ATLAS Fast Calorimeter Simulation

Xiaozhong Huang
on behalf of the ATLAS collaboration

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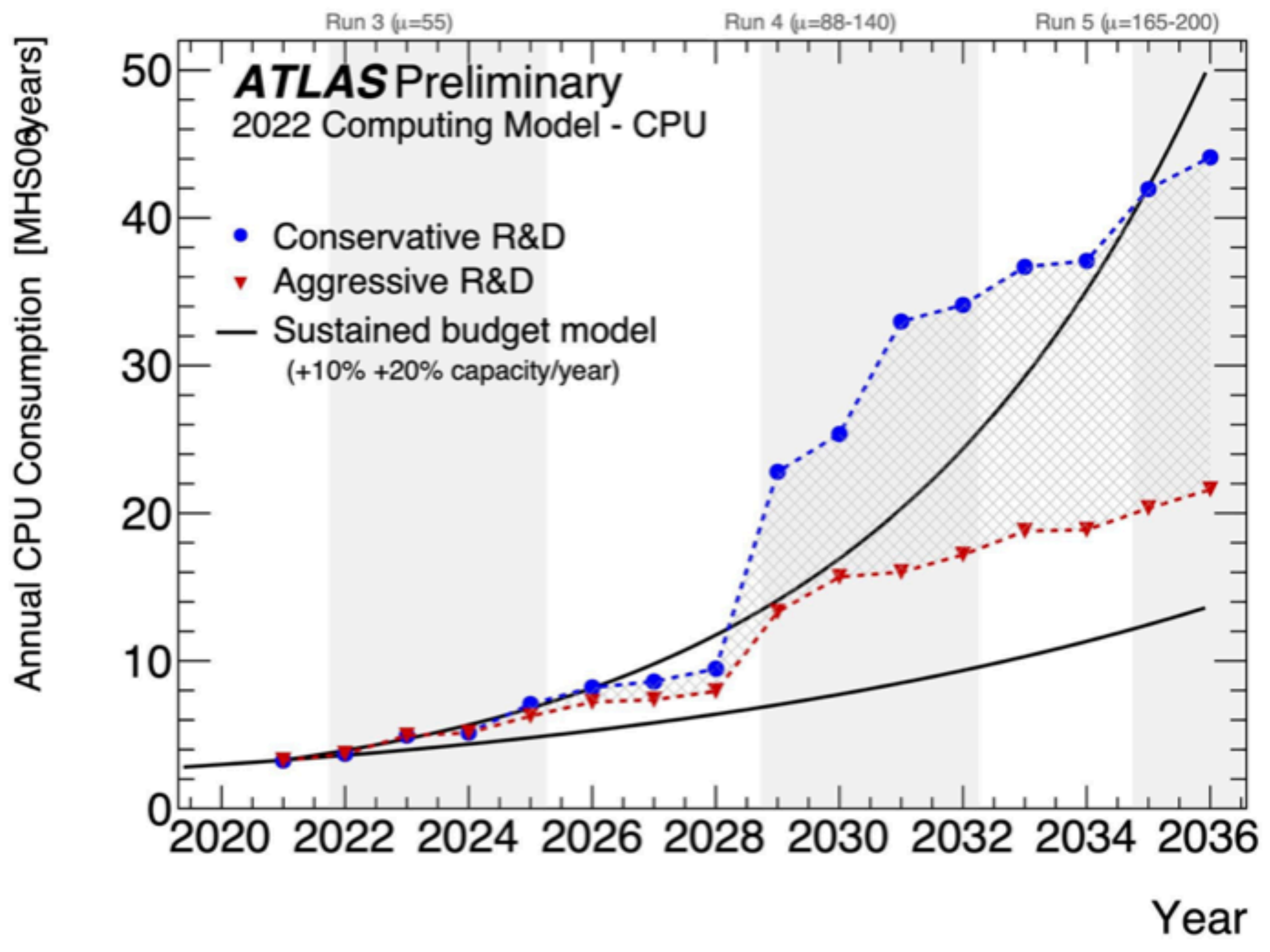
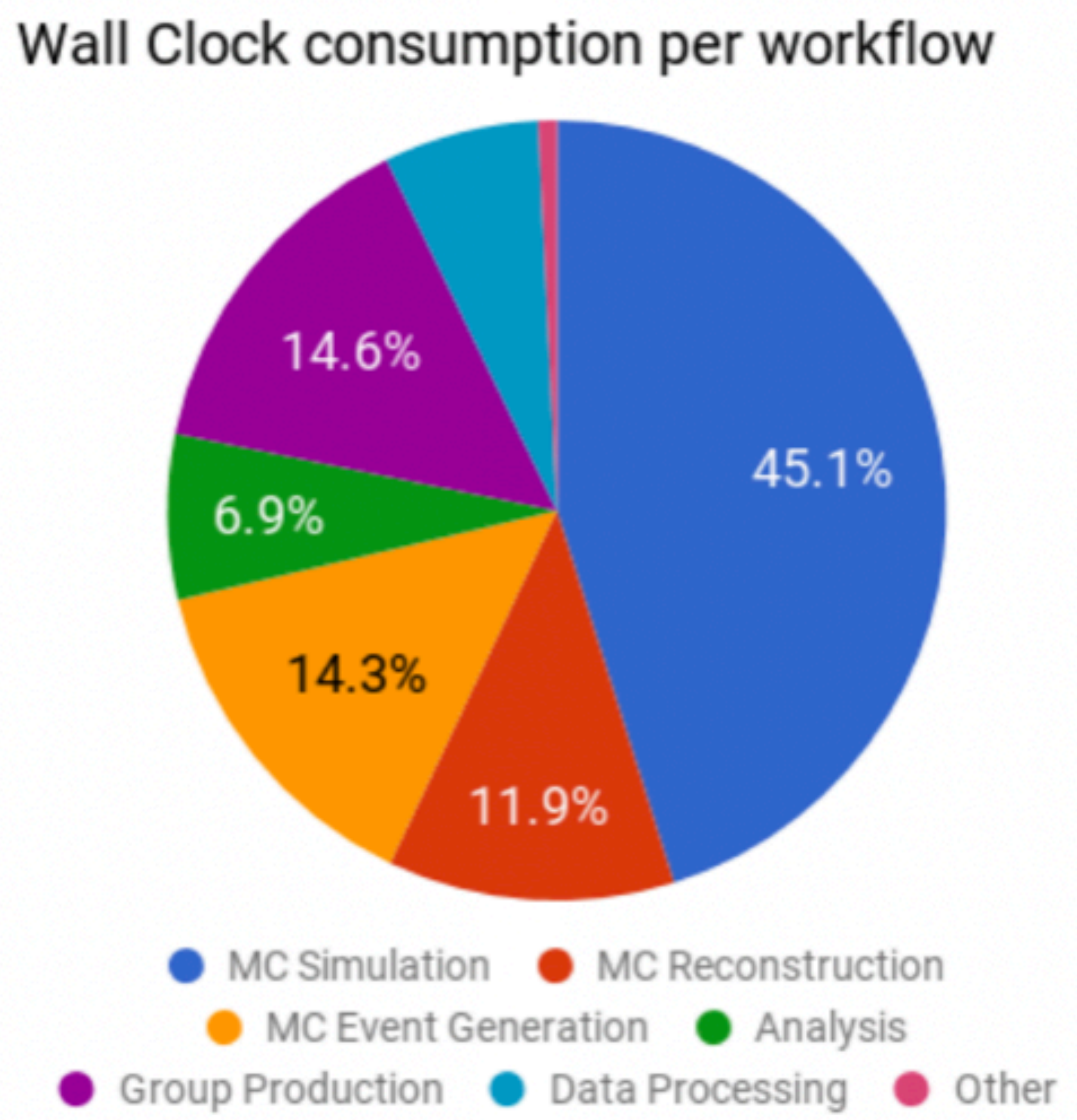
Why Fast Calorimeter Simulation ?

- HL-LHC ⟶ enormous computing resources
- Top CPU consumer: MC simulation, dominated by **calorimeter**
- Fast calorimeter simulation: an important approach to help overcome the computational challenge



ATLAS Software and Computing HL-LHC Roadmap



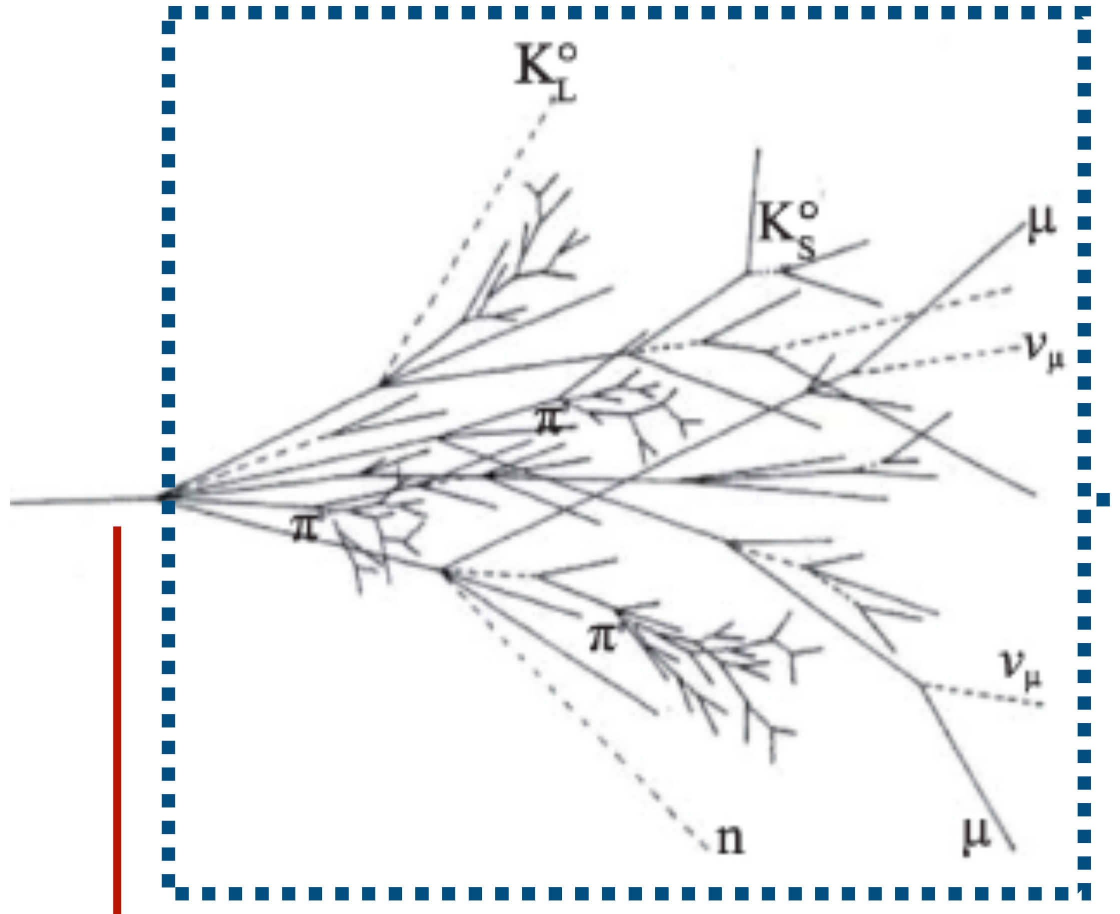
ATLAS 2017 number

Calorimeter Simulation

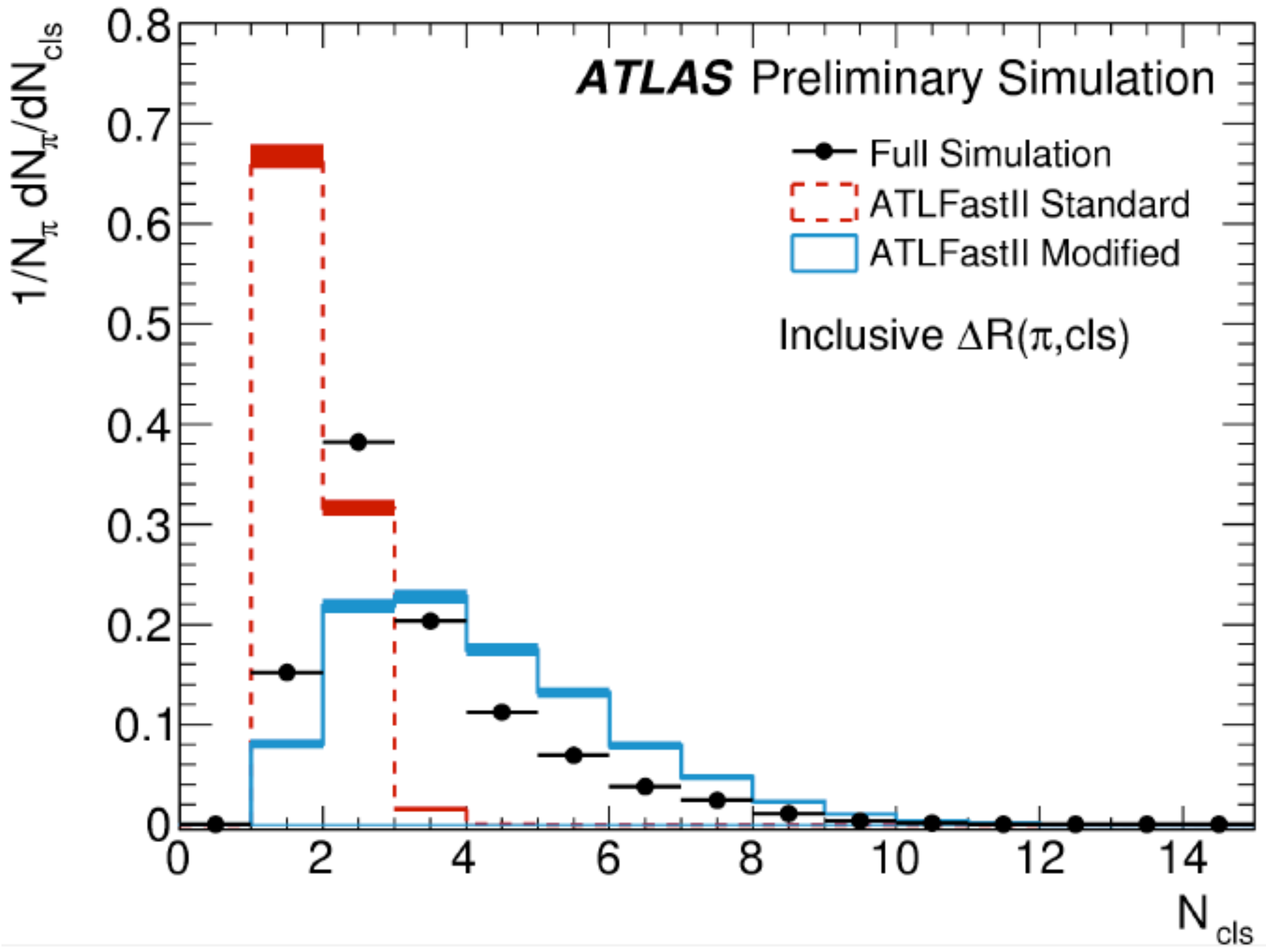
- Geant4: CPU intensive
  - complex geometry
  - number of secondary particles grows exponentially

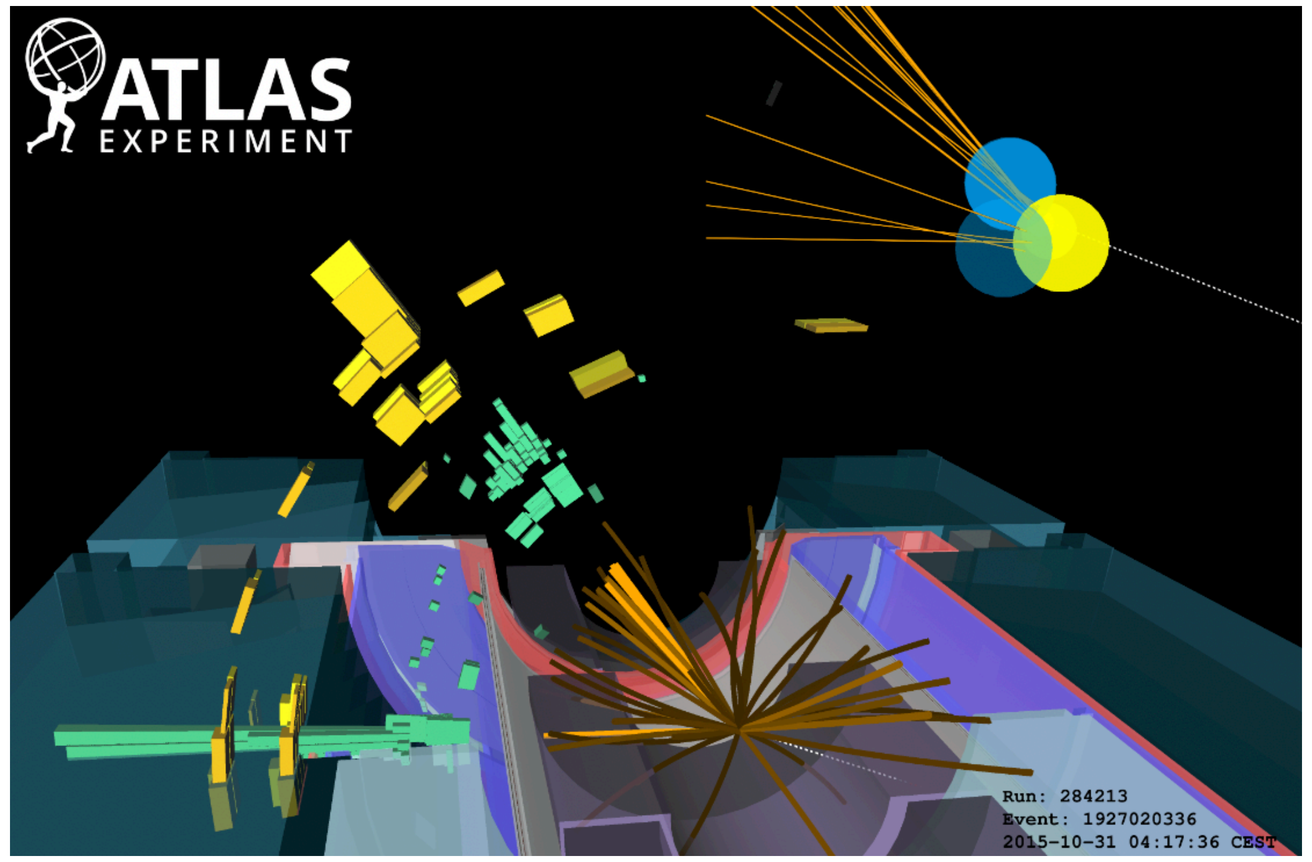
- AF2, fast simulation tool used in ATLAS (Run1 & Run2)
  - simplified geometry
  - classical parameterization
  - complex variables not well modeled, e.g. jet substructures
  - Run2: AF2 account for ~50% of all simulation

Geant4



Fast

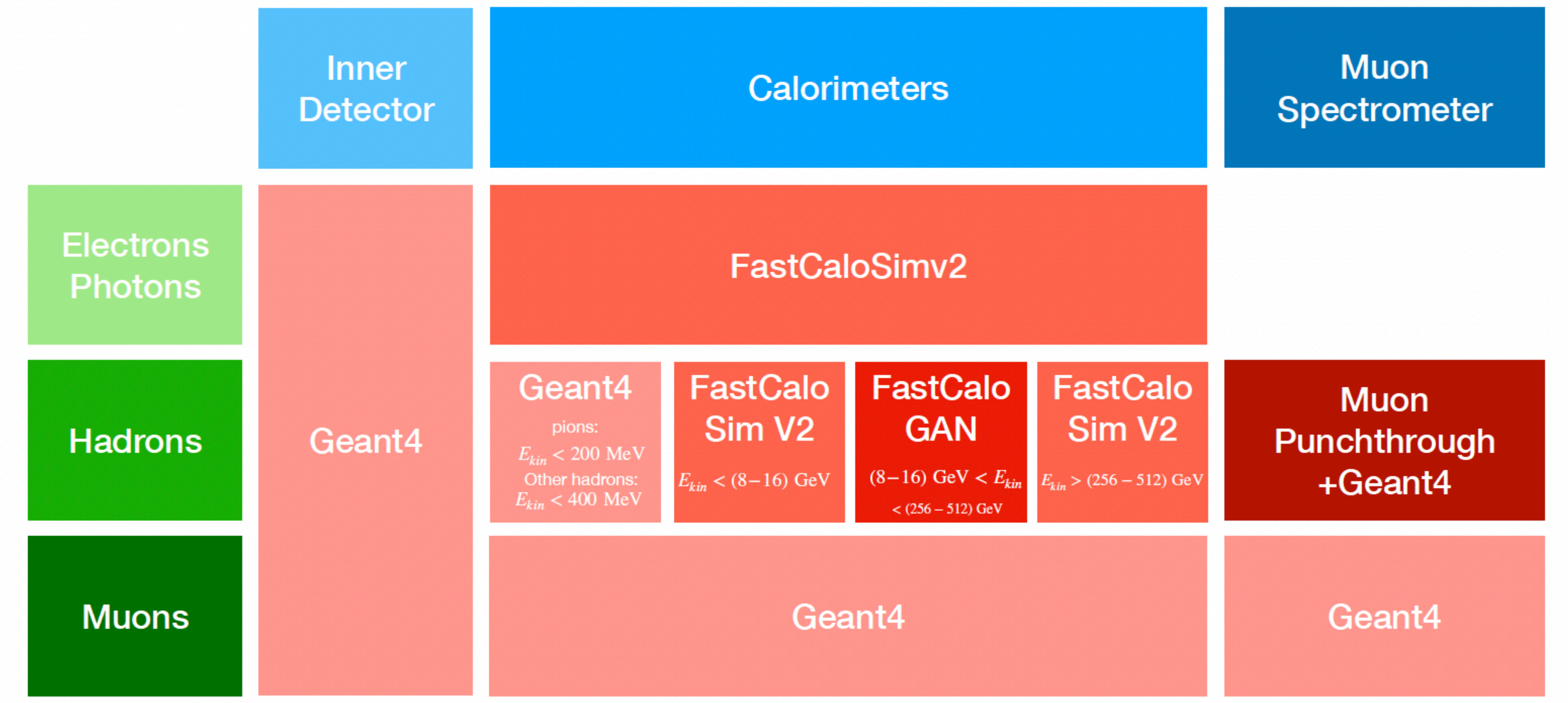




Overview of AtlFast3 (AF3)

- AF3 combines the strength of the **FastCaloSimV2** and **FastCaloGAN**
  - FastCaloSimV2: classical approach based on parameterization
  - FastCaloGAN: machine learning approach based on GANs

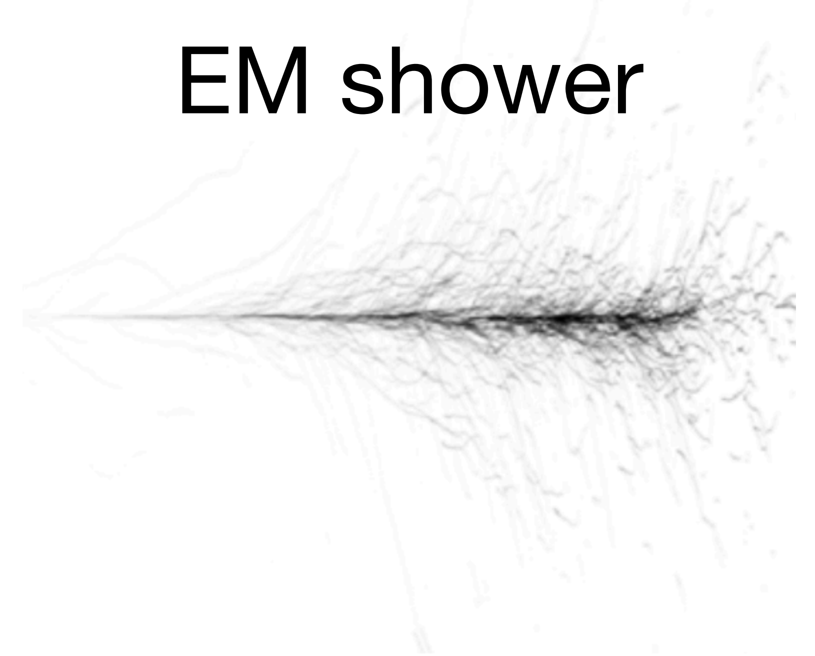
- Muon punch-through: secondary particles created in hadronic showers can escape through the back of calorimeter



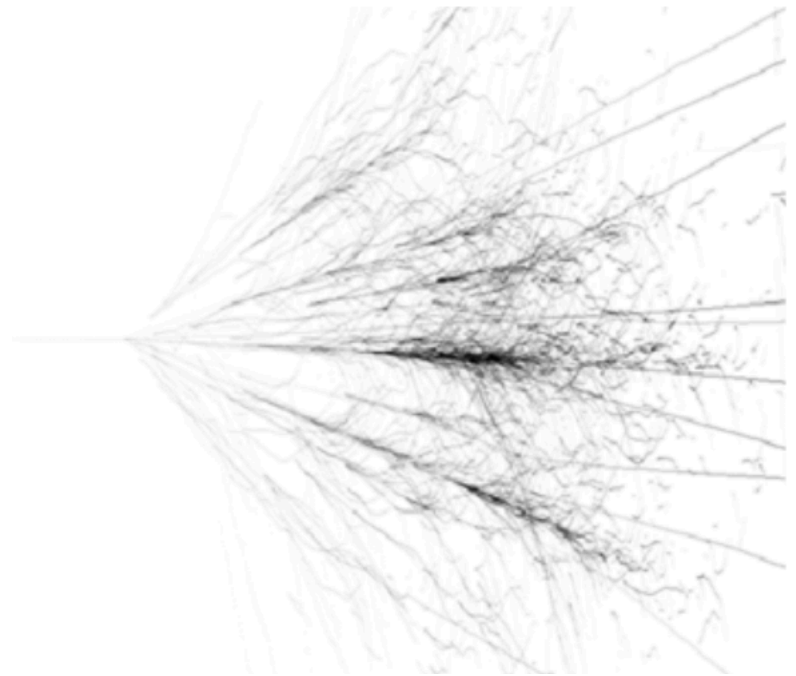
Input Datasets for AF3 Modeling

- Single particles generated at calorimeter surface
  - photons and electrons: electromagnetic showers
  - pions: hadronic showers
- Samples are sliced by momentum and η
- Special G4 configuration: smaller simulation steps
- Electronic noise and cross-talk between neighboring cells are turned off in digitization

