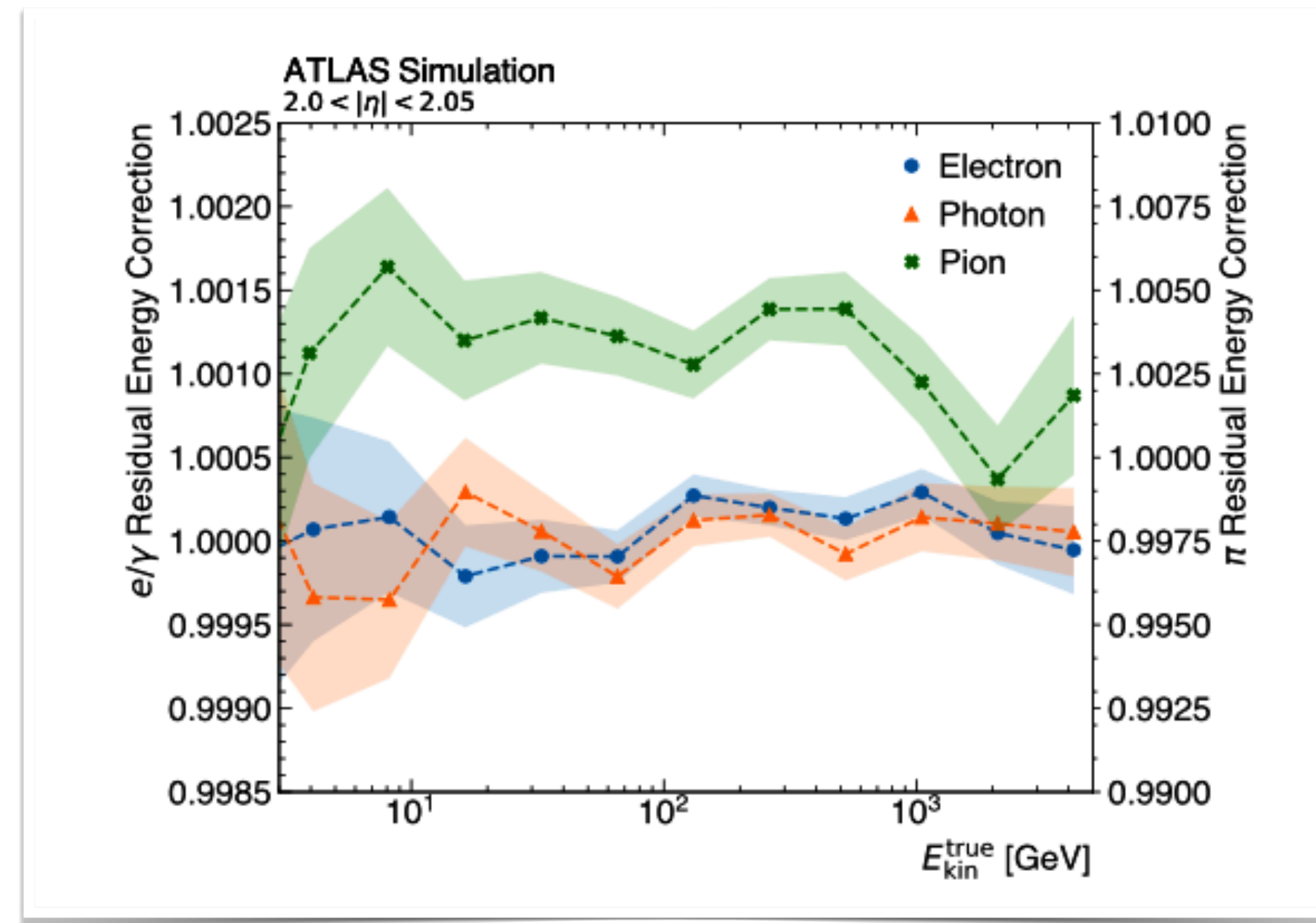
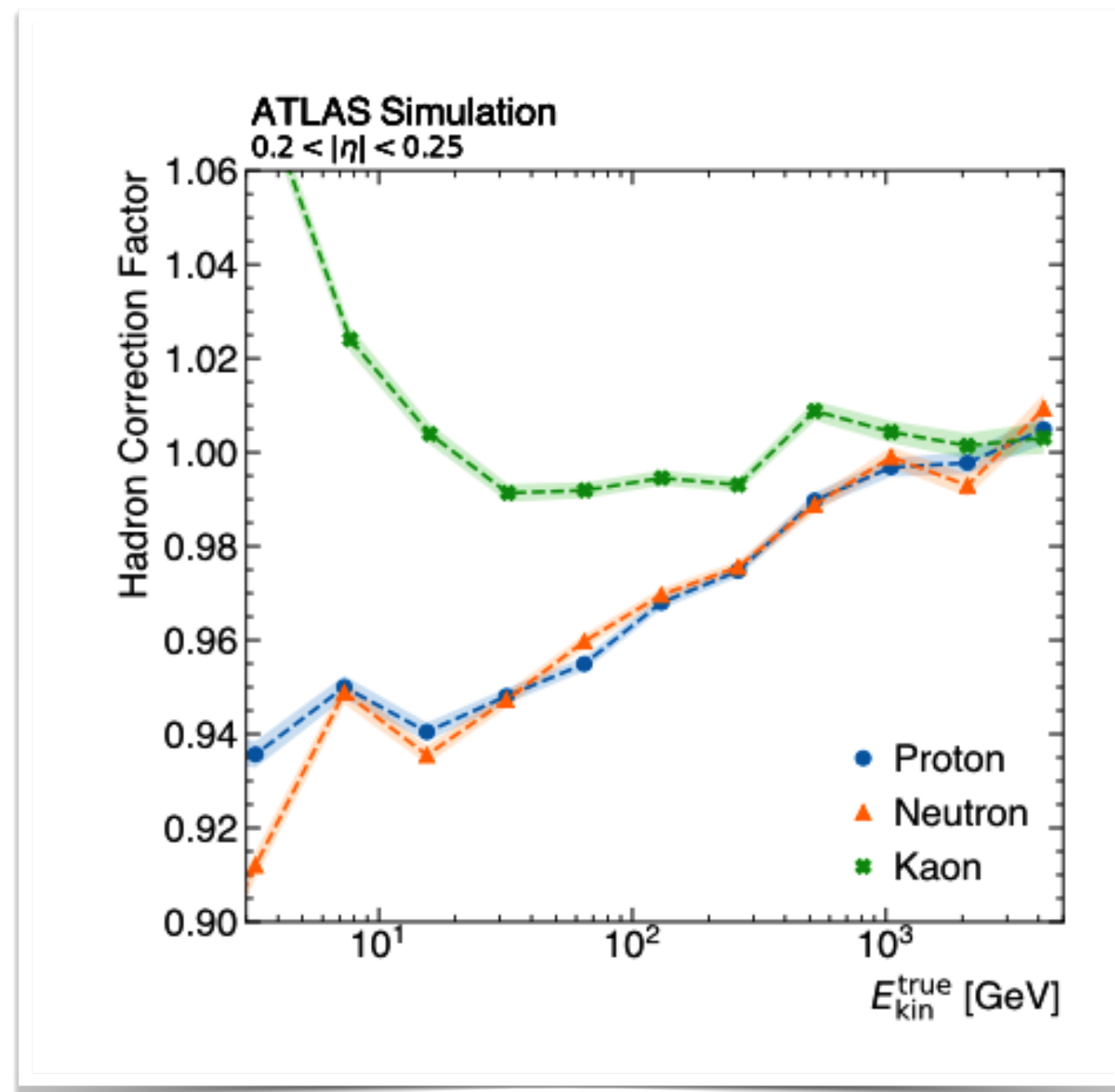


- ◆ There is a **modulation of energy in the phi direction** in the input G4 due to accordion structure in Liquid Argon (LAr) calorimeter which is not modeled in AF3.
- ◆ The Geant4 inputs are corrected before parametrization to “flatten” the phi modulation.



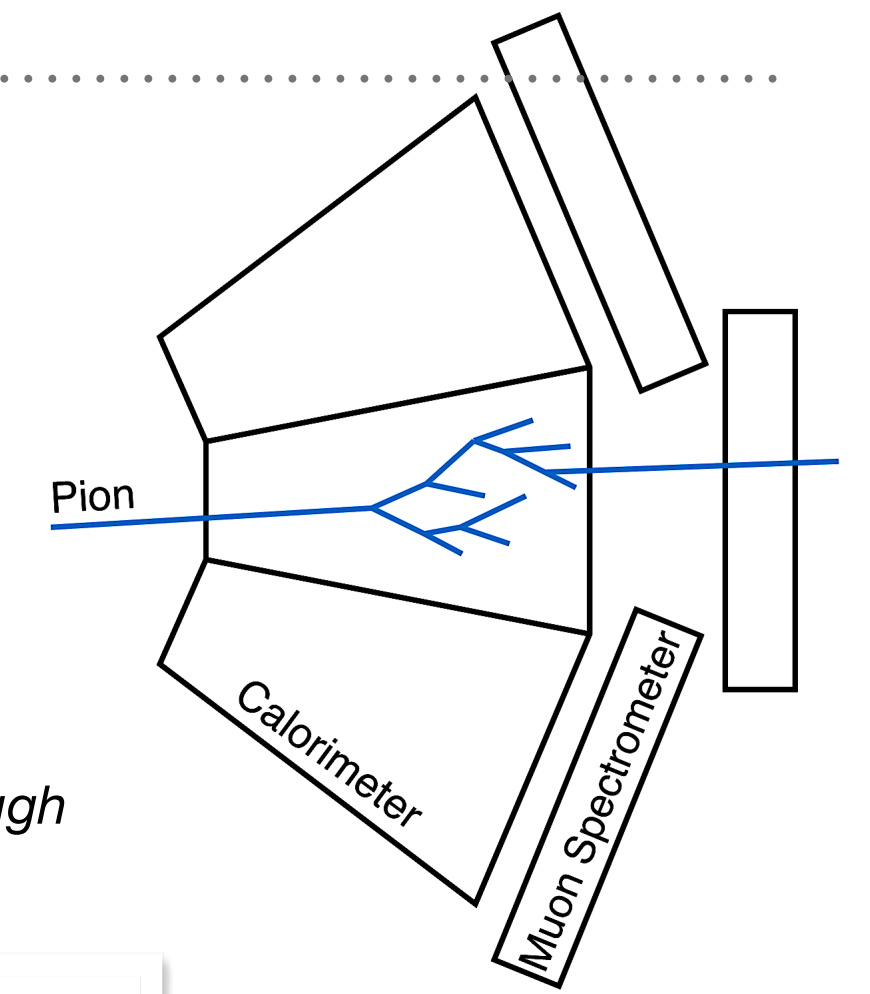
# Corrections to improve mean energy

- ◆ Small residual differences in energy response simulation in electron , photon and pion:
  - ◆ derive correction factors  $\bar{E}_{G4}/\bar{E}_{AF3}$  for each energy and  $\eta$  points with linear interpolation in between
  - ◆ for photons & electrons the corrections are applied if the correction factor is statistically significant
- ◆ Hadron showers simulated with pion parametrization has an intrinsic energy difference:
  - ◆ derive  $\bar{E}_{G4}^{\text{Hadron}}/\bar{E}_{G4}^{\pi}$  correction factors scaled by  $E_{\text{kin,true}}^{\pi}/E_{\text{kin,true}}^{\text{Hadron}}$
  - ◆ the correction factors are linearly interpolated in between the discrete energy points



