S&C Week: Fast Calorimeter Simulation Group Progress Report

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On behalf of FastCaloSim Group

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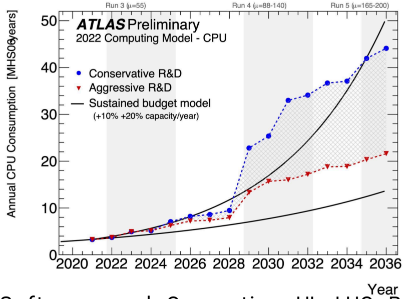
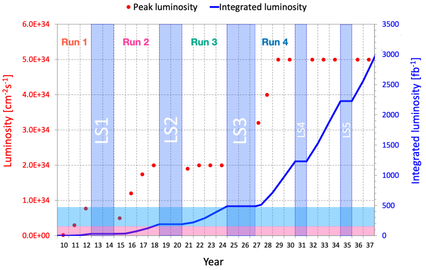
ATLAS Future Program

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

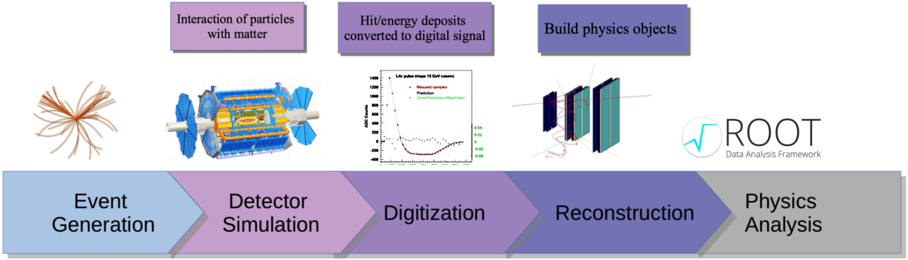


ATLAS_Software_and_Computing_HL_LHC_Roadmap

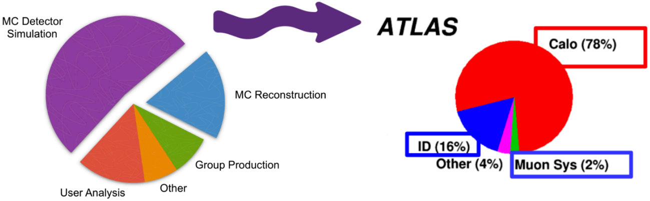


- CPU requirements will increase due to luminosity
- Rely on MC events – stats several times data luminosity
- **Fast Simulation** – for majority of events in **Run3** and **HL-LHC**

Simulation in ATLAS



- Largest proportion of CPU time spent on **Detector Simulation**
- **80%** of Geant4 simulation time is spent in calorimeters [1]

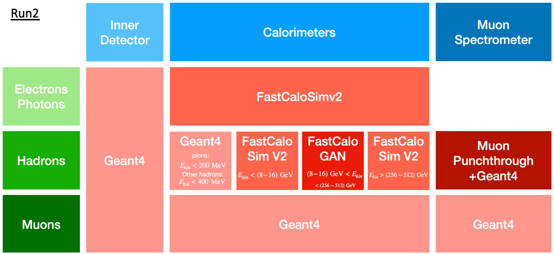


[1]ATLFAST3(2022)

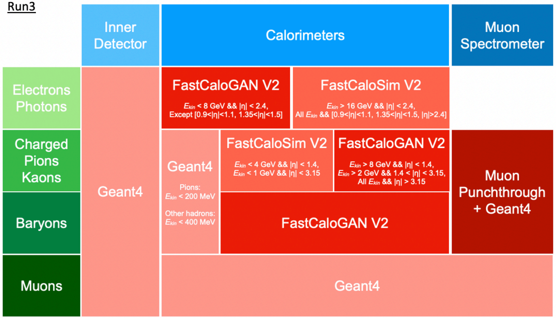
AtlFast3 (AF3)

- Fast simulation suite employed in ATLAS for Run3, distinct shower generation mechanism: **3x - 15x faster** than Geant4 in many processes.
- Improves physics performance significantly over AF2 (Run1 & Run2).
- Three main components for calorimeter simulation:
  - **FastCaloSimV2** - parameterised modelling
  - **FastCaloGANV2** - Deep learning using GANs
  - **MuonPunchthrough**