EM shower



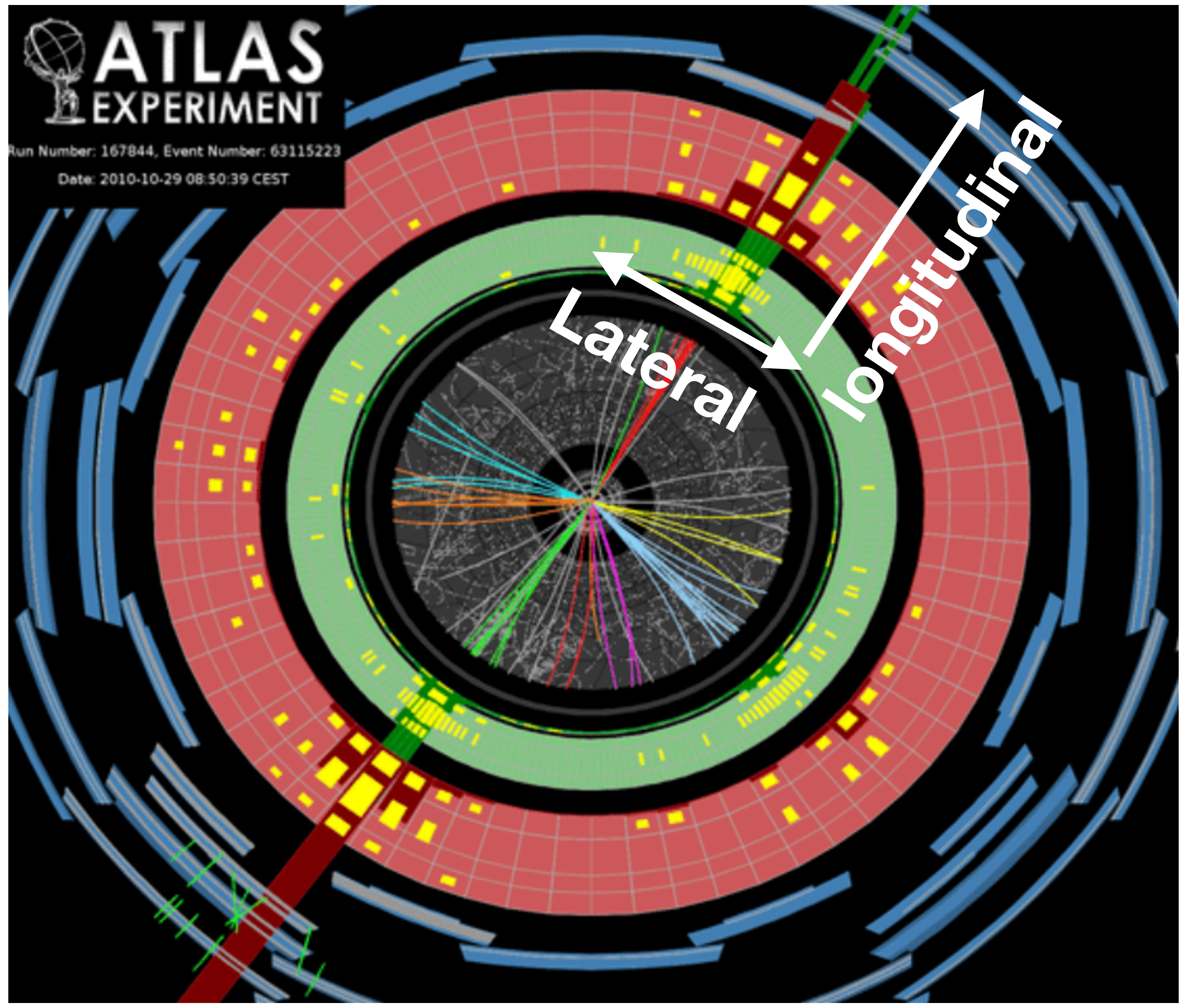
Hadronic shower

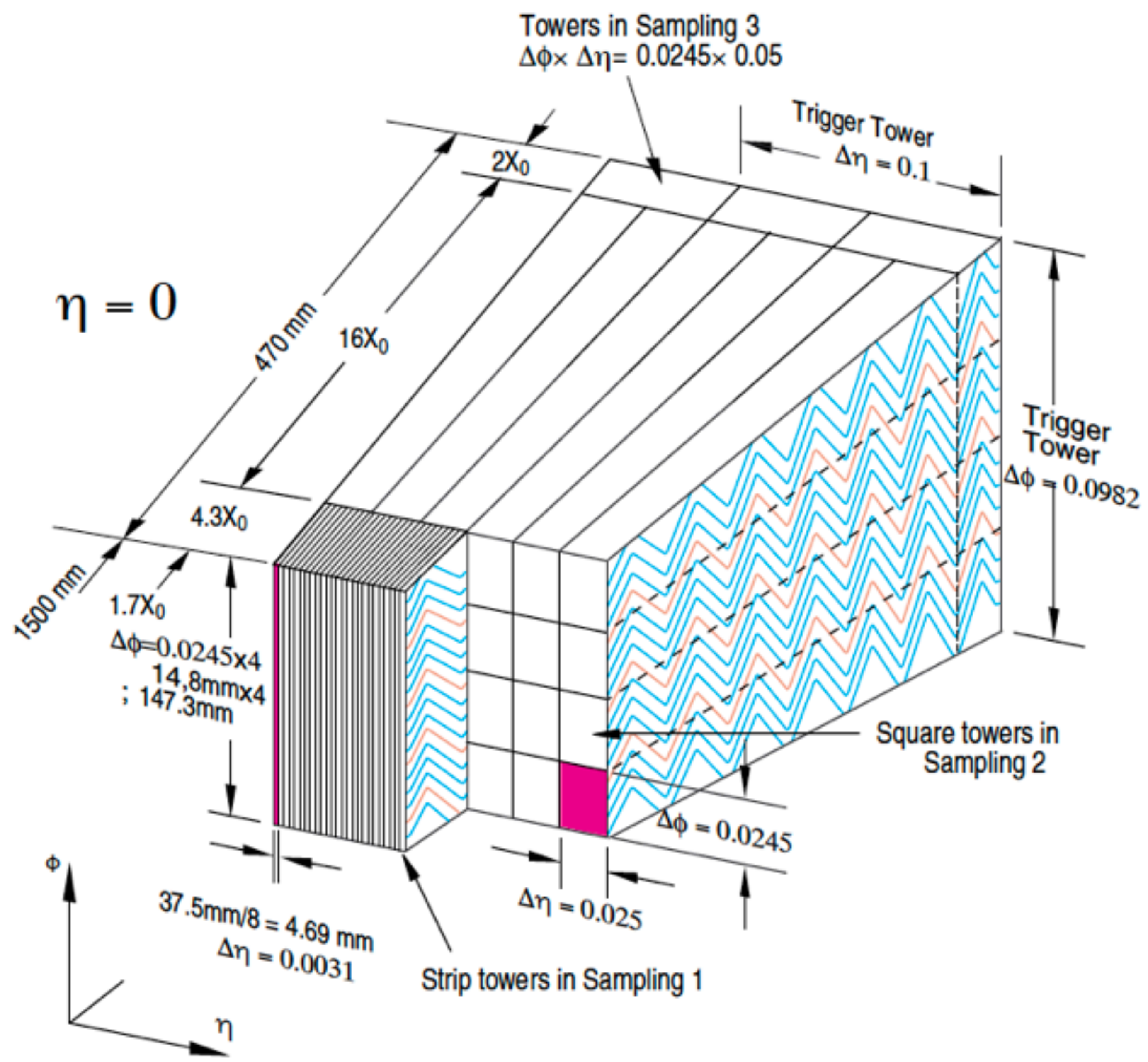


Overview of FastCaloSimV2

- Parameterize the single particle shower development in longitudinal and lateral directions **separately**
  - longitudinal direction: energy deposition in each layer
  - lateral direction: shower shape

- Simplified geometry: cuboid cell instead of accordion structure

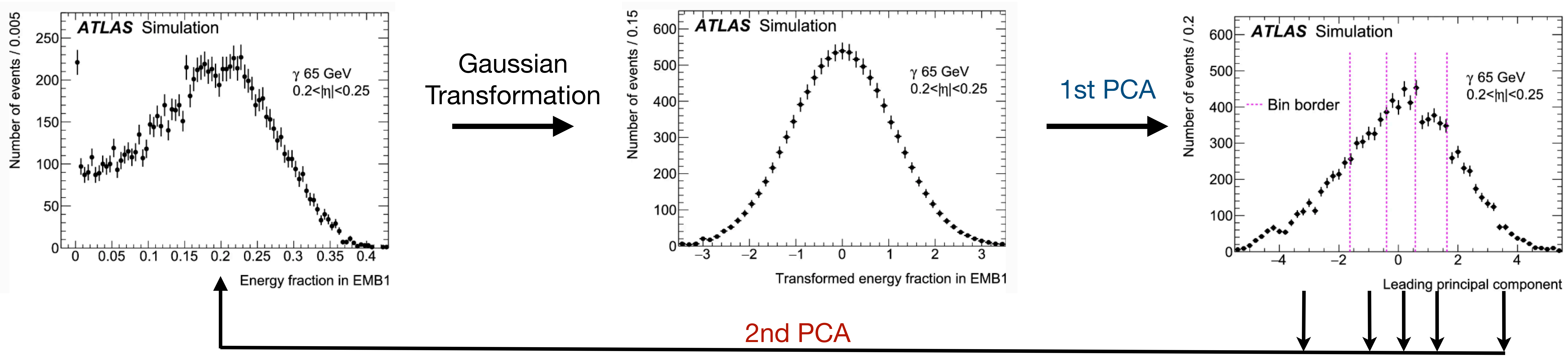




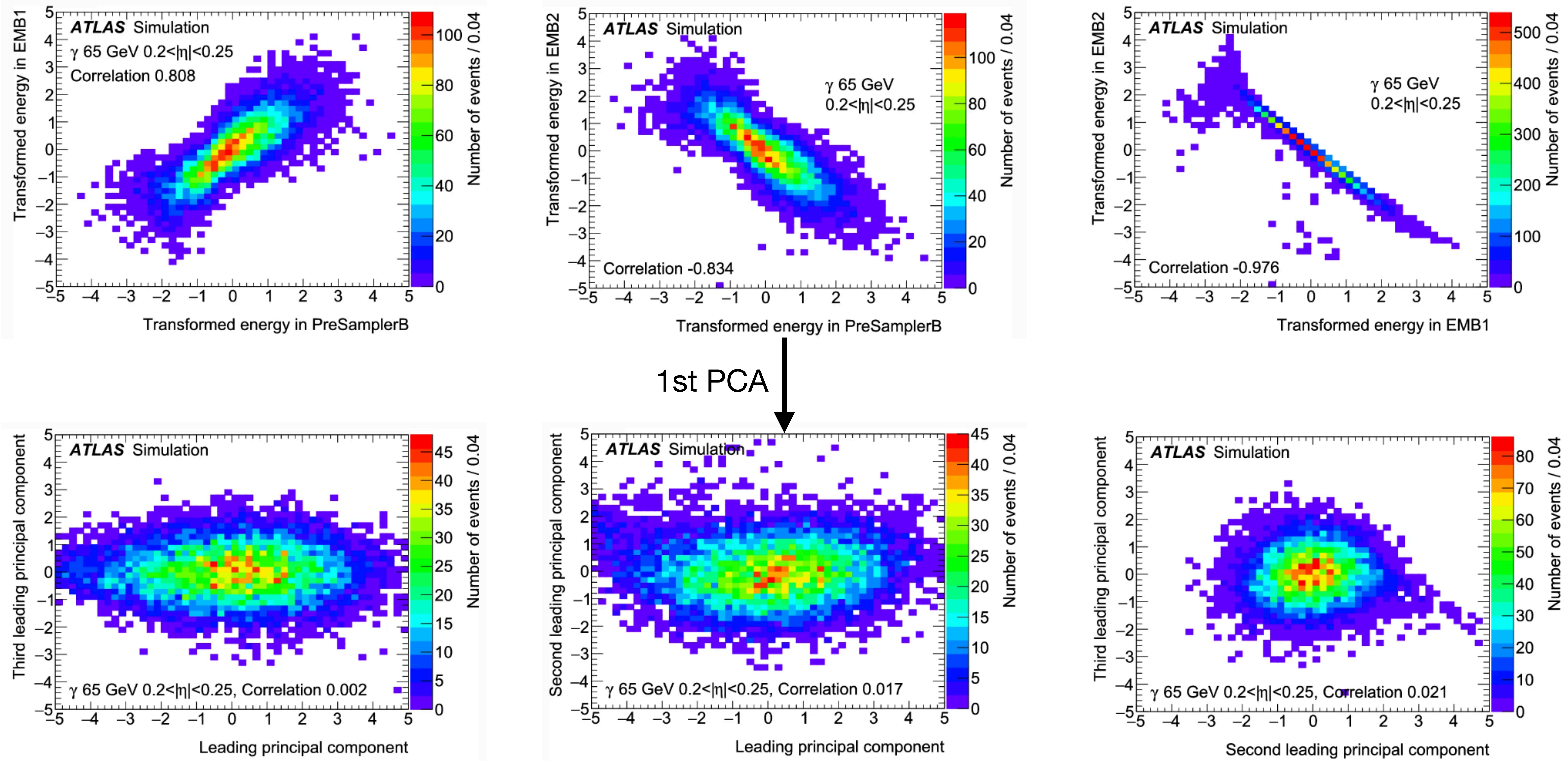
Longitudinal Energy Parameterization

- PCA to remove the energy correlation between layers
  - input: total energy, the energy fraction of each layer
  - gaussian transformation is performed for each input variable

- PCA performed **twice**
  - 1st PCA to divide the G4 samples
  - 2nd PCA to achieve a better decorrelation
  - correlated energy deposition in layers →uncorrelated random variables

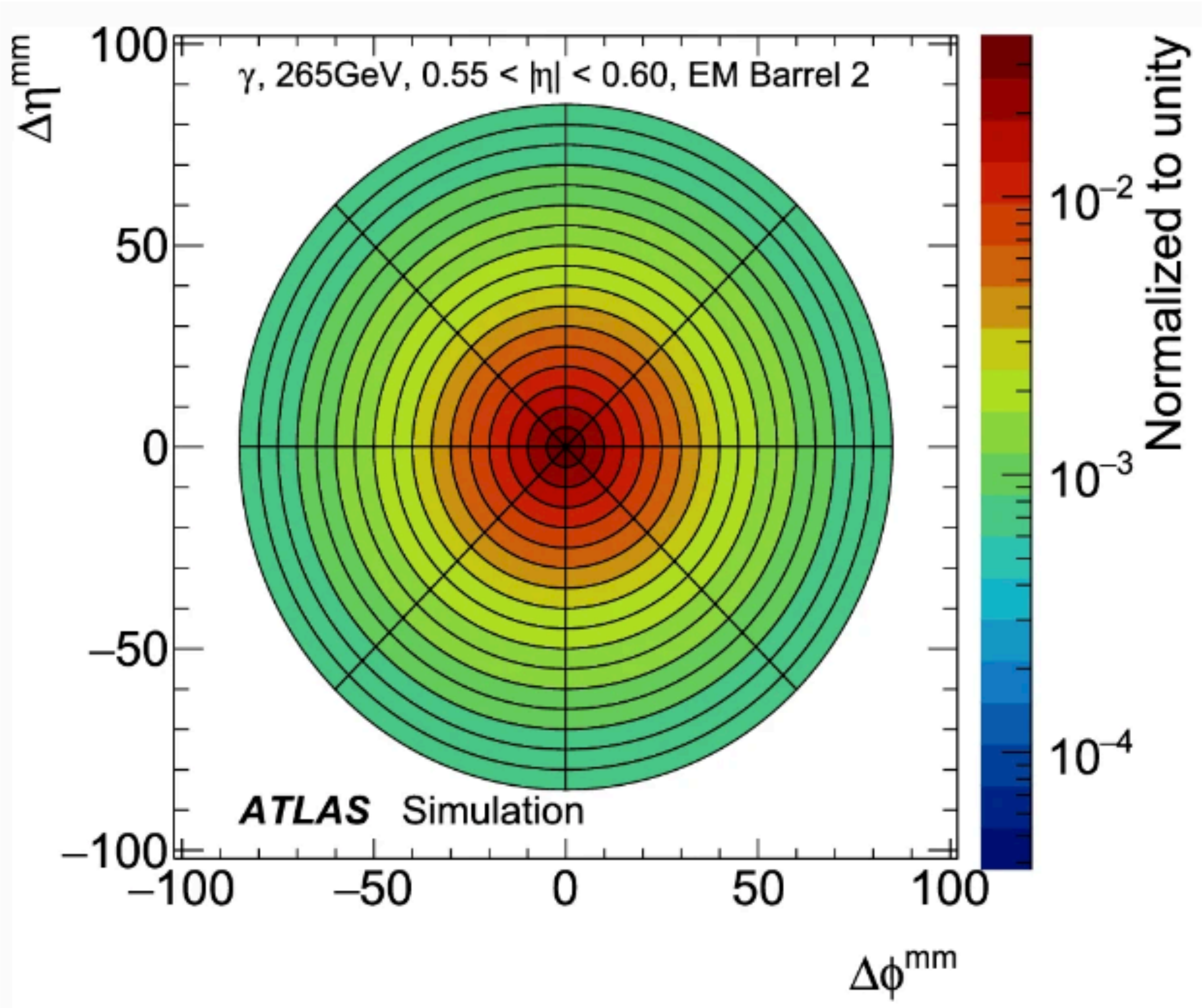


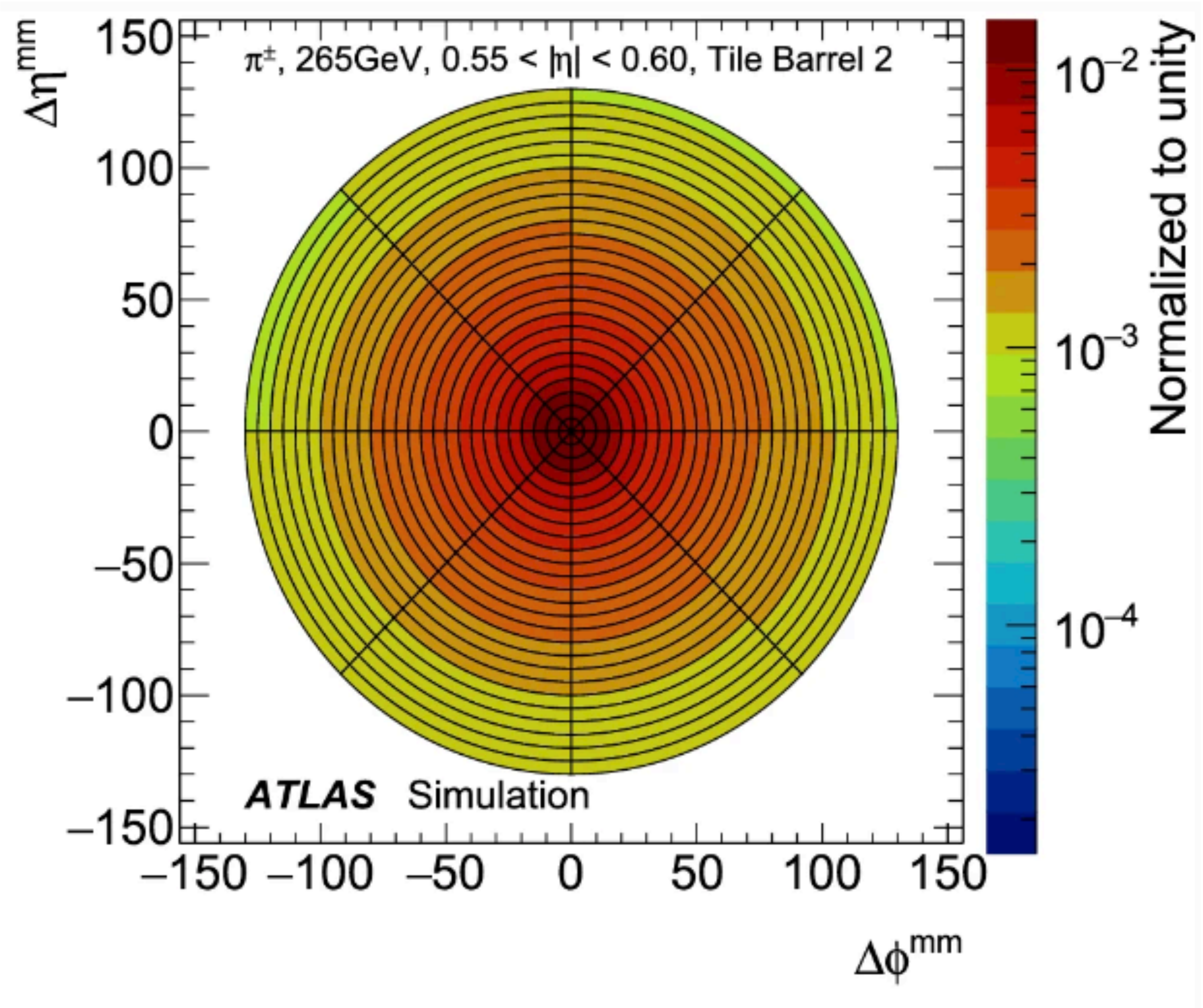
Validation of 1st PCA



Lateral Shower Shape Parameterization

- The average shower energy in **radial and angular direction** as a PDF (hits are **voxelized**)
- Derived in each layer for each PCA bin for each sample

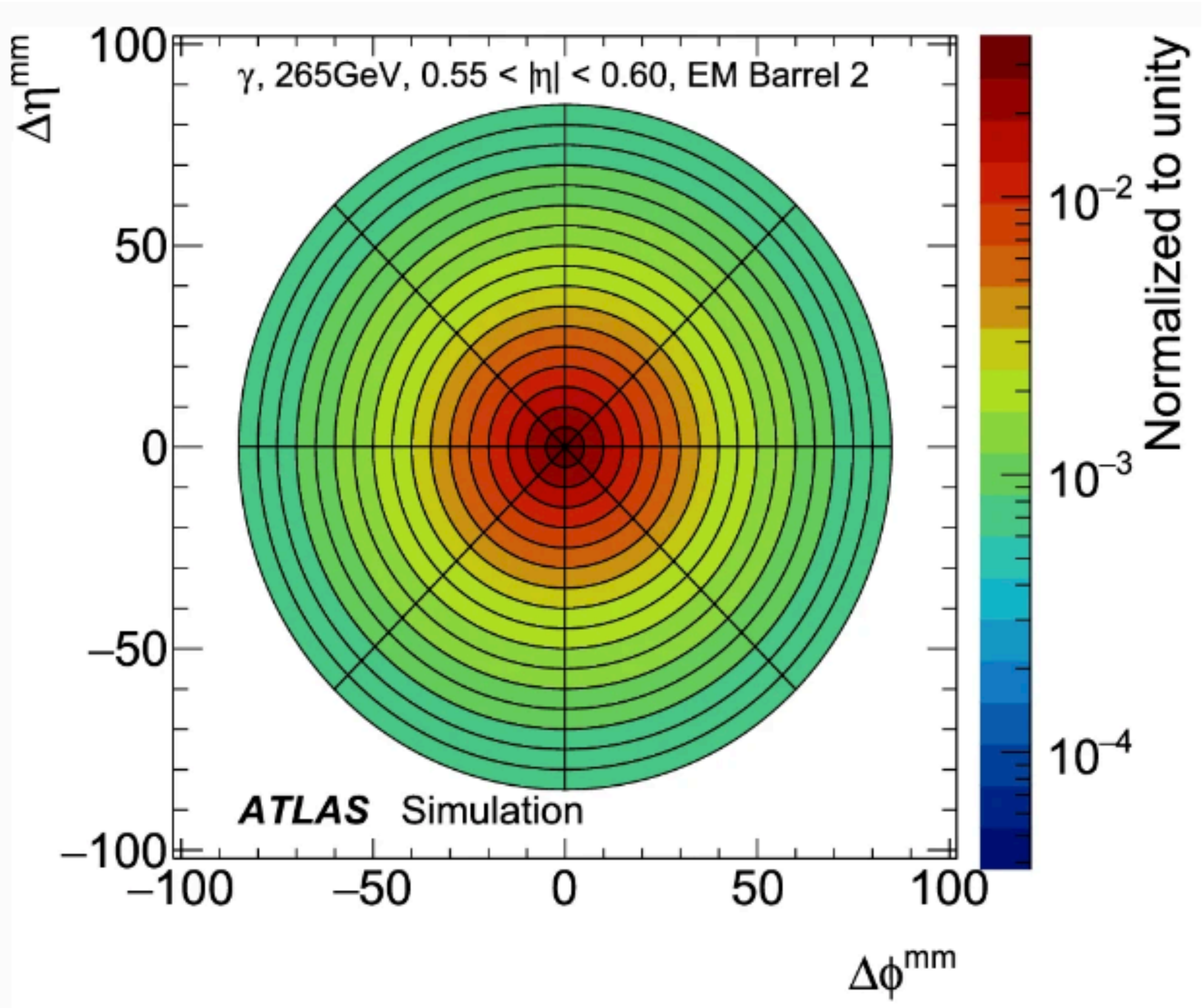




Lateral Shower Simulation

- Shower generation is a stochastic process given the lateral shower parameterization