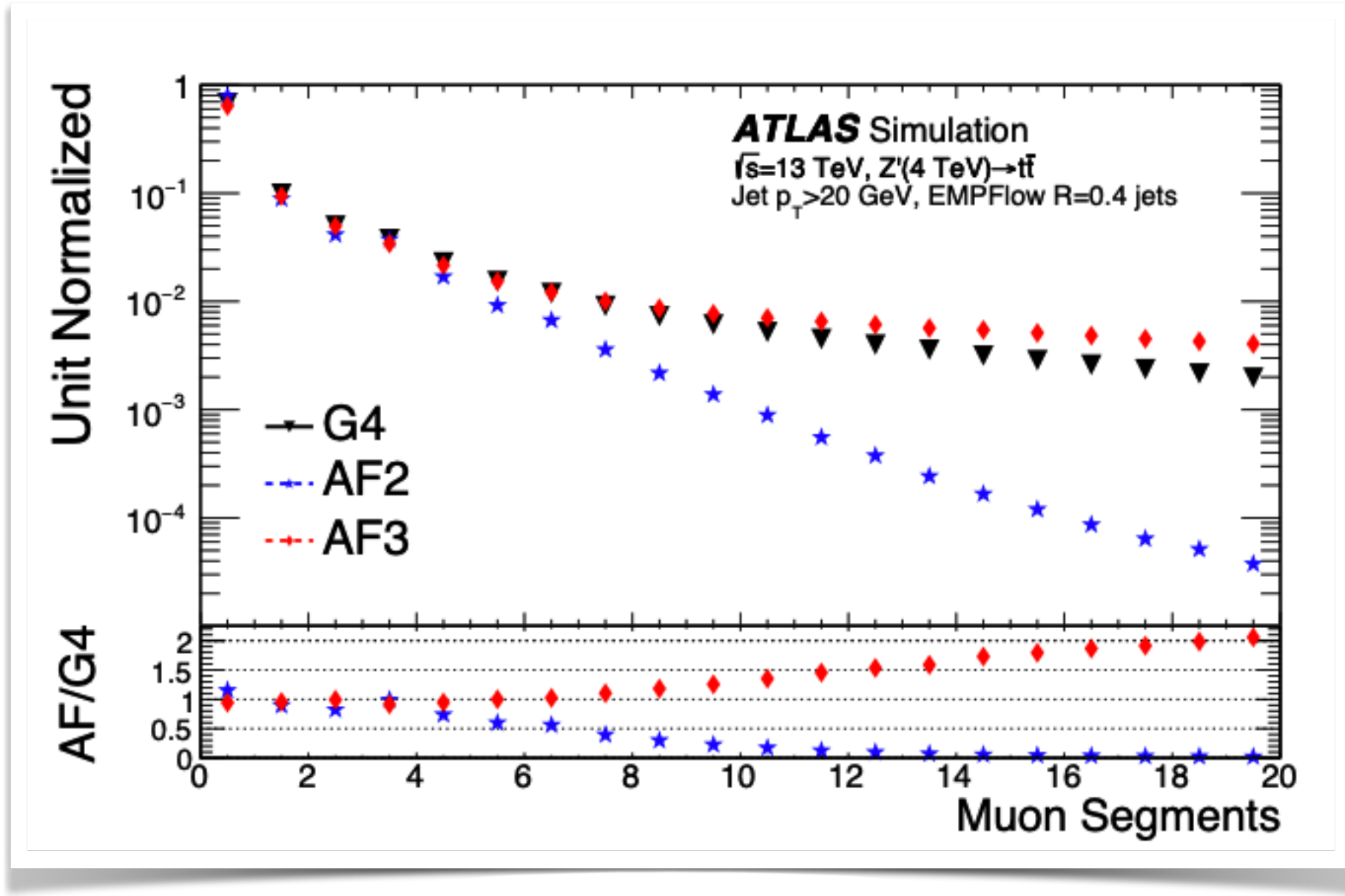
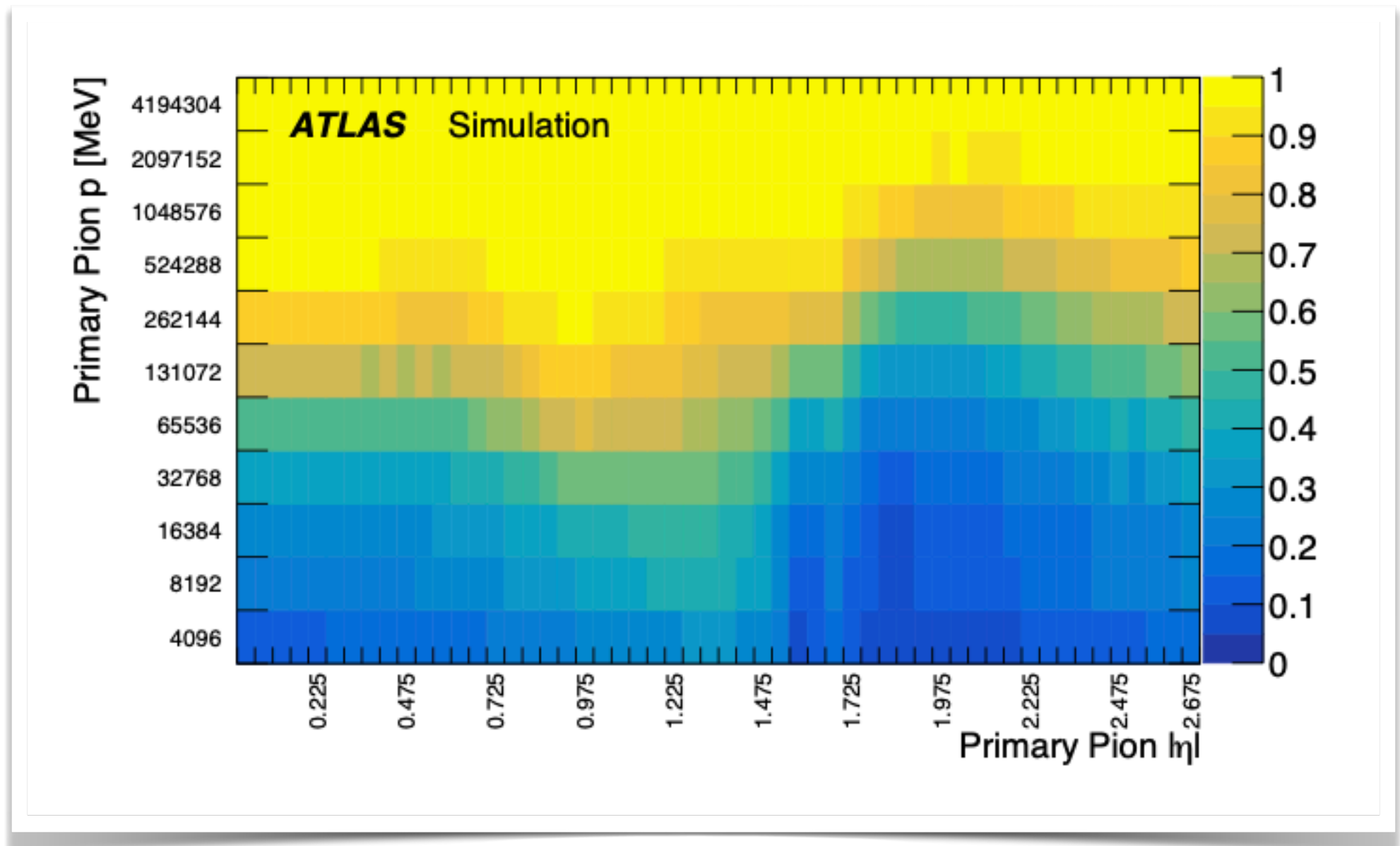
# Parametrization of particles escaping to the muon systems

- ◆ Particles that **punch through to the MS** are reconstructed as a fake muon.
- ◆ AF3 includes a dedicated parametrization to model the **secondary particles** (e,  $\gamma$ ,  $\pi$ ,  $\mu$ ,  $p$ )
- ◆ Depending on the momentum and  $\eta$  for a pion entering the calorimeter volume, the punch through particles are generated and **passed to Geant4**.



probability of a single pion to produce at least one punch-through particle of at least 50 MeV

muon segments results from particles punching through the calorimeter as well as real muons