Run2



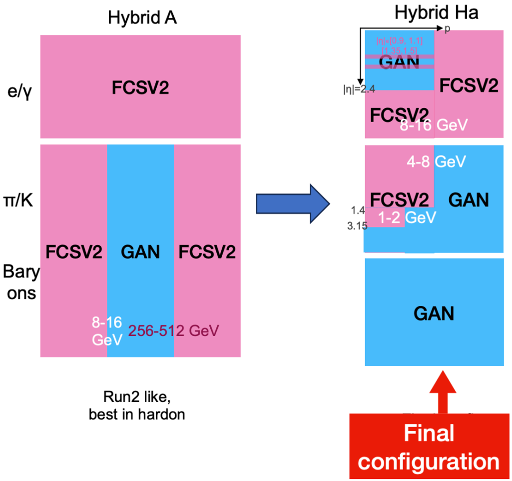
Run3



News/Recap

- **AF3** configuration finalised & **released**: ATLPHYSVAL-970
- Latest production MC23d campaign: link, link2
- **Today**: progress since last S&C Week SC_03Oct2023

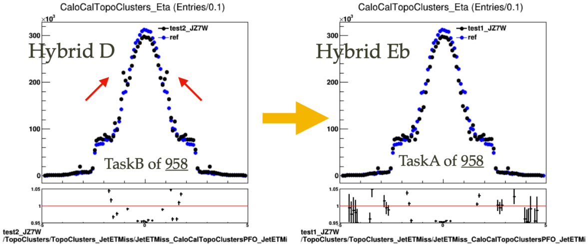
AF3 Release

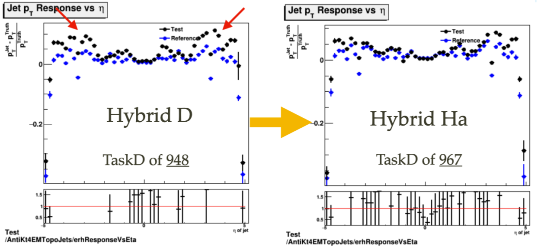


- How did we come to this? SimMeeting_20230912,
- 5 PhysVal and 10 configurations later...
- Final AF3 configuration w/ pileup, tuned for e/γ, hadron, π/K cluster, transition region spikes and maximise GAN...
- Introduced p GANs for dealing better with baryons...

Model Tuning: e/γ

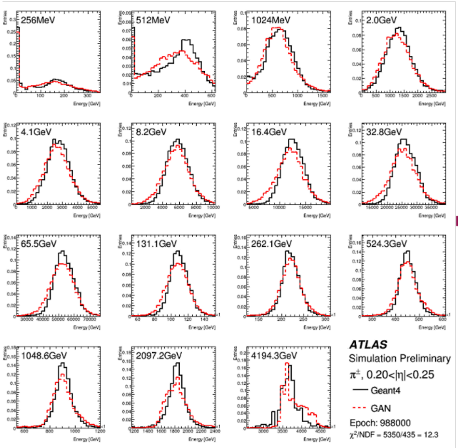
- Spikes at $|\eta| \sim 1$, add additional FCSV2 for harder to model (GAN) slice.
- Extend range of FCSV2 to $|\eta| > 2.4$ to suppress jet p_T response.





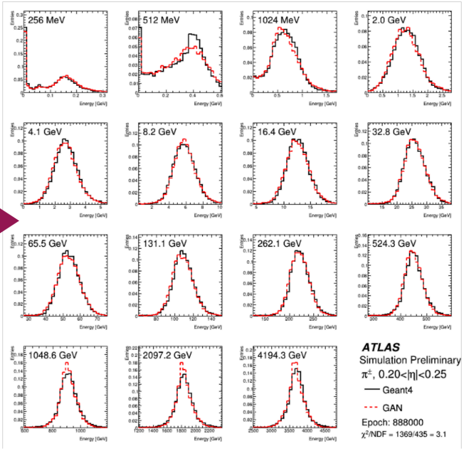
FastCaloGANV2 ($\pi^{\pm}$)