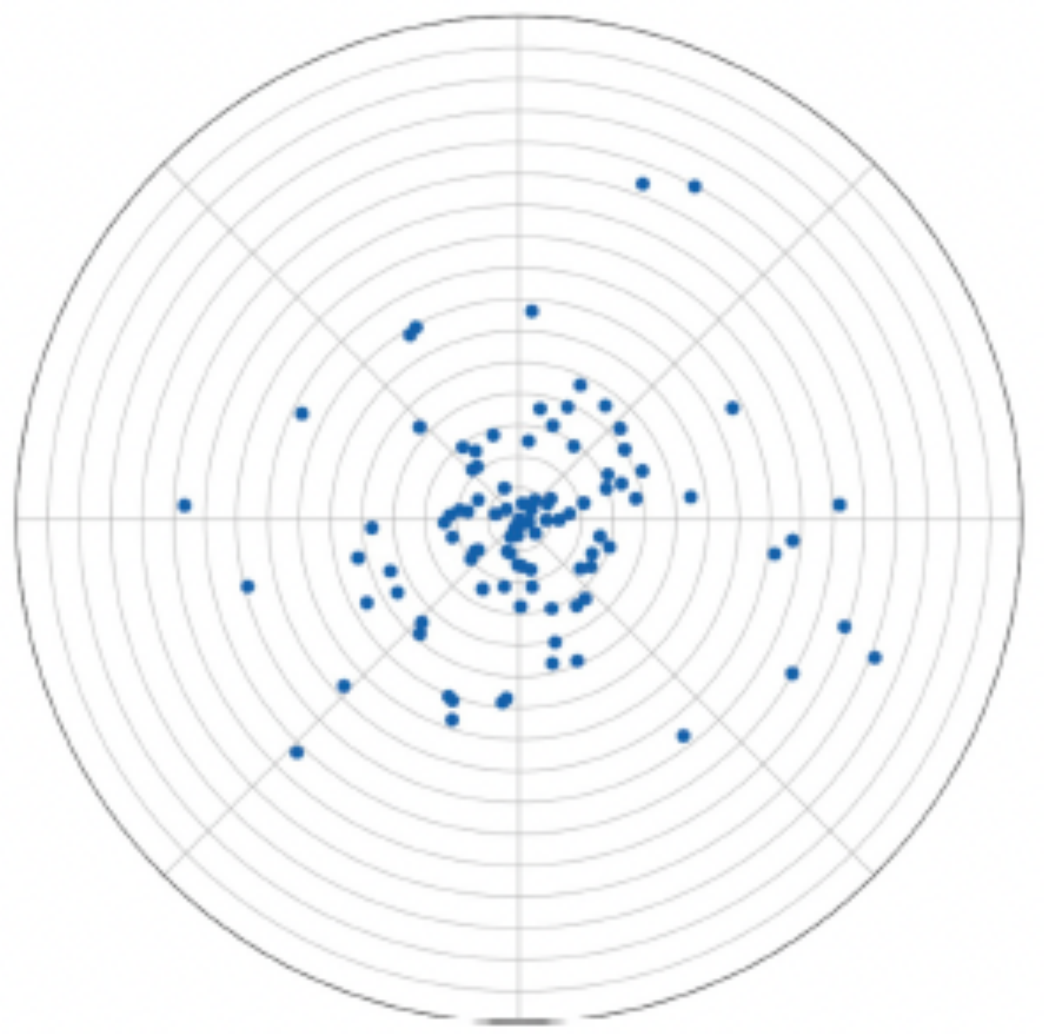
- Throw N_{hit} hits based on the average lateral shower shape
  - electromagnetic shower: equal hit energy ($E_{\text{hit}} = E_{\text{layer}}/N_{\text{hit}}$)
  - hadronic shower: weighted hit energy



$$N_{\text{hit}} \sim \text{Poisson}(1/(\sigma_{\text{E}}/\text{E})^2)$$

$$\sigma_{\text{E}}/E = a/\sqrt{(E/\text{GeV})} \oplus c$$

Energy resolution of the calorimeter

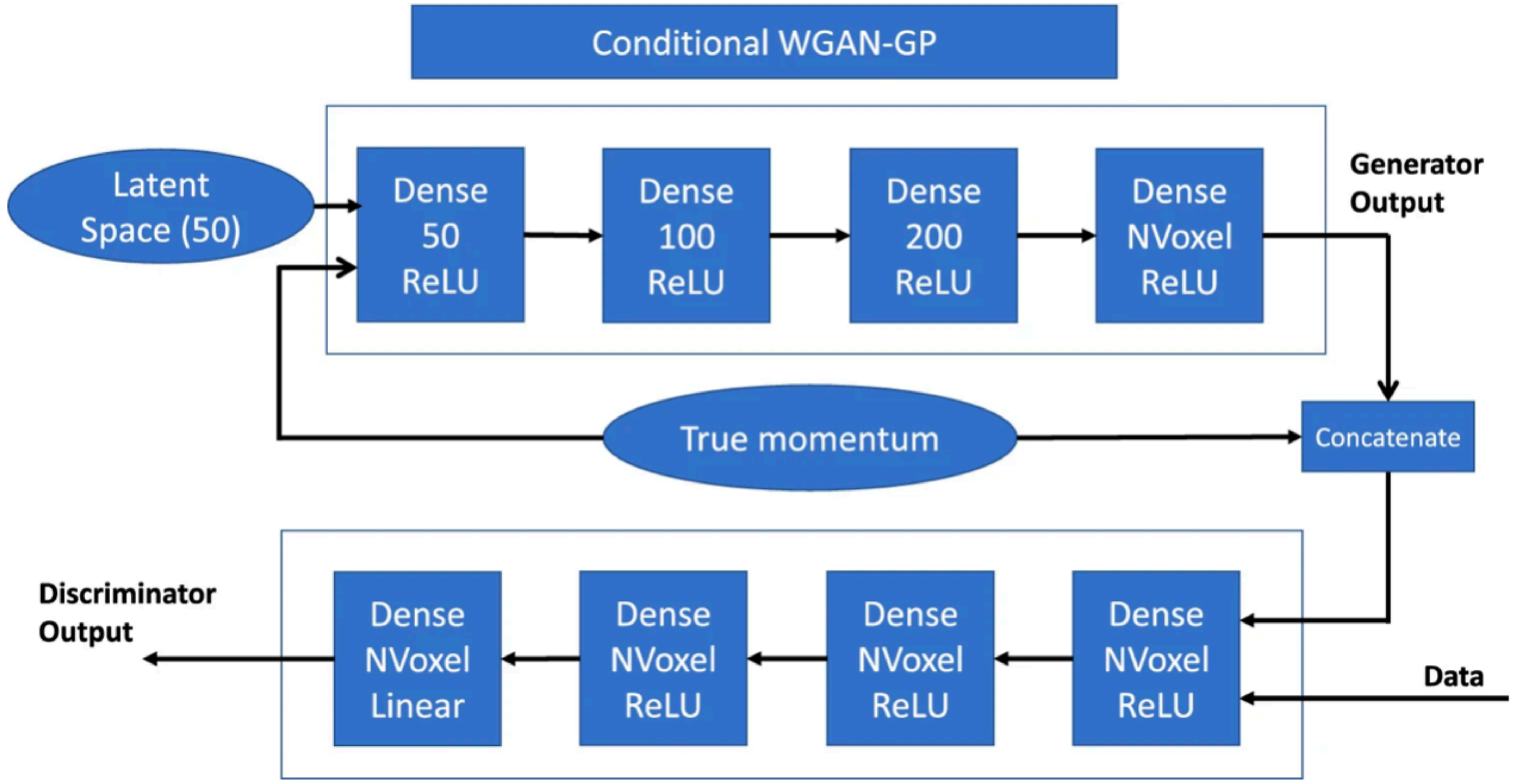


Overview of FastCaloGAN

- Simulate shower development in the longitudinal and lateral direction **simultaneously**

- Architecture: WGAN with GP, conditioned on the truth momentum, output the energy deposition in each voxel (reduce the dimension)

- One GAN for each η slice (100 GANs for pions)



NVoxel	Number of voxels
Generator nodes	50, 50, 100, 200, NVoxel
Discriminator nodes	NVoxel, N[illegible]Voxel, 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 (λ)	10

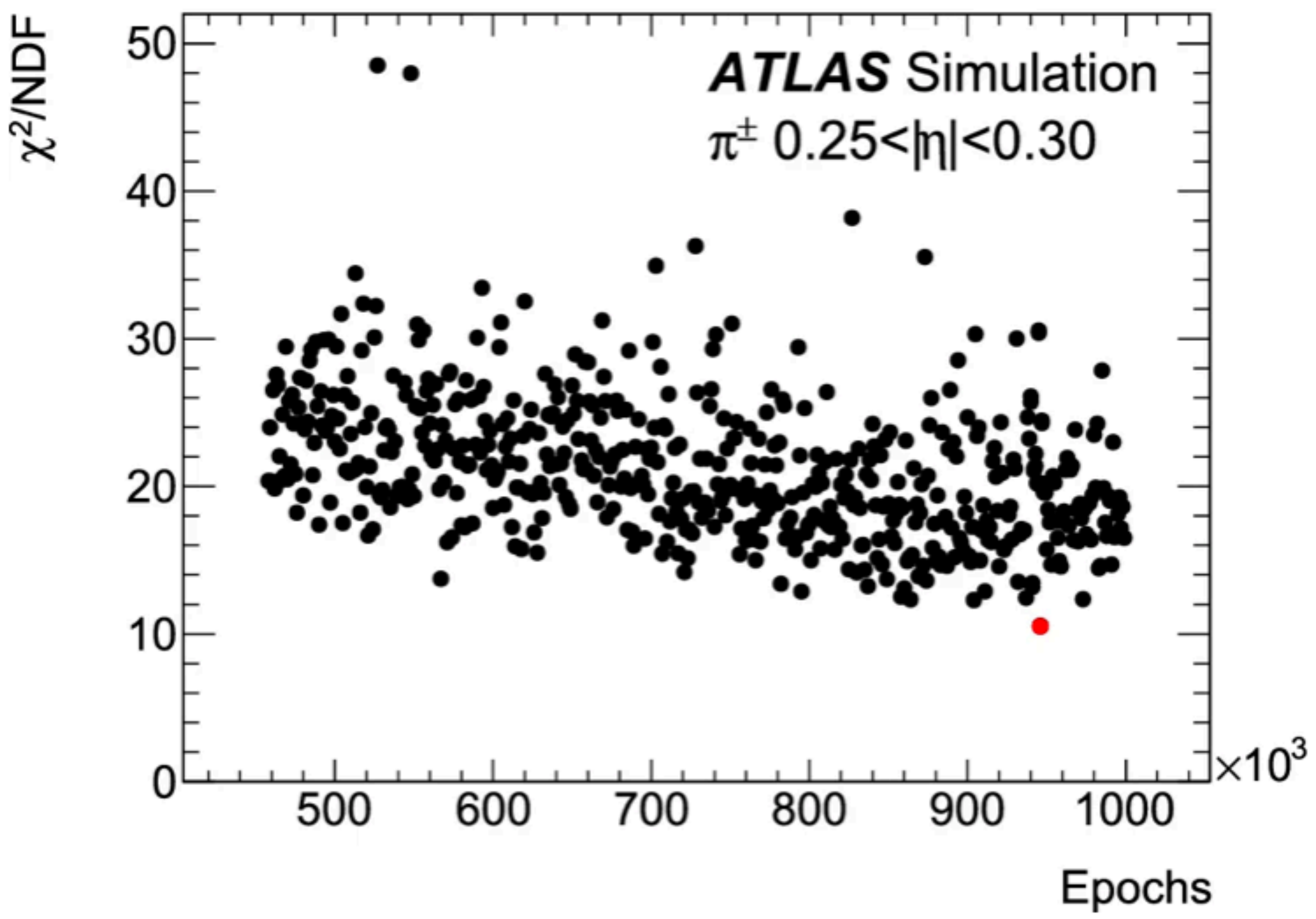
Training Strategy

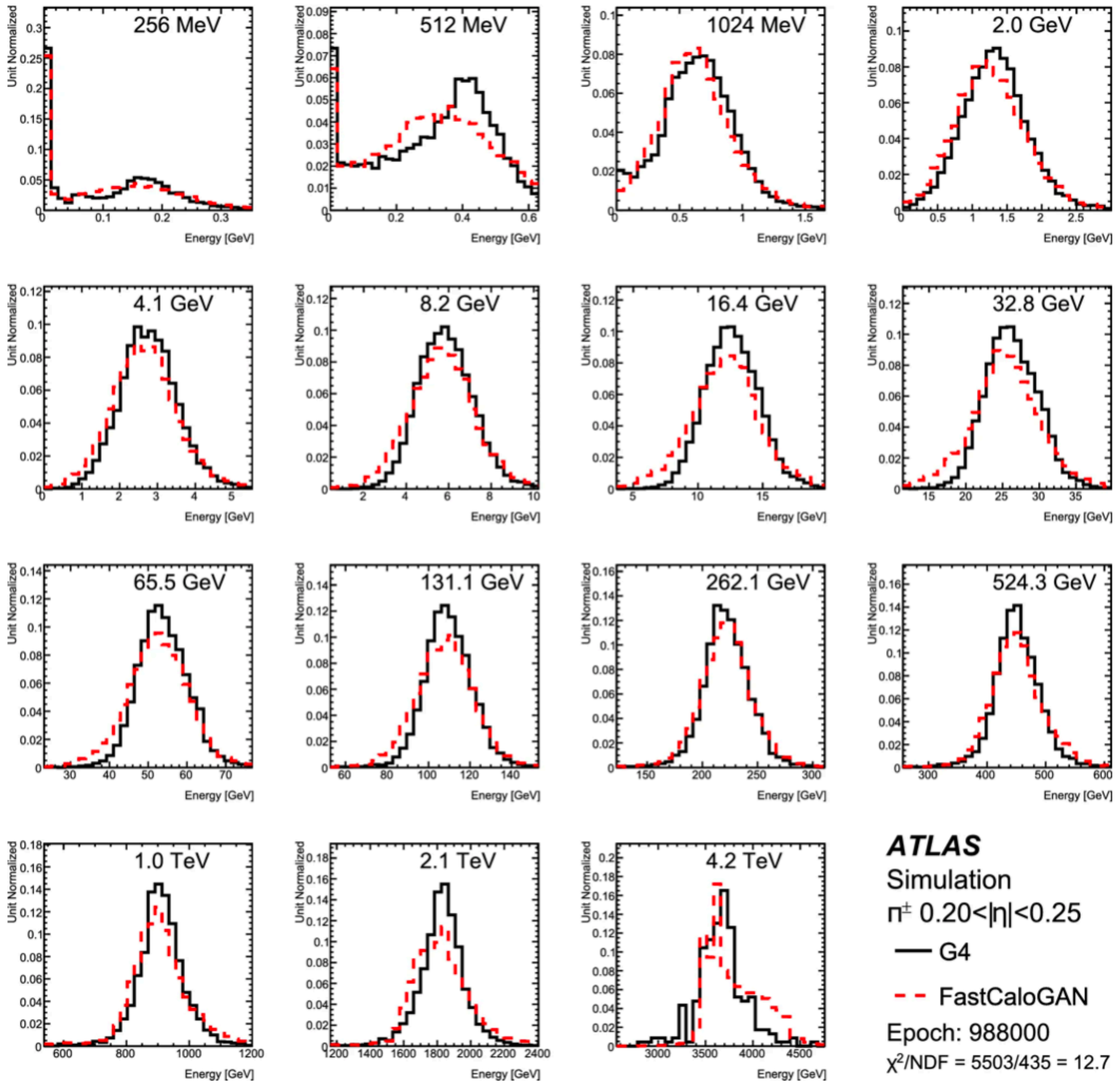
- GAN is **first** trained on a single energy point, then **progressively** add other energy points
  - train the first 50k epochs with a middle energy sample (32 GeV)
  - every 20k epochs add a new sample, alternating between higher and lower energy
  - Once all energy points have been added, continue training with all samples
- 1 million epochs (limited by the available resources)
- Training time for each GAN: **~8 hours** on the NVIDIA V100 **GPUs**

Best Epoch Performance

- Figure of merit: χ^2 of the total energy between the reference samples and generated samples

- Select epoch with lowest χ^2

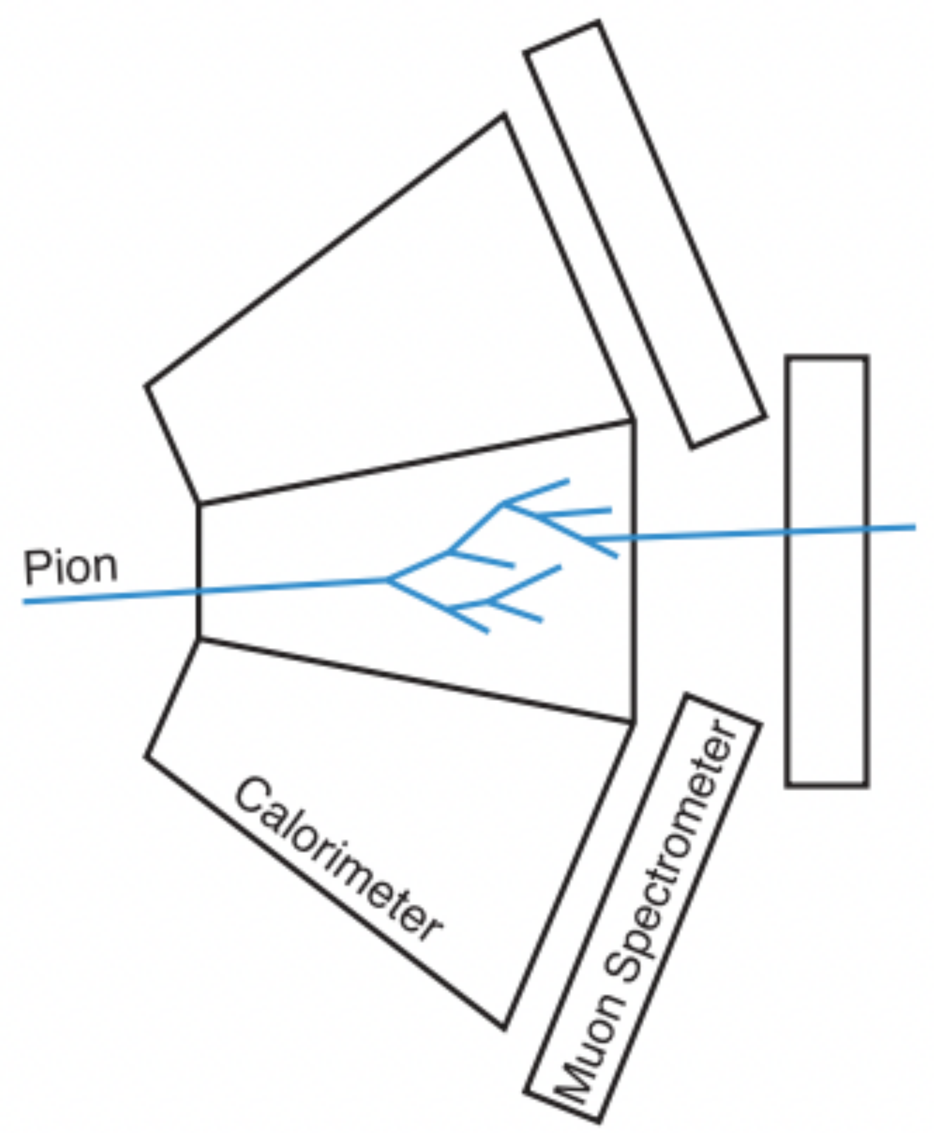


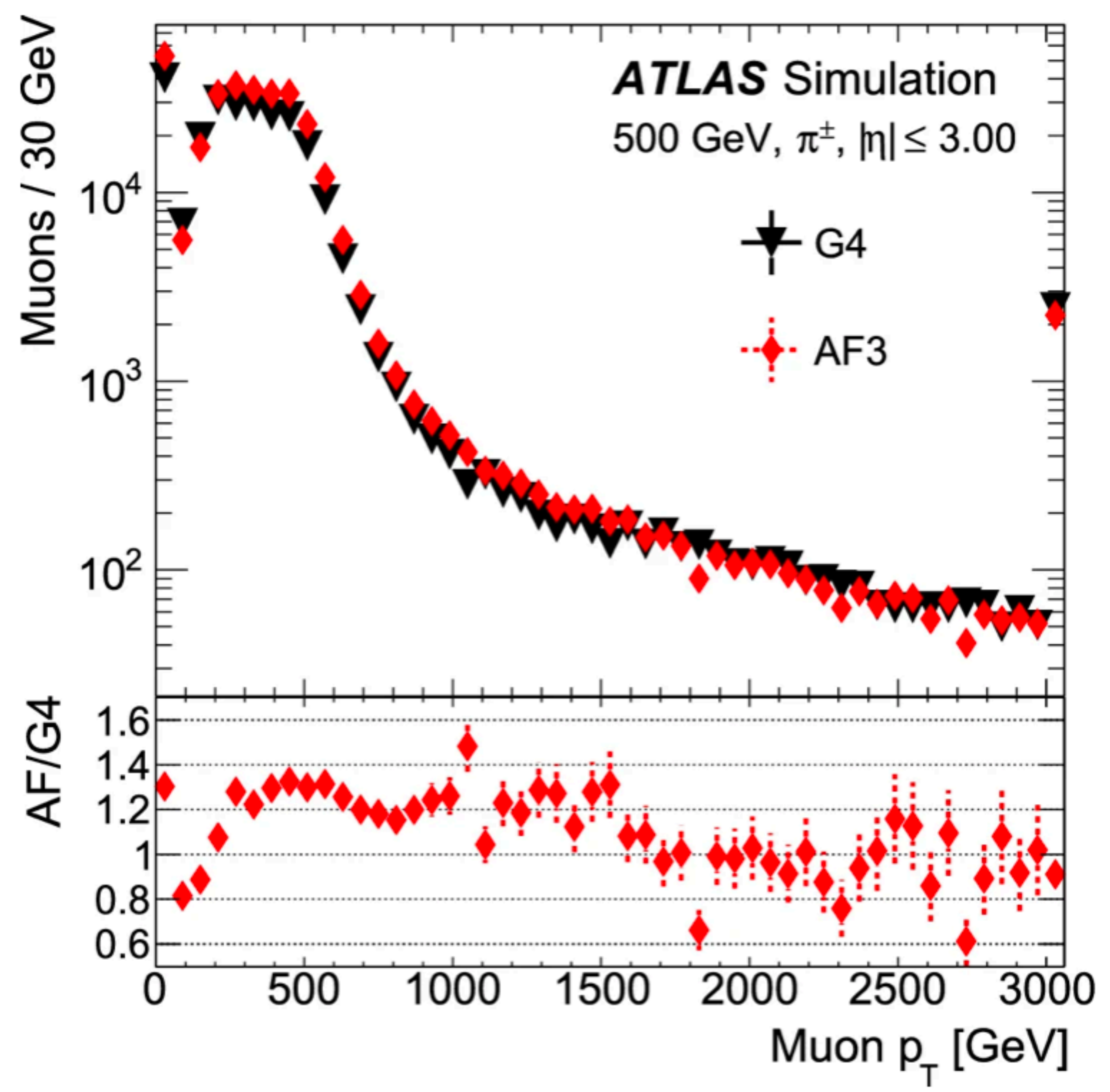


Muon Punch-Through

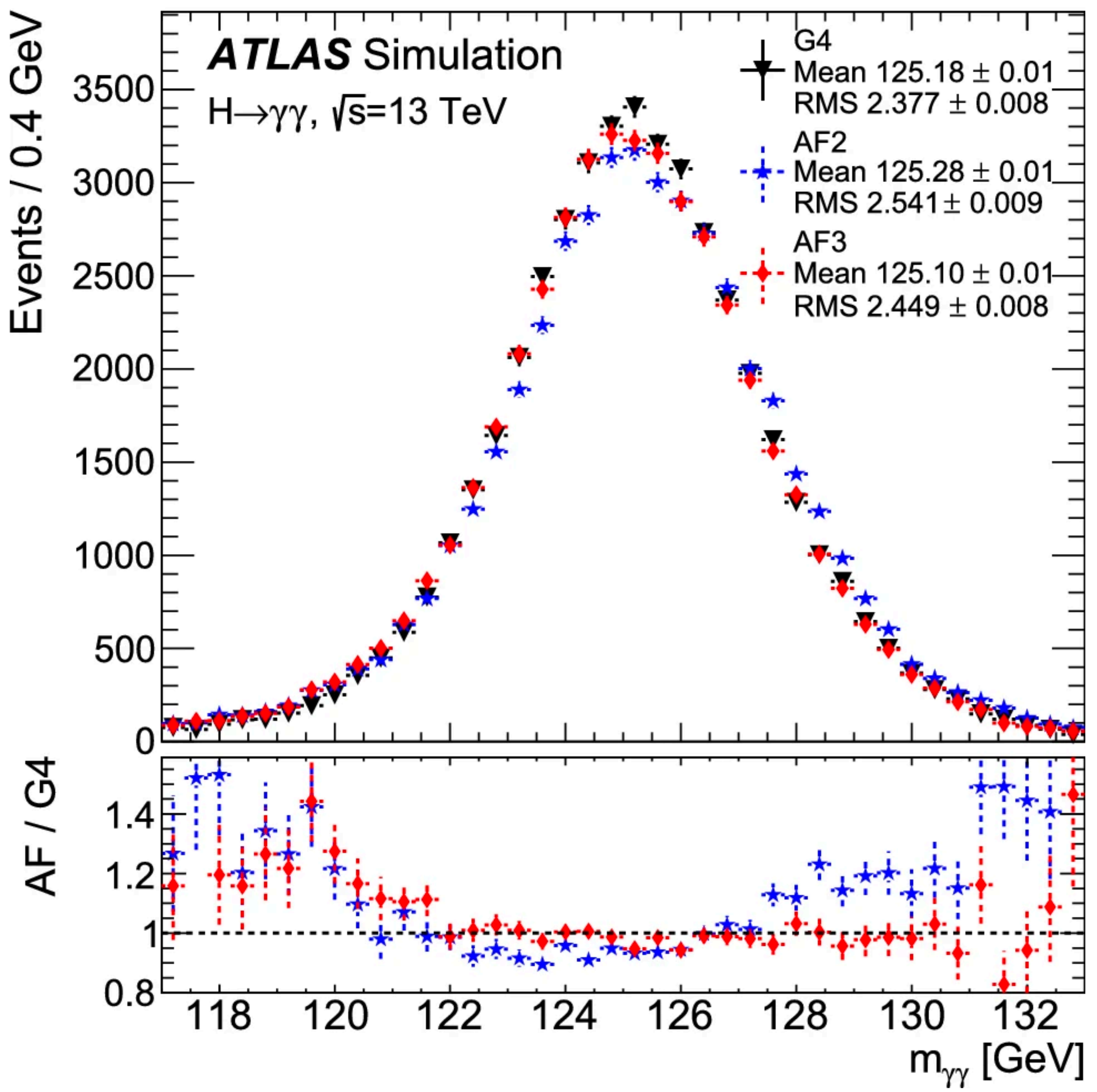
- Secondary particles can escape the calorimeter and generate hits in the muon spectrometer
  - new in AF3
  - need to be well modeled to describe the backgrounds of muons