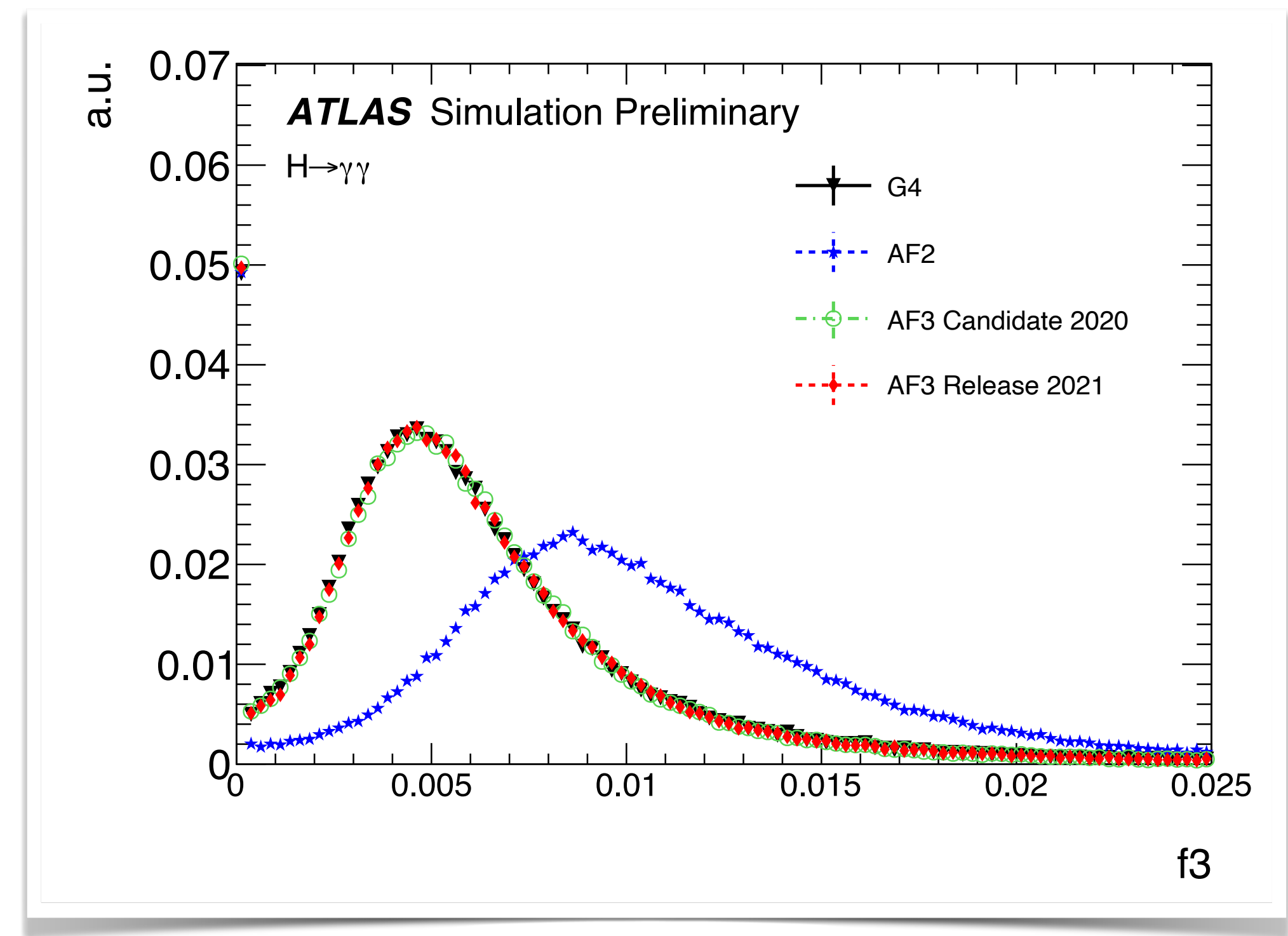
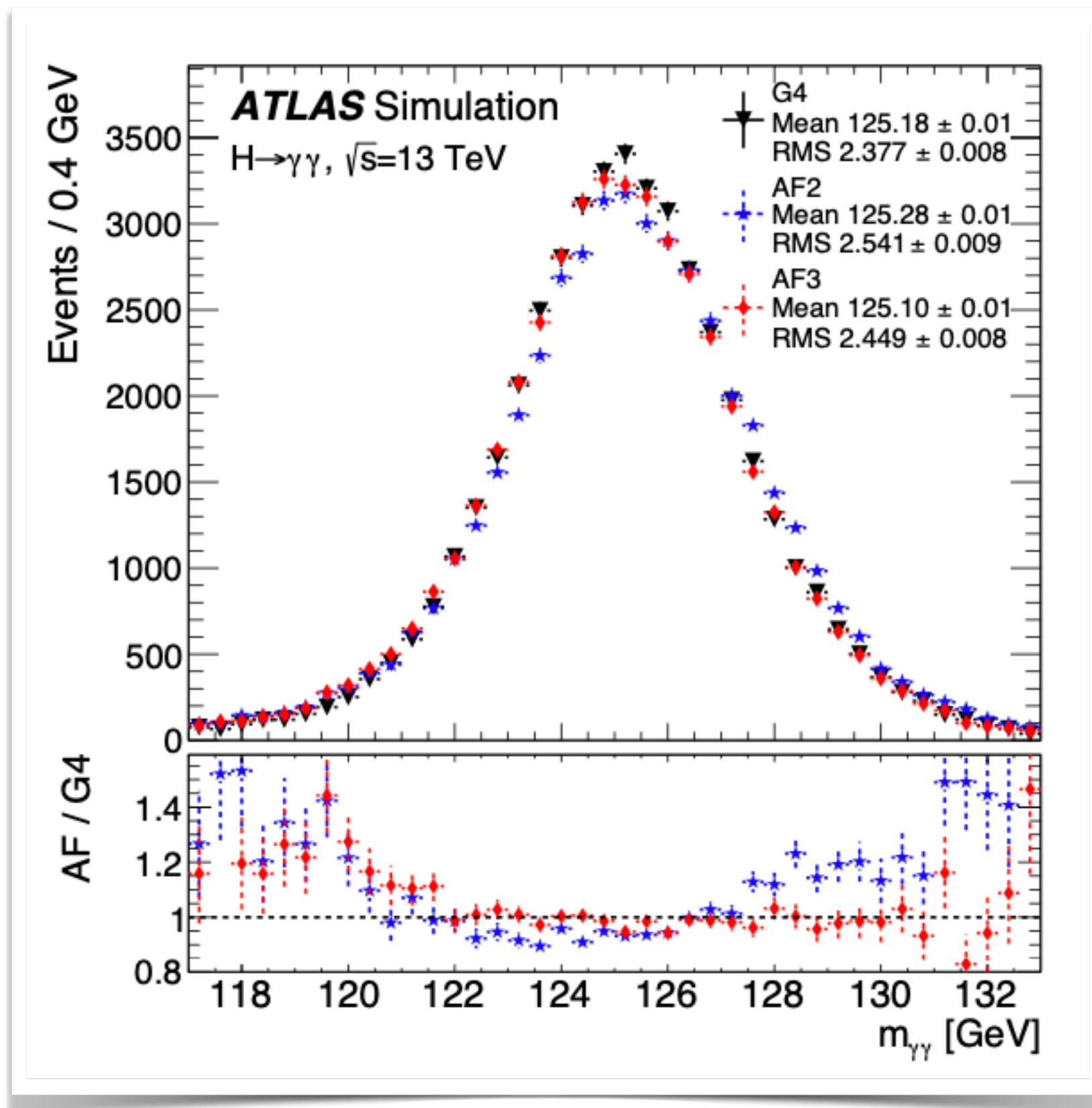


Improves modeling of muons significantly compared to AF2!



# Performance of AF3: reconstructed photons & electrons

- ◆ Photons and electrons are reconstructed from clusters of energy deposits in EM calorimeter.
- ◆ The objects are selected with identification criteria with high purity as used in physics analyses.

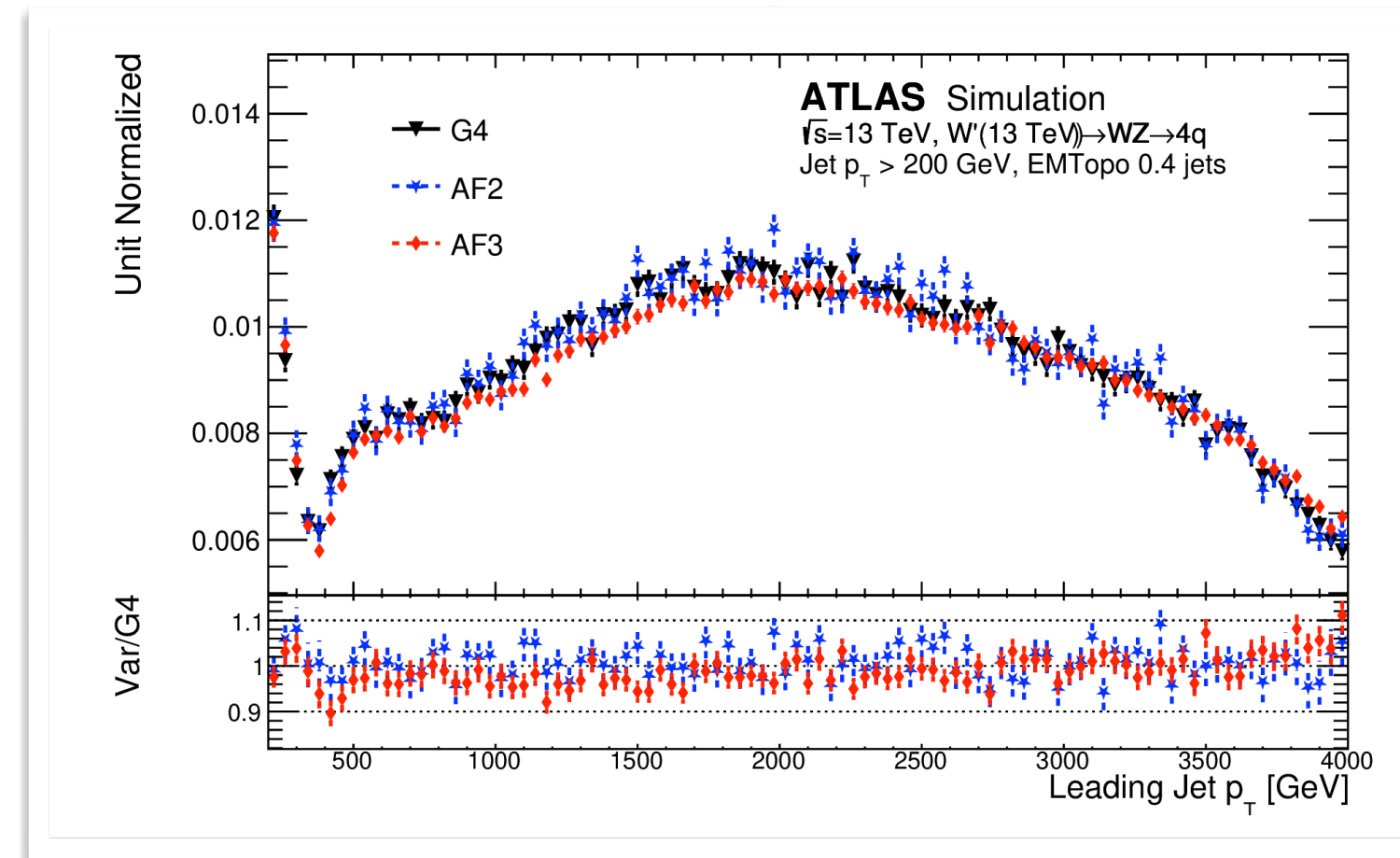
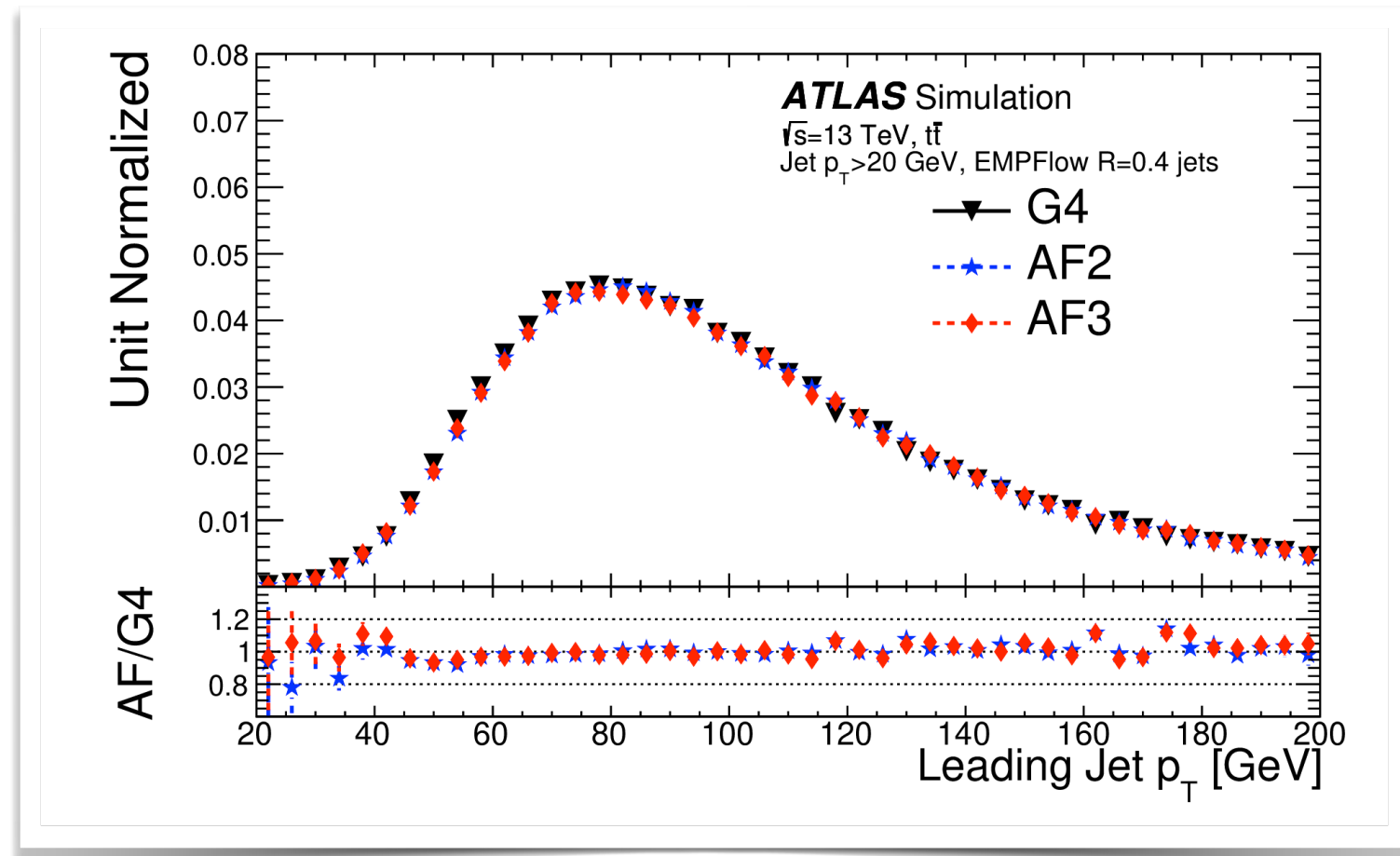