Run 2



χ^2/NDF = 12.3

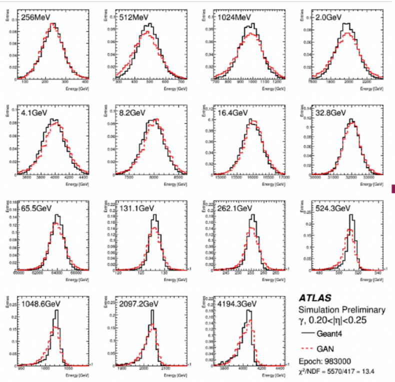
Run 3



χ^2/NDF = 3.1

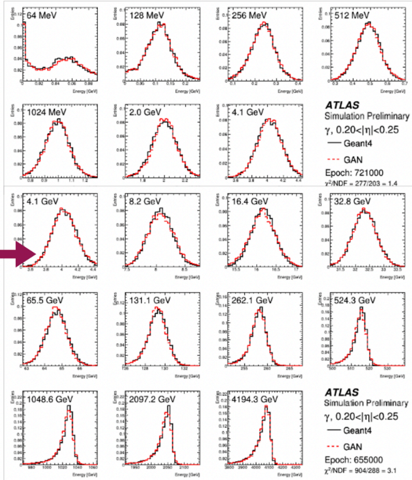
FastCaloGANV2 (γ)

Run 2



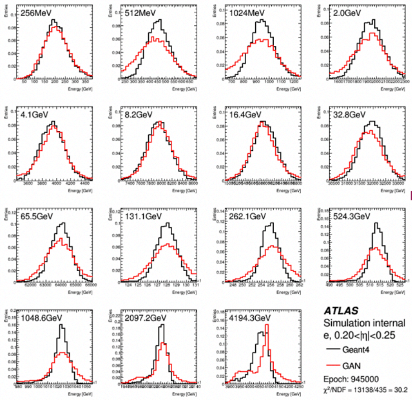
$\chi^2/\text{NDF} = 12.3$

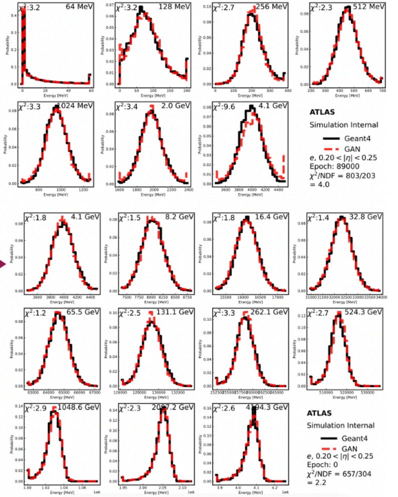
Run 3



$\chi^2/\text{NDF} = (277+904) / (203+288) = 2.4$

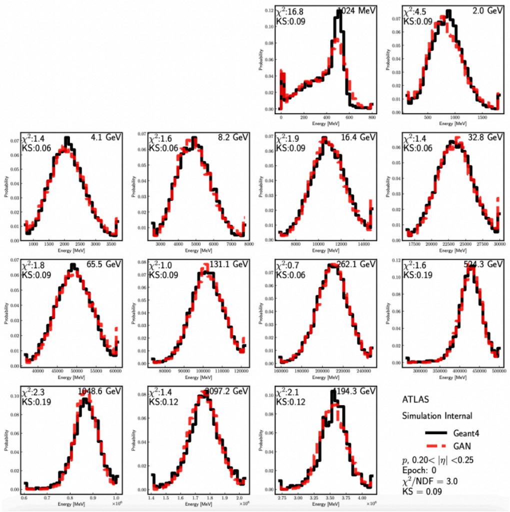
FastCaloGANV2 (e)





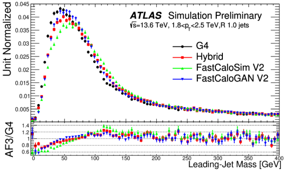
$\chi^2/\mathrm{NDF} = (803+657) / (203+304) = 2.9$