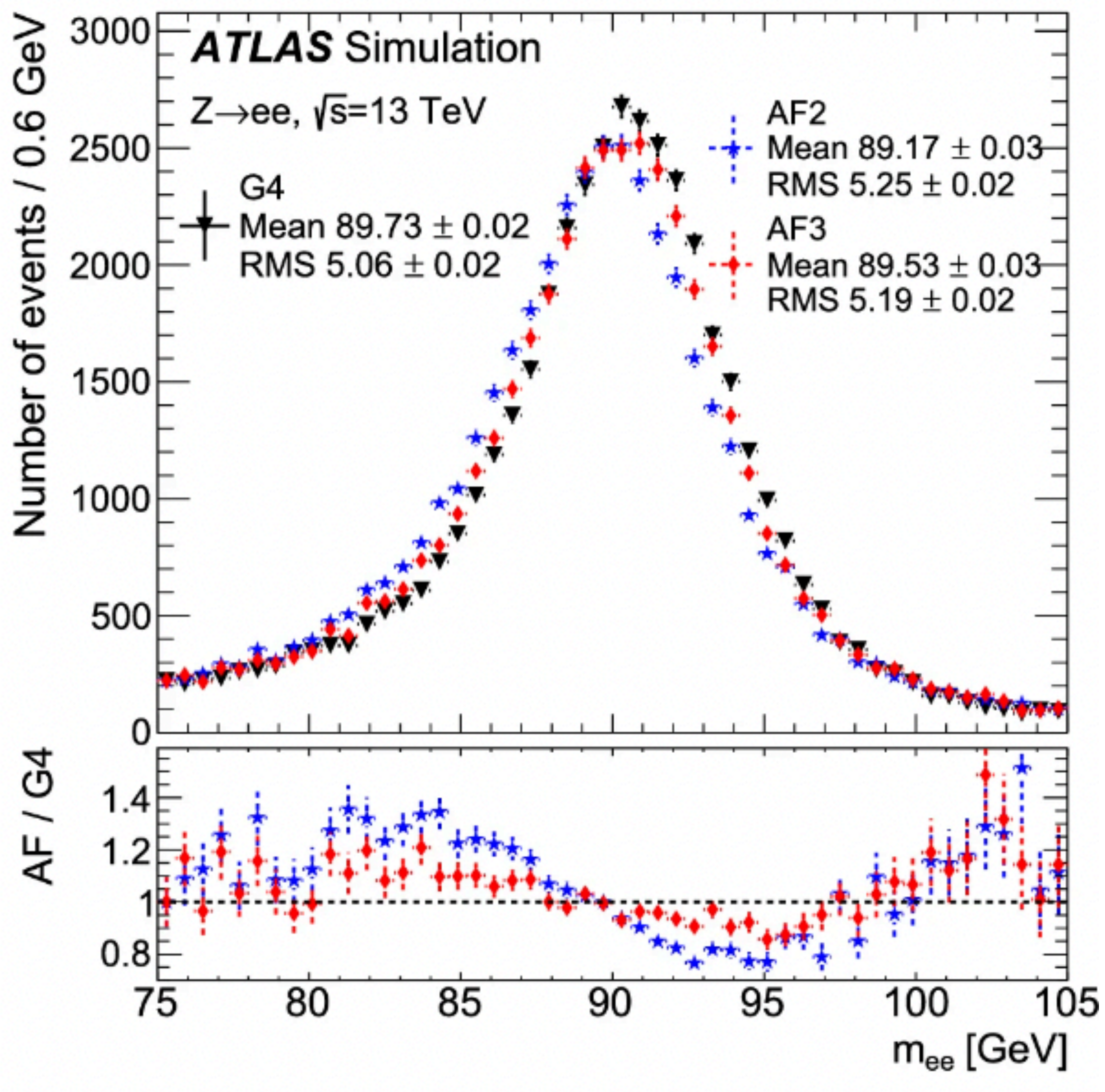
- Number of secondaries and their energy, position and momentum are parameterized





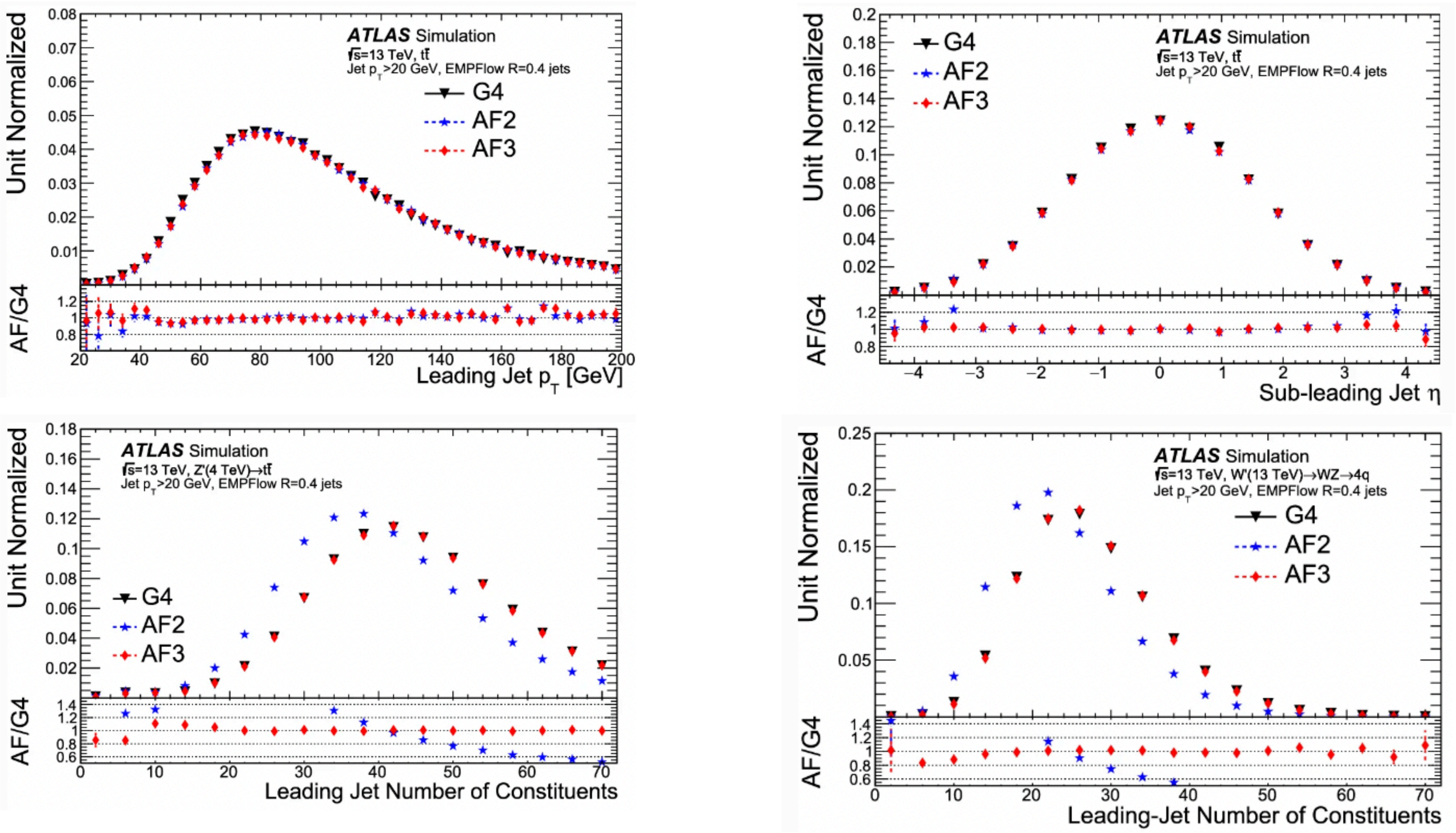
Performance: Photons & Electrons





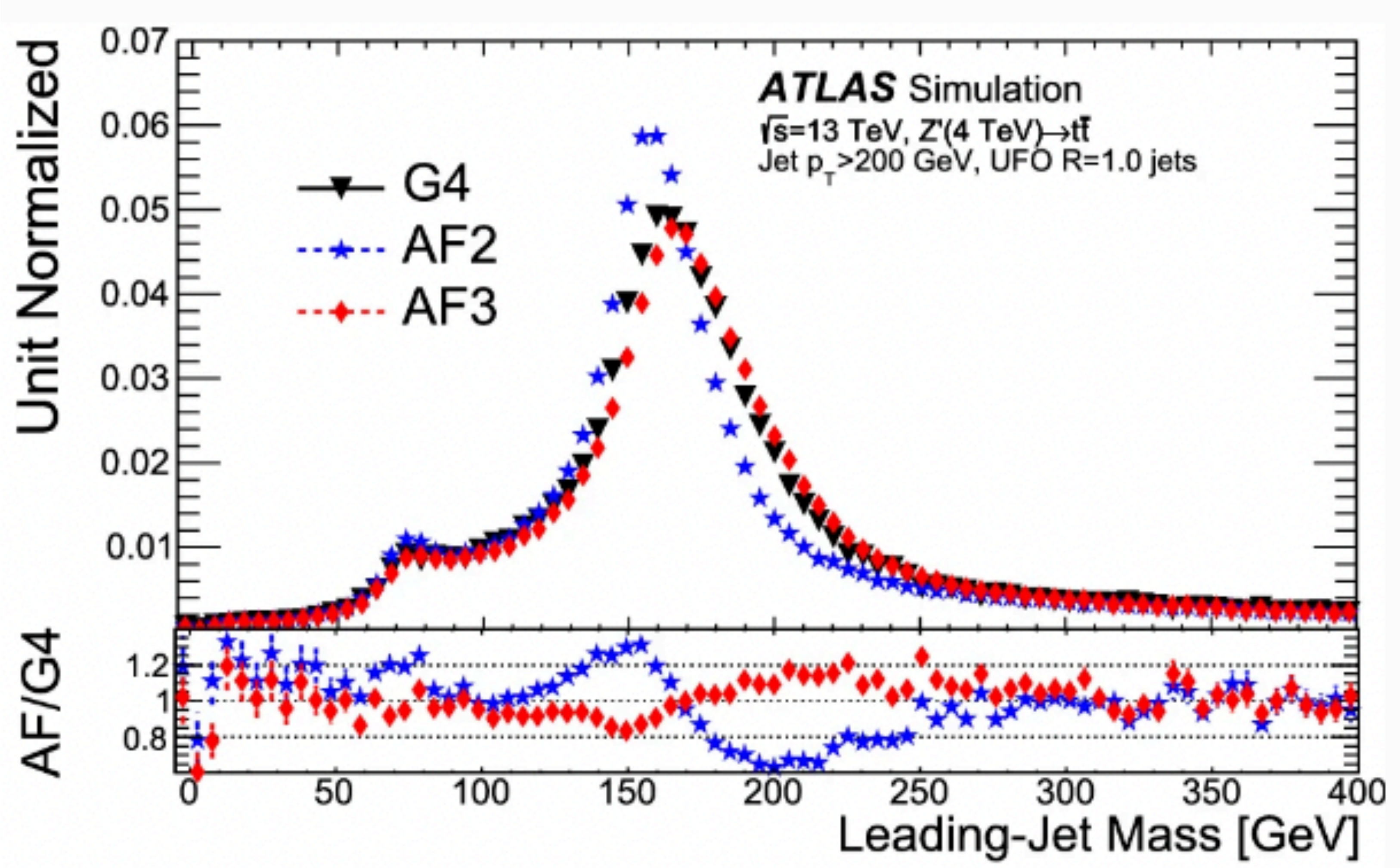
Good modeling for photons and electrons

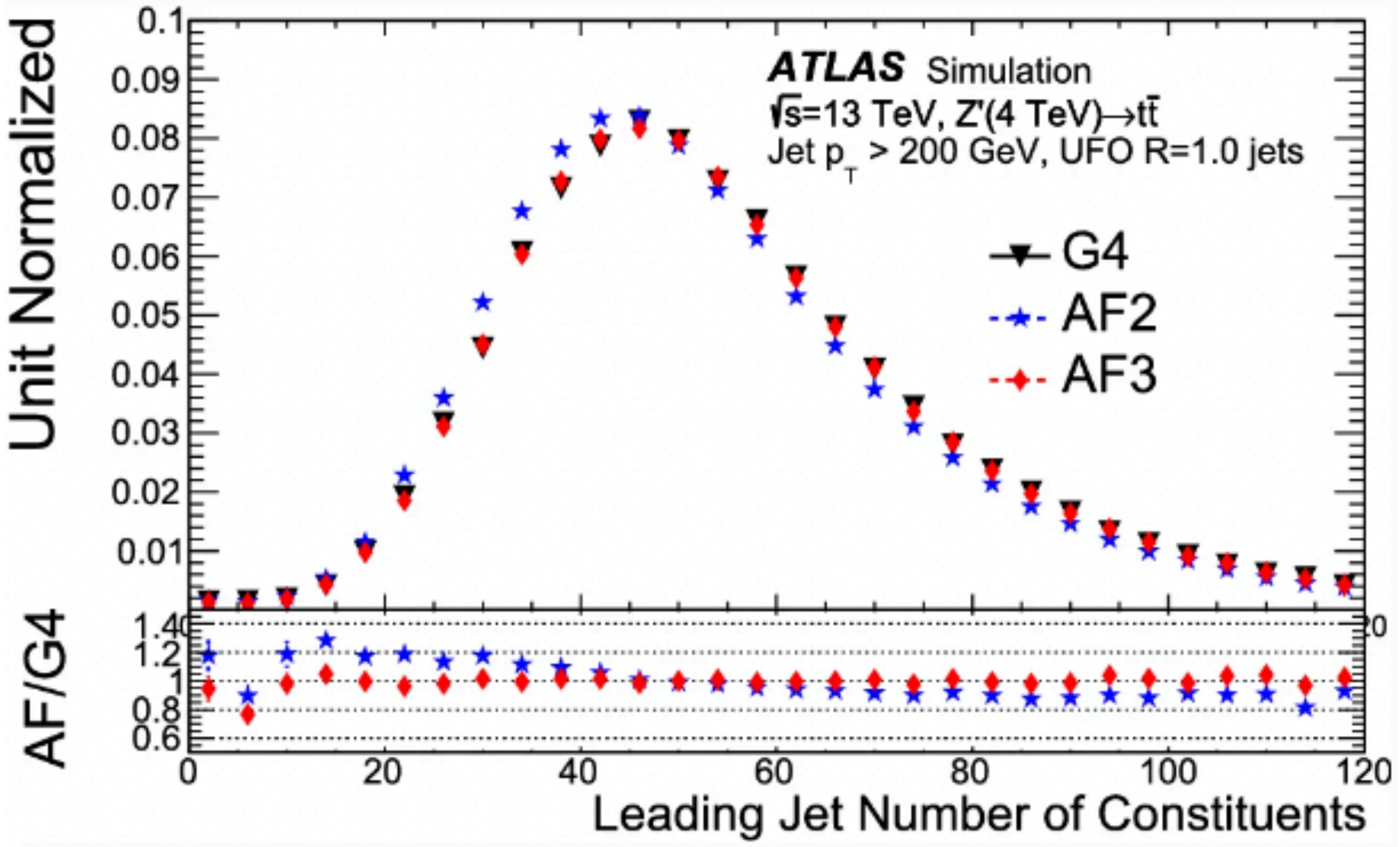
Performance: R=0.4 Jets

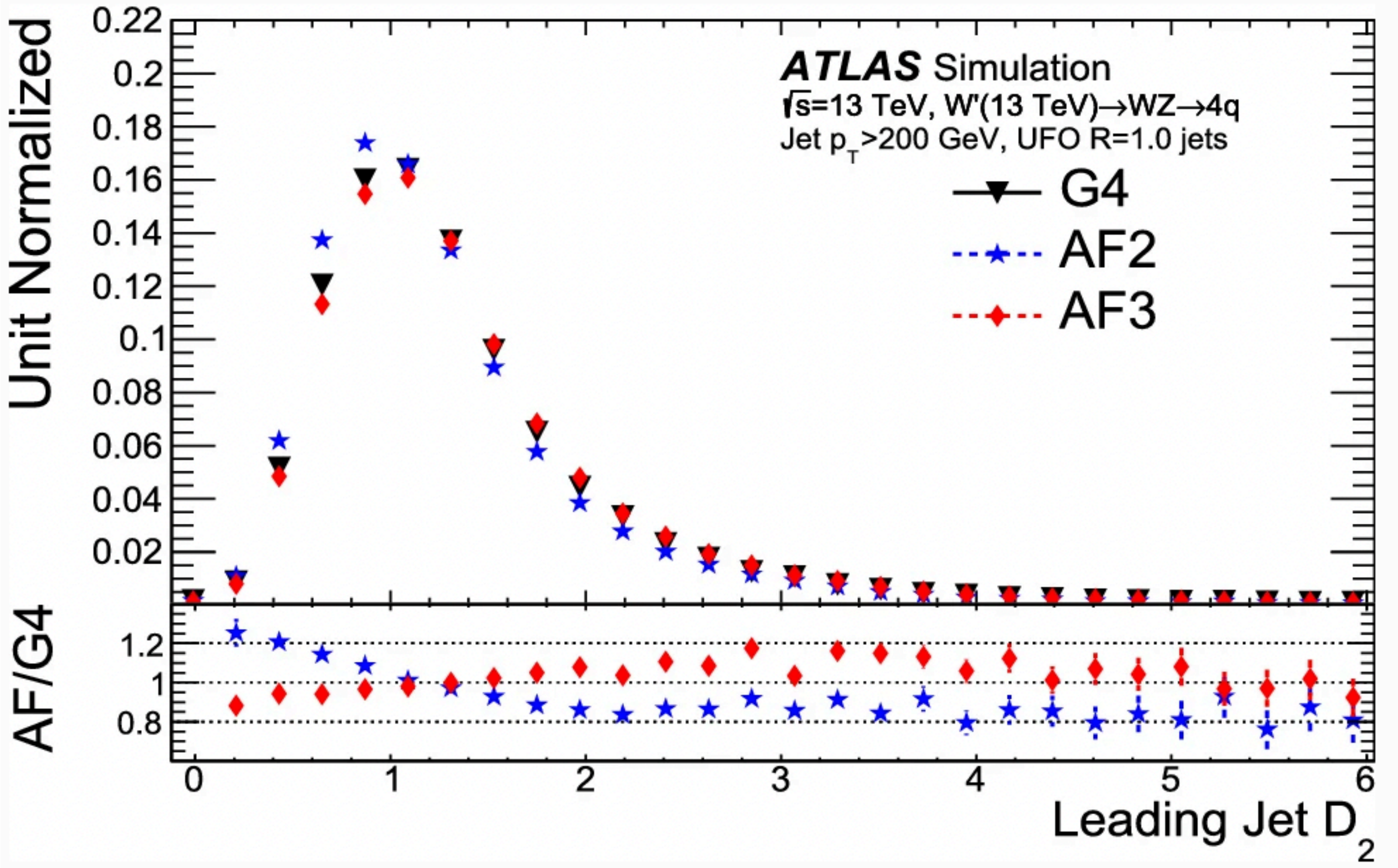


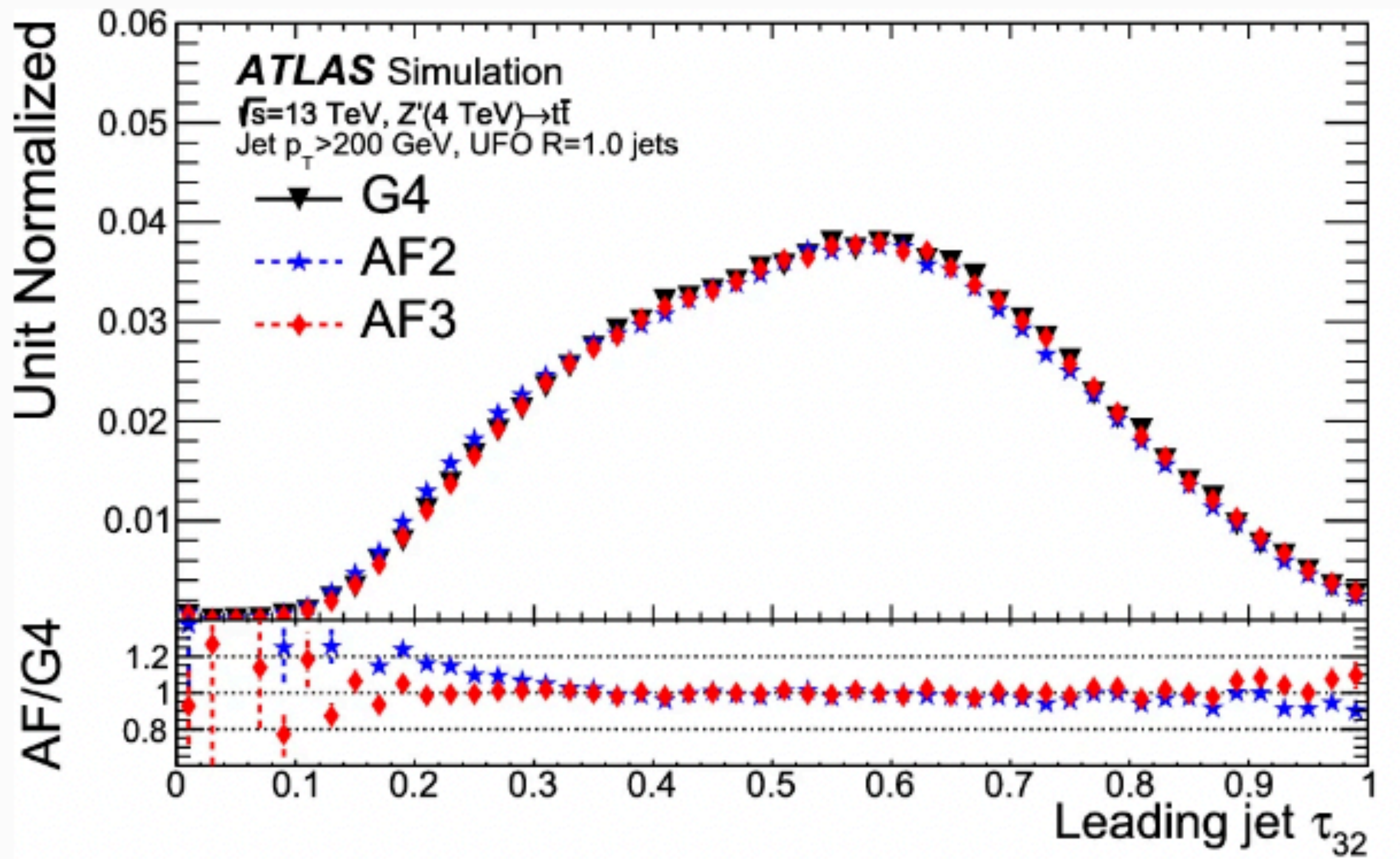
Improved modeling for R=0.4 Jets

Performance: R=1.0 Jets









Improved modeling for R=1.0 Jets

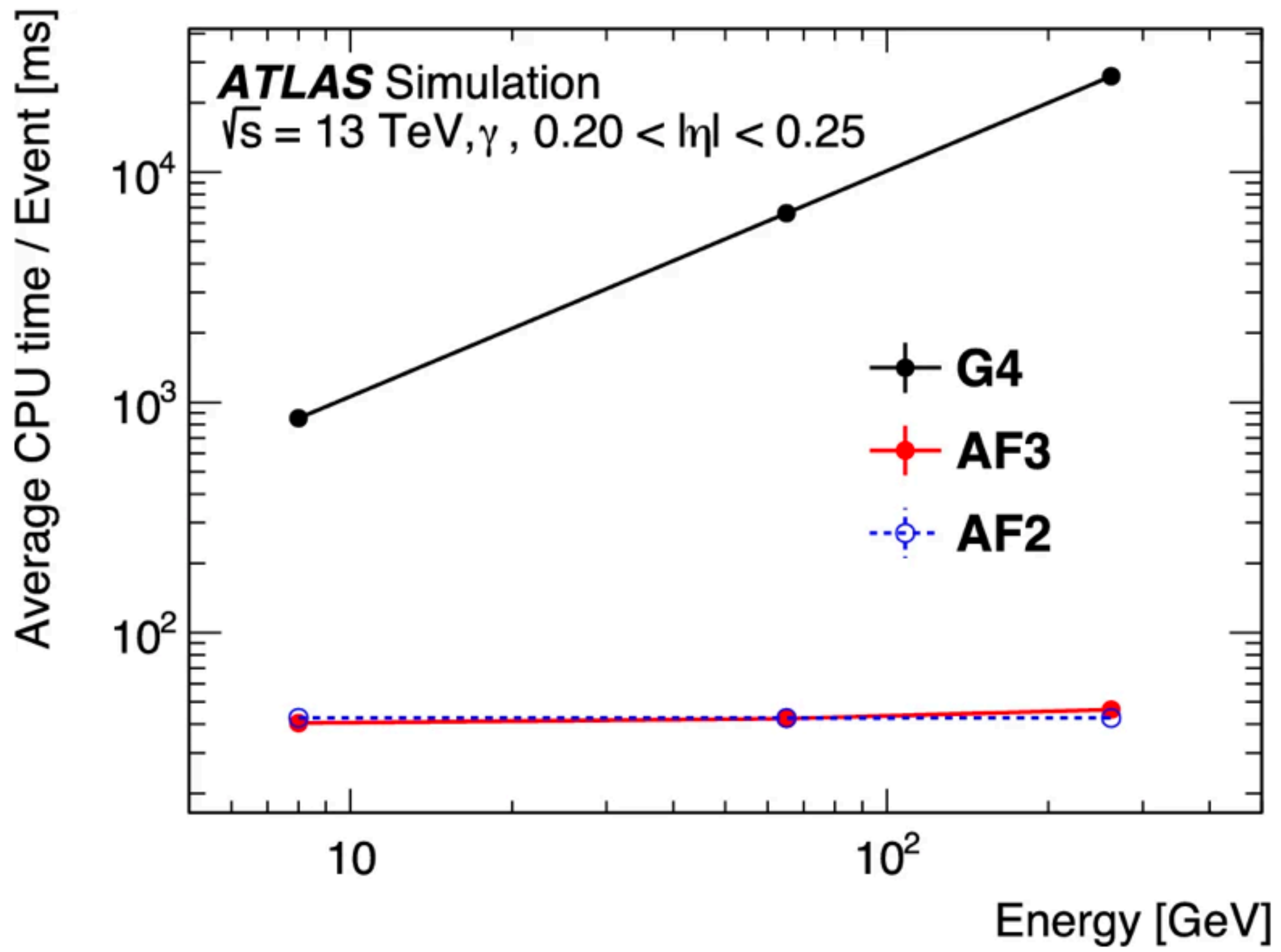
Conclusion

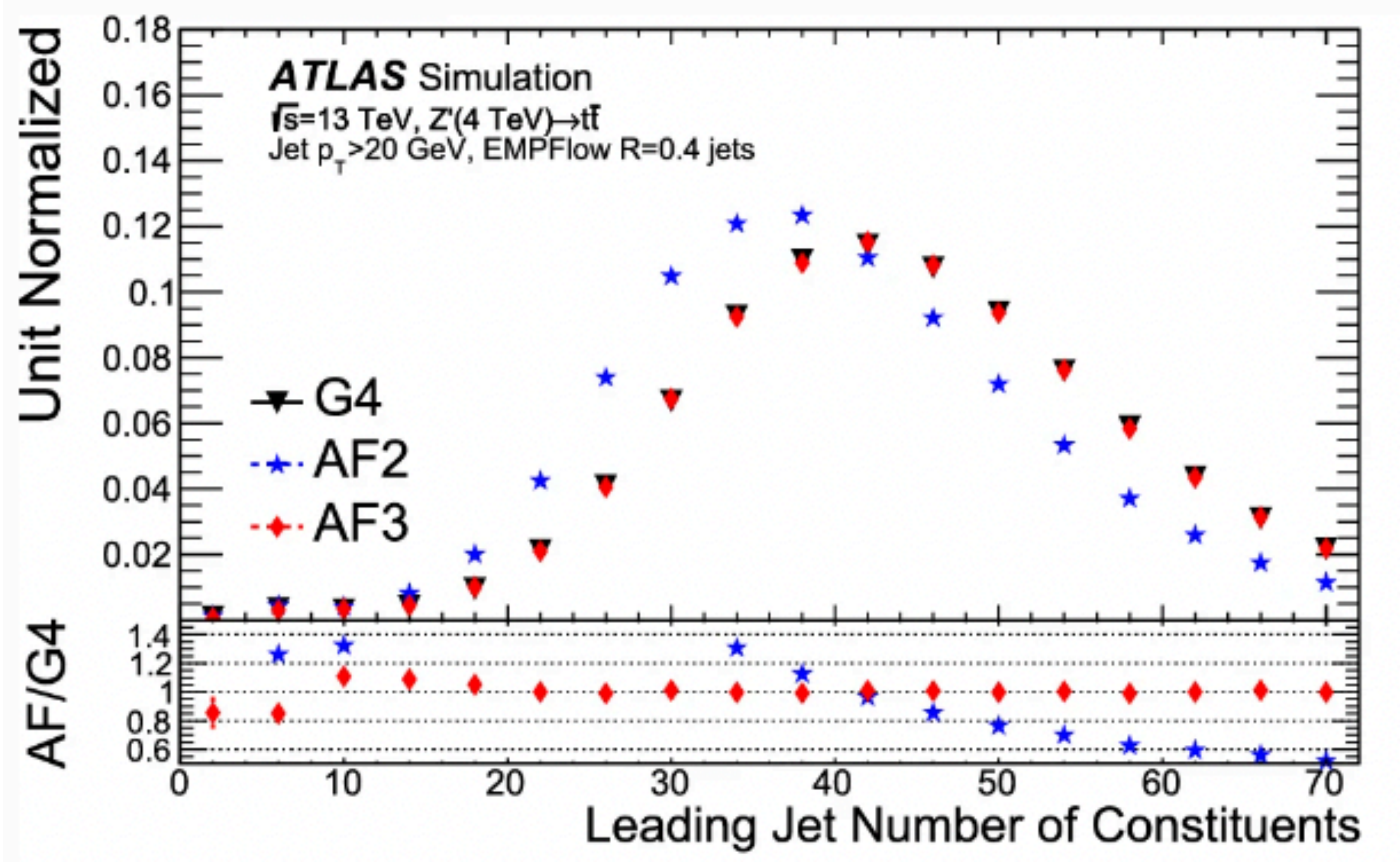
- AF3: next generation of fast simulation in ATLAS
  - FastCaloSimV2: classical parameterization
  - FastCaloGAN: machine learning
  - Muon punch-through: fake muon