*Invariant mass of Higgs (left) and energy fraction in sampling 3 of the EM calorimeter (right) in  $H \rightarrow \gamma\gamma$  events*

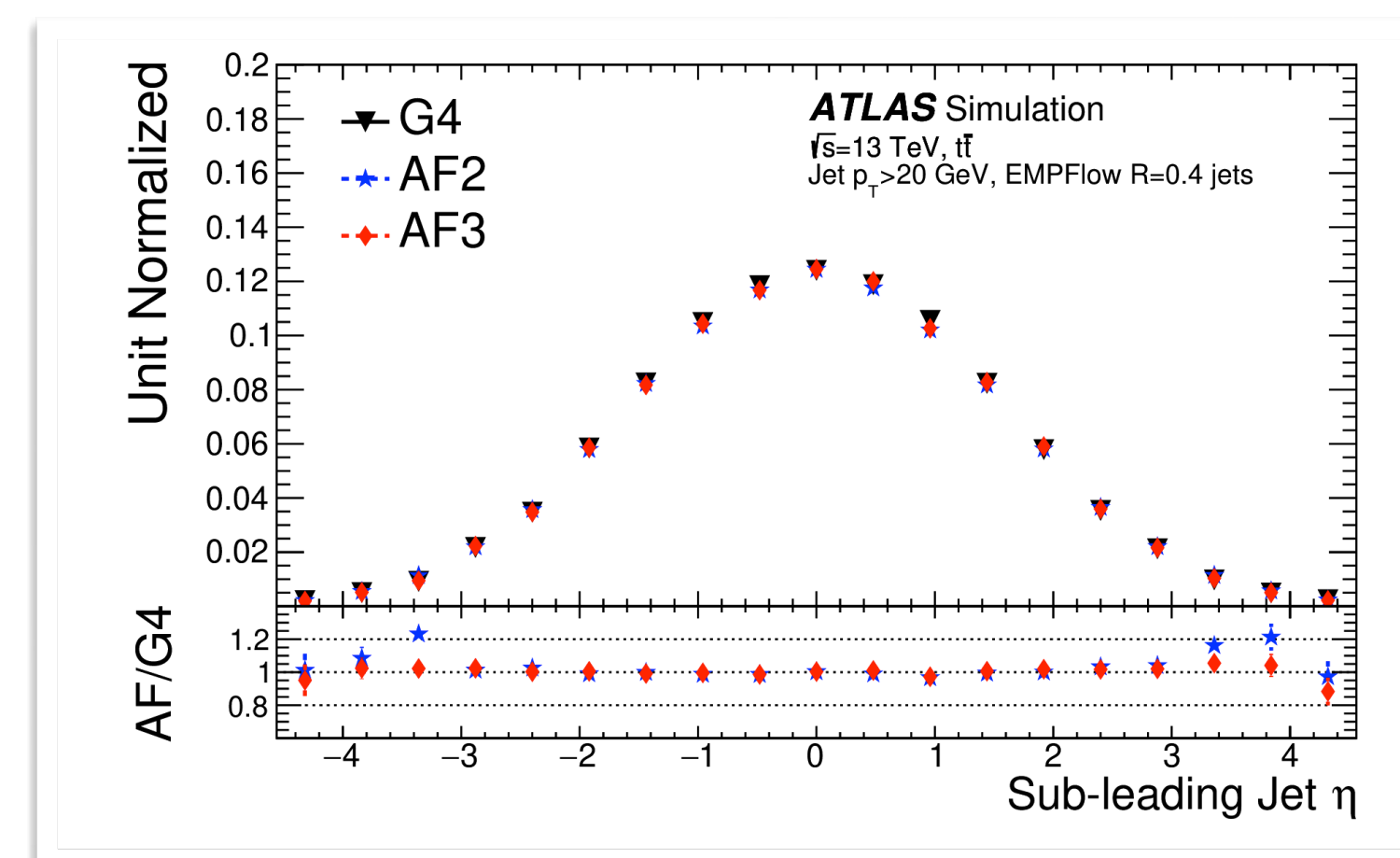
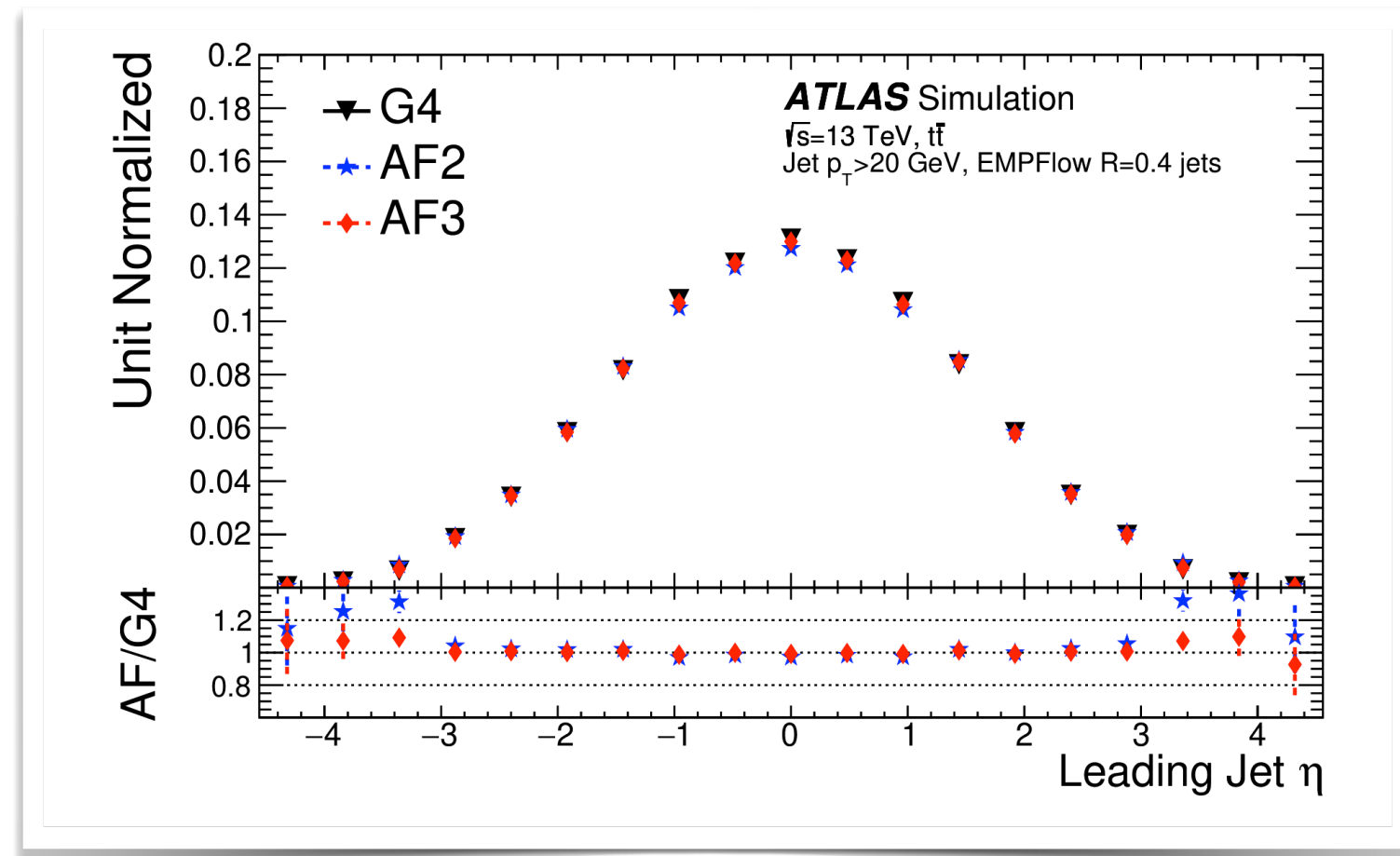
Very good modeling for all electron/photon variables!

