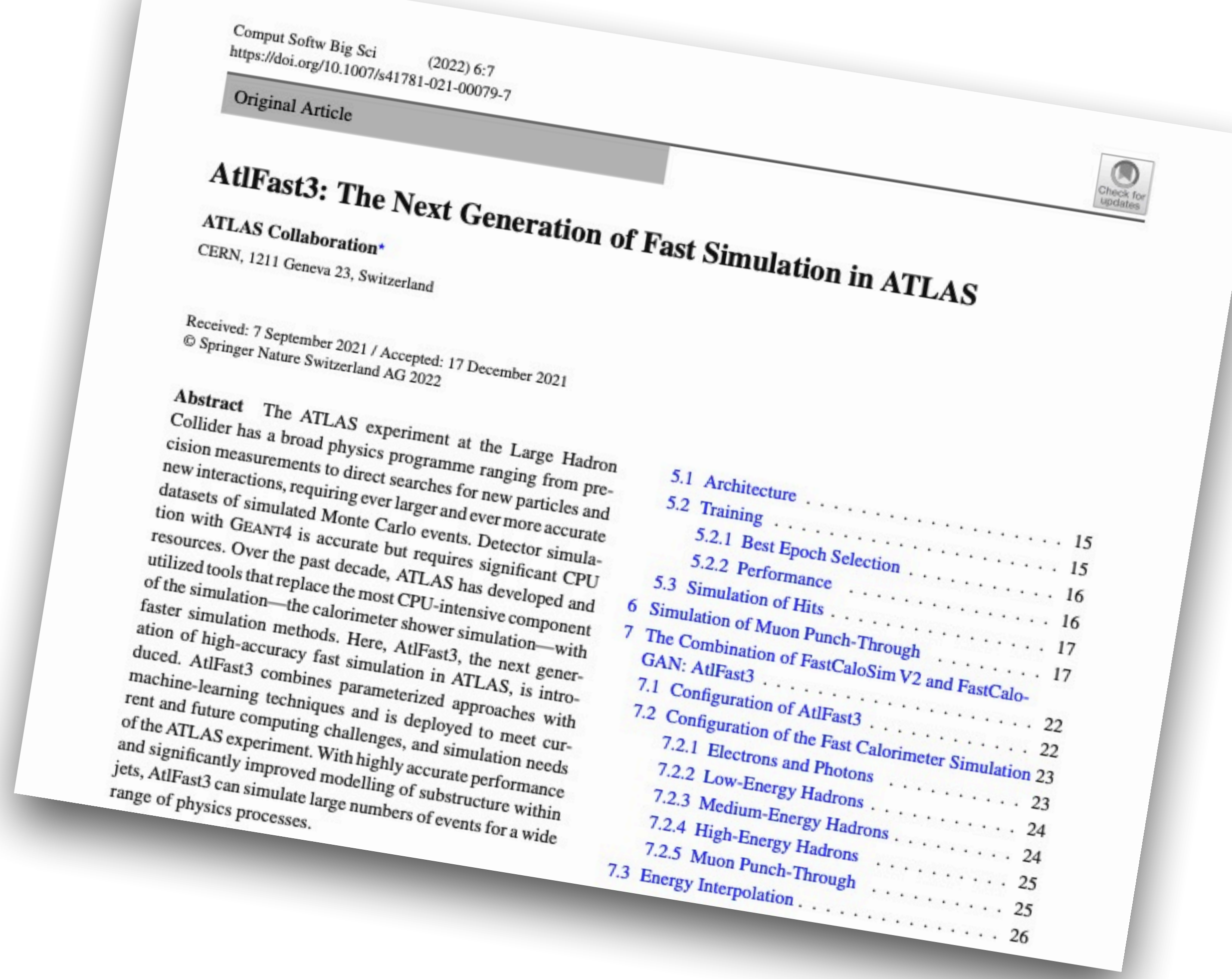

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Original Article

AtlFast3: The Next Generation of Fast Simulation in ATLAS

ATLAS Collaboration*
CERN, 1211 Geneva 23, Switzerland

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Abstract The ATLAS experiment at the Large Hadron Collider has a broad physics programme ranging from precision measurements to direct searches for new particles and new interactions, requiring ever larger and ever more accurate datasets of simulated Monte Carlo events. Detector simulation with GEANT4 is accurate but requires significant CPU resources. Over the past decade, ATLAS has developed and utilized tools that replace the most CPU-intensive component of the simulation—the calorimeter shower simulation—with faster simulation methods. Here, AtlFast3, the next generation of high-accuracy fast simulation in ATLAS, is introduced. AtlFast3 combines parameterized approaches with machine-learning techniques and is deployed to meet current and future computing challenges, and simulation needs of the ATLAS experiment. With highly accurate performance and significantly improved modelling of substructure within jets, AtlFast3 can simulate large numbers of events for a wide range of physics processes.

AtlFast3:

The Next Generation of Fast Simulation in ATLAS

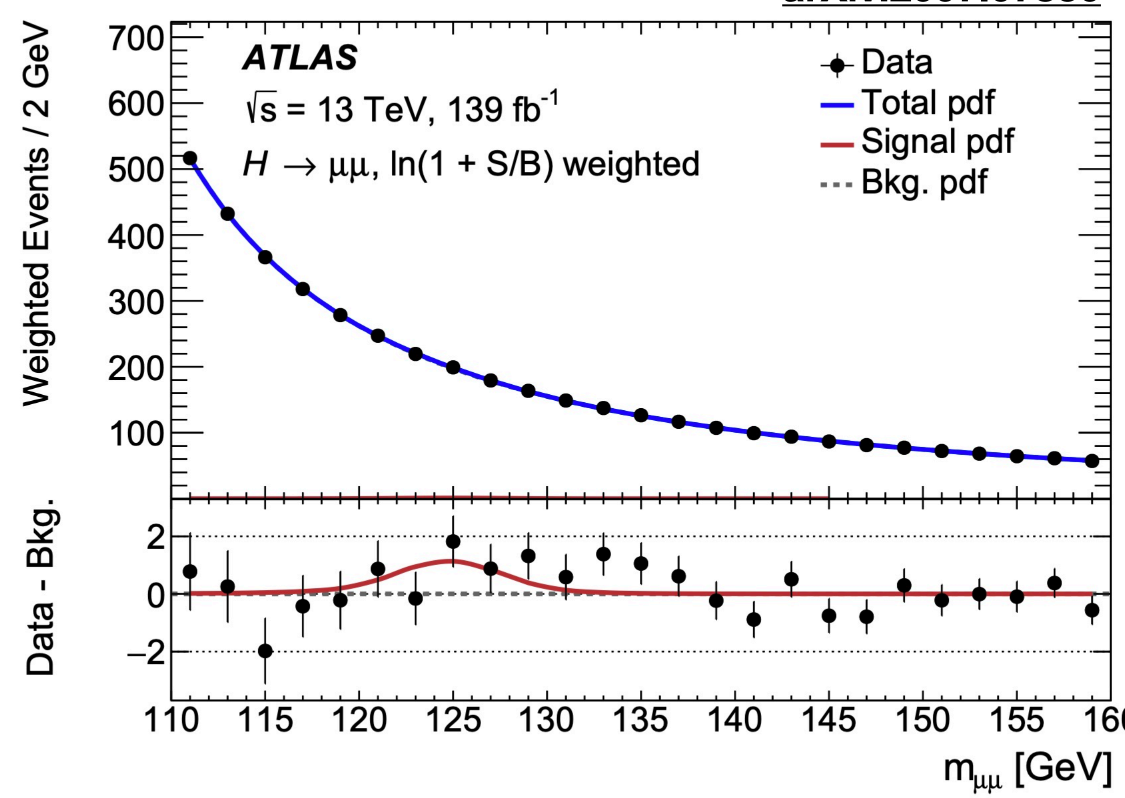
ICHEP 2022

Tom Carter : thomas.michael.carter@cern.ch

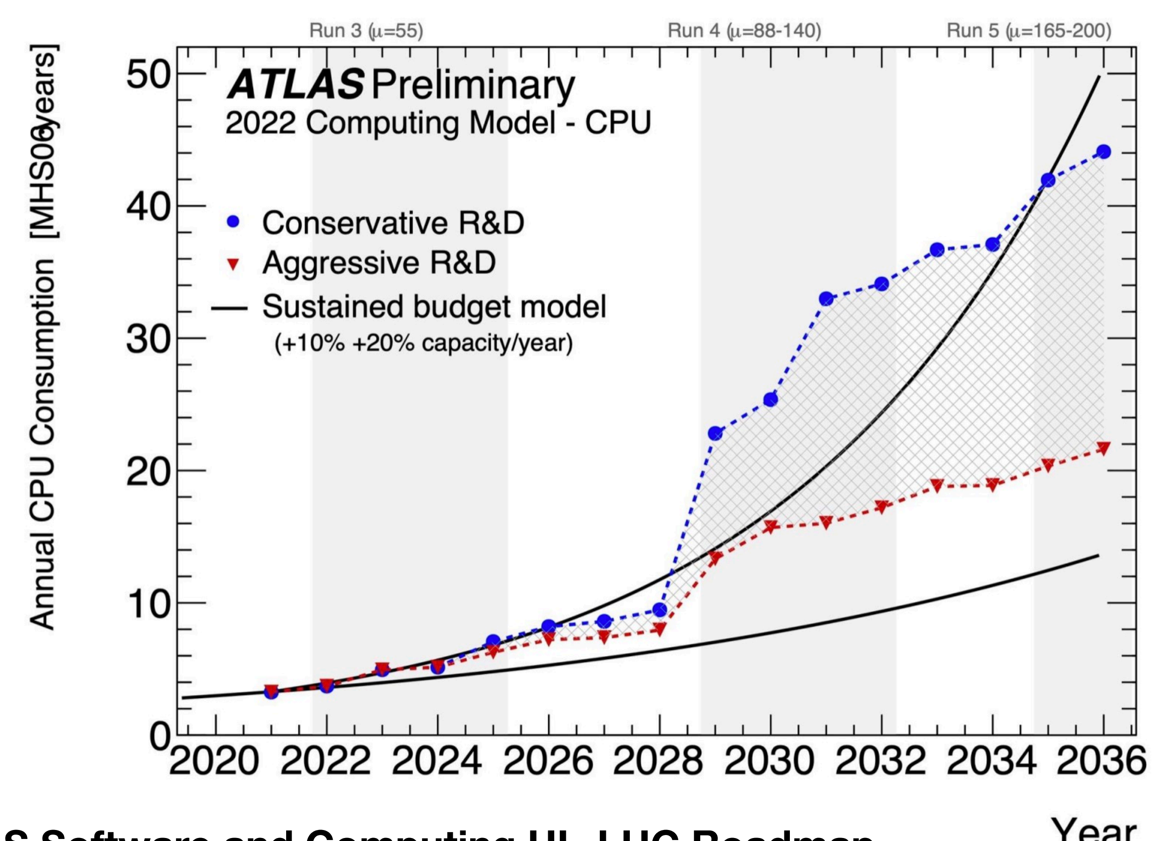
ATLAS Future Program

- Wide ranging physics program - precision measurements to BSM searches.
- **Run3** - Increased $\sqrt{s}$ and pileup
- **HL-LHC** - Increased pileup

arXiv:2007.07830



- CPU requirements will increase due to luminosity
- Rely on MC events - stats several times data luminosity.
- **Fast Simulation** for majority of events in **Run3** and **HL-LHC**



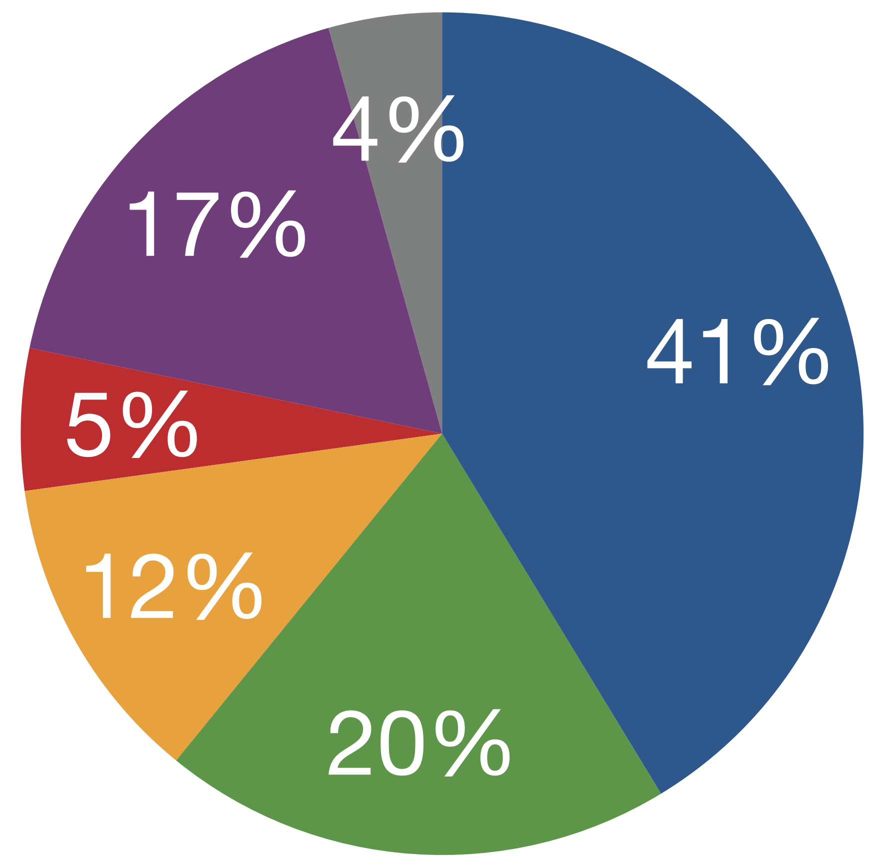
ATLAS Software and Computing HL-LHC Roadmap

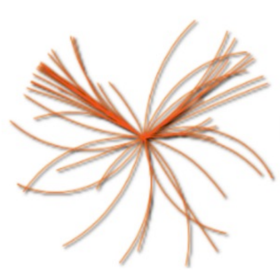
Simulation in ATLAS

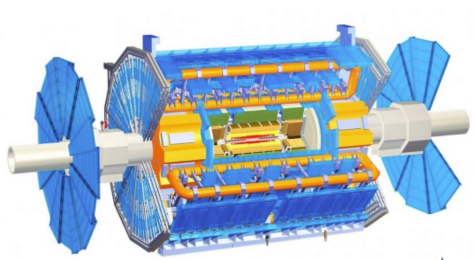
- Largest proportion of CPU time spent on **Detector Simulation**

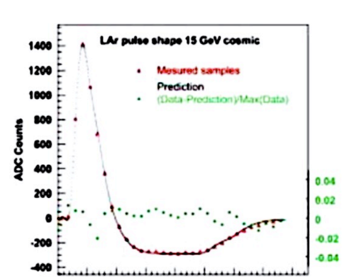
- **80%** of Geant4 simulation time is spent in calorimeters [1]

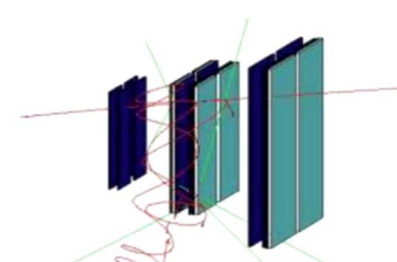
CPU Wall Time 2018 [1]