- Similar CPU consumption as AF2, improved modeling

- Default simulator for Run3 and HL-LHC
  - Run3: >50%, targeting 70%
  - HL-LHC: 90%

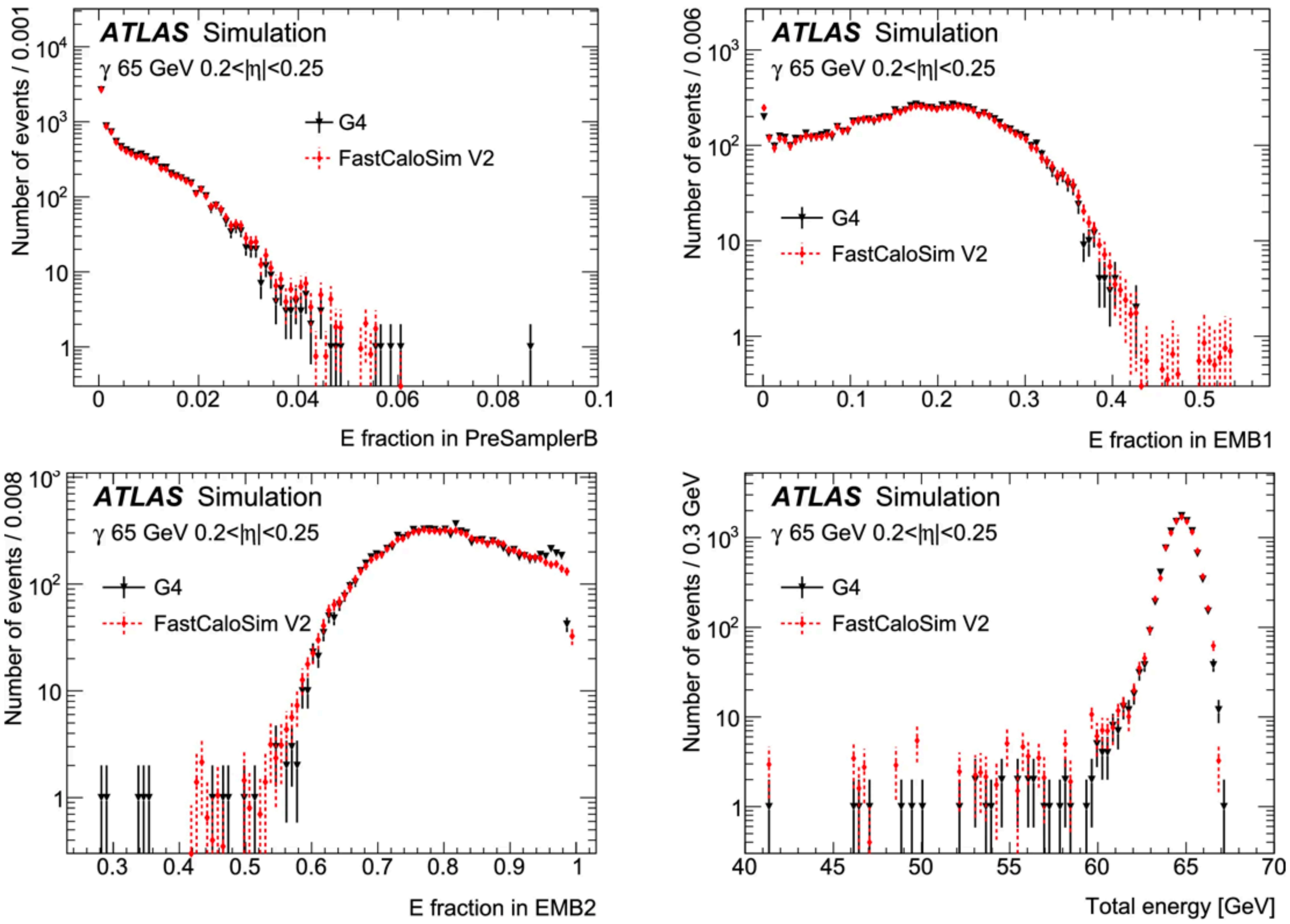
Thank You !





Backup

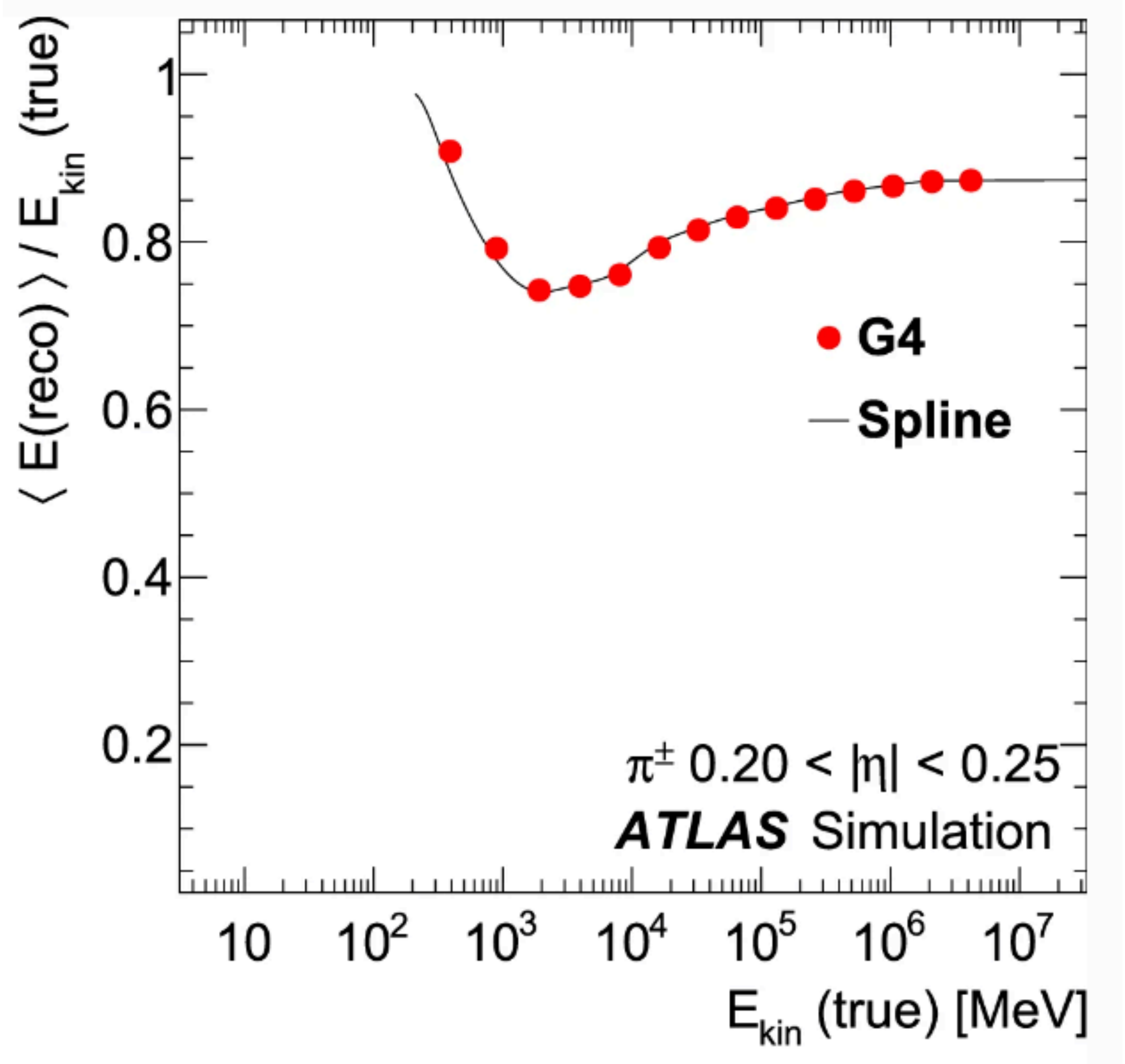
Validation of the Longitidinal Energy Parameterization

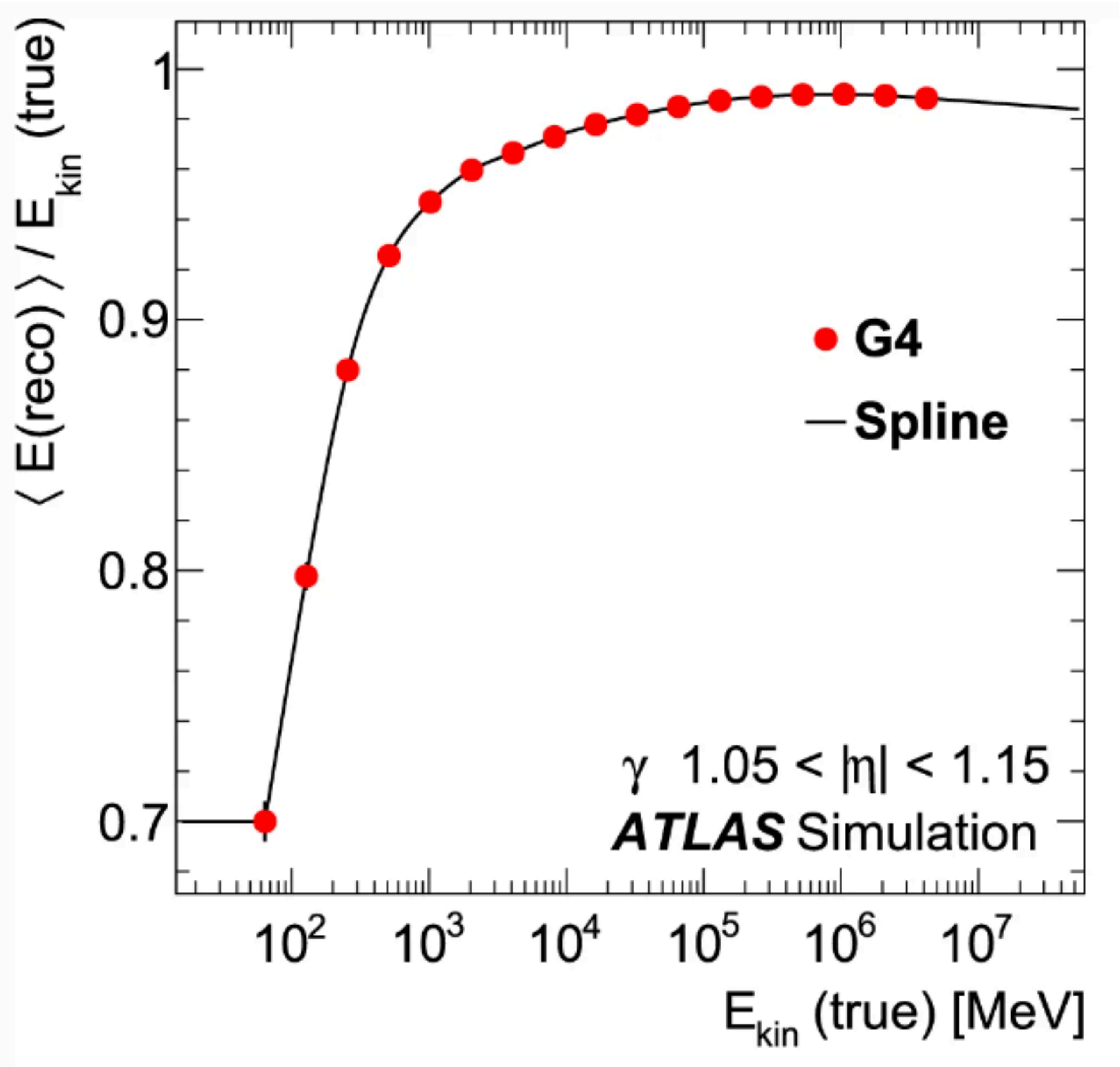


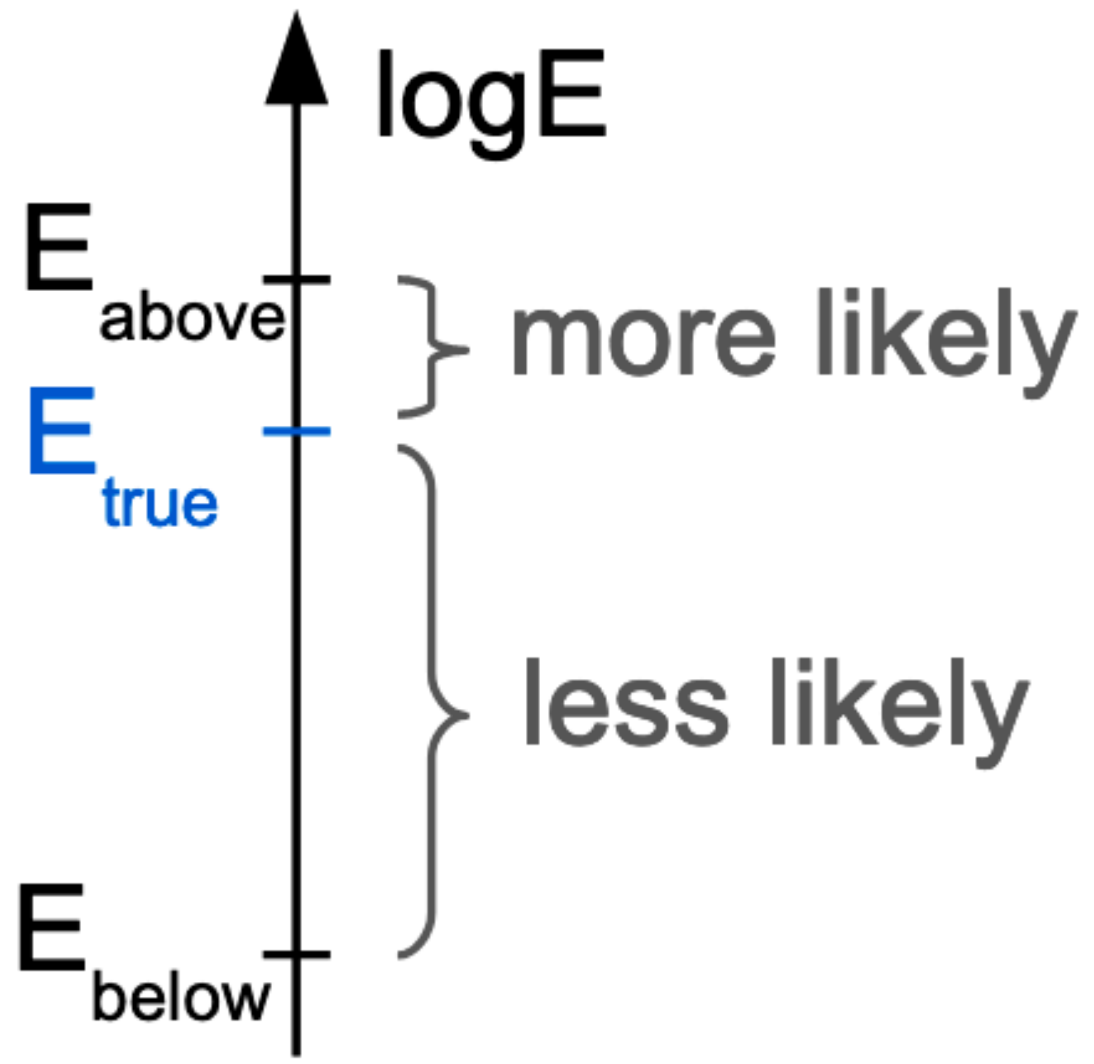
Longitude Energy Simulation

- During simulation, inverse PCA to obtain the energy in each layer
  - uncorrelated random variables → correlated energy deposition in layers

- Interpolation used to simulate particles of all energies
  - energy response: spline interpolation
  - parameterization: randomly selected based on the logarithm distance







Energy Resolution of Calorimeter

EM shower

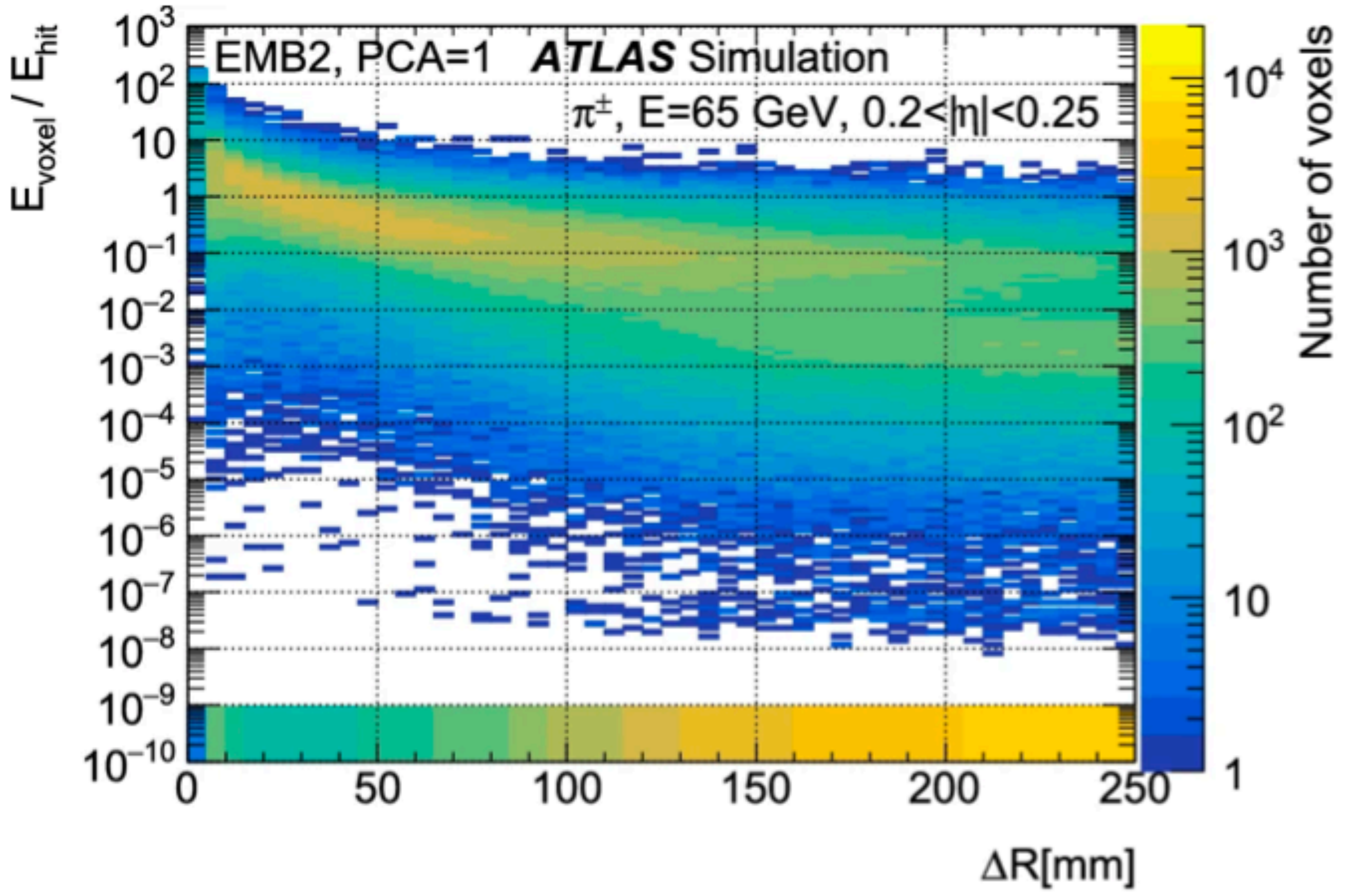
Calorimeter technology	Stochastic term *a*	Constant term *c*
LAr EM barrel and endcap	10.1%	0.2%
Tile	56.4%	5.5%
LAr hadronic endcap	76.2%	0
FCal	28.5%	3.5%