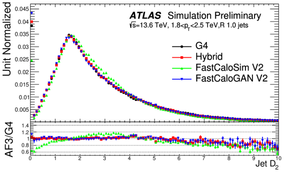
FastCaloGANV2 (p)

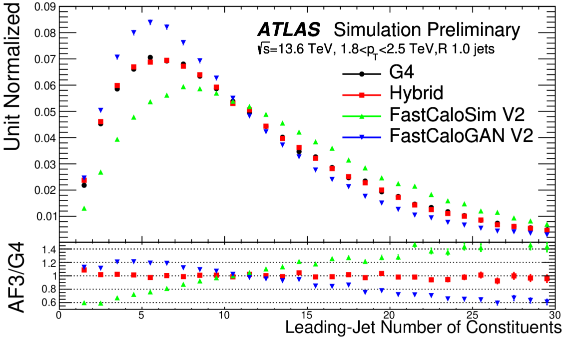


χ^2/NDF = 3.0

AF3: Physics Modelling (JZ7)



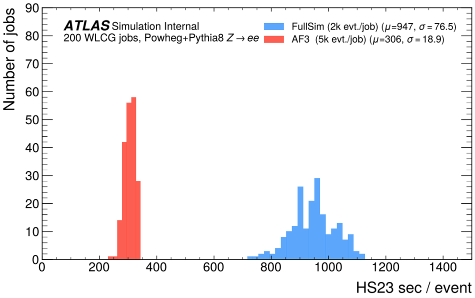


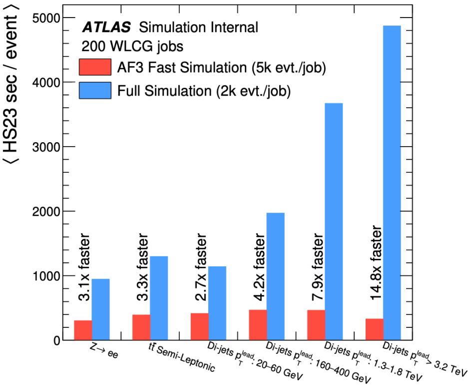


Atlas/GROUPS/PHYSICS/PLOTS/SIM-2023-004

AF3 Performance

- **Much faster** than fullsim! (especially in high energy dijets with more particle showers)

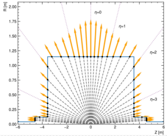


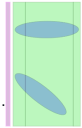


Challenges and Opportunities

Angle of entry

See more here



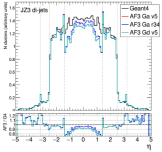


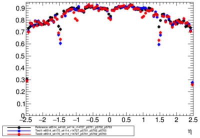
Tilted shower shows less energy in third layer and more energy in the first layer

- Particles used for parametrization generated at ID-Calo boundary with momentum pointing away from origin
- Particles extrapolated according to incident direction, but bending in magnetic field may introduce small bias in simulation for charged particles
- Could capture average B-field effect from average $\Delta\phi$ of single particles at ID-Calo boundary

Transition regions

See more here

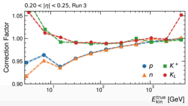


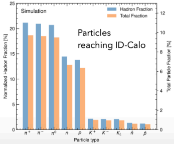


- Modelling in transition regions in some cases problematic:
  1. $\eta \sim 1.4$ - barrel to end-cap
  2. $\eta \sim 3.1$ - end-cap to FCal transition
- Not well understood - requires more investigation
- Could try to increase the η granularity in the transition region

Other hadrons

See more here





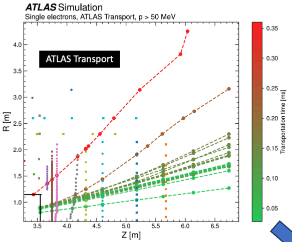
- Dedicated GANs for pions and protons
- Energy corrections for $K^{\pm}$ and K_L
- Neutrons and other hadrons: simulated as protons (accounting for mass differences)
- More GANs could be trained per hadron species

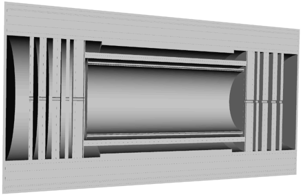
Recent Developments