# Performance of AF3: kinematics of reconstructed jet

- ◆ Good modeling of jet kinematics for jets of cone 0.4 reconstructed with EMPFlow or EMTopo algorithms
- ◆ Jets with  $p_T > 200$  GeV shows better agreement in AF3 compared to AF2
- ◆ Dedicated parametrization in forward calorimeter also improves the modeling for  $|\eta| > 3$



*all jets  $p_T$  distribution - (left) for  $p_T < 200$  GeV in  $t\bar{t}$  and (right) for  $p_T > 200$  GeV in  $W'(13\text{TeV}) \rightarrow WZ \rightarrow 4q$*

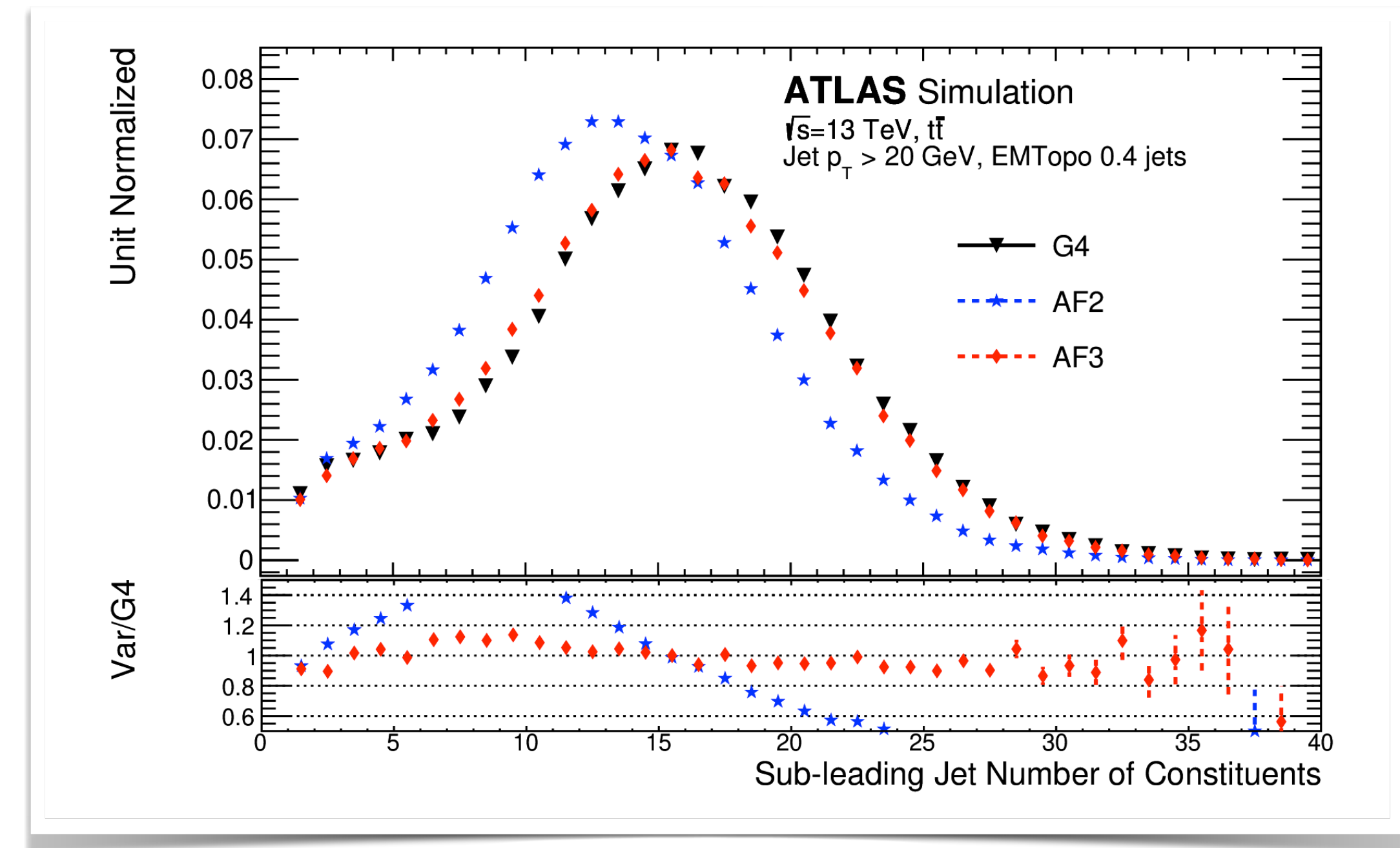
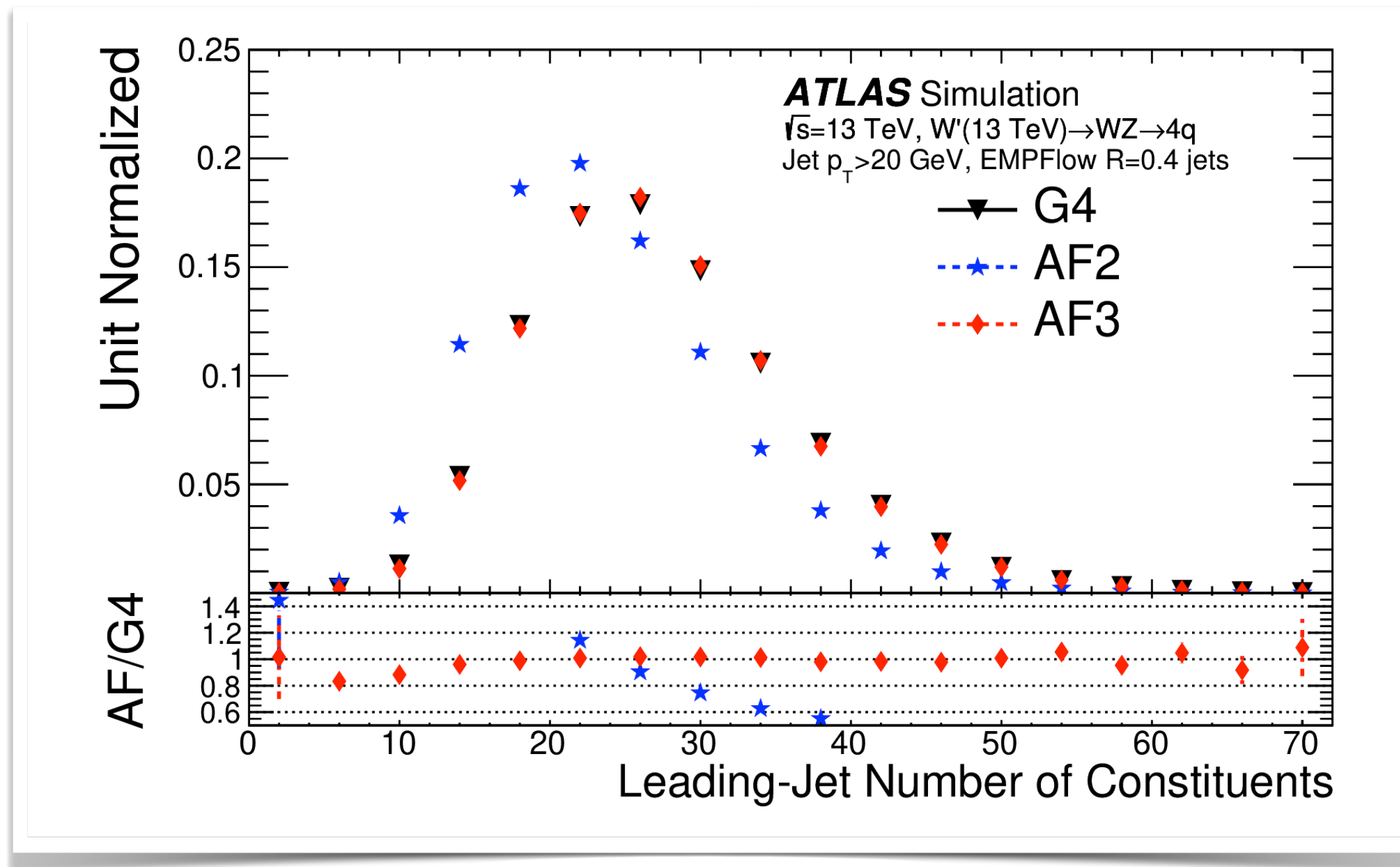


*jet  $\eta$  distribution - (left) for leading and (right) sub-leading jet in  $t\bar{t}$*



# Jet performance: small-R jet number of clusters

- ◆ Number of constituents inside a **jet of cone 0.4** for leading ( $p_T > 200$  GeV) and sub-leading ( $p_T > 20$  GeV)
- ◆ Jets reconstructed with EMPFlow algorithm