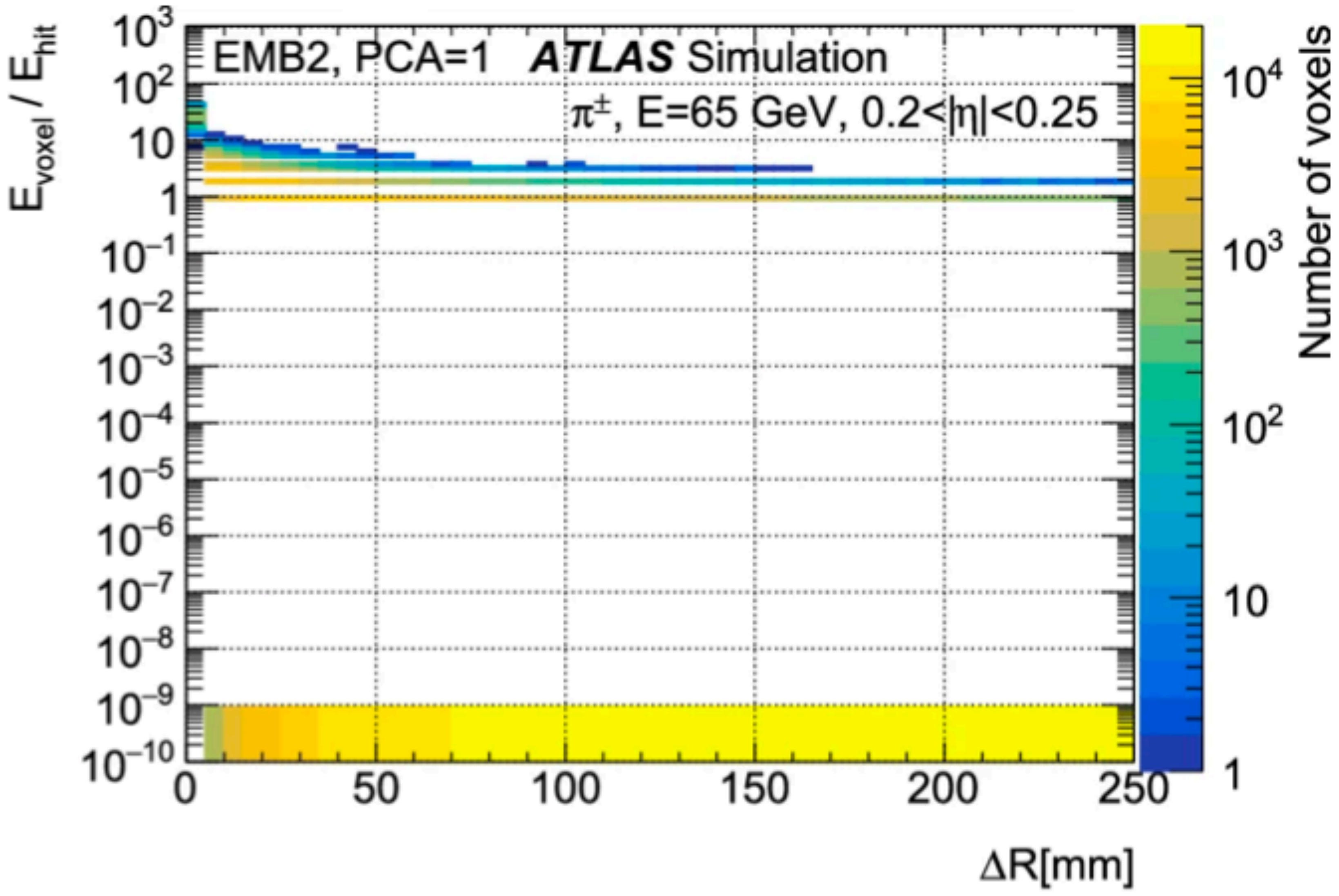
Hadronic shower

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

Weighted Hit

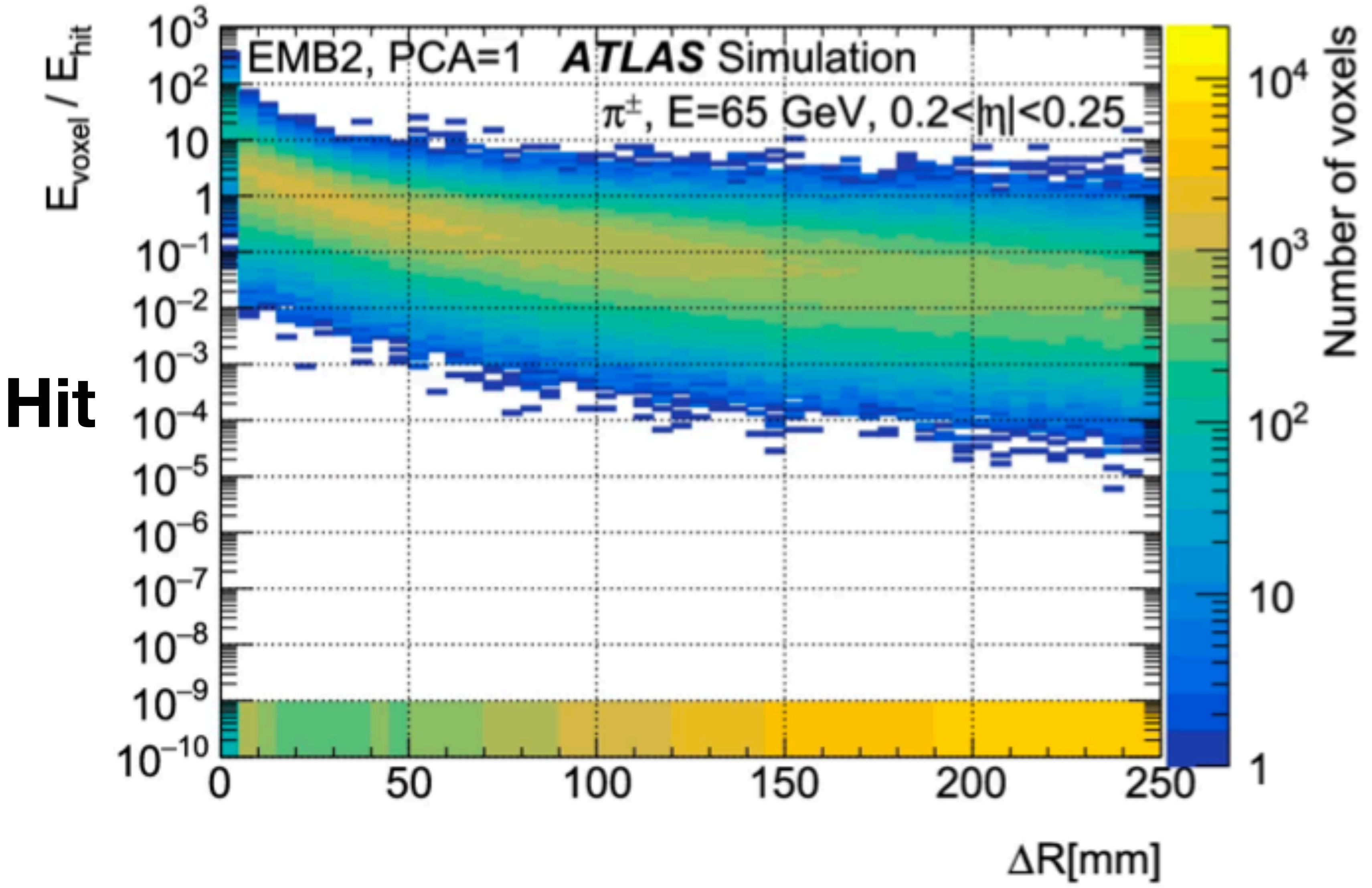
G4

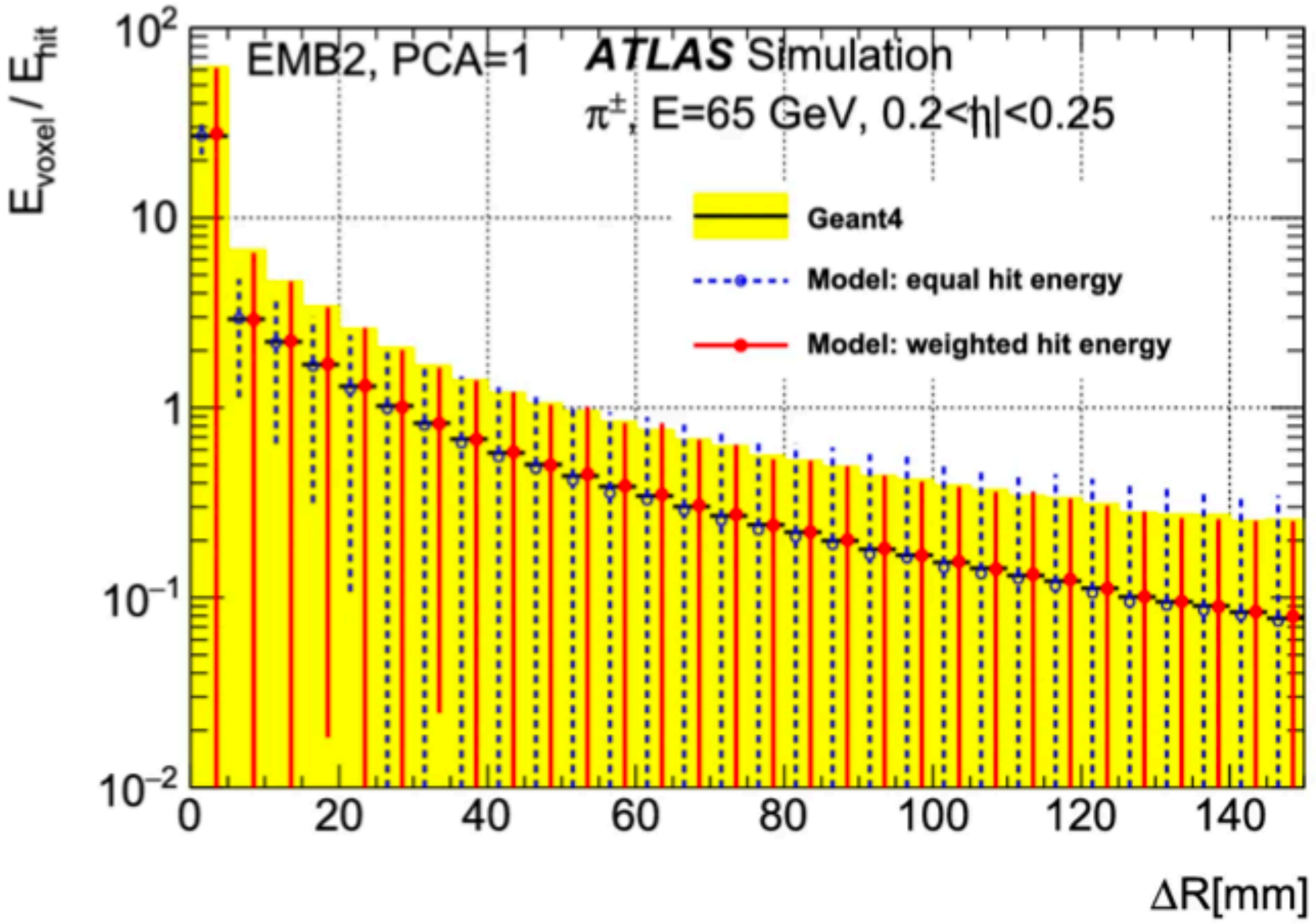




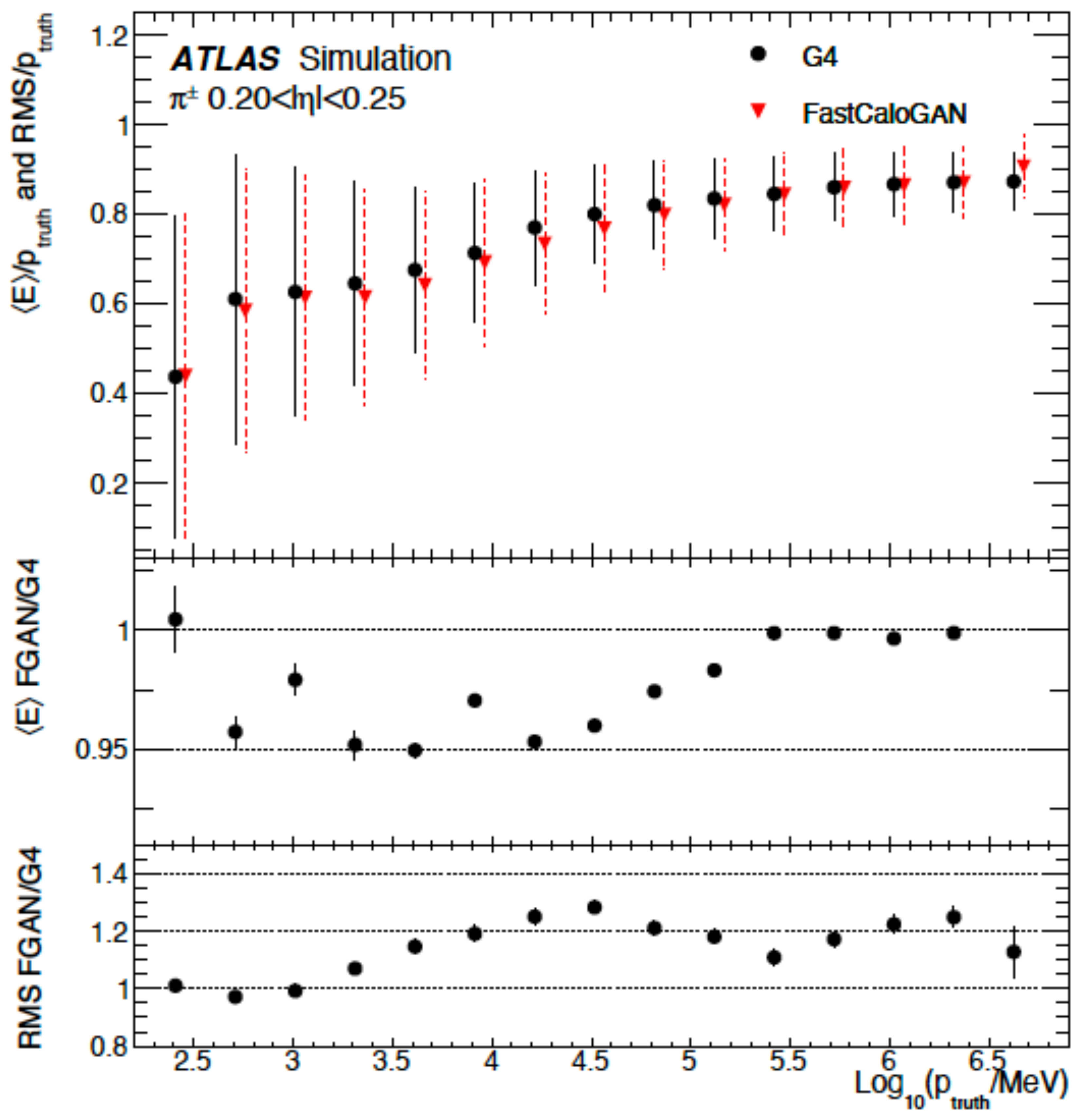
Equal Hit

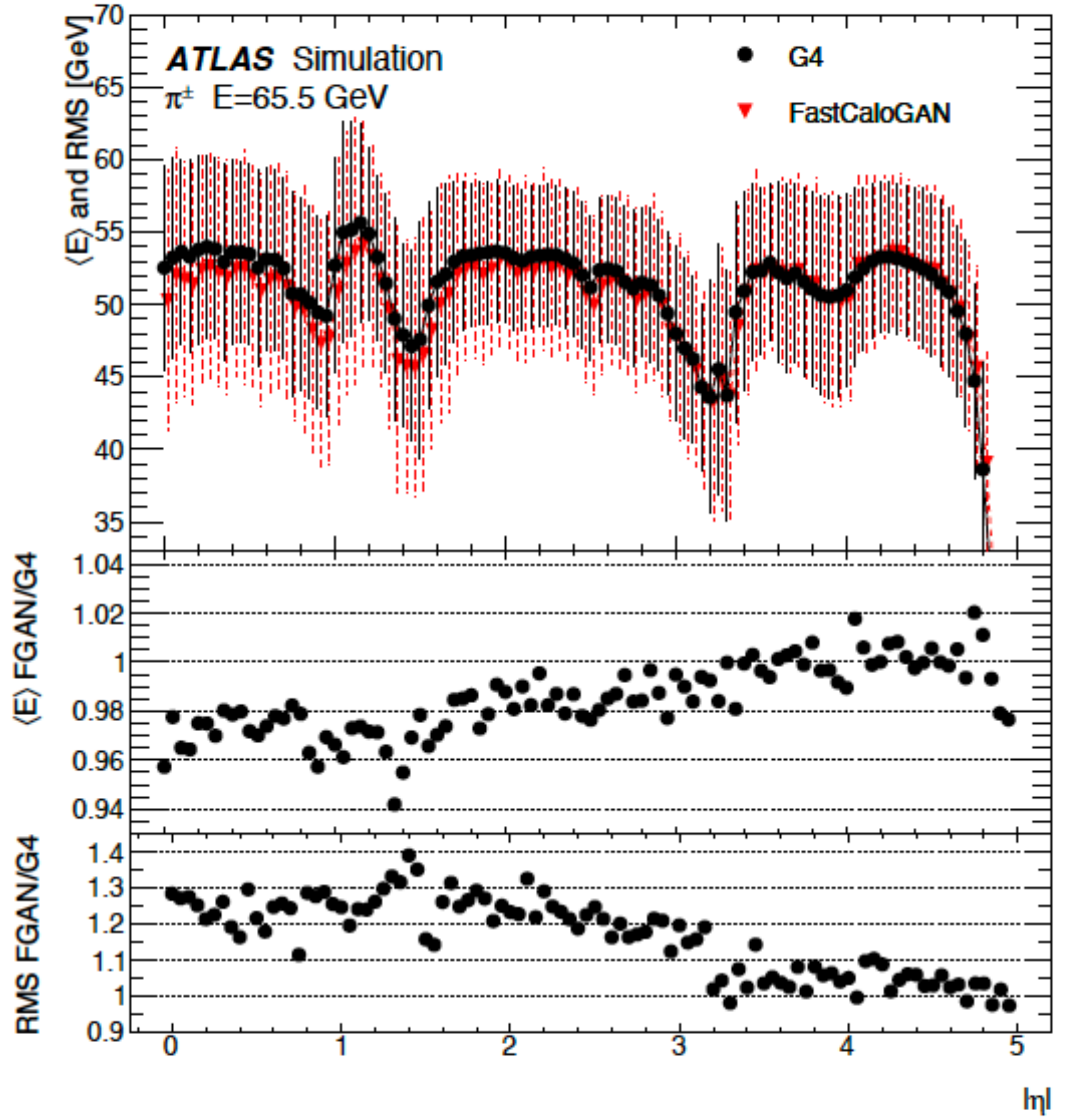
Weighted Hit



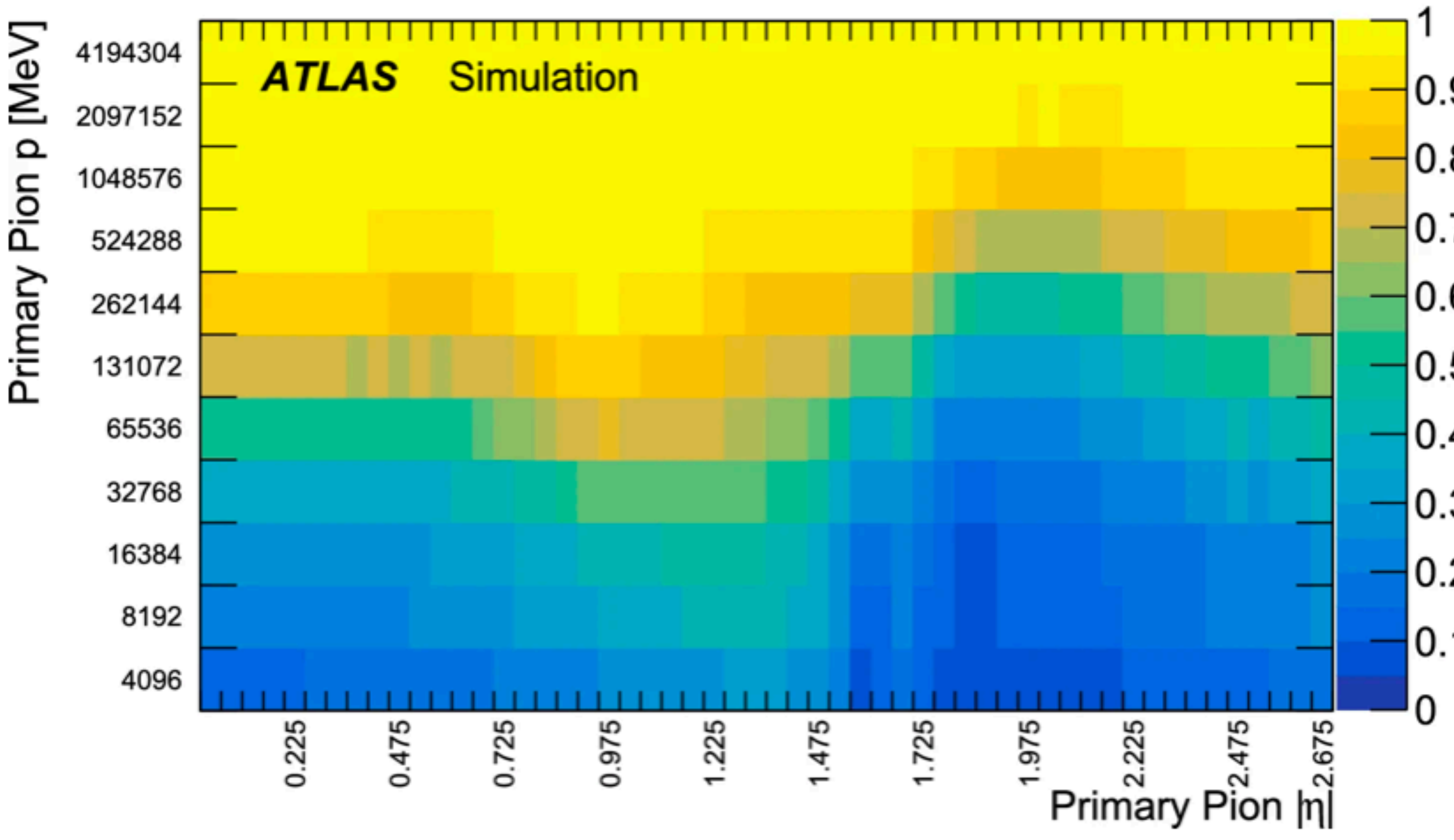


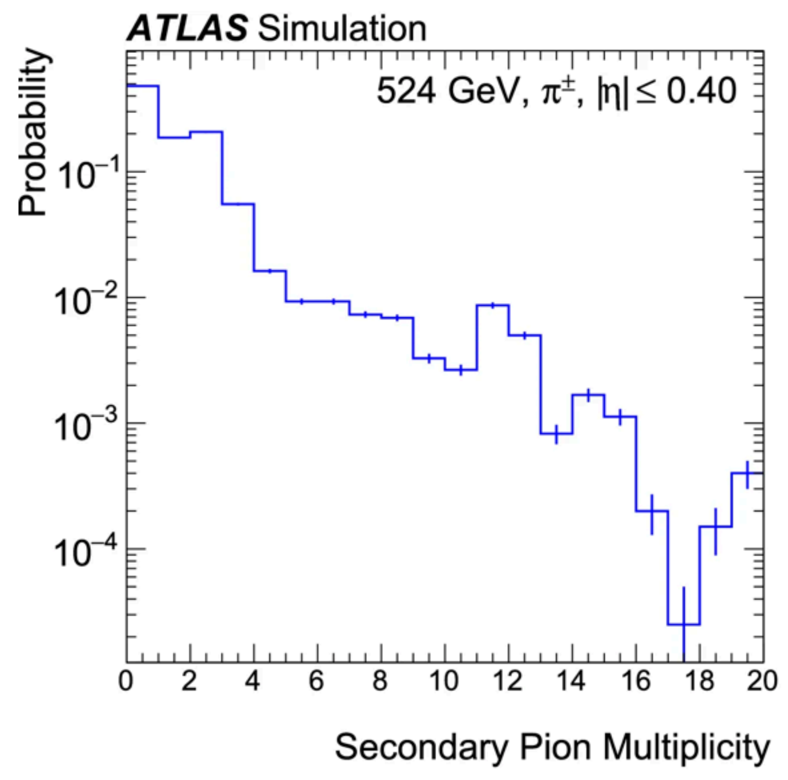