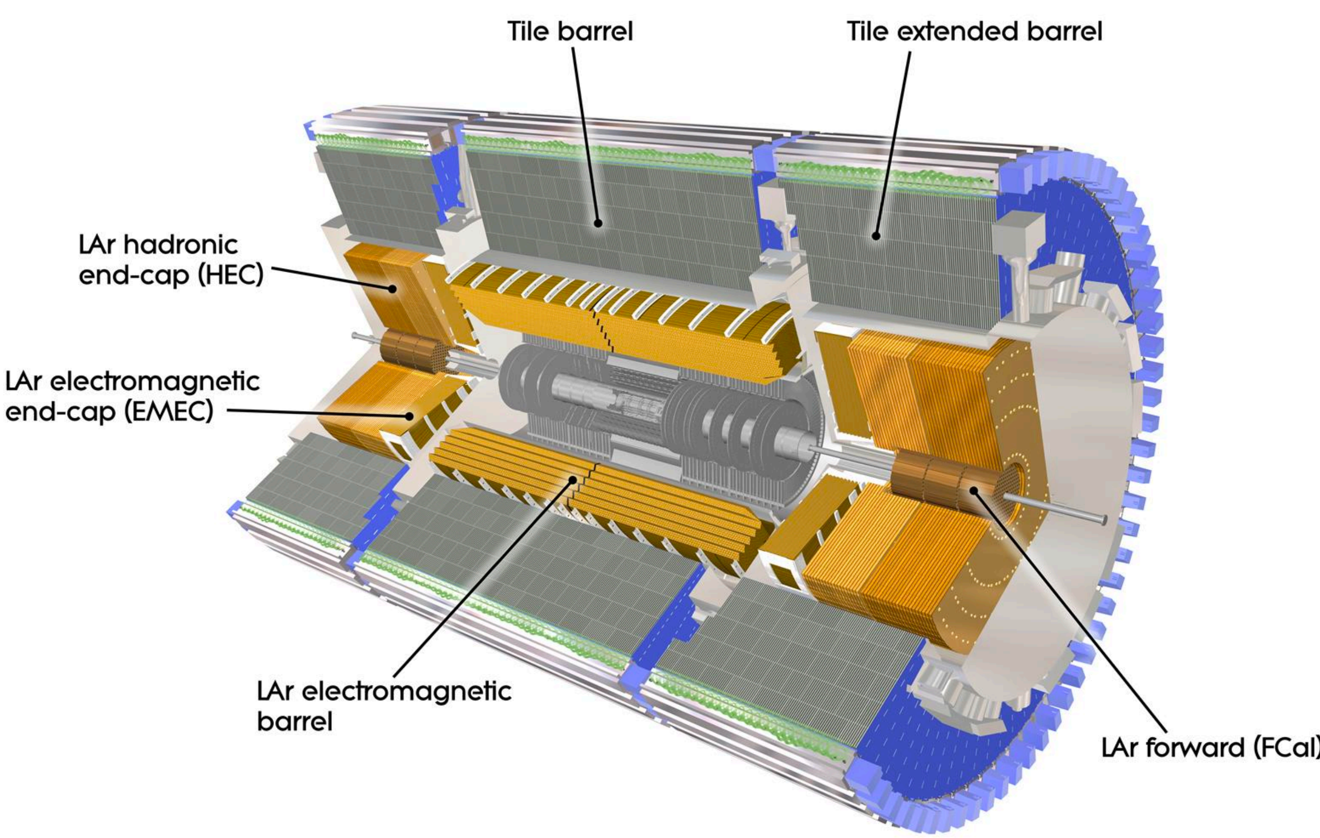
ROOT Data Analysis Framework

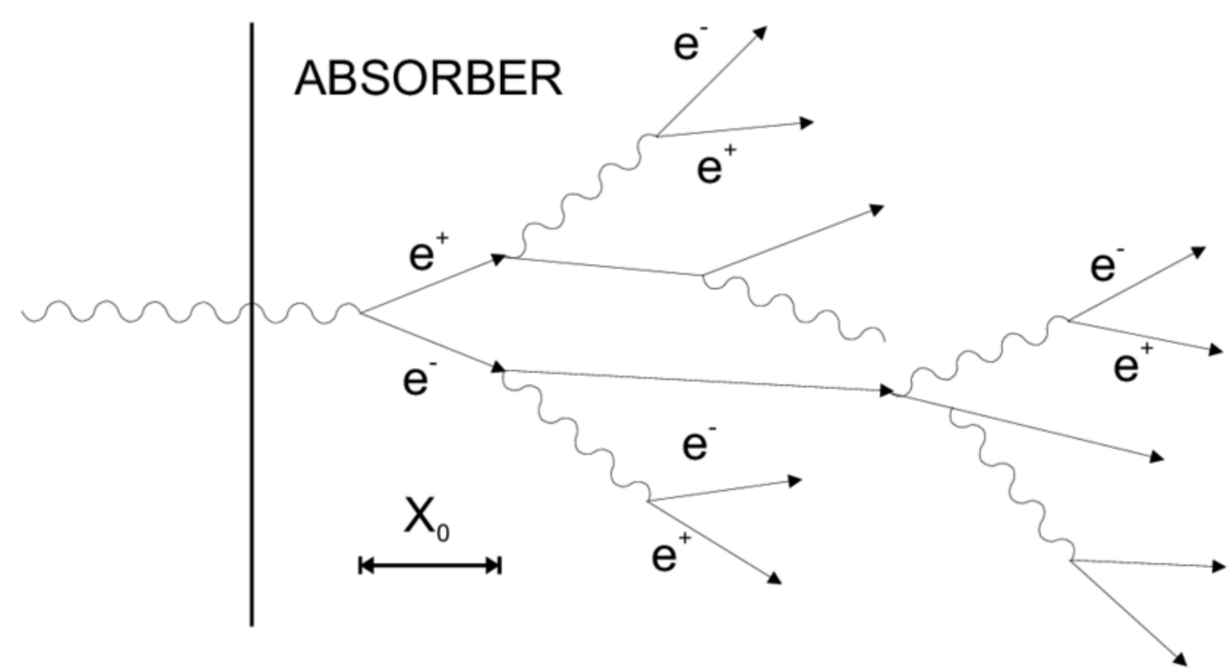
Event Gen → Detector Simulation → Digitization → Reconstruction → Group Prod → Analysis

[1] arXiv:2109.02551

Calorimeter Simulation

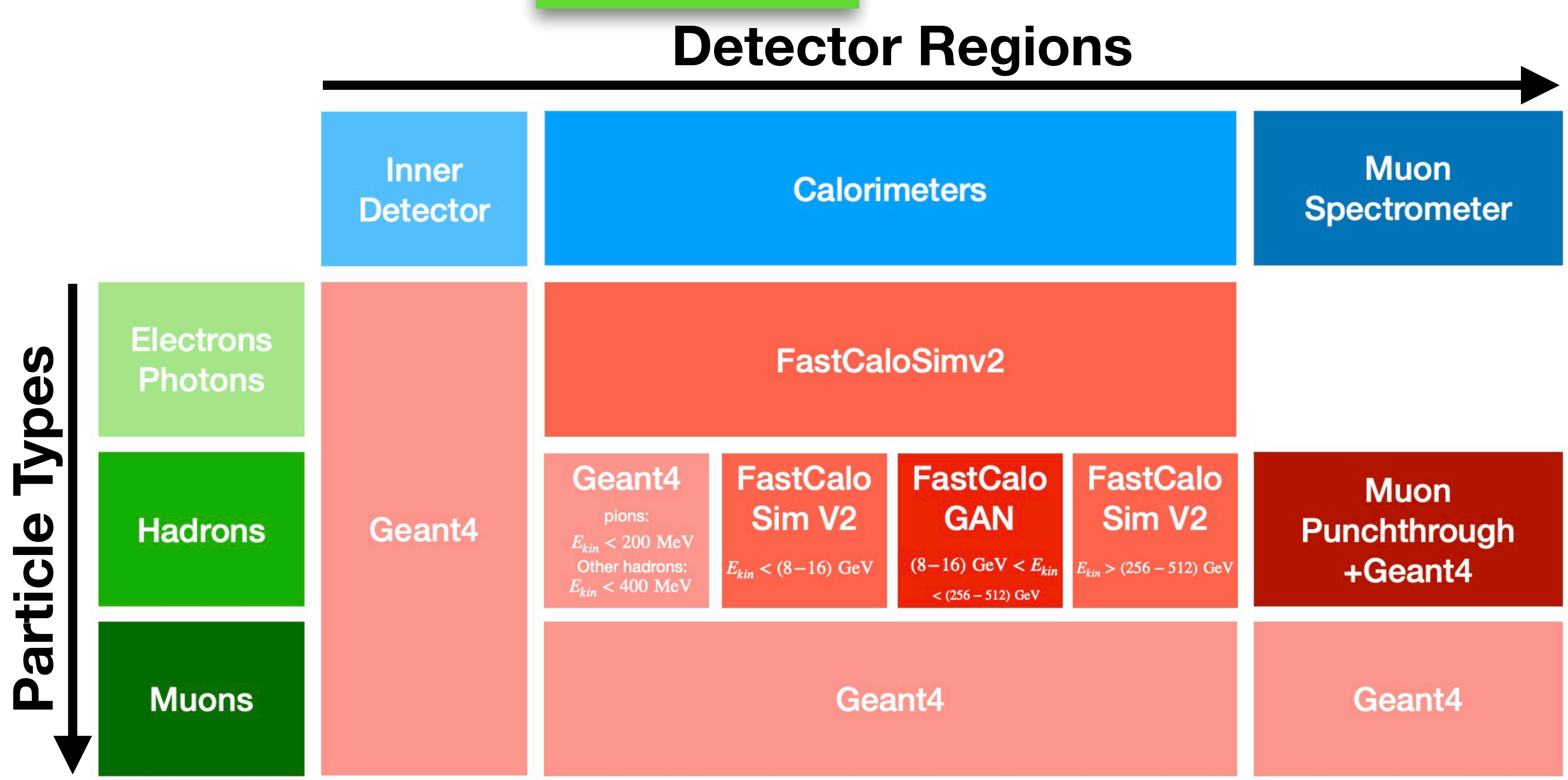
- **Electromagnetic Calo** - Electron and Photon ID
- **Hadronic Calo** - Jets and E^{T}_{miss}
- Complex geometries and boundaries - large simulation time
- Geant4 simulates particle "steps" ∝ simulation time





AtlFast3 (AF3)

- Parameterised calorimeter simulation - **500x faster** than Geant4 in calorimeter
- Improves physics performance significantly over AtlFast2 (AF2) (Run1 & Run2)
- Three main components for calorimeter simulation:
    - **FastCaloSimV2** - Classical parameterisation Improved for AF3!
    - **FastCaloGAN** - Deep learning using GANs New for AF3!
    - **MuonPunchThrough** New for AF3!

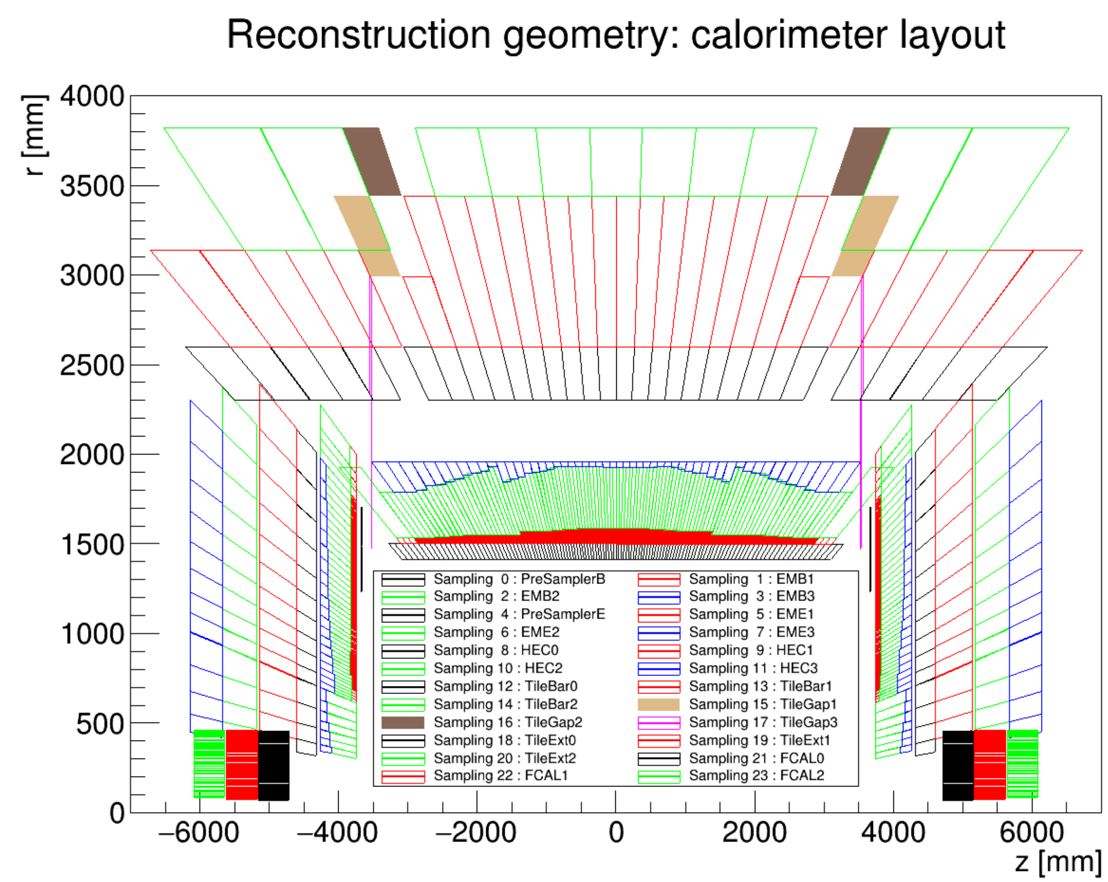


[1] arXiv:2109.02551

Input Datasets for AF3 modelling

- Geant4 simulated single particles generated at the calorimeter surface
  - **Single Photons** - for photon shower
  - **Single Electrons** ($e^{\pm}$) - for electron shower
  - **Single Pions** ($\pi^{\pm}$) - for hadronic shower
- Record energy deposit in calo **layers** and **cells**
- Simulated in grid of η and **incoming momentum**

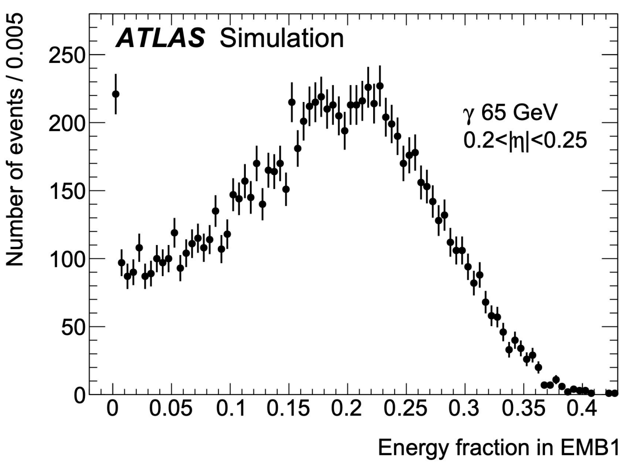
[1] arXiv:2109.02551



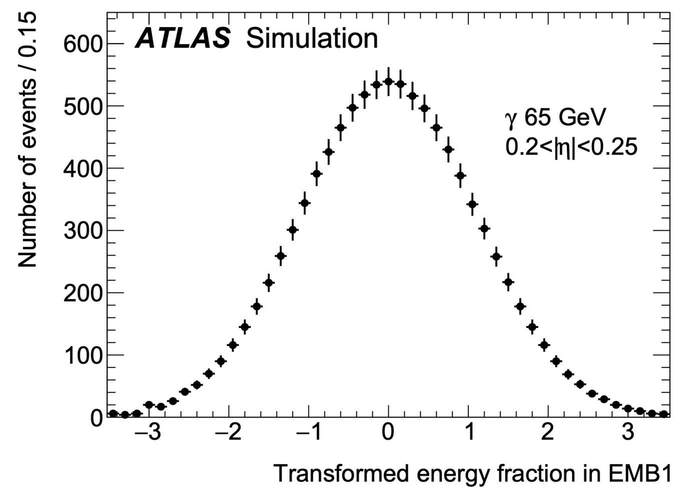
FastCaloSimV2: Longitudinal Shower

New for FCSv2!