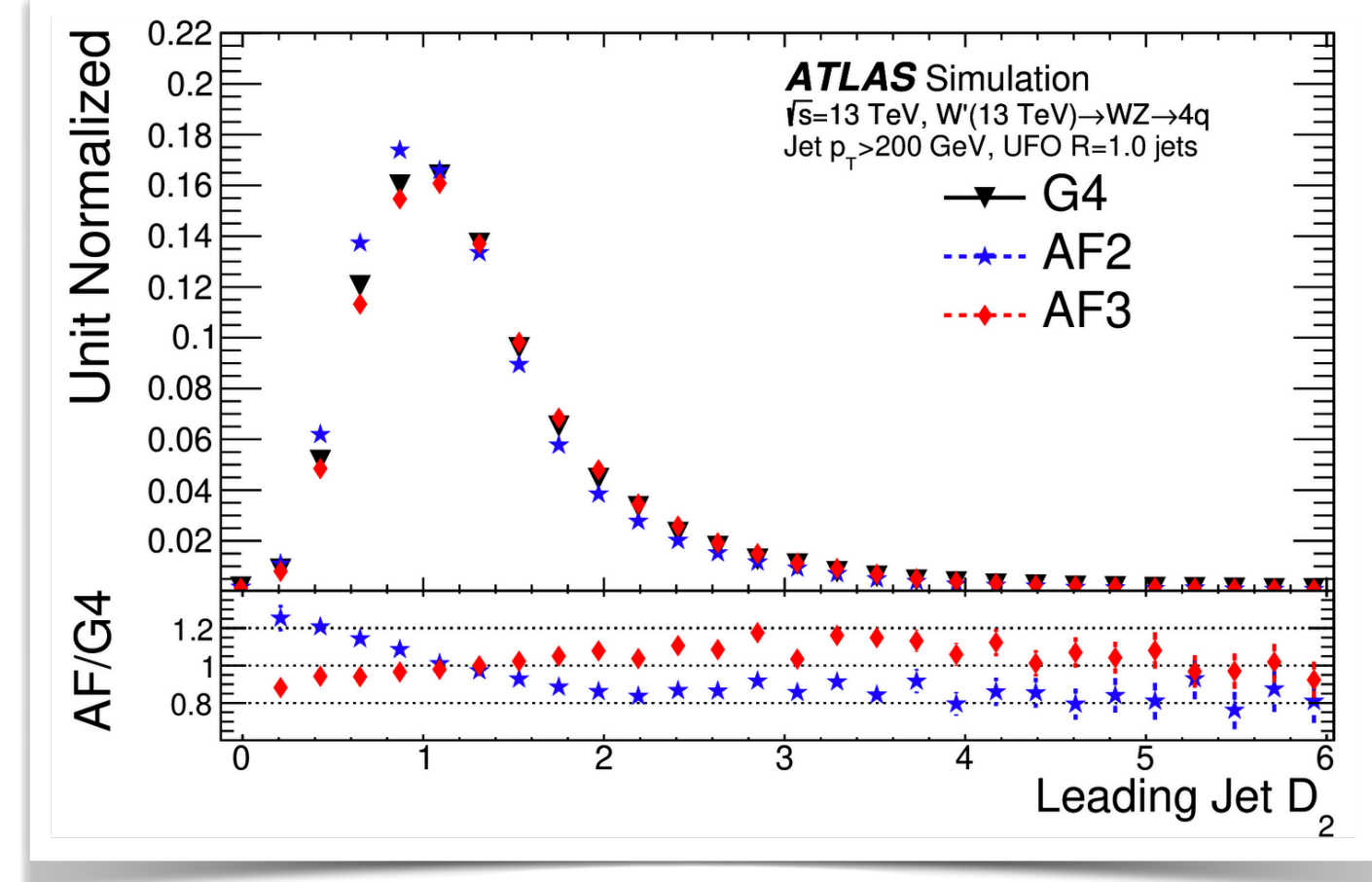
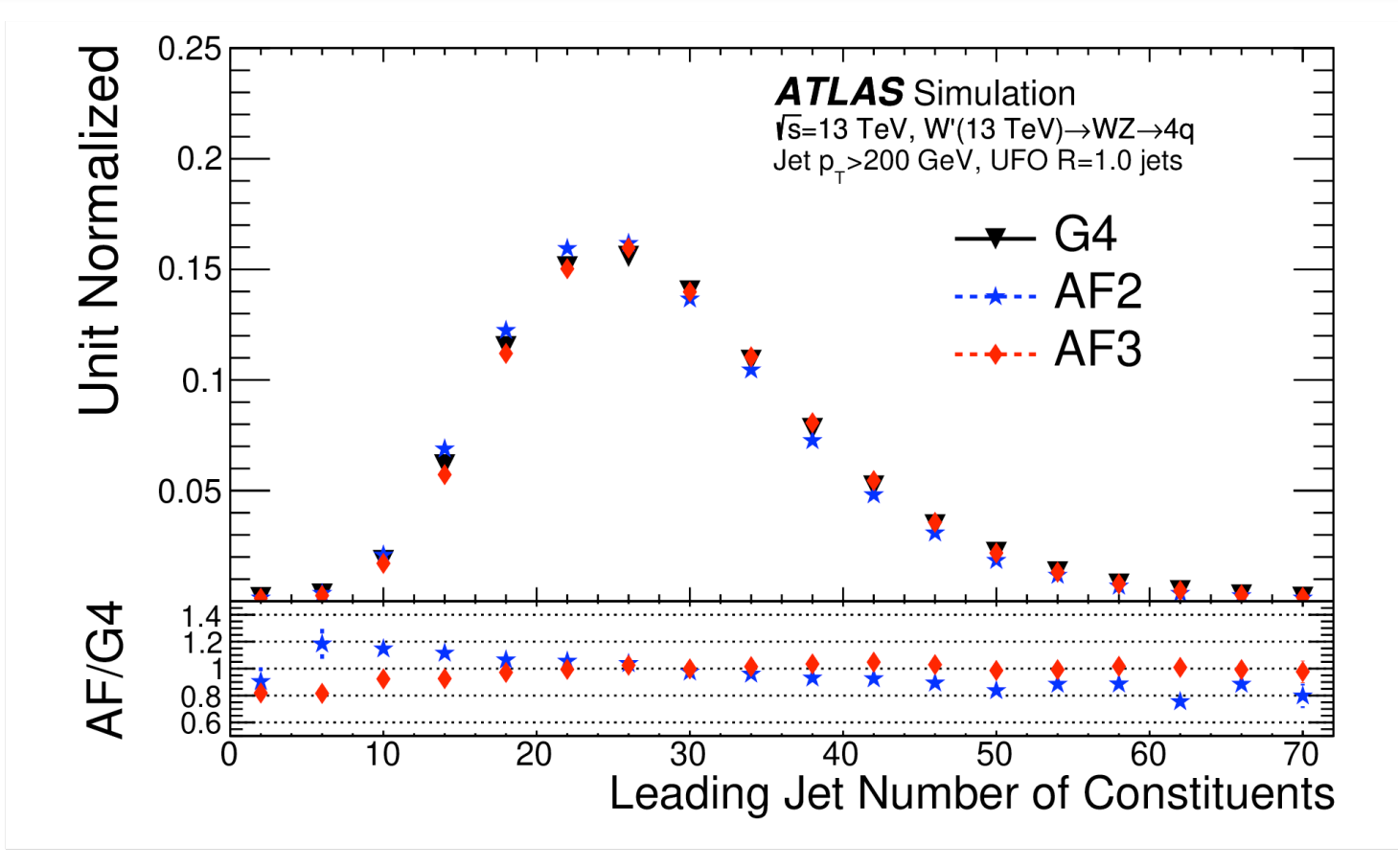


Number of constituents - (left) leading jet in  $W'(13\text{TeV}) \rightarrow WZ \rightarrow 4q$  and (right) sub-leading jet in  $t\bar{t}$  events

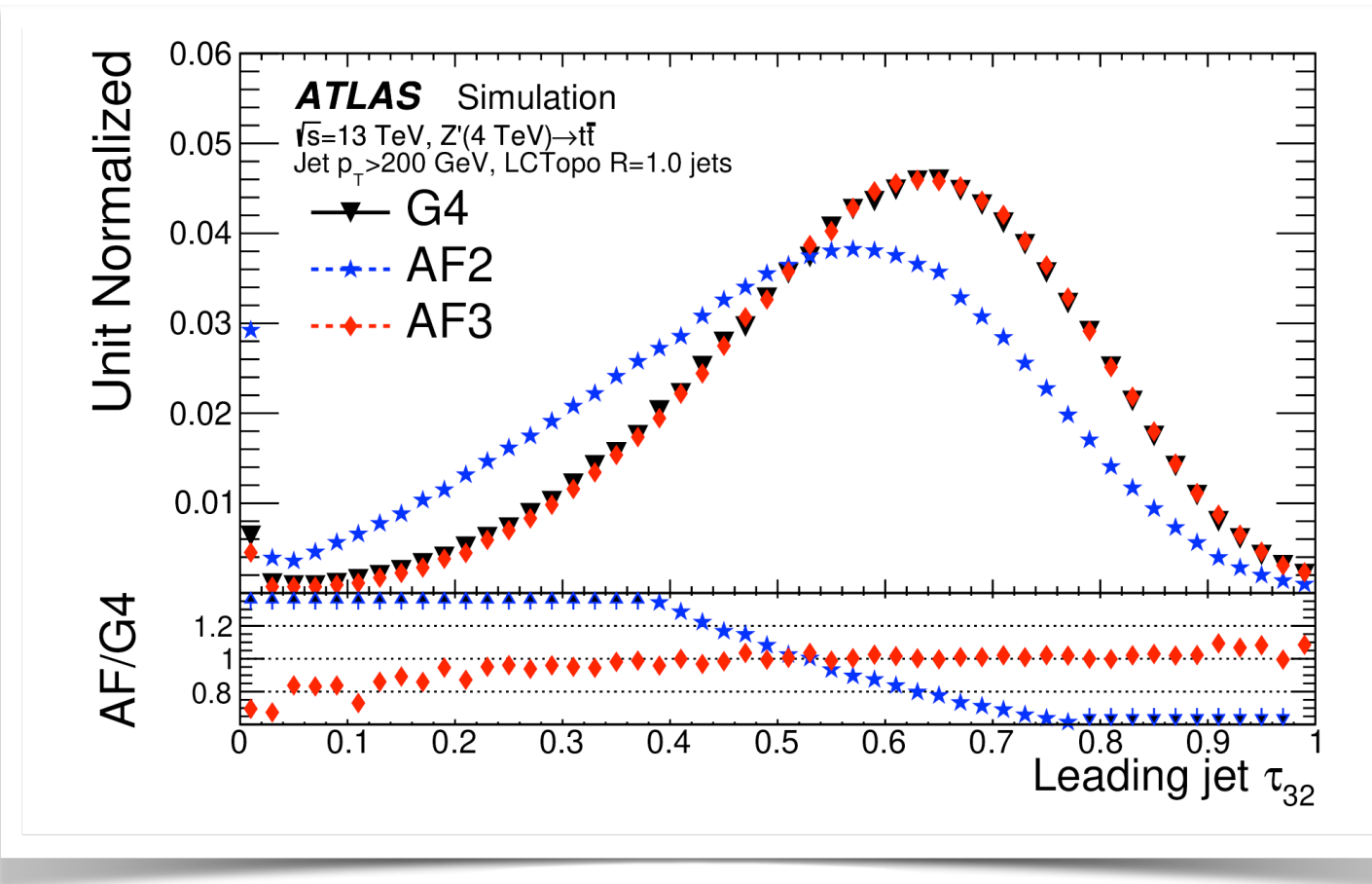
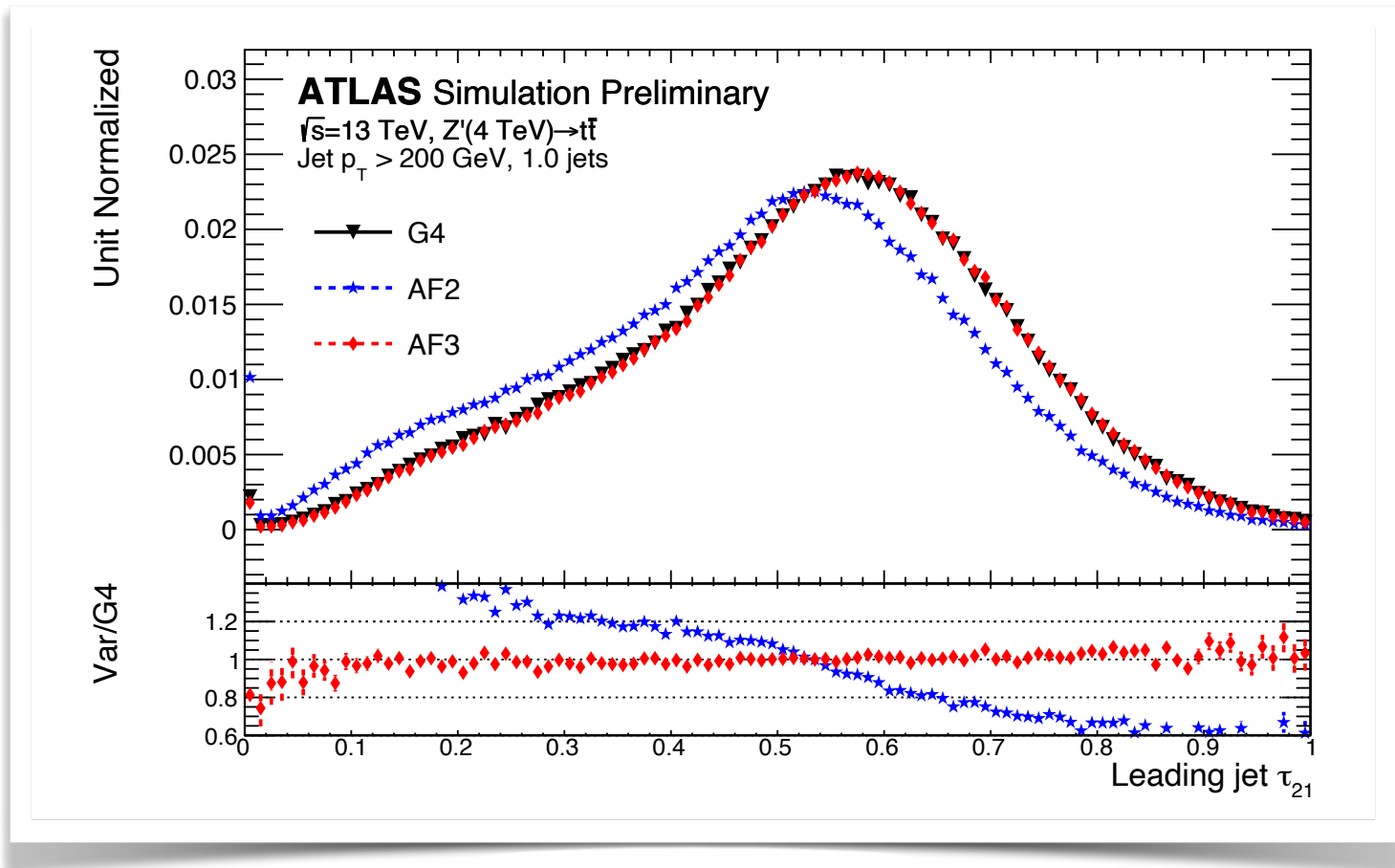
Significant improvement over AF2 leading to improvements in other observables!