FastCaloGAN

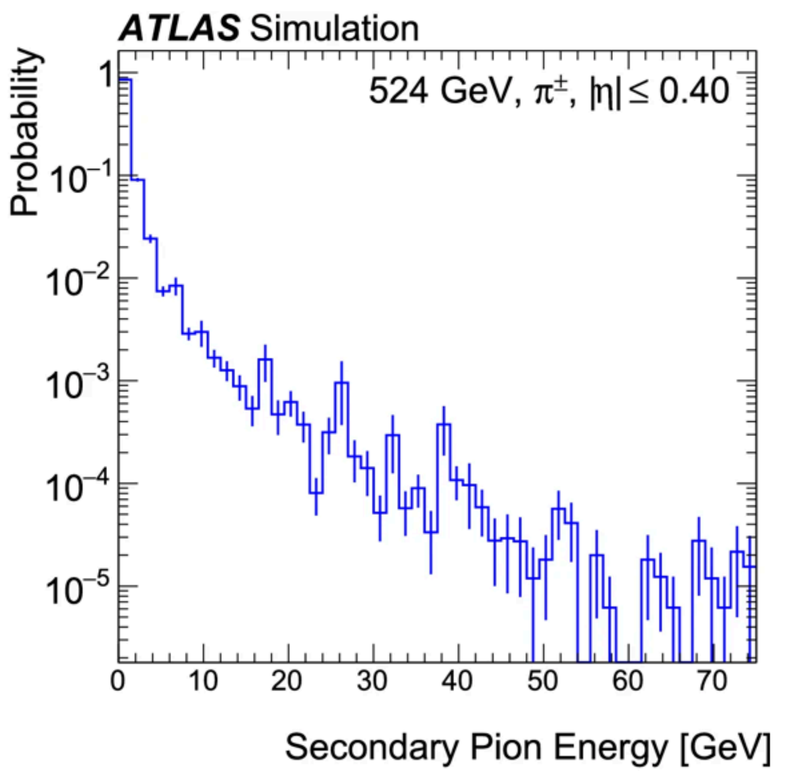


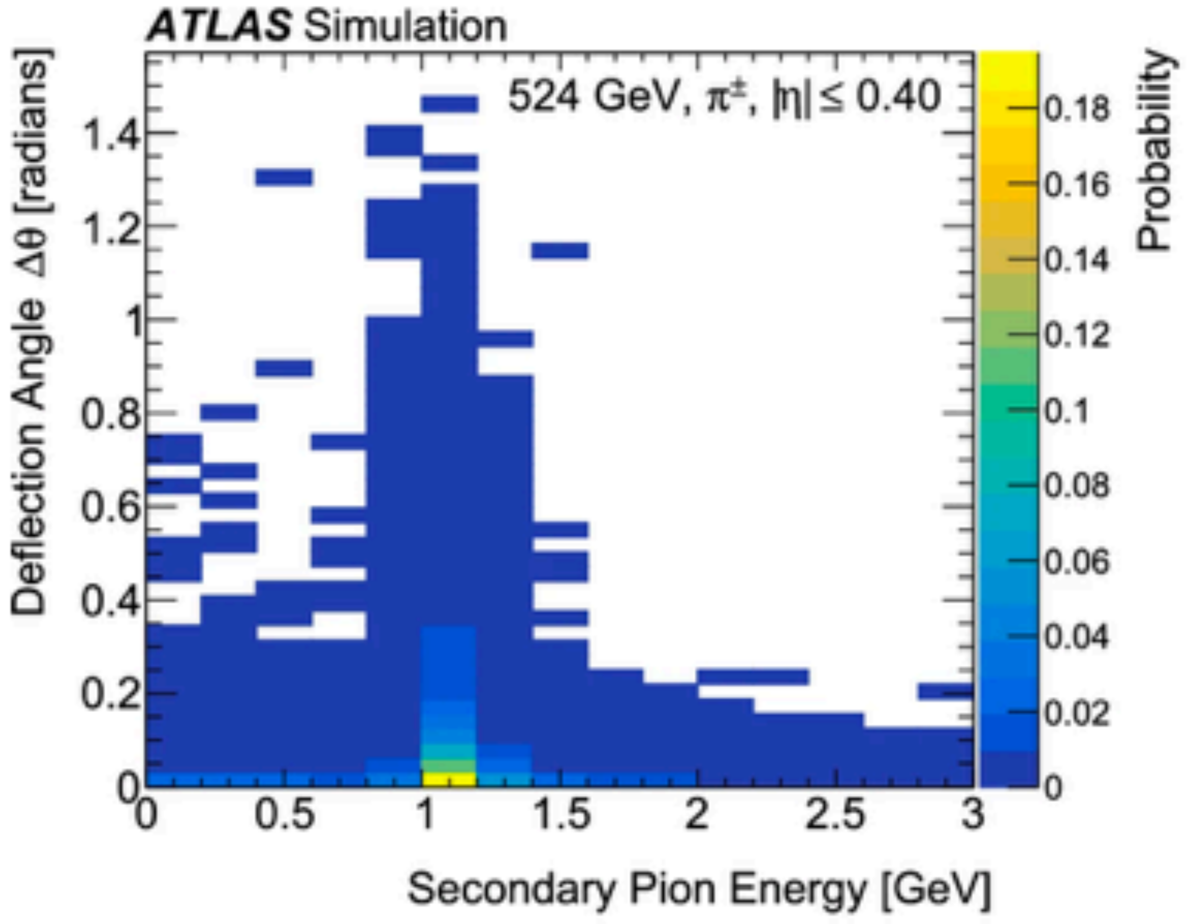


Muon Punch-Through Parameterization

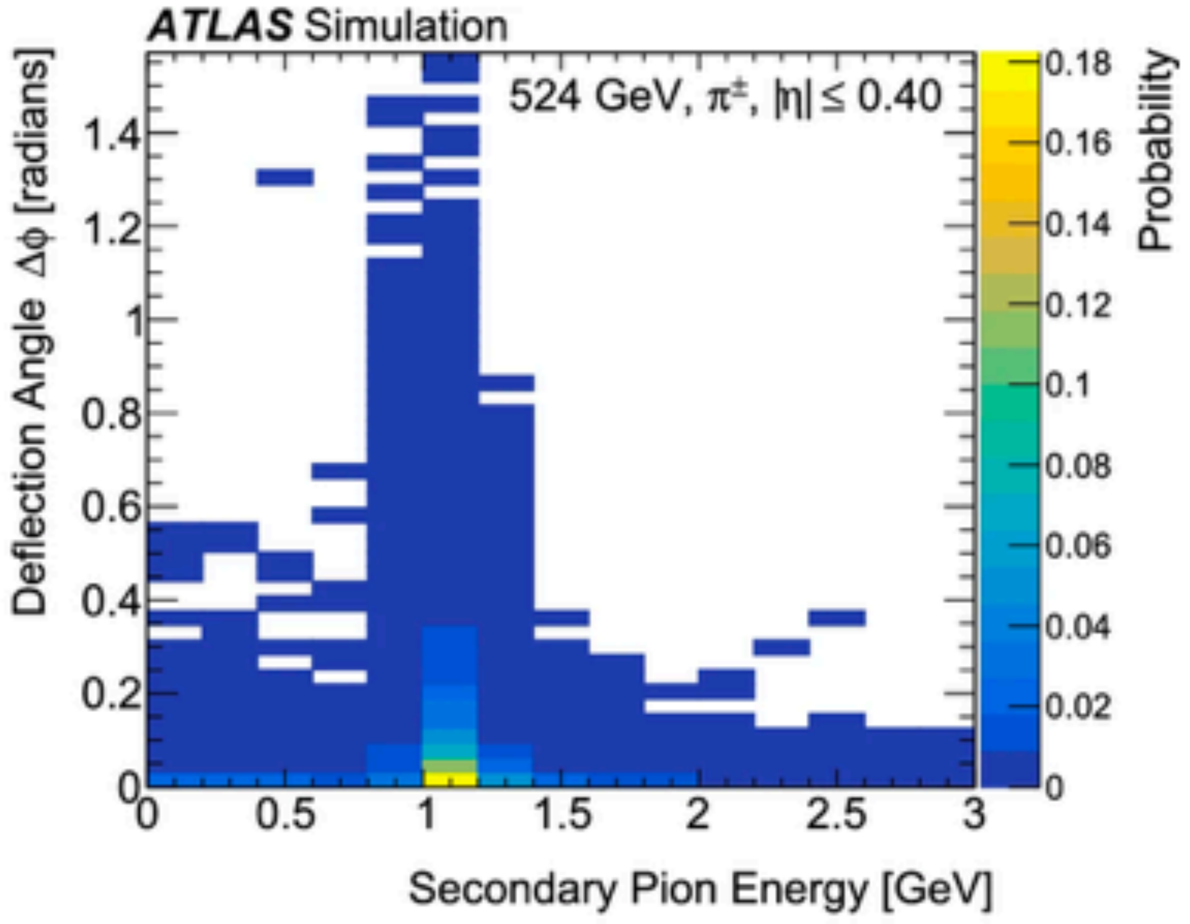




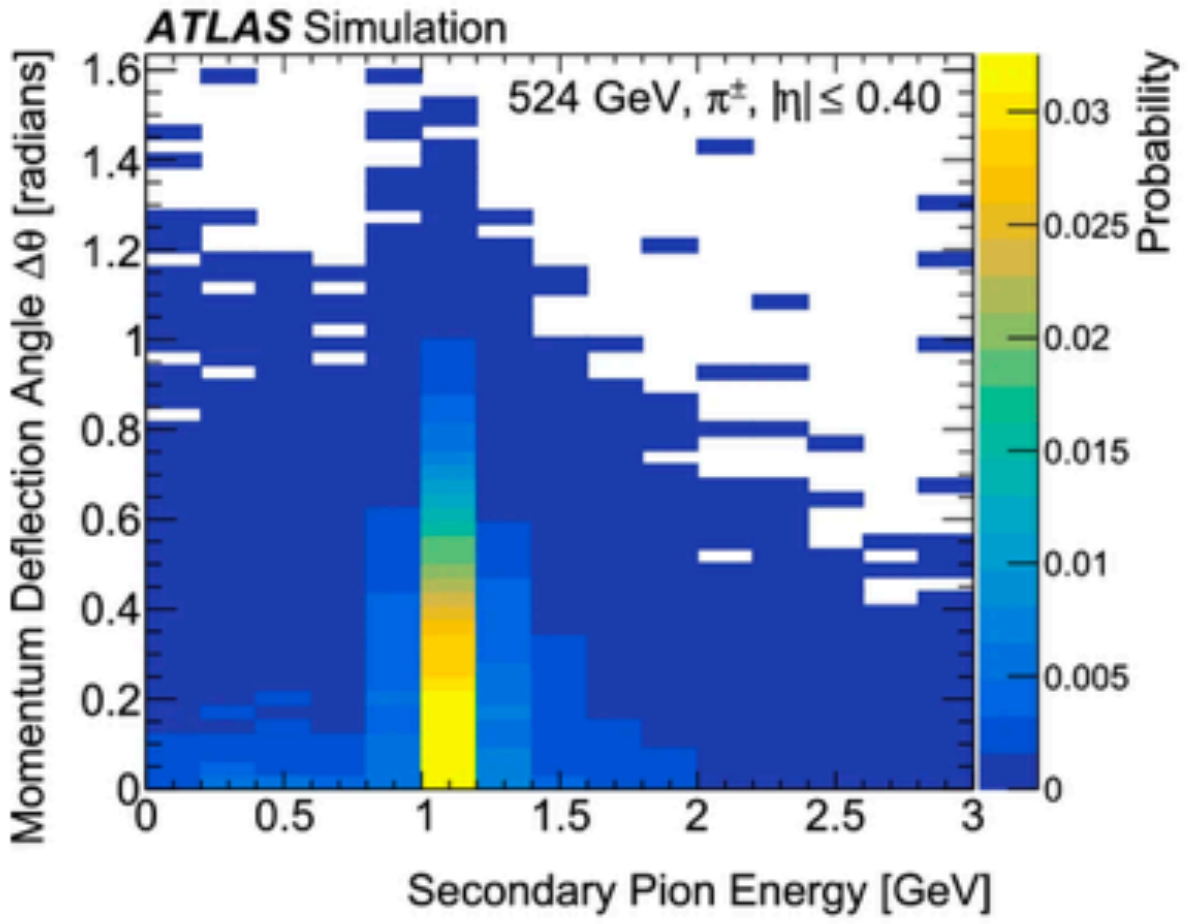




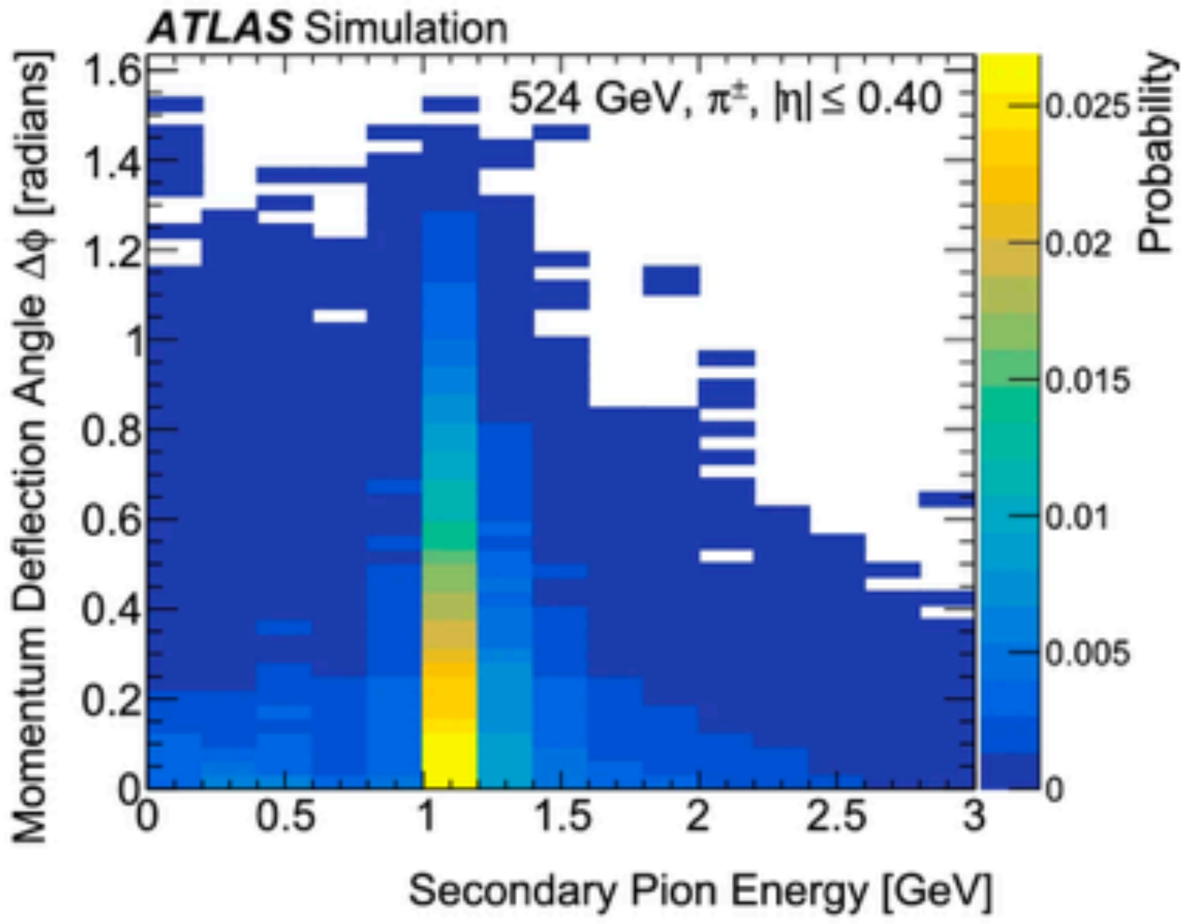
(a)



(b)

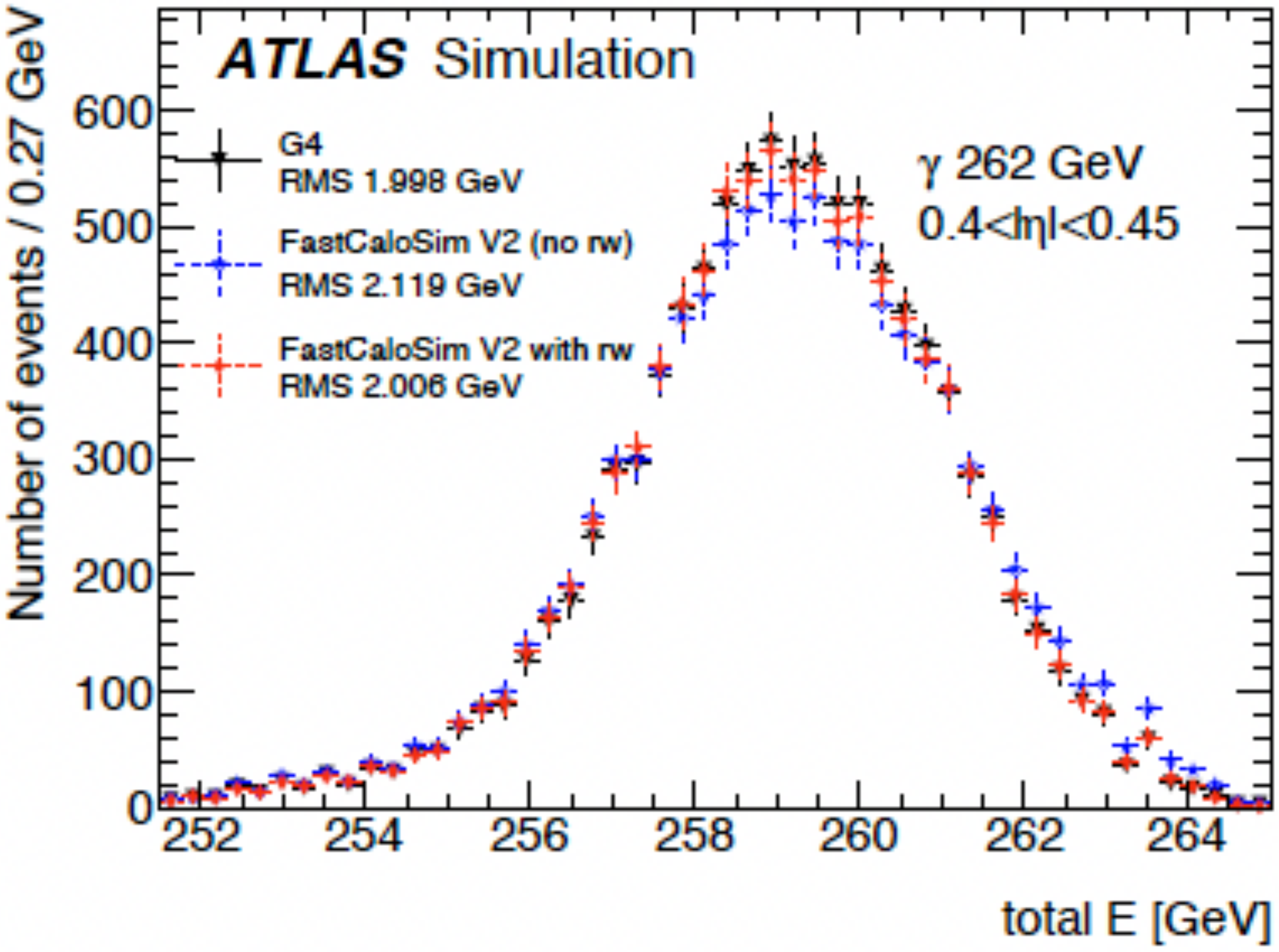


(c)

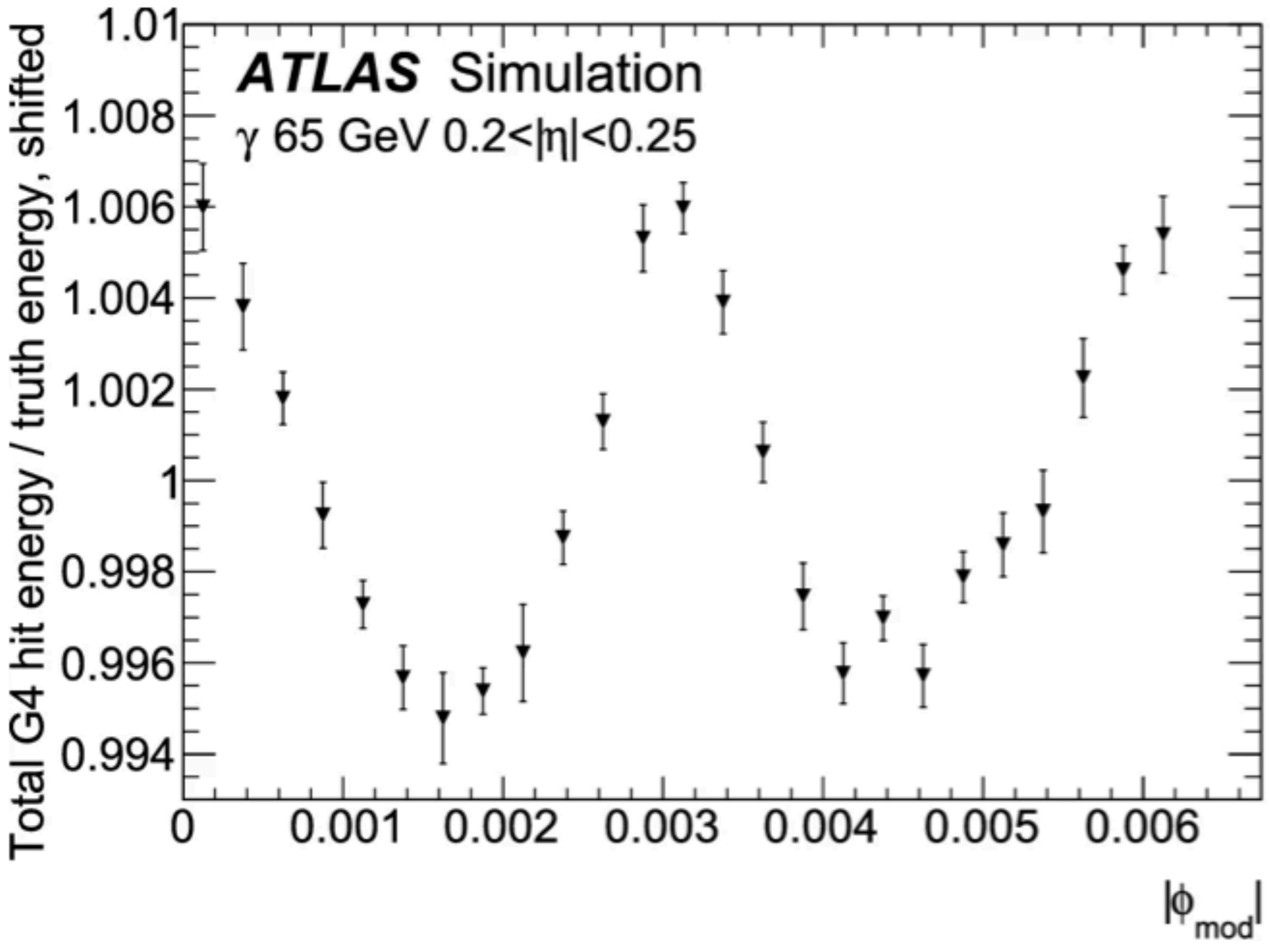


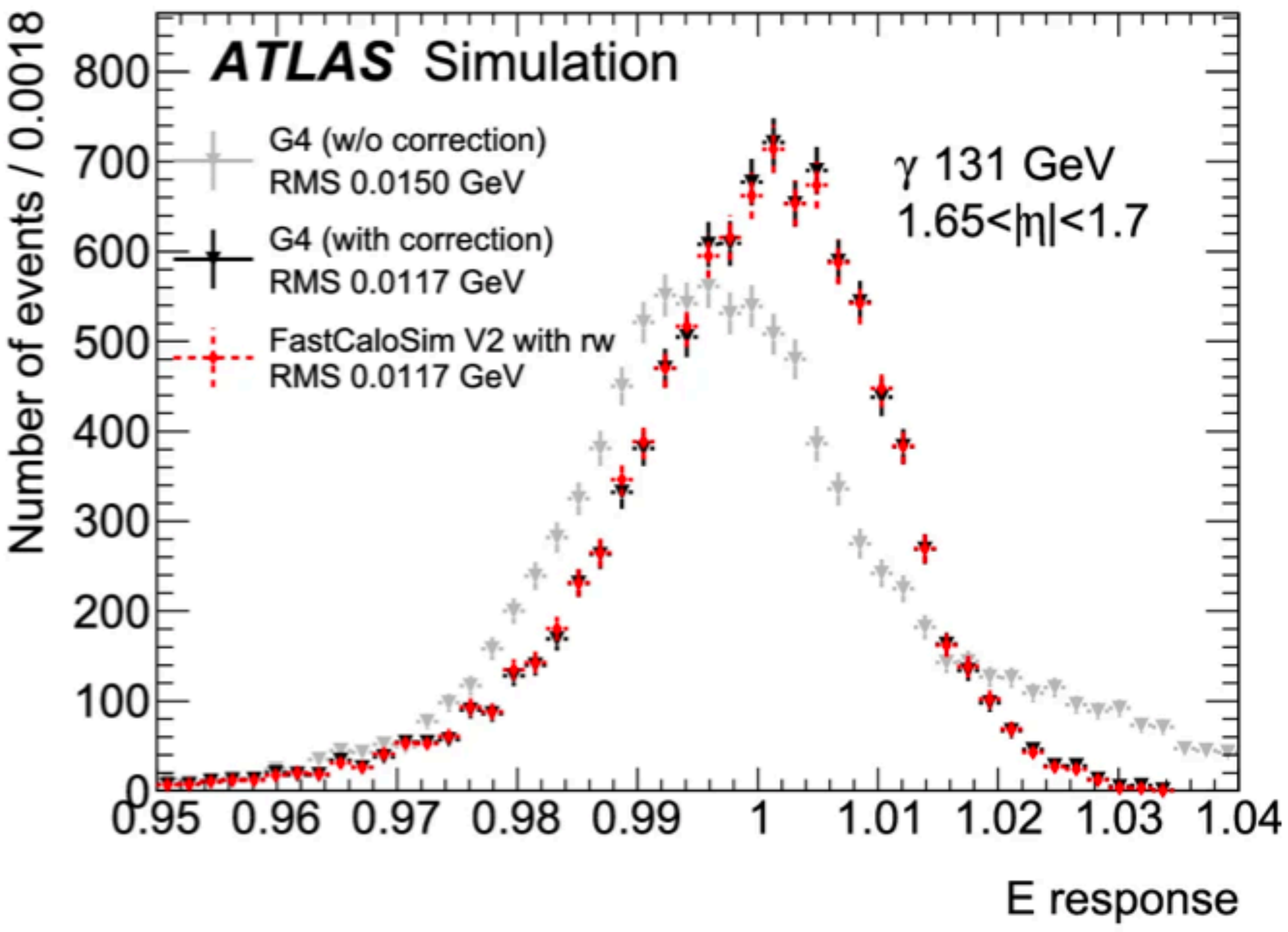
(d)