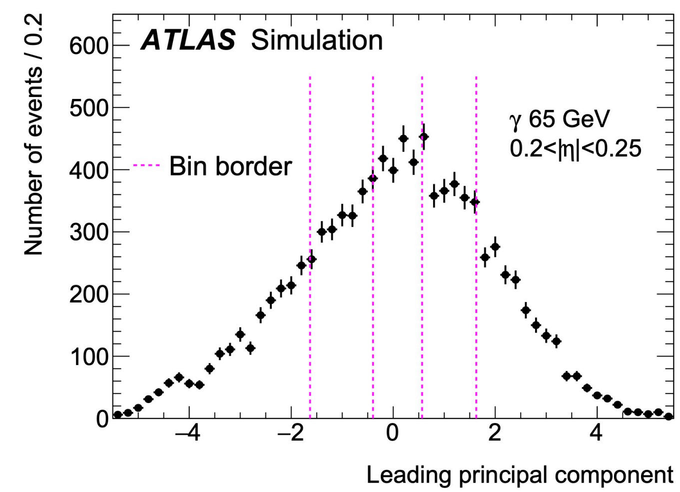
Energy in Each Layer



Transform to Gauss



Apply PCA1

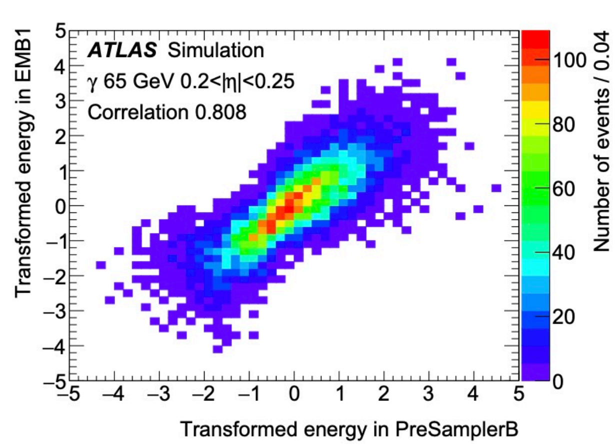


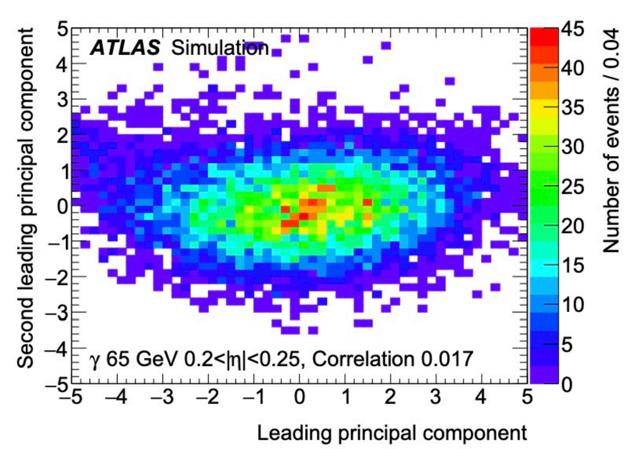
Categorize

Apply PCA2

Set of Gaussian distributions

PCA1 Effectiveness





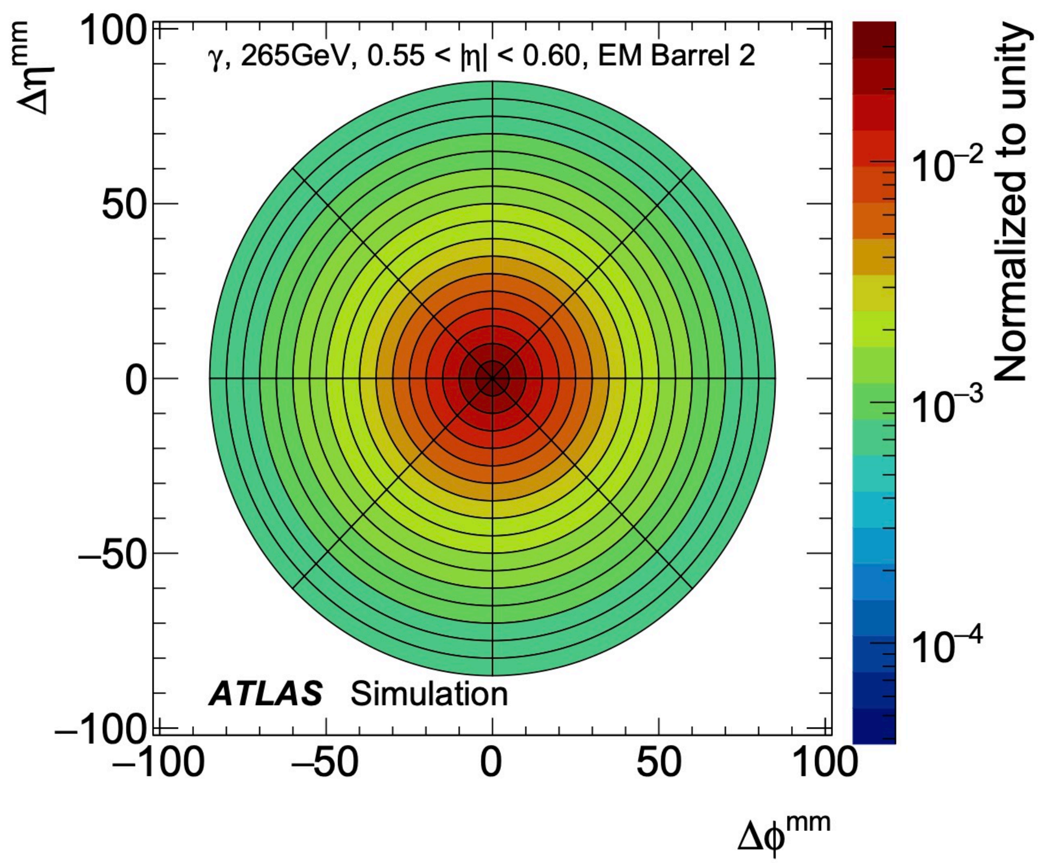
[1] arXiv:2109.02551

PCA = Principal Component Analysis

FastCaloSimV2: Lateral Shower

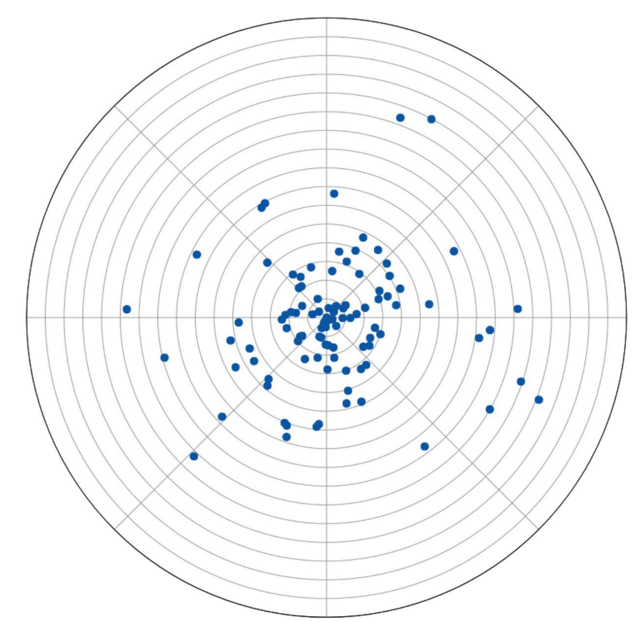
Improved for FCSv2!

- Average radial energy distribution in each calo layer is used as a **PDF**
- N_{hits} is calculated to give the same **Poisson RMS** as the resolution of the calorimeter layer.
- Hadronic energy deposits are **weighted** to account for fluctuations.



$$\sigma_E/E = a/\sqrt{E/\mathrm{GeV}} \oplus c$$

$$N_{hits}^{layer} \sim Poisson\left(\frac{1}{\sigma_E^2}\right)$$



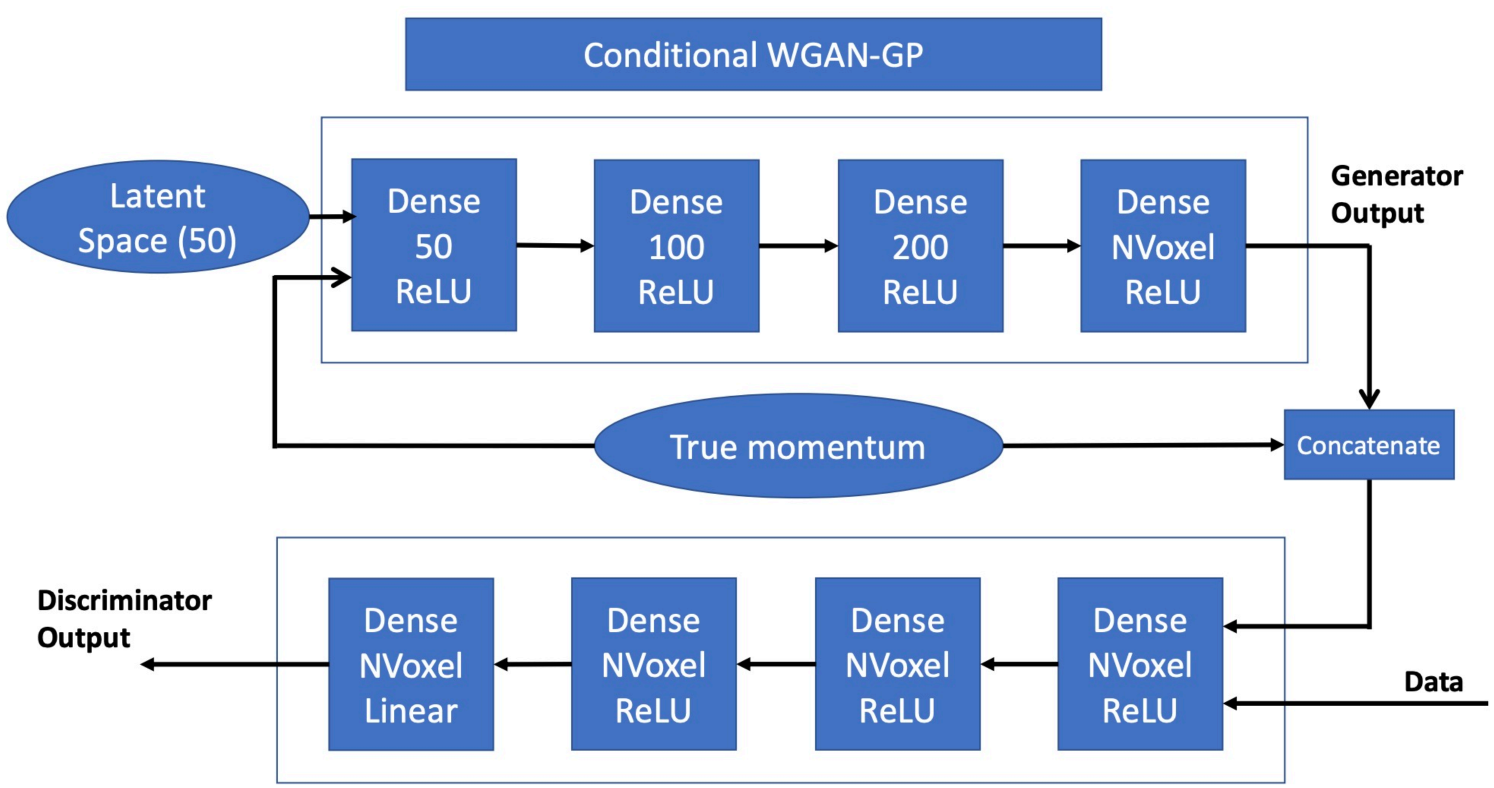
$$E_{hit} = E_{layer}/N_{hits}$$

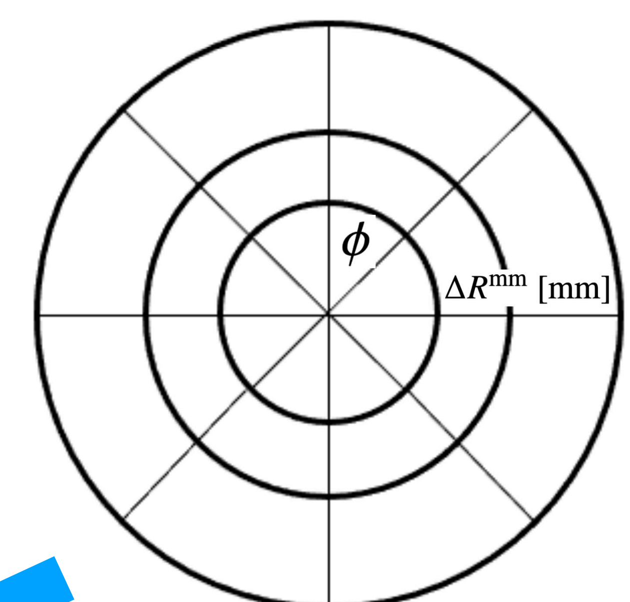
[1] arXiv:2109.02551

FastCaloGan: GAN Setup

New for AF3!

- **Generative Adversarial Network (GAN)** using **TensorFlow2** to generate showers
- Incorporates longitudinal and lateral modelling, and correlations
- Calorimeter deposits are **voxelized** in ΔR and ϕ
- One GAN is trained for each η region, inclusive in truth momentum
- Wasserstein GAN with gradient penalty (WGAN - GP) conditioned on truth momentum





[1] arXiv:2109.02551

FastCaloGan: GAN Training

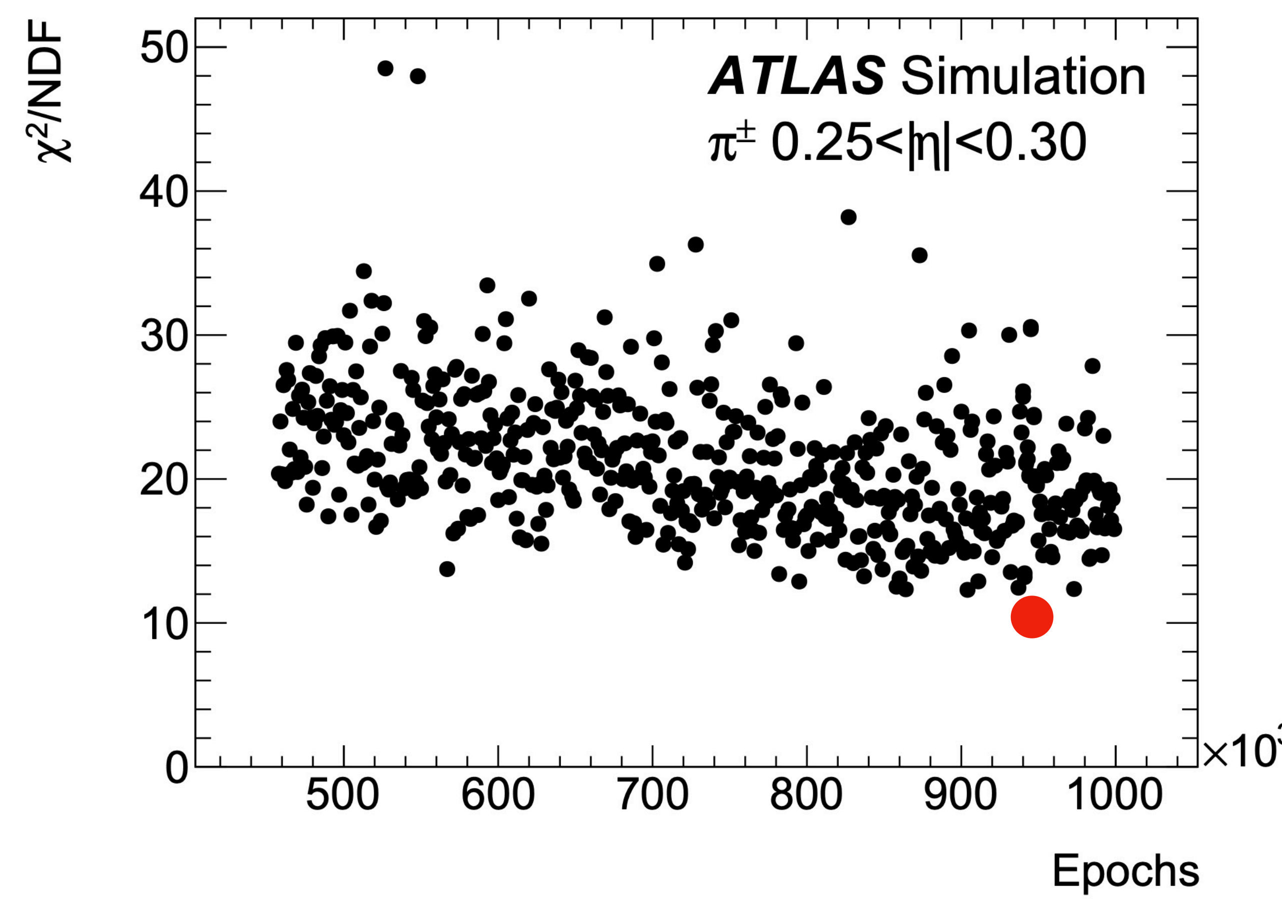
New for AF3!