# Jet performance: large-R jet substructures

- ◆ Jet substructure variables for high energetic jets inside a cone of 1.0
- ◆ Reconstructed with trimmed UFO or LCTopo algorithm



*Number of constituents - (left) and dipolarity (right) in  $W(13\text{ TeV}) \rightarrow WZ \rightarrow 4q$  events*



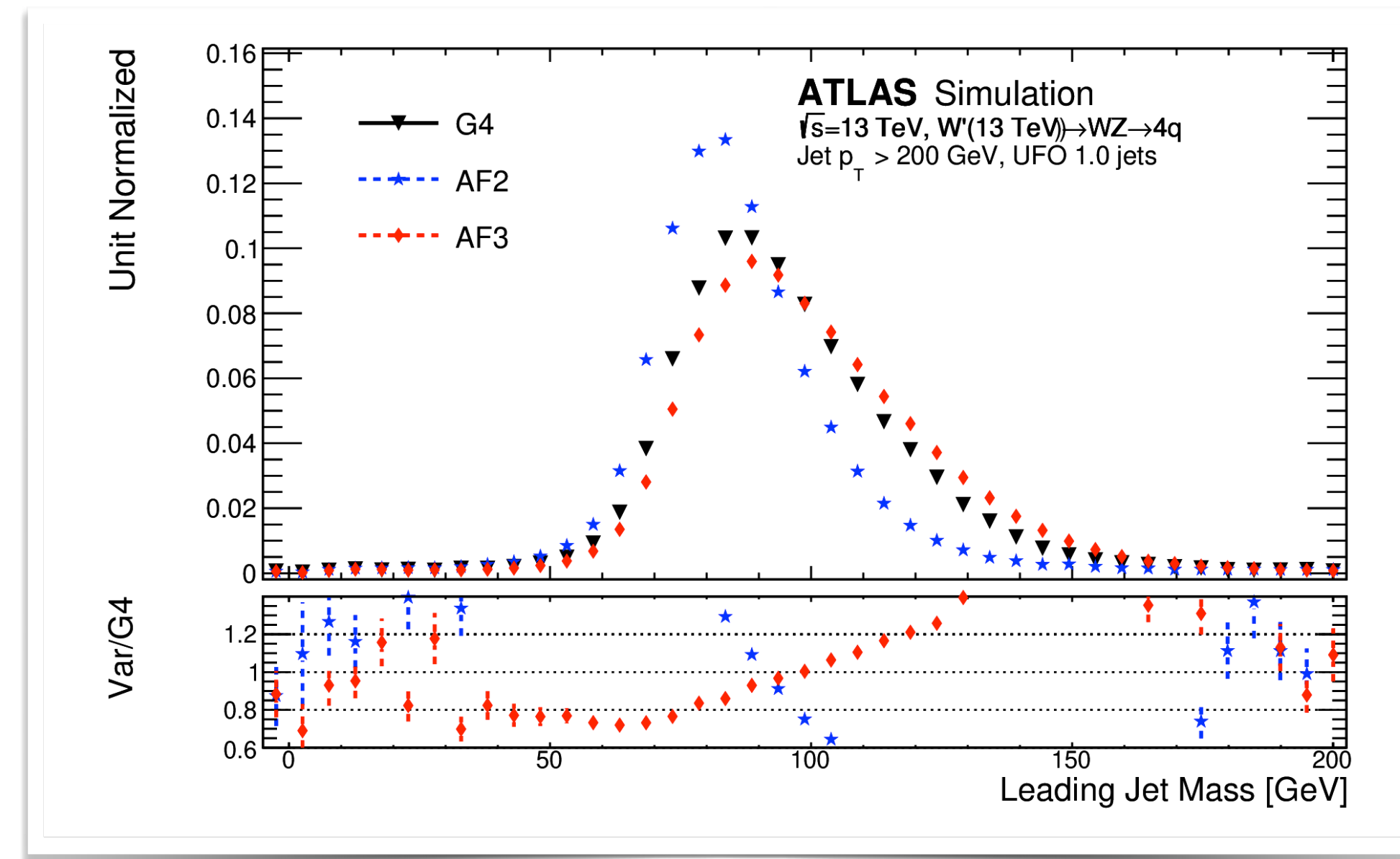
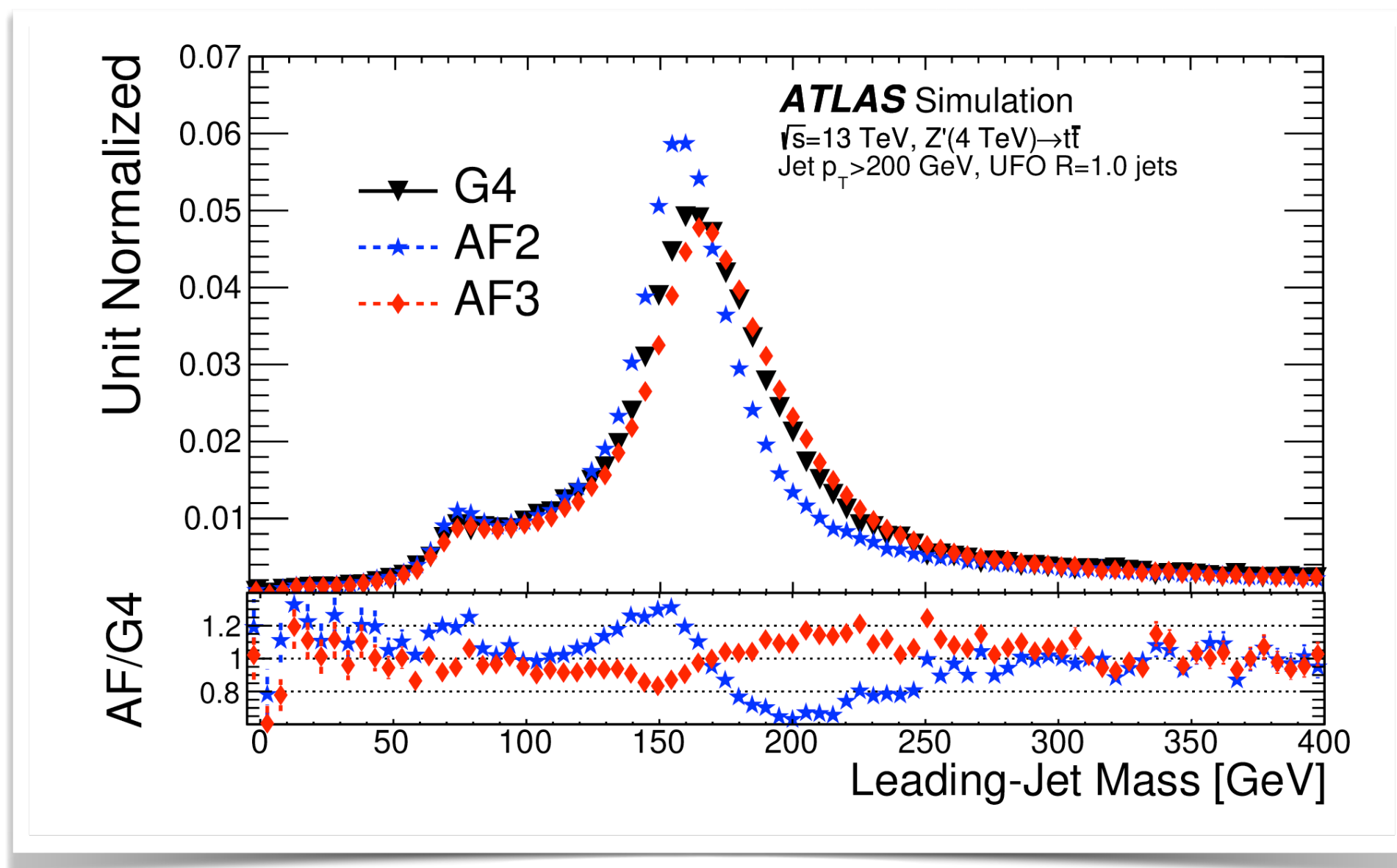
*sub-jetiness variables -  $\tau_{21}$ , (left) and  $\tau_{32}$  (right) in  $Z(4\text{ TeV}) \rightarrow t\bar{t}$  events*

Improvements of these variables in AF3 over AF2 will allow more analyses to use fast simulation!