Energy Resolution Correction

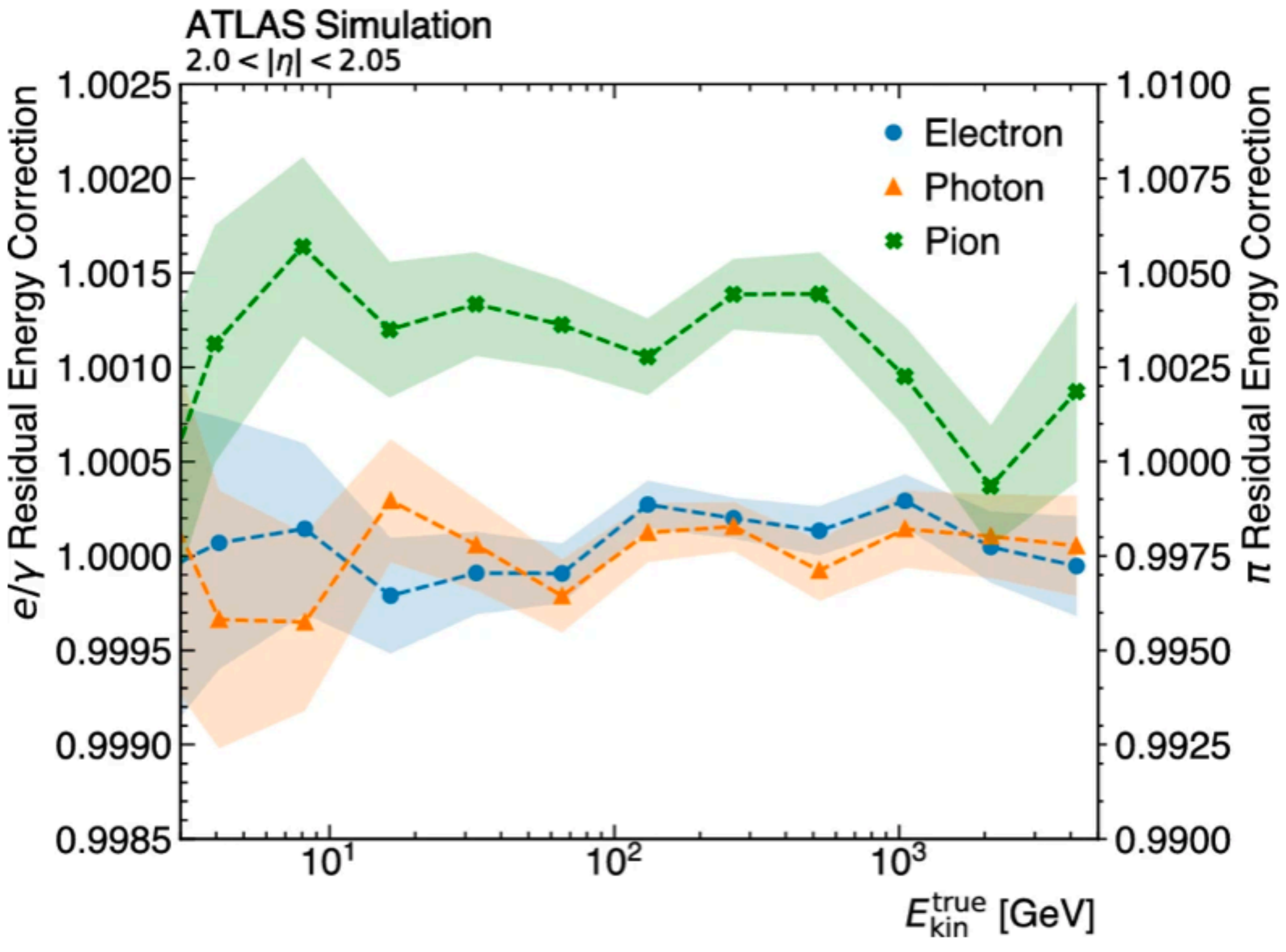


Phi Modulation

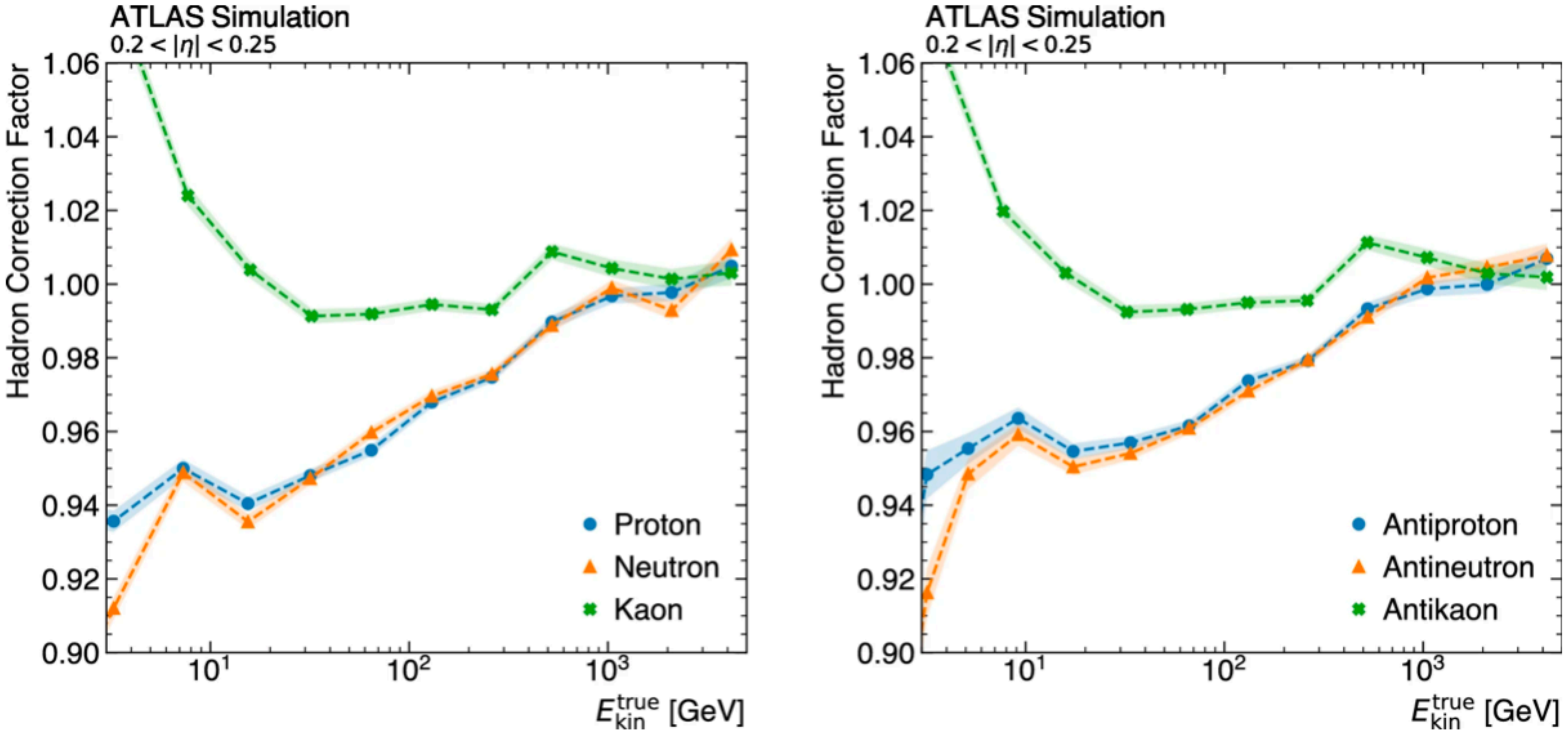




Energy Correction

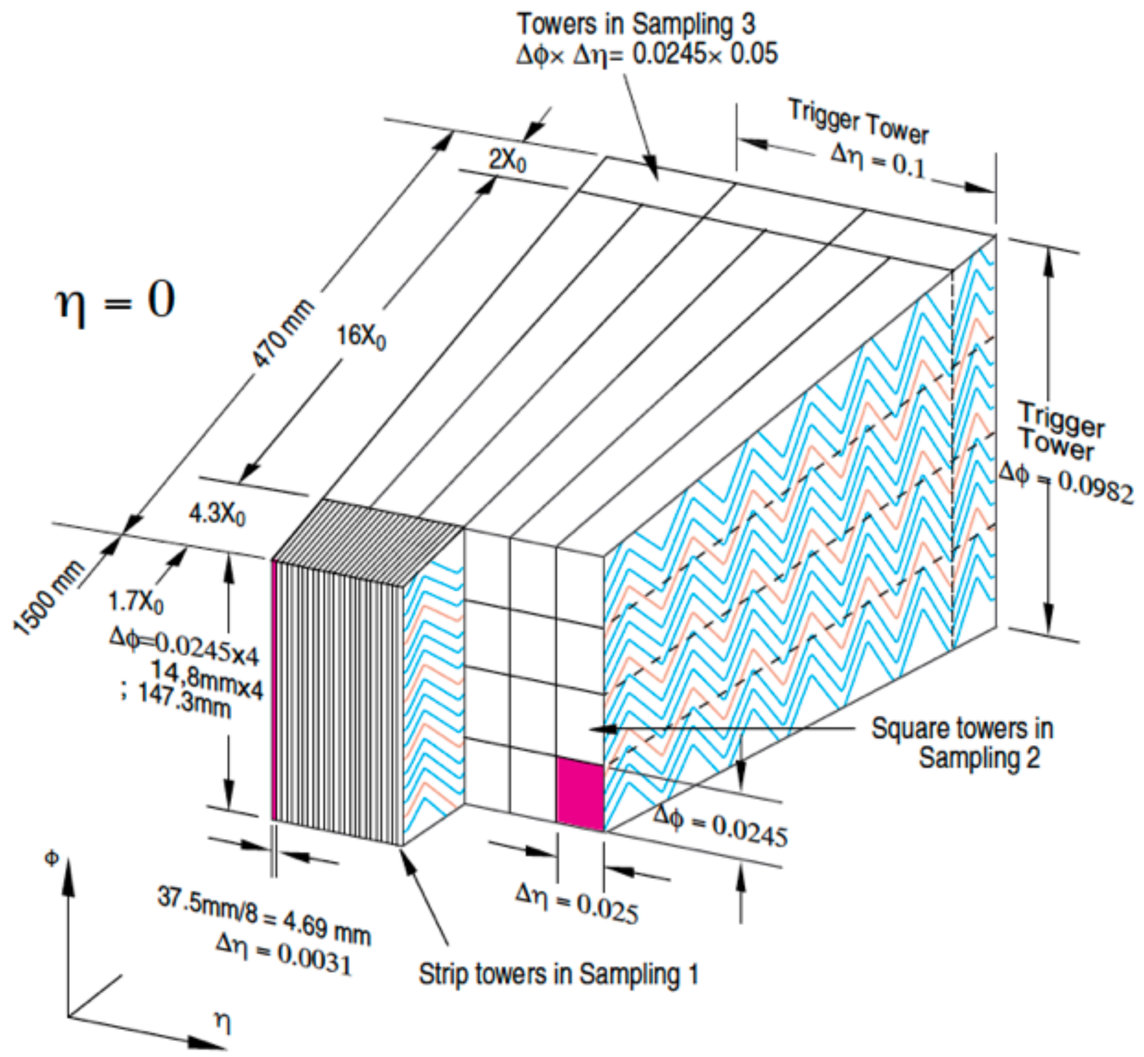


$$\frac{E_{\mathrm{G4}}}{E_{\mathrm{AF3}}}$$

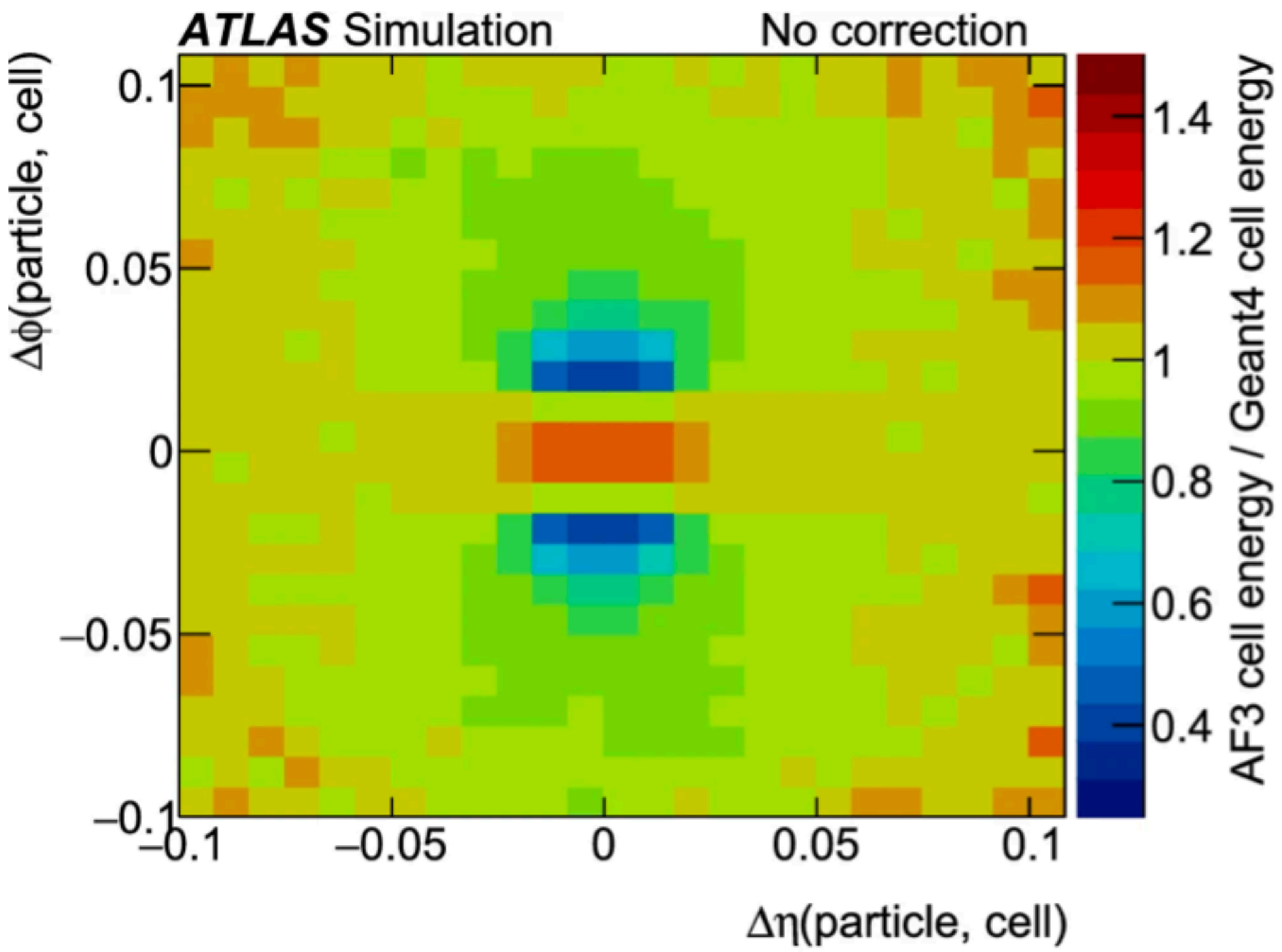


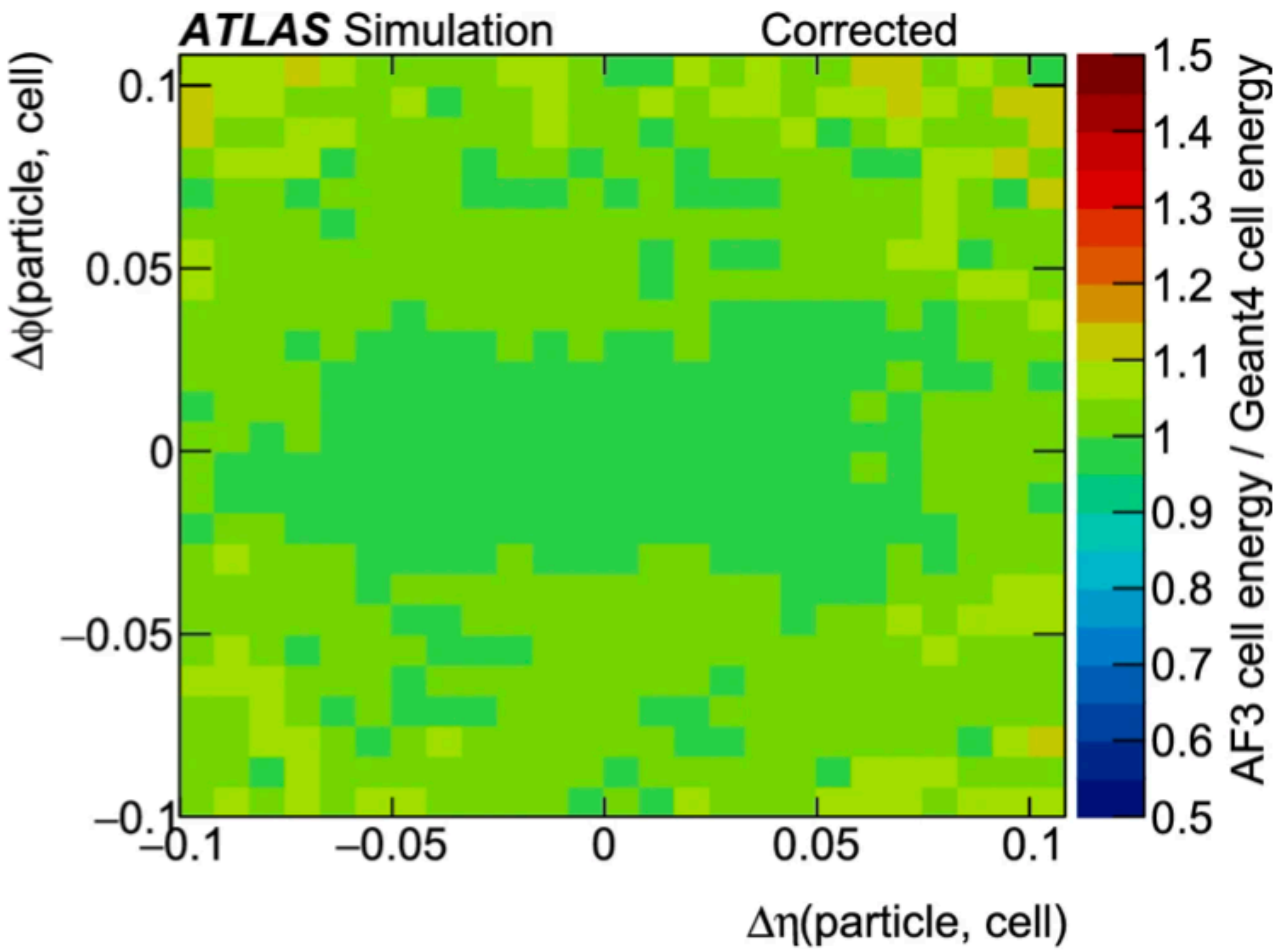
$$\frac{E^{\mathrm{h}}_{\mathrm{G4}}}{E^{\pi}_{\mathrm{G4}}} \times \frac{E^{\pi,\mathrm{true}}_{\mathrm{kin}}}{E^{\mathrm{h,true}}_{\mathrm{G4}}}$$

Simplified Geometry Correction

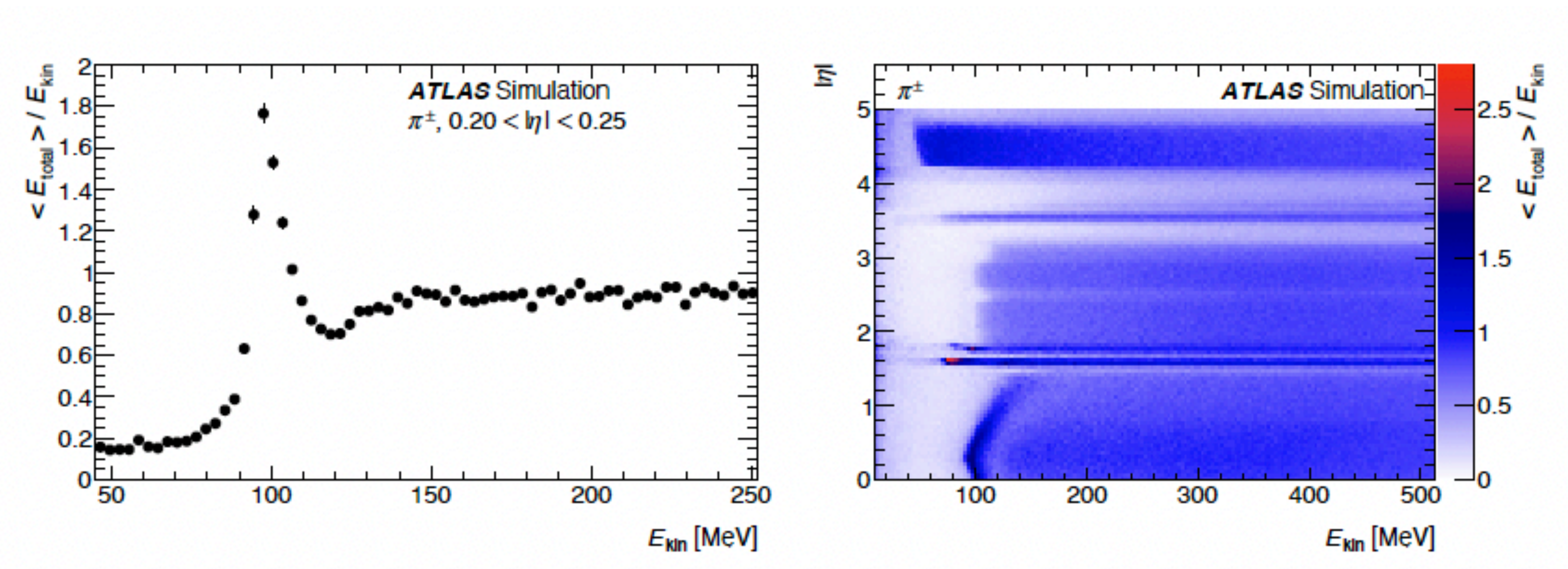


1. Change the geometry: use the accordion geometry
2. Shift the hit in the phi direction



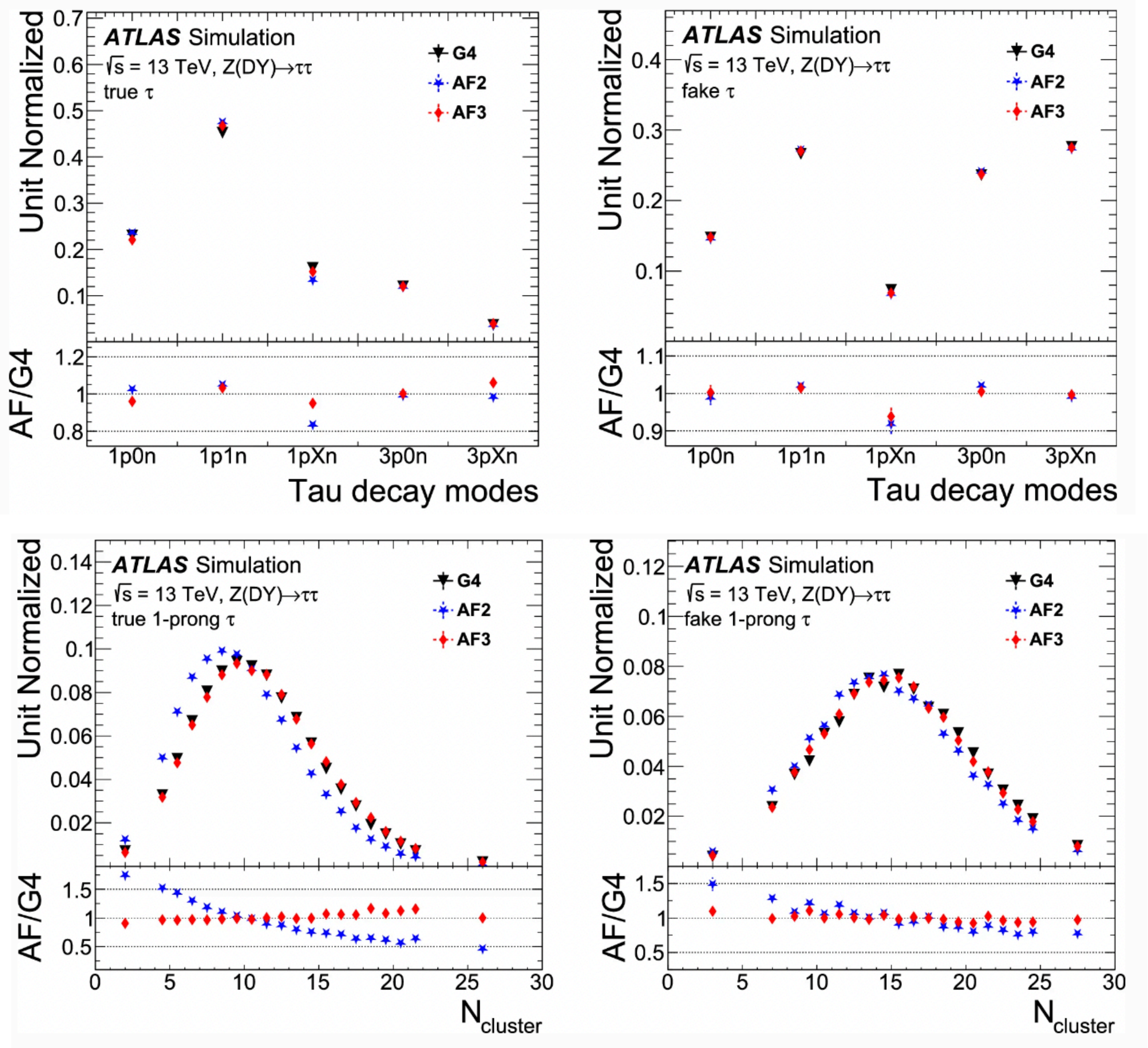


Low Energy Hadron



Presampler, calibrated using high energy particles

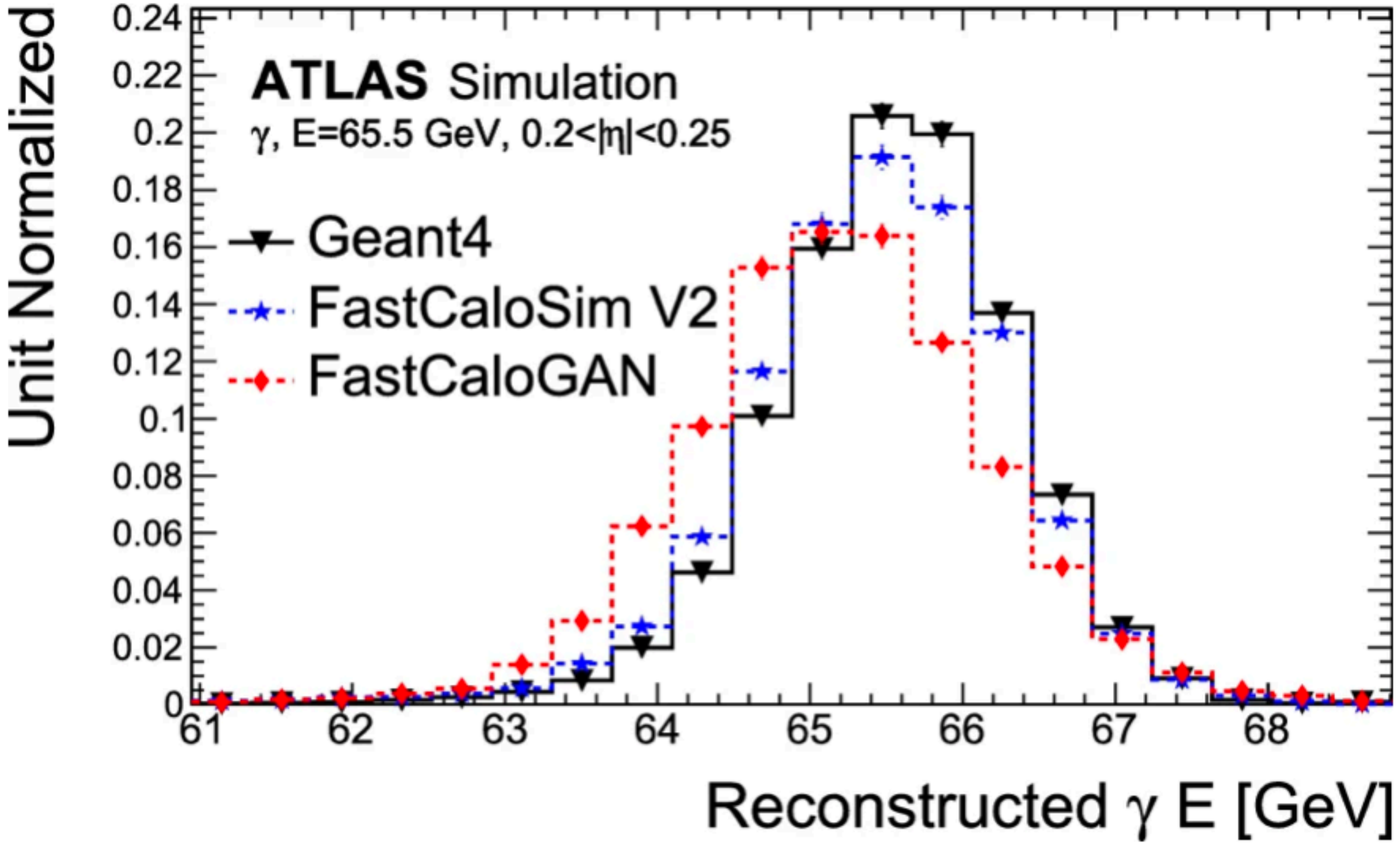
Performance: Taus



- $Z^\star/\gamma^\star \rightarrow \tau\tau$ sample (2.0 - 2.25 TeV)
- Look at hadronically decaying taus
- Tau decay modes
  - number of charged tracks: 1p/3p
  - number of neutral particles: 0n/1n/Xn
- Number of clusters, similar as number of constituents in jets

Improved modeling for taus

G4 vs FastCaloSimV2 vs FastCaloGAN



G4 vs FastCaloSimV2 vs FastCaloGAN