Strategy

- An **incremented** training strategy is used:
  - start with 32 GeV and train for 50K epochs
  - add new incoming momentum points every 20K epochs
- In total each GAN is trained for 1M epochs, checkpoint saved every 1k

Checkpoint selection

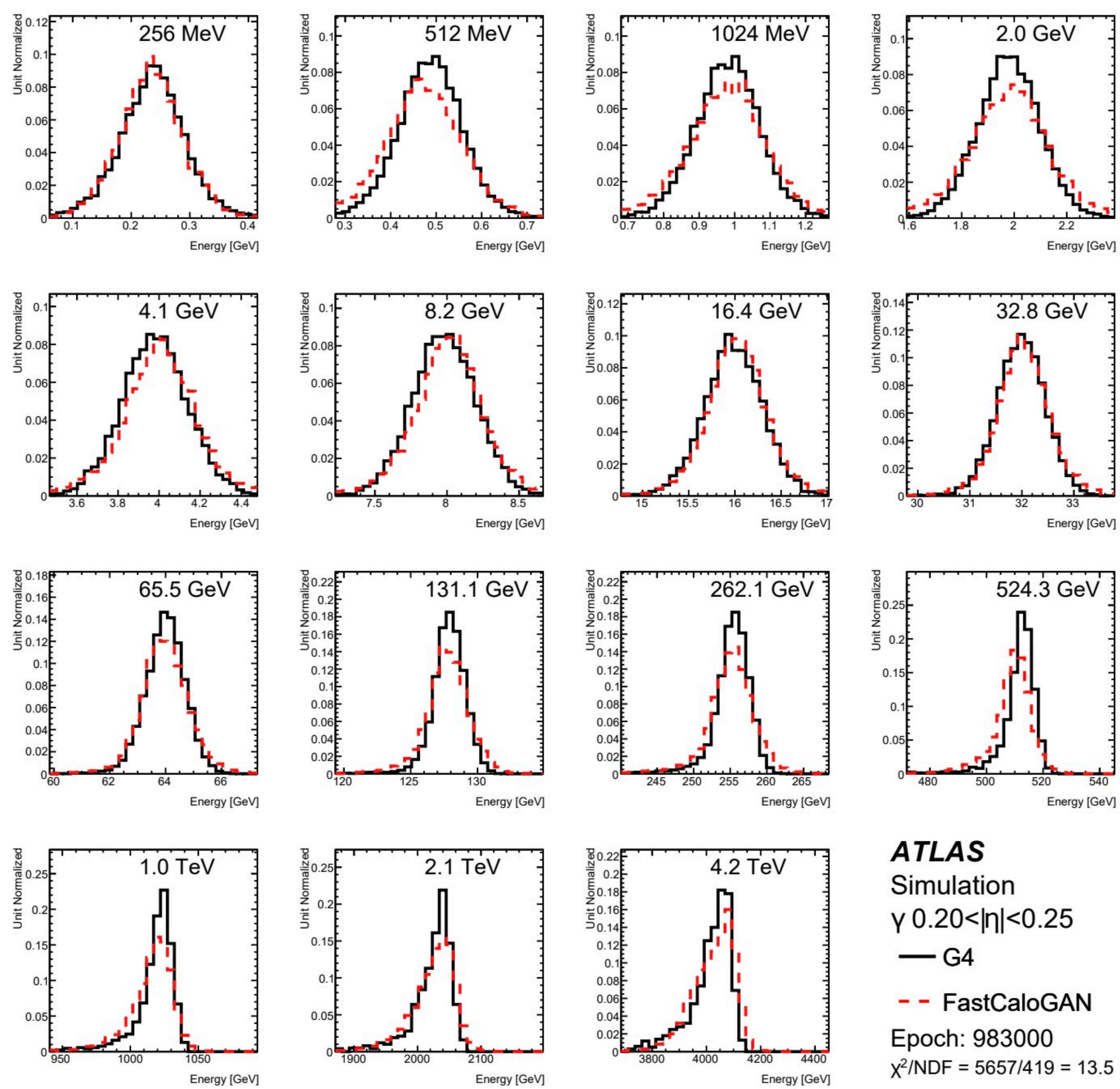
- **Best performing** epoch needs to be selected.
- χ^2 between total energy generated by GAN and Geant4 is used as metric
- Select epoch with lowest χ^2

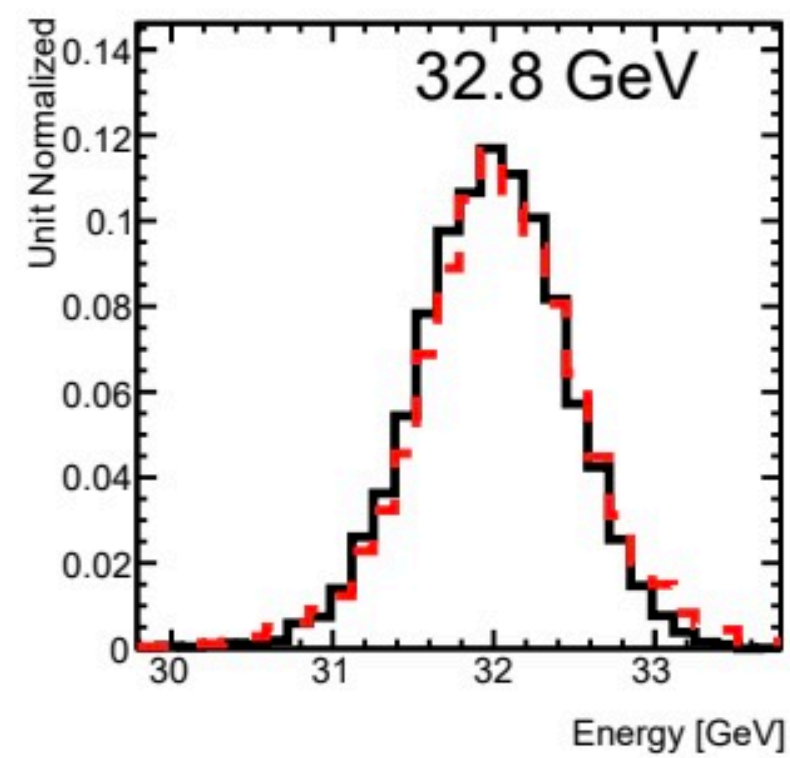


[1] arXiv:2109.02551

FastCaloGan: Best Epoch Performance

New for AF3!



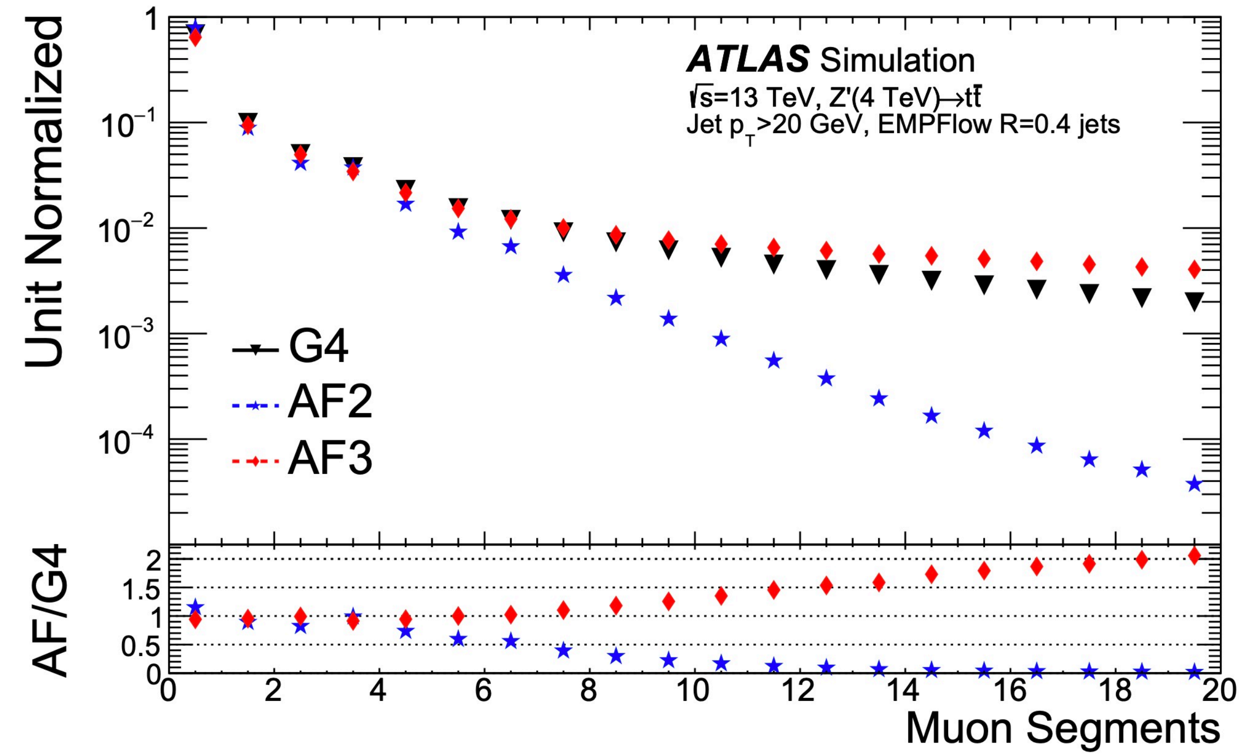


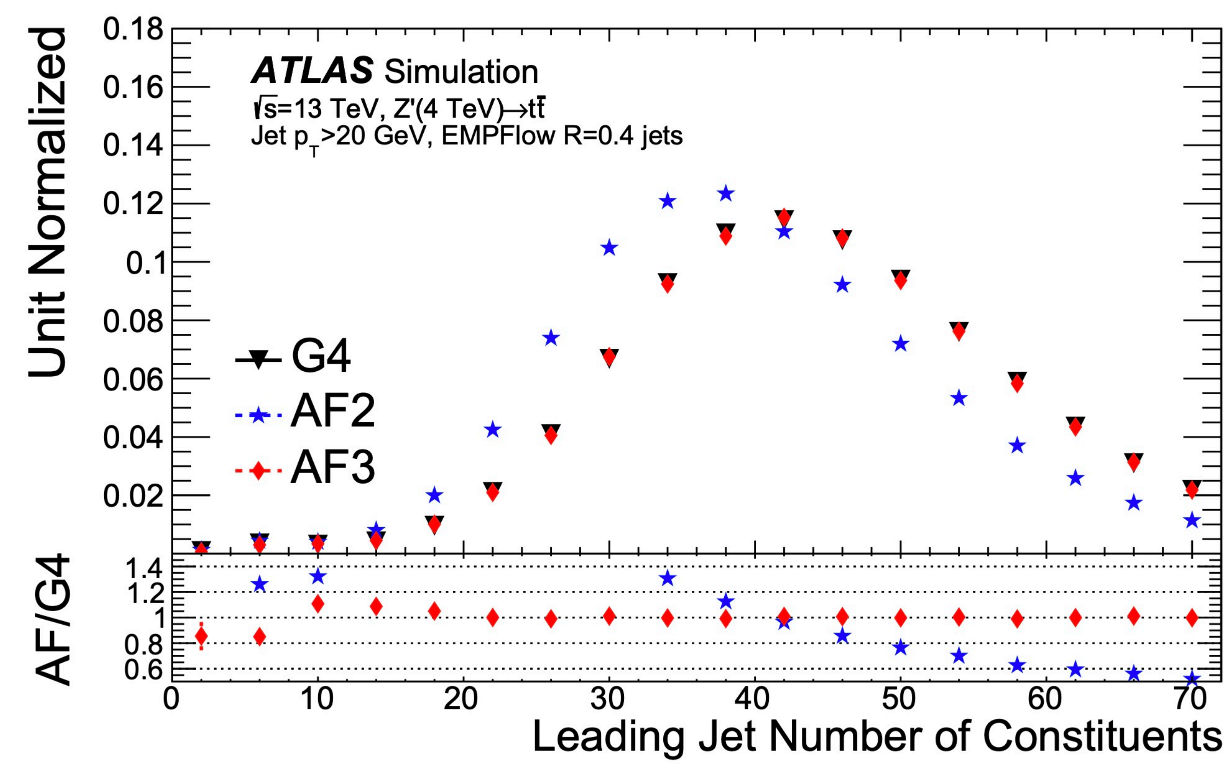
[1] arXiv:2109.02551

Physics Modelling

Improvements

- **FCSv2** - Improved correlation and shower depth modelling from PCA1
- **FCSv2** - Improved lateral modelling and correlations
- **FastCaloGAN** - Better correlations, and sub-structure modelling
- **MuonPunchThrough** - Modelling of fake muons



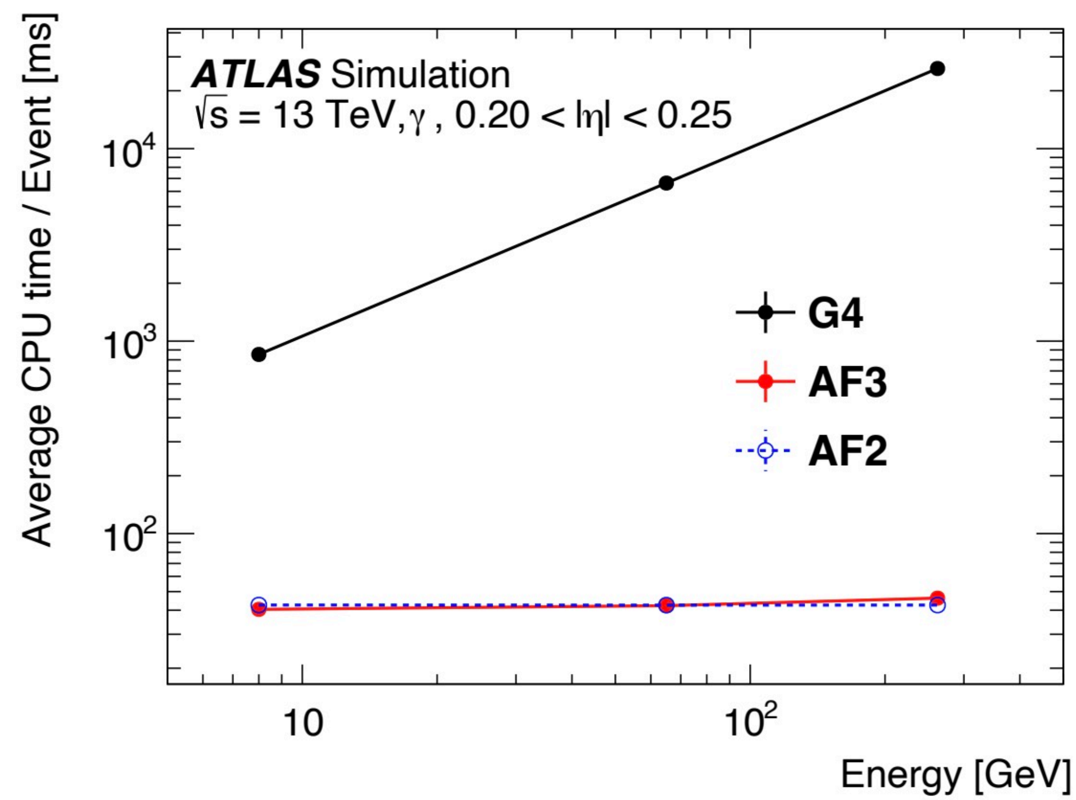


[1] arXiv:2109.02551

Summary

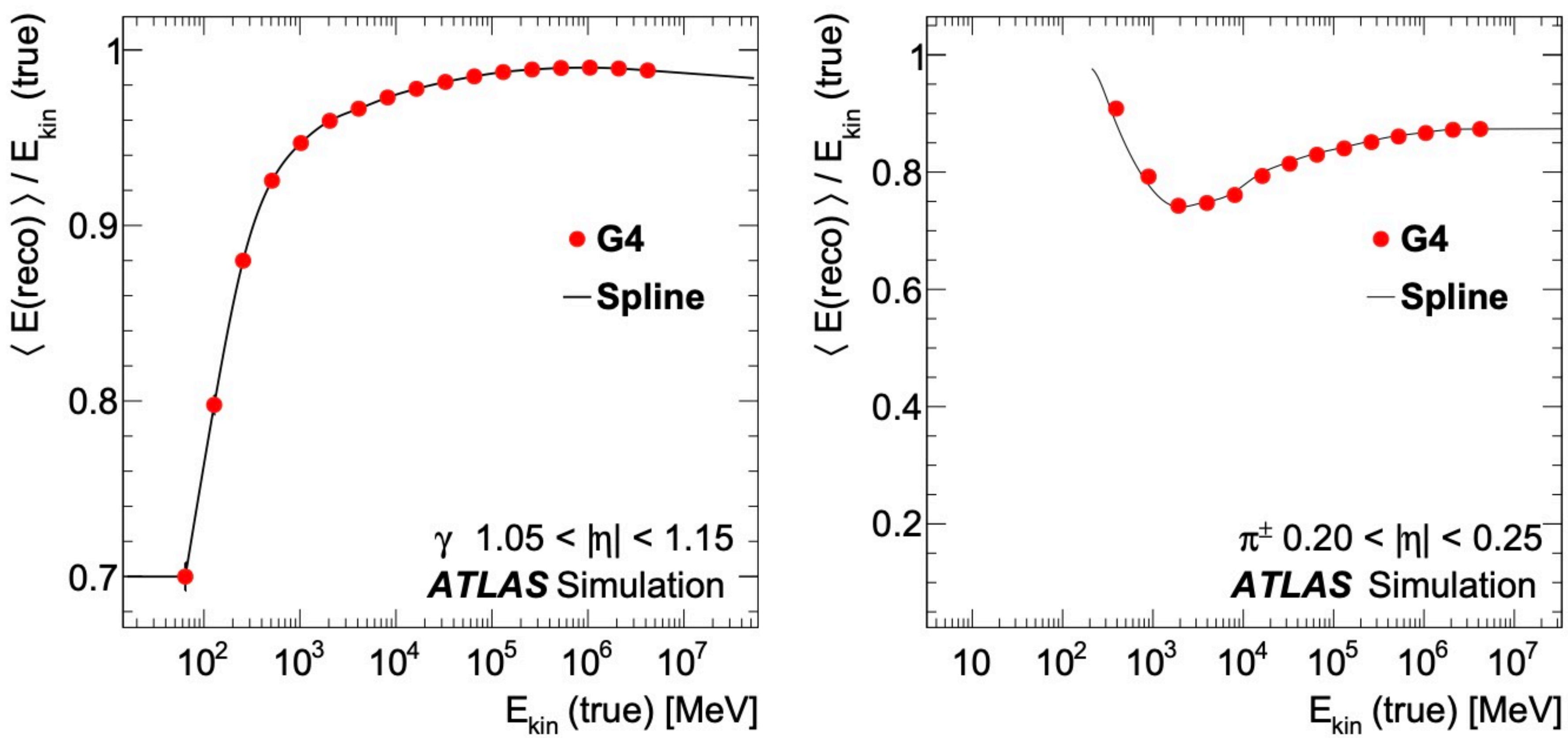
- **FastCaloSimV2** - electrons, photons and low/high energy hadrons.
- **FastCaloGAN** - medium energy hadrons.
- **MuonPunchThrough** - punch through modelling (fake muons).
- Excellent physics modelling!