# Jet performance: scope for improvement

- ◆ High energetic jets inside **a cone of 1.0** reconstructed with trimmed UFO algorithm
- ◆ AF3 shows some discrepancy for jet mass - although improves upon AF2
- ◆ The discrepancies are in the **tails of the high energetic jets**



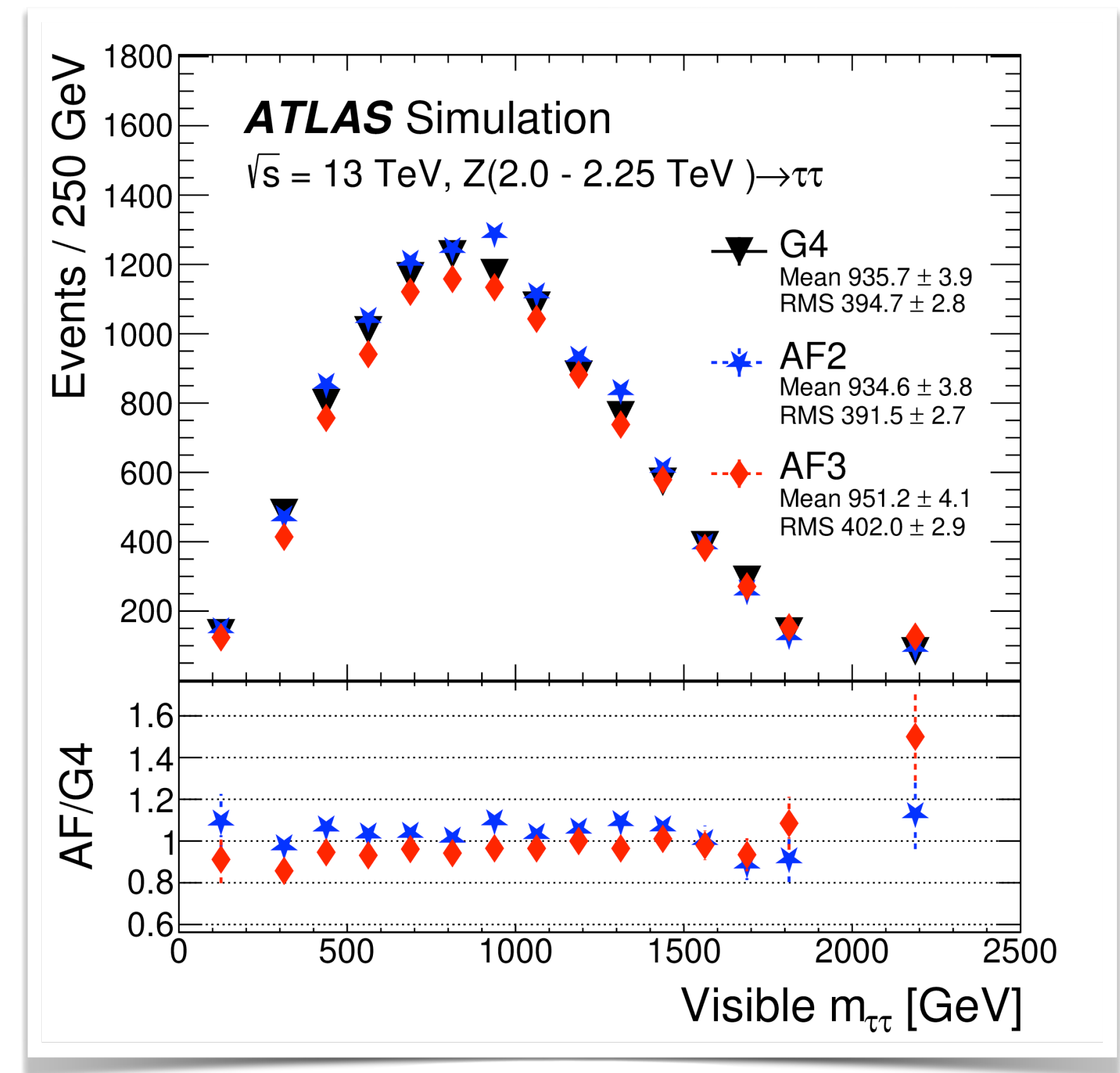
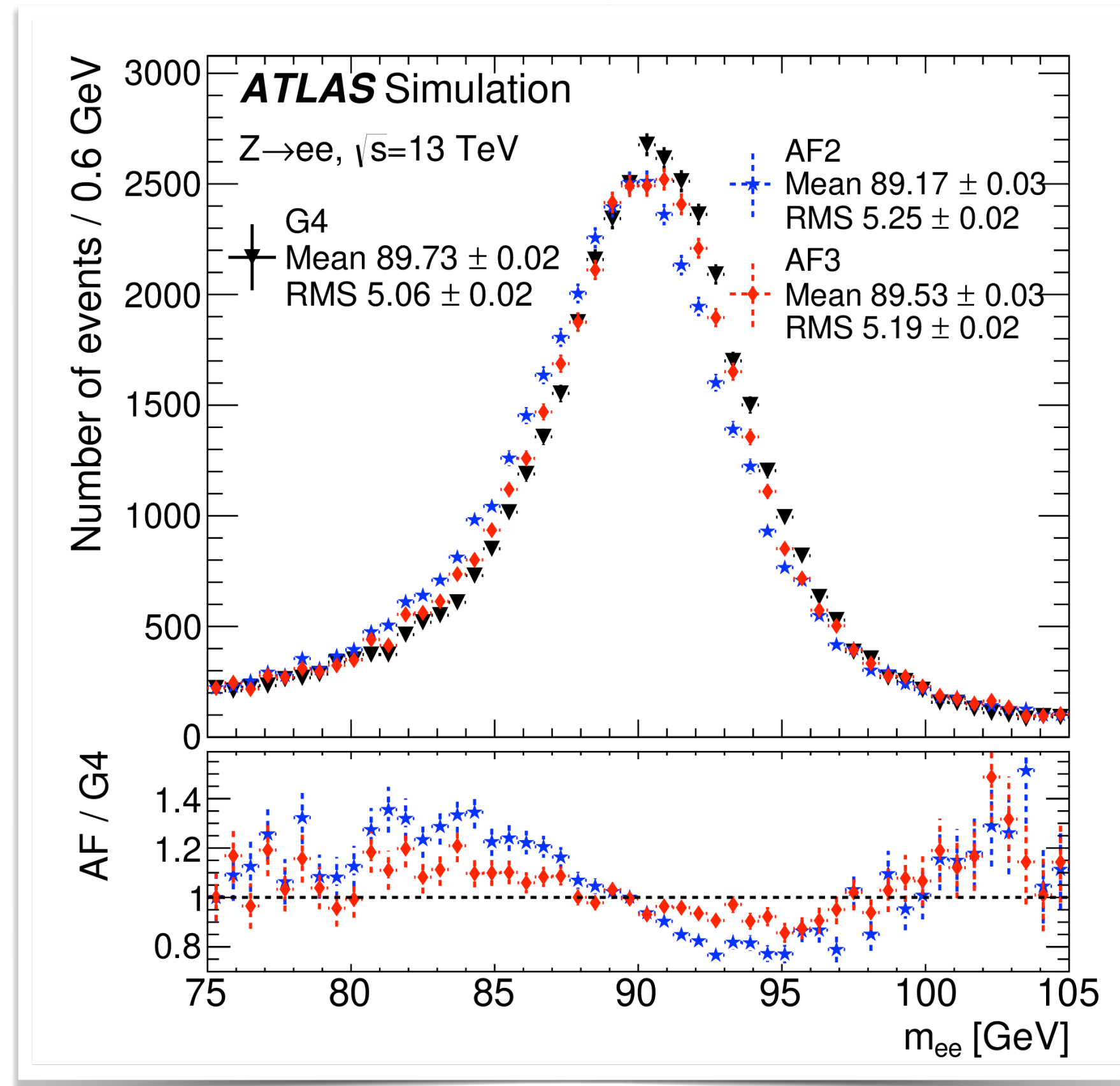
leading jet mass - (left) in  $Z'(4\text{ TeV}) \rightarrow t\bar{t}$  and (right) in  $W'(13\text{ TeV}) \rightarrow WZ \rightarrow 4q$  events

Most physics analyses are not affected!

# Performance of AF3: reconstructed electrons & hadronic taus

- ◆ Invariant di-electron and di-tau masses show good agreement

*Invariant mass distribution from a selection targeting events with a Z boson decaying into () two electrons with  $p_T > 25$  GeV and  $|\eta| < 1.37$  or  $1.52 < |\eta| < 2.47$ , and the visible part of the invariant mass of two hadronically decaying  $\tau$ -leptons in  $Z \rightarrow \tau\tau$  DY events filtered for an off-shell mass of 2.0--2.25 TeV*



AF3 shows good performance for both electrons and taus !



# Summary

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- ◆ AF3 is the next generation of fast simulation in ATLAS - successfully deploying complex parametrized and deep learning algorithms.
- ◆ AF3 achieved very good modeling for all reconstructed observables compared to Geant4 even for complex variables such as jet substructure.
- ◆ The CPU performance of AF3 is only limited by the ID simulation (Geant4), but a factor of  $O(10)$  speed up is sufficient to meet the CPU needs for Run 3.
- ◆ ATLAS used AF3 to re-simulate 8 billion events from Run 2.
- ◆ An update of the current AF3 version is expected for Run 3 - current performance seems sufficient to produce a large fraction of ATLAS Run 3 Monte Carlo events.

*Thank you!*



**BACKUP**