- **500x** speed up in calorimeter simulation vs Geant4
- Will be default simulator for **Run3** and **HL-LHC**
  - **>50%** for **Run3**, targeting **70%**
  - **90%** for **HL-LHC**



[1] arXiv:2109.02551

FCSv2 - Energy Interpolation

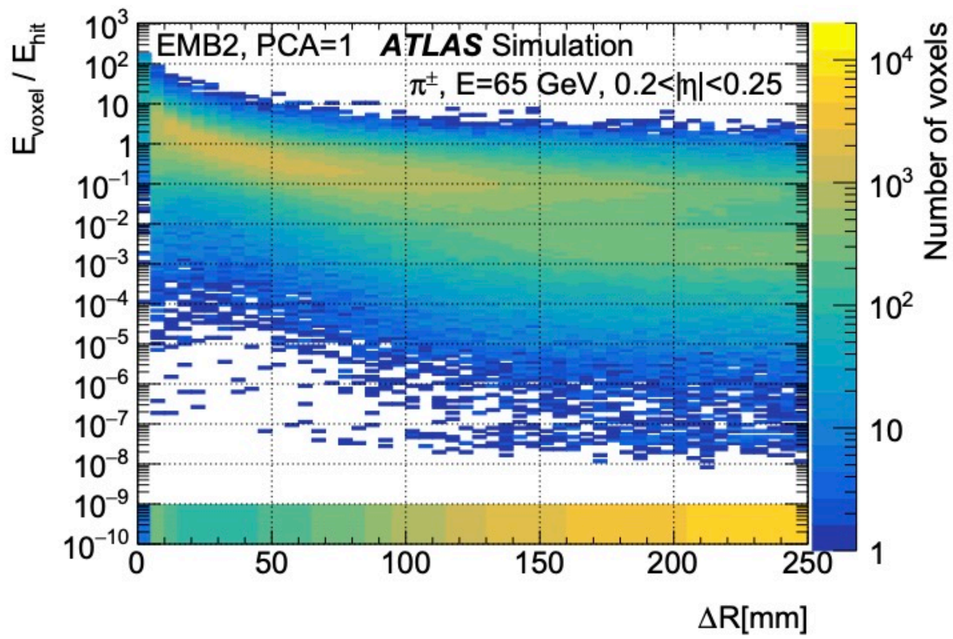


(a) Photons

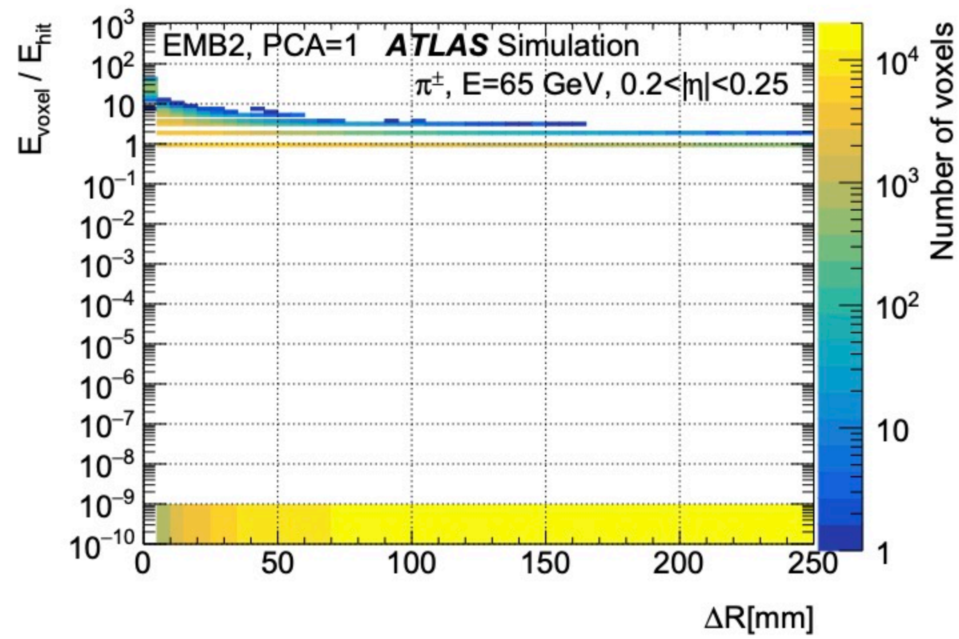
(b) Pions

Figure 22: Energy response, defined as the ratio of the reconstructed energy in the calorimeter cells to the kinetic energy of the particle, for (a) photons in $1.05 < |\eta| < 1.10$ and (b) pions in $0.20 < |\eta| < 0.25$. The red dotted points represent the response derived at discrete energies, using GEANT4 simulated single particles. The black line is a spline fit used to interpolate between discrete energy points. The statistical uncertainties are shown but are similar in size to the points or smaller.

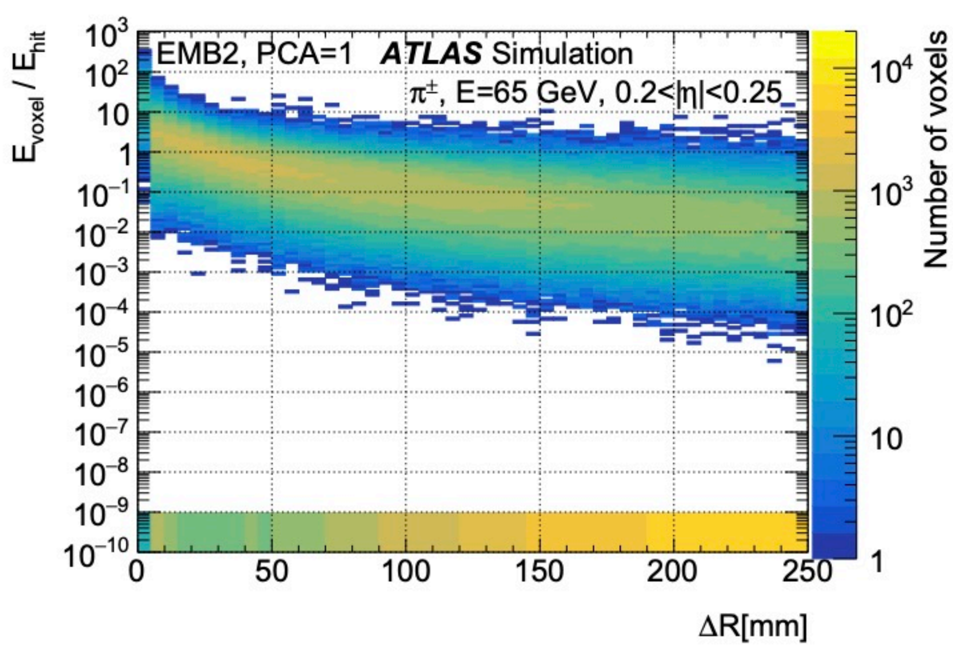
FCSv2 - Weighted hits

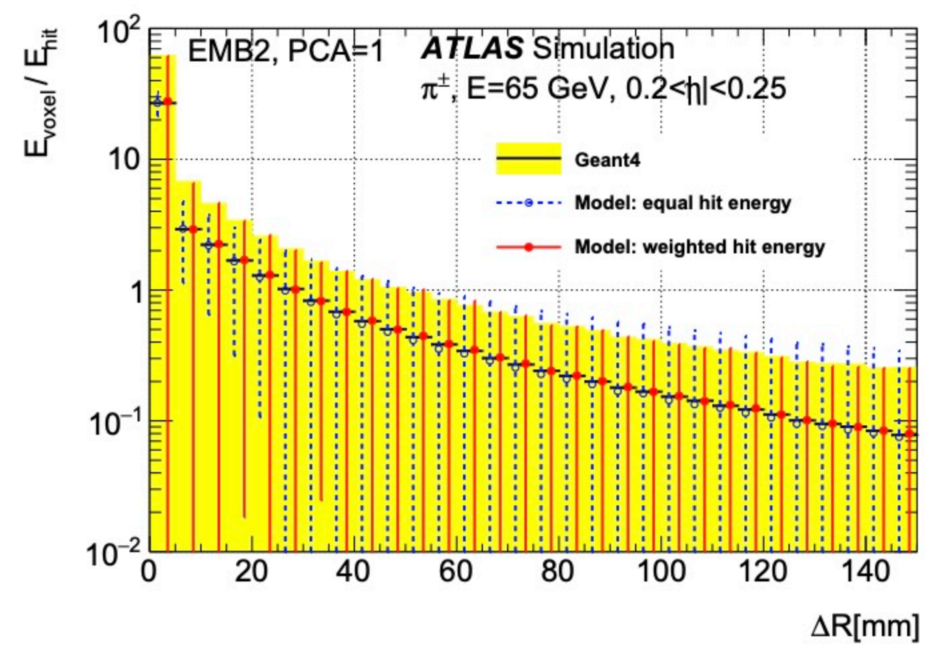


(a) GEANT4

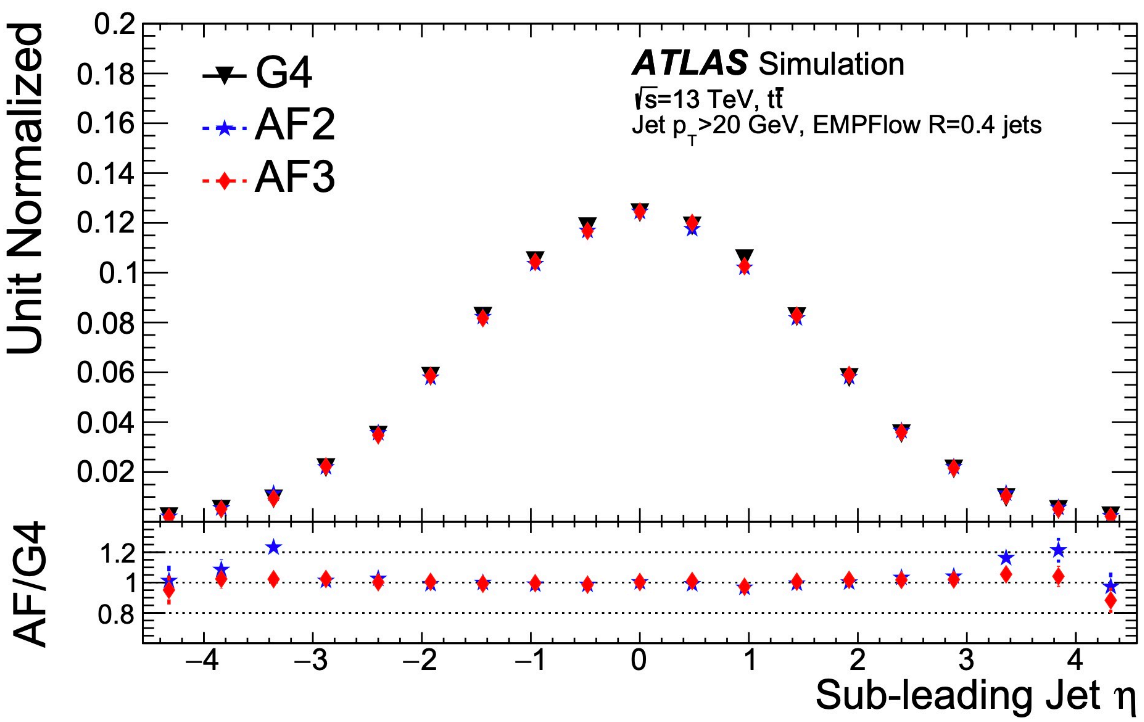


(b) Model: equal hit energy

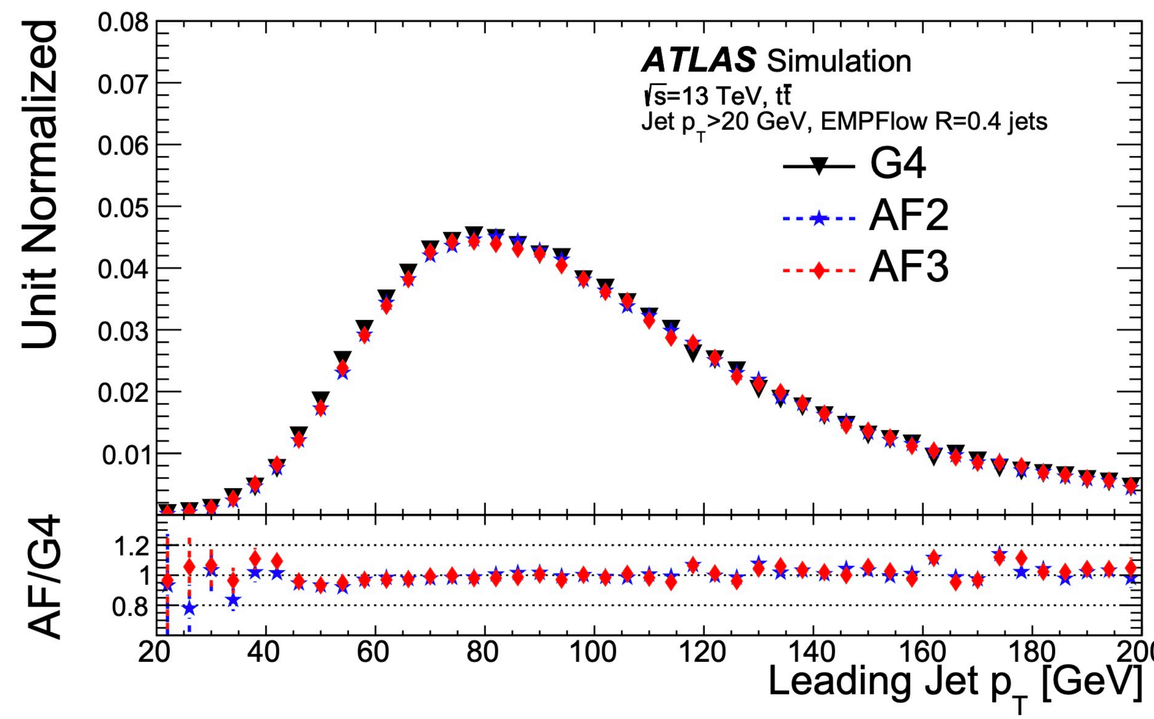




$t\bar{t}$

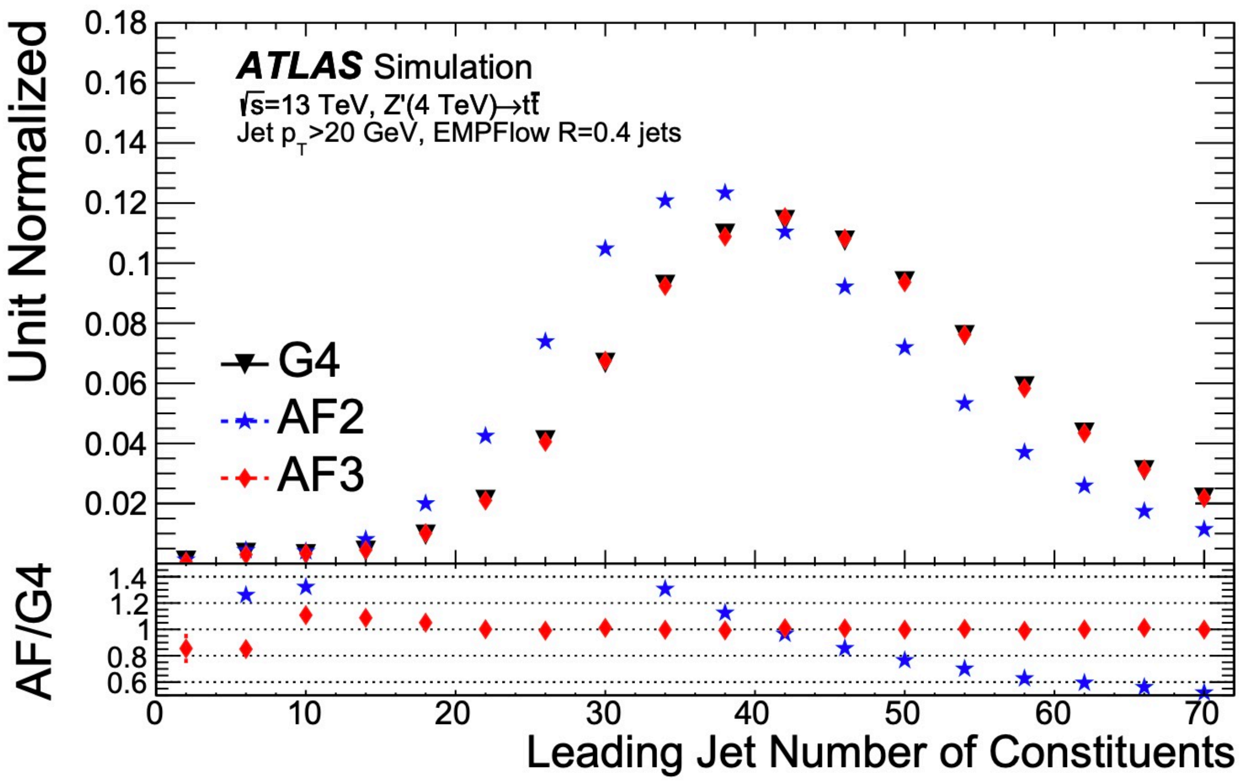


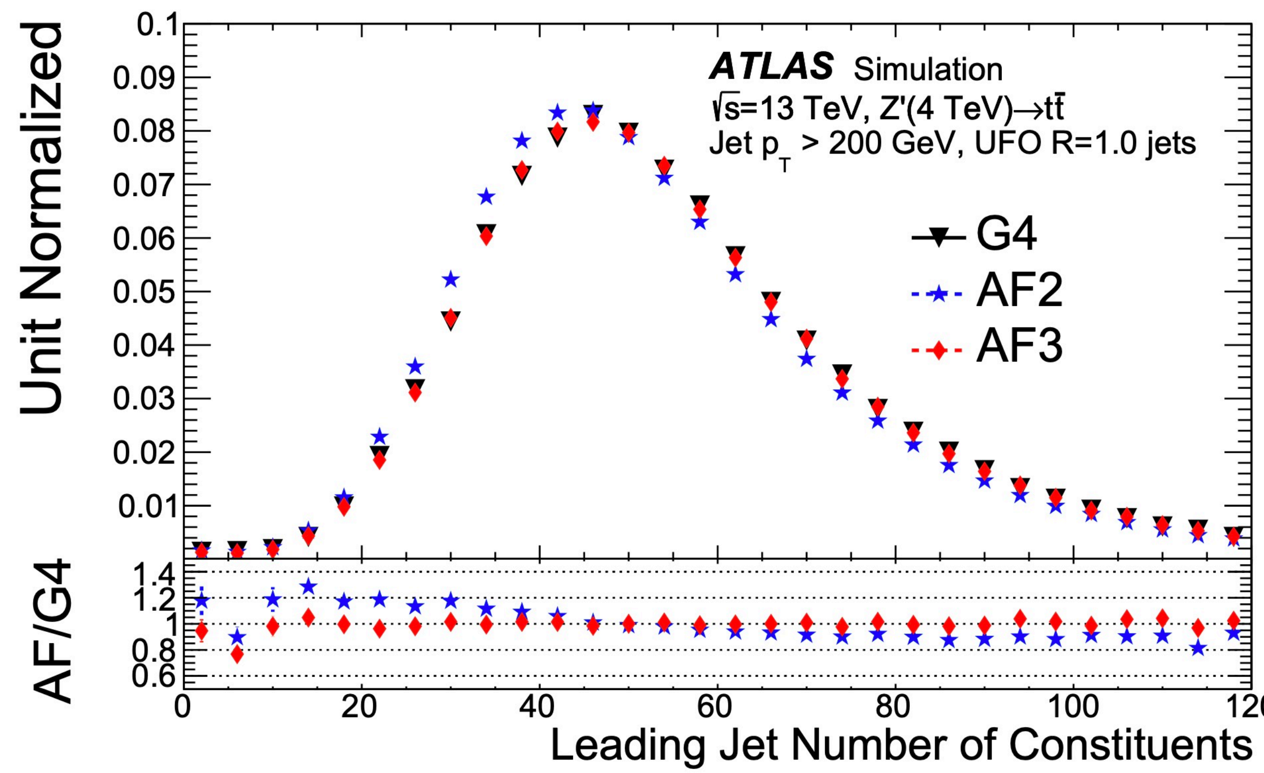
G4
AF2
AF3
ATLAS Simulation
√s=13 TeV, tt̄
Jet p_T>20 GeV, EMPFlow R=0.4 jets
Unit Normalized
AF/G4
Sub-leading Jet η



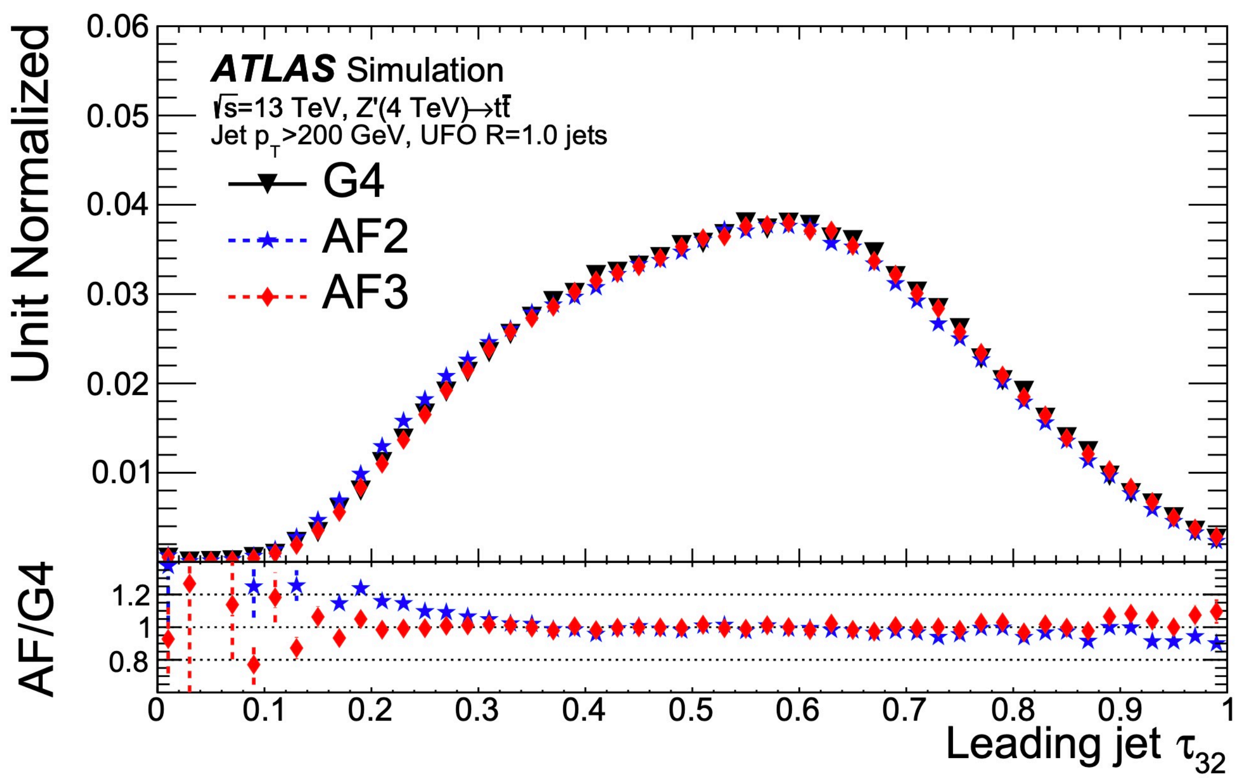
ATLAS Simulation
√s=13 TeV, tt̄
Jet p_T>20 GeV, EMPFlow R=0.4 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading Jet p_T [GeV]

Z’(4 TeV)→$t\bar{t}$

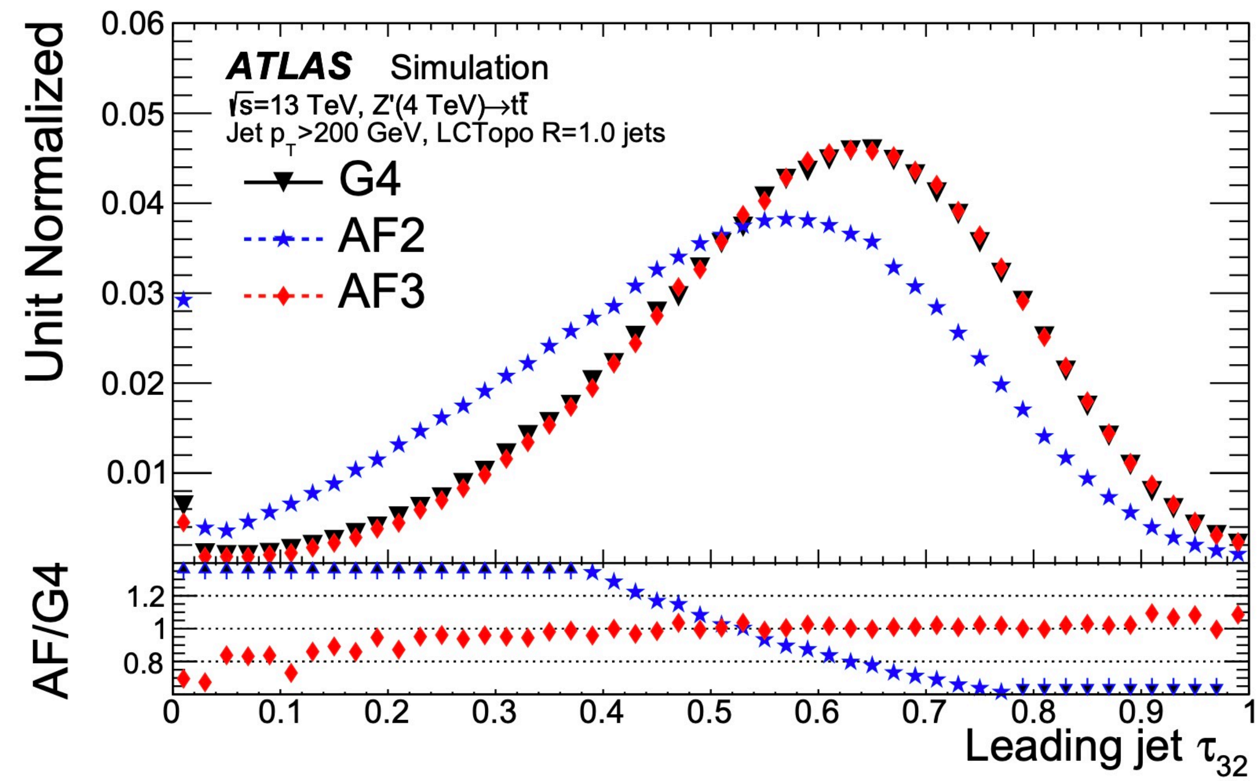

ATLAS Simulation
√s=13 TeV, Z'(4 TeV)→tt̄
Jet p_T>20 GeV, EMPFlow R=0.4 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading Jet Number of Constituents


ATLAS Simulation
√s=13 TeV, Z'(4 TeV)→tt̄
Jet p_T > 200 GeV, UFO R=1.0 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading Jet Number of Constituents

Z'(4 TeV)→$t\bar{t}$

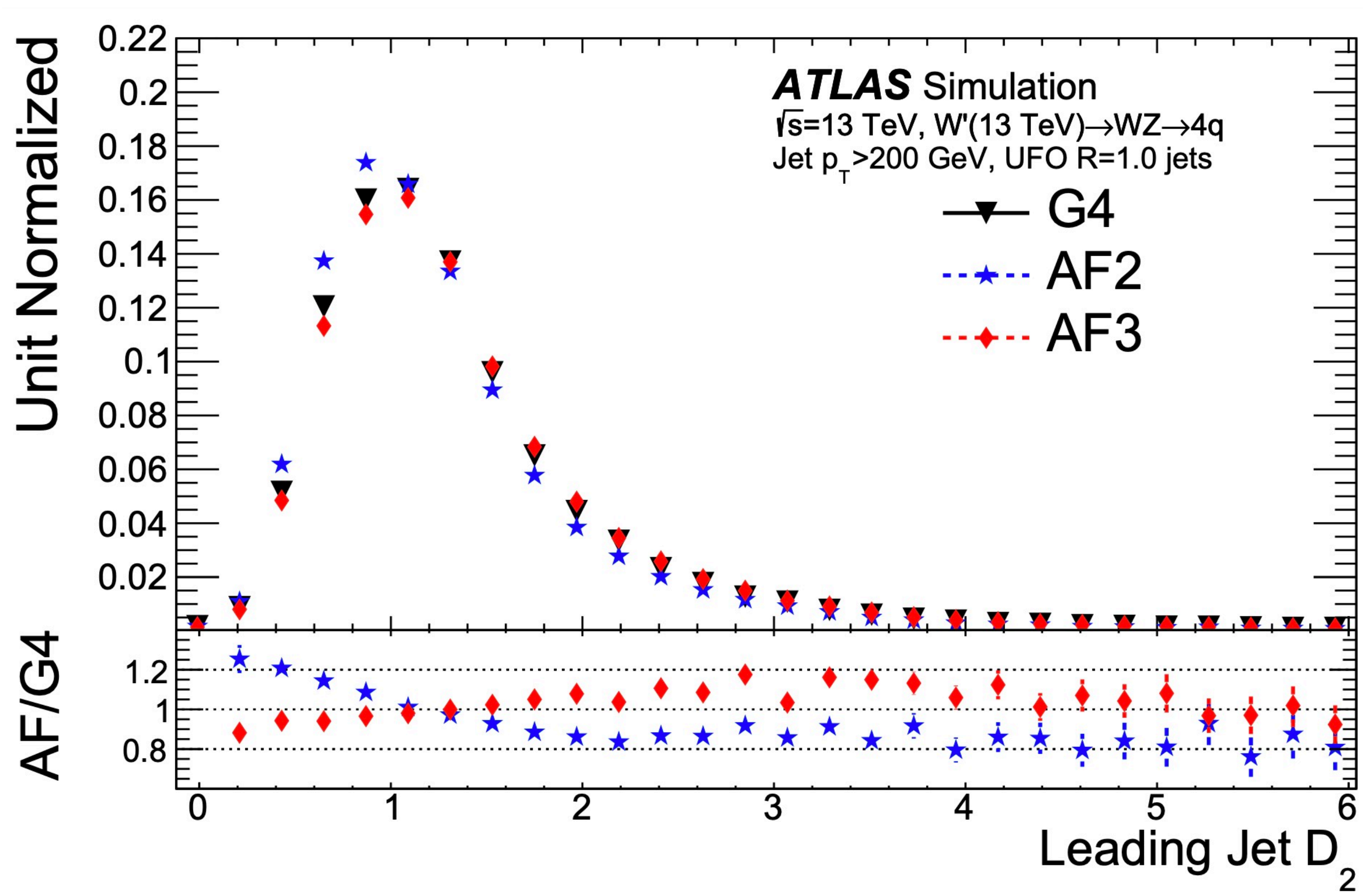


ATLAS Simulation
√s=13 TeV, Z'(4 TeV)→tt̄
Jet p_T>200 GeV, UFO R=1.0 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading jet τ32



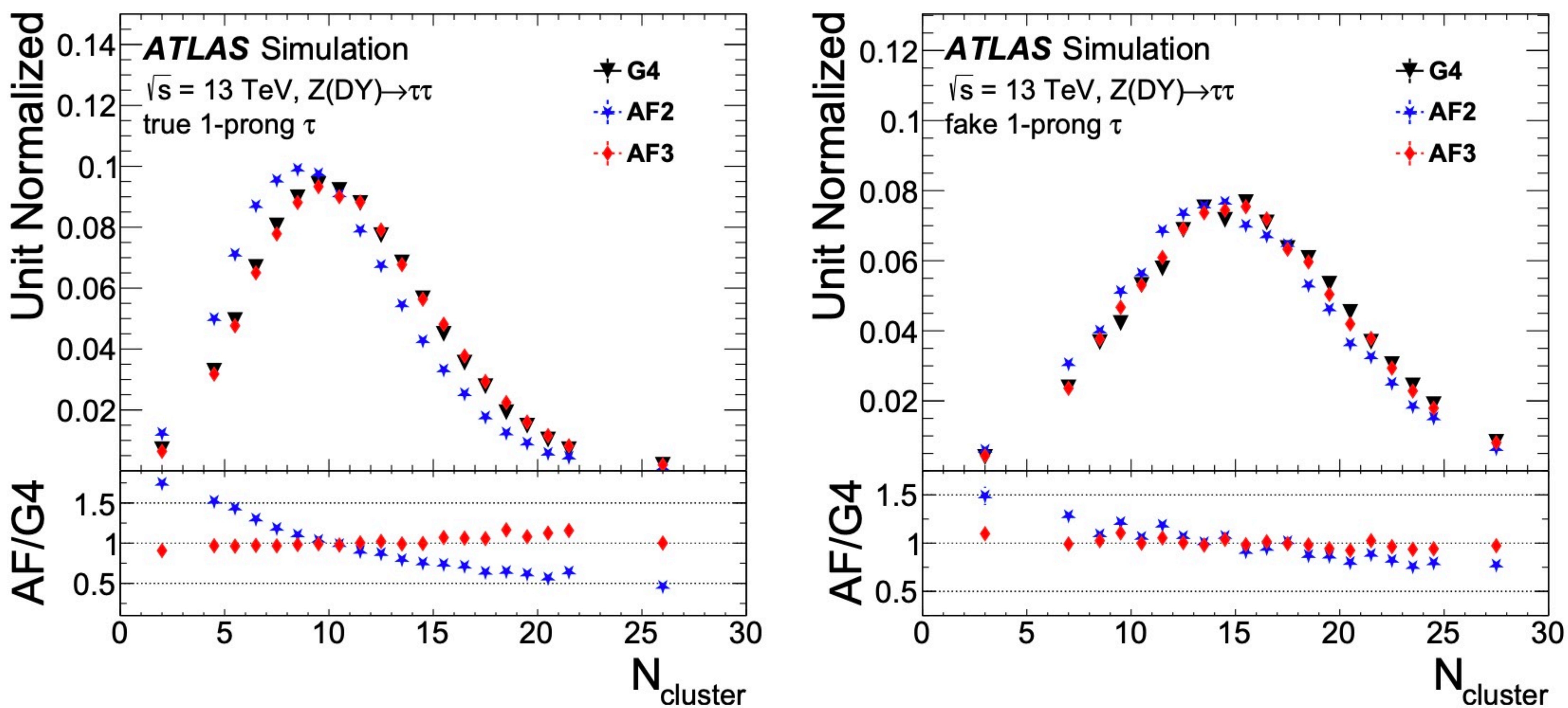
ATLAS Simulation
√s=13 TeV, Z'(4 TeV)→tt̄
Jet p_T>200 GeV, LCTopo R=1.0 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading jet τ32

Z’(13 TeV)→WZ→4q

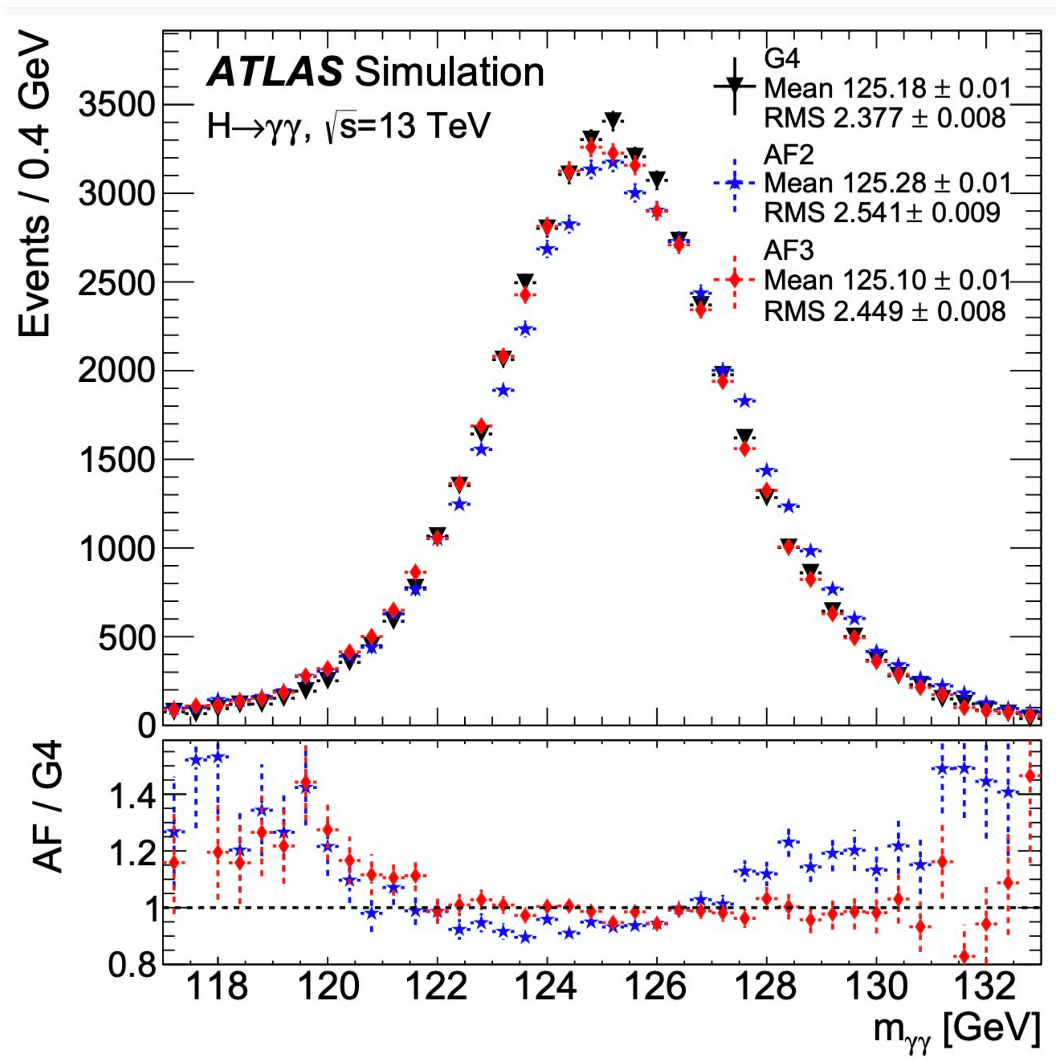


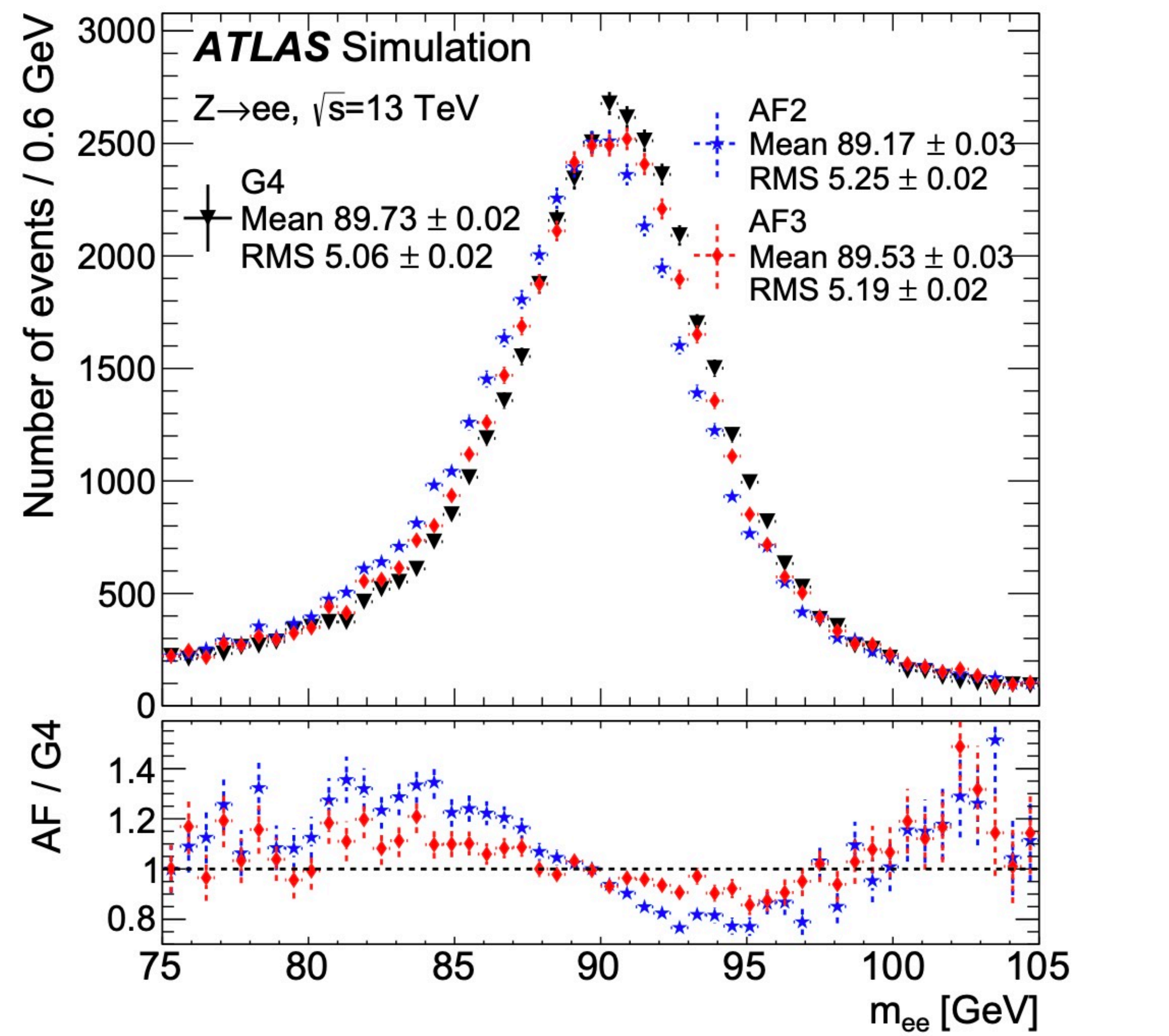
ATLAS Simulation
√s=13 TeV, W'(13 TeV)→WZ→4q
Jet p_T>200 GeV, UFO R=1.0 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading Jet D_2

Taus

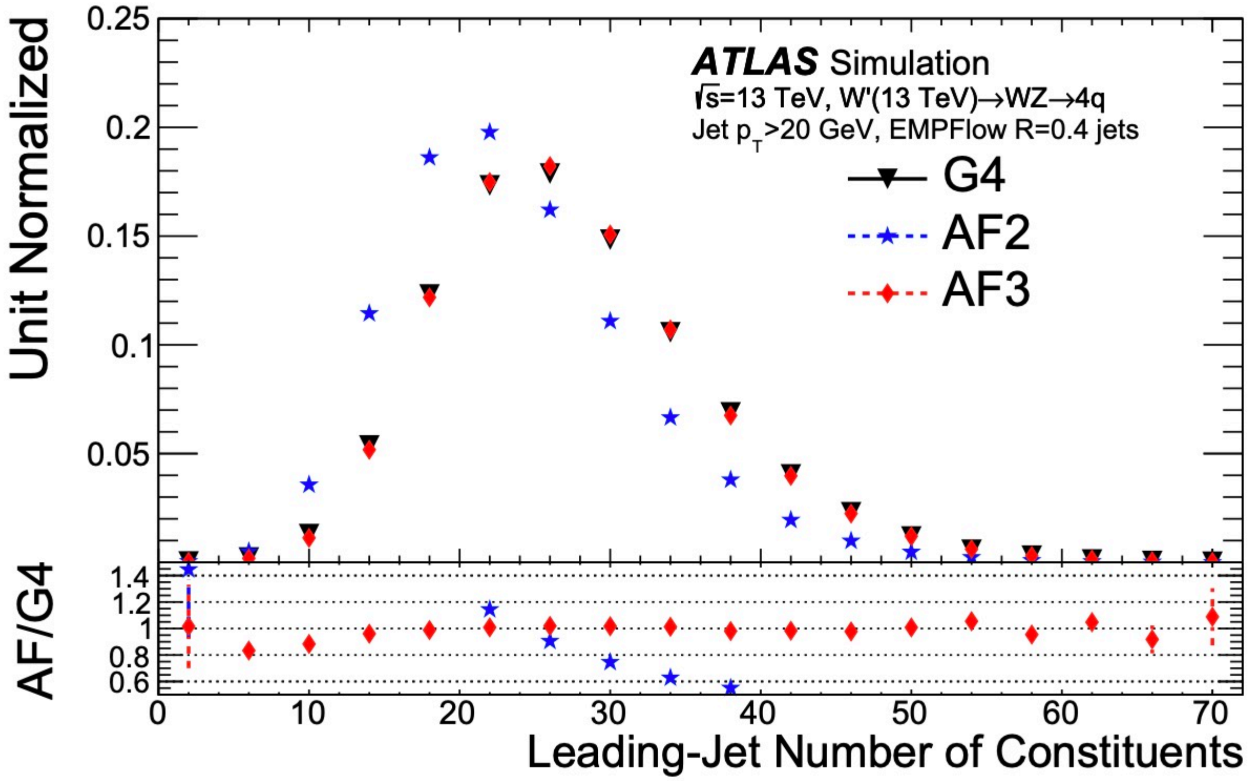

ATLAS Simulation
√s = 13 TeV, Z(DY)→ττ
true 1-prong τ
G4
AF2
AF3
Unit Normalized
AF/G4
N_cluster
ATLAS Simulation
√s = 13 TeV, Z(DY)→ττ
fake 1-prong τ
G4
AF2
AF3
Unit Normalized
AF/G4
N_cluster

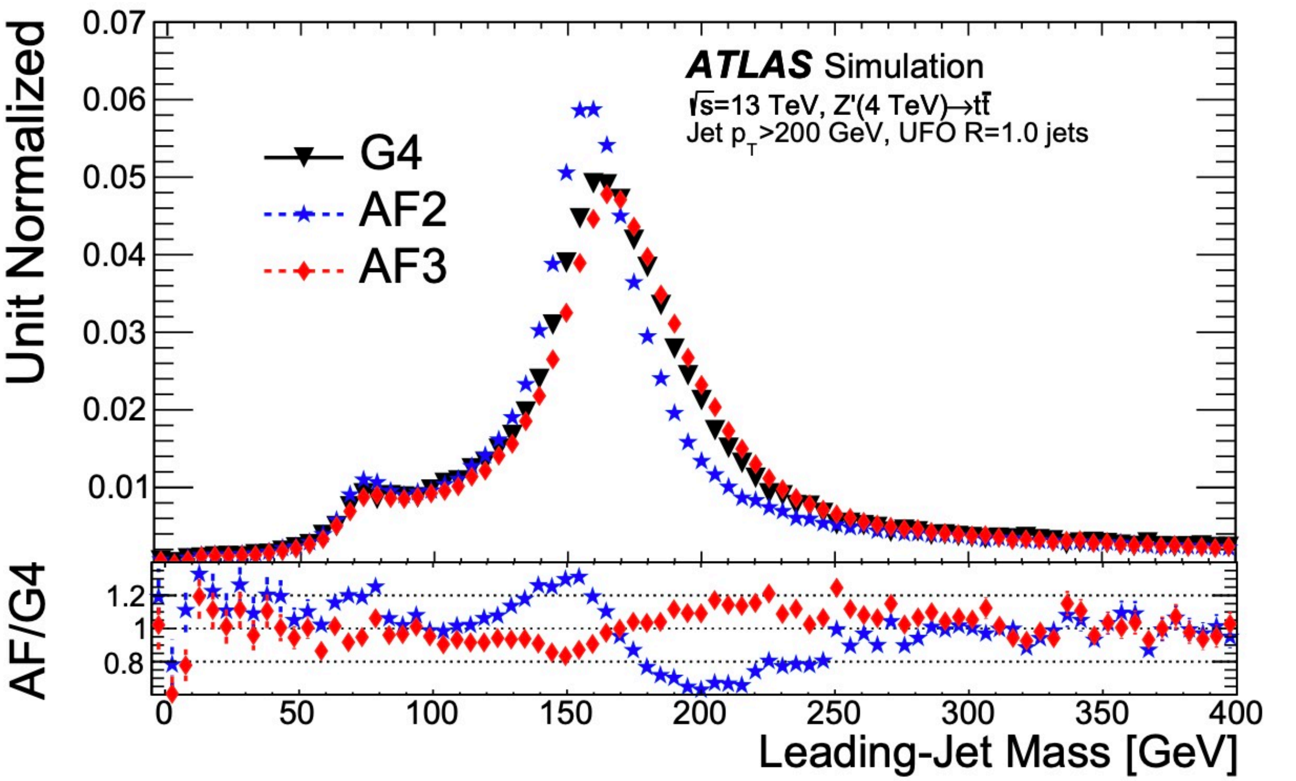
Analysis Distributions





W’ and Z’

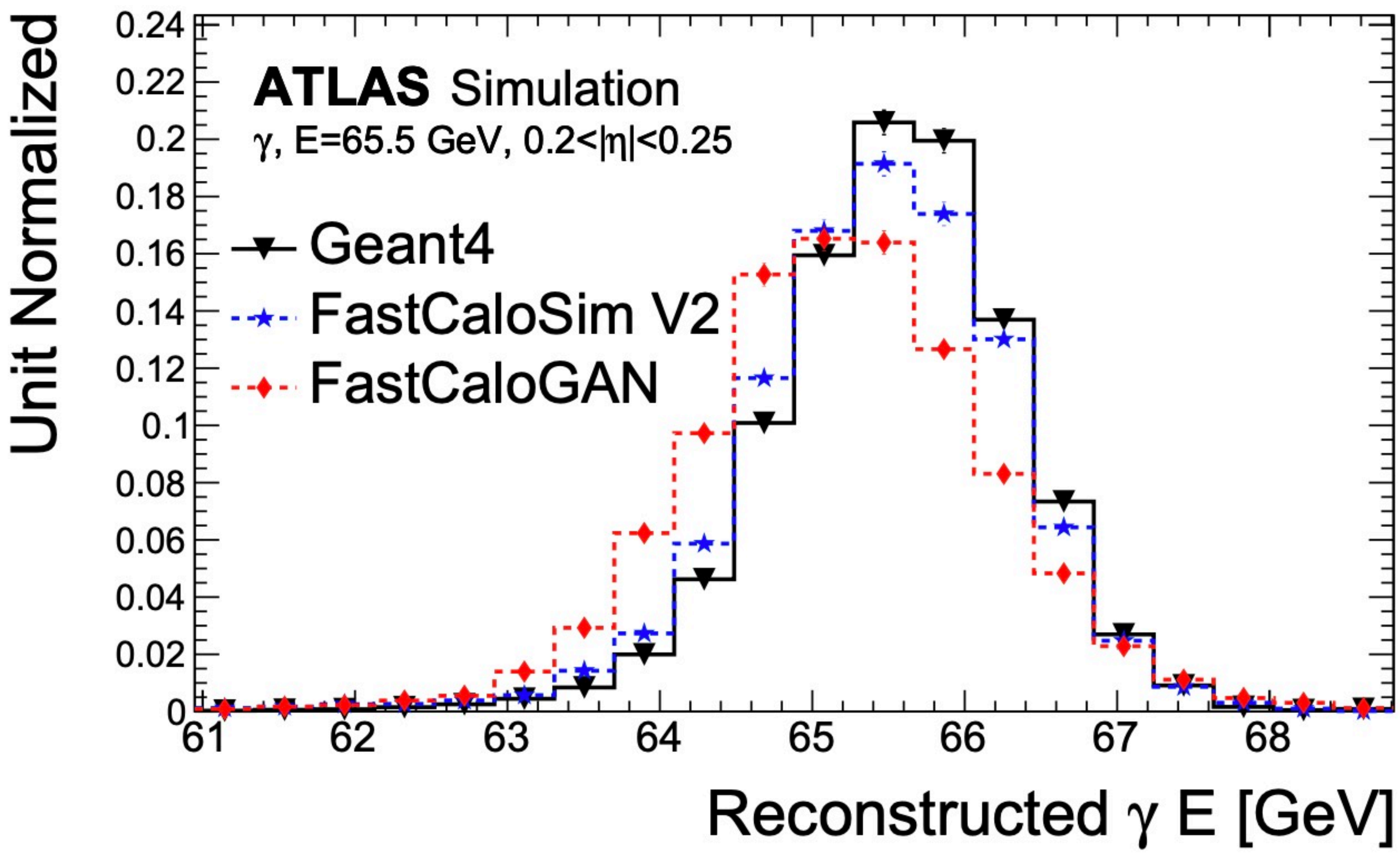

ATLAS Simulation
√s=13 TeV, W'(13 TeV)→WZ→4q
Jet p_T>20 GeV, EMPFlow R=0.4 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading-Jet Number of Constituents


ATLAS Simulation
√s=13 TeV, Z'(4 TeV)→tt̄
Jet p_T>200 GeV, UFO R=1.0 jets
G4
AF2
AF3
Unit Normalized
AF/G4
Leading-Jet Mass [GeV]

FastCaloSimv2 vs FastCaloGAN

Electrons and photons

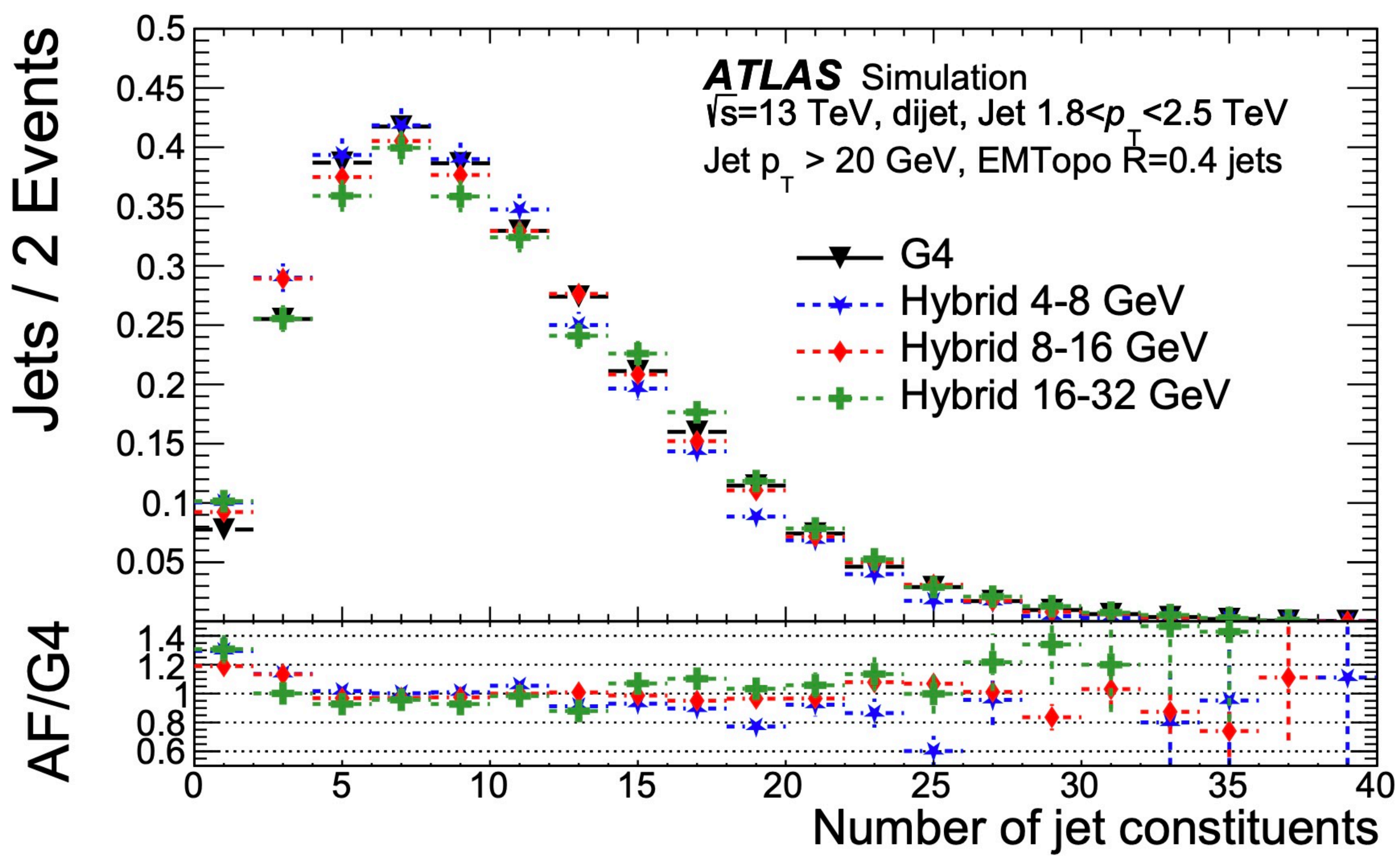
- FCSv2 shows better total energy performance
- FCSv2 is used to simulate all photons and electrons



FastCaloSimv2 vs FastCaloGAN

Medium energy hadrons

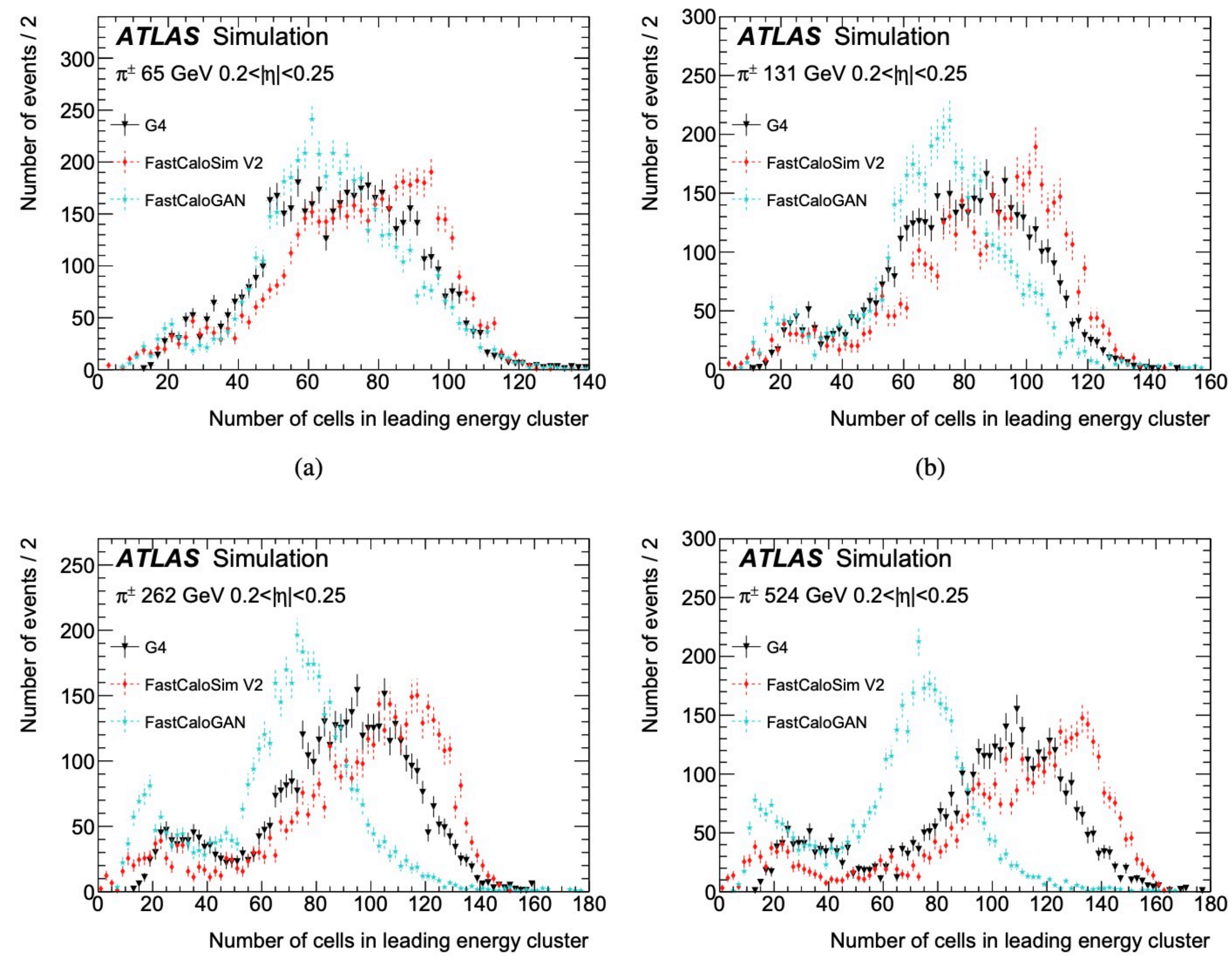
- FastCaloGAN shows better jet constituent modelling for medium energy hadrons.
- Transition threshold of 8-16GeV is chosen.



FastCaloSimv2 vs FastCaloGAN

High energy hadrons

- FastCaloGAN mis models at high energy.
- Transition back to FCSv2 at threshold 256 - 512 GeV

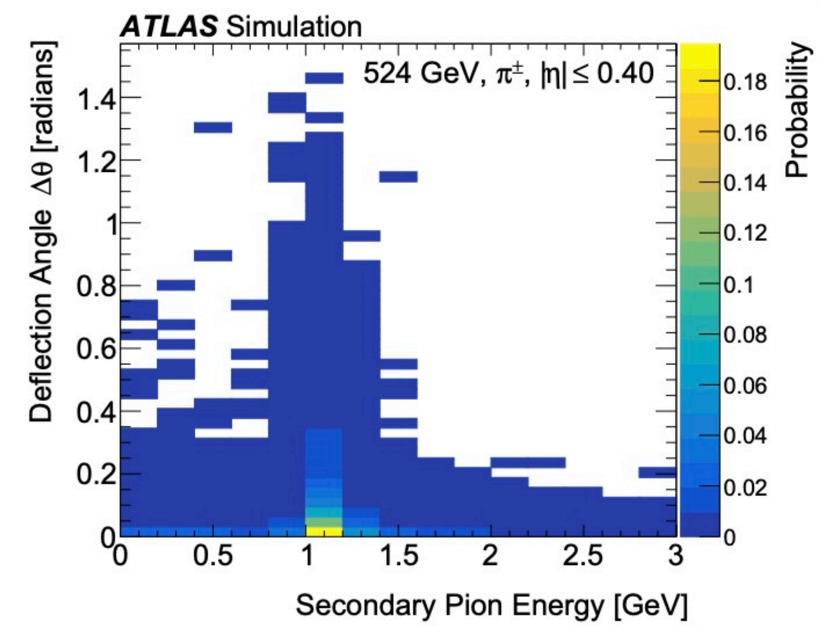


(a) (b)

Muon Punch Through

New for AF3!

- Store parameterisation of punch through particles and their kinematics
- Draw from param for when particles entering calorimeter
- Pass punch through particles to G4 for simulation in MS



(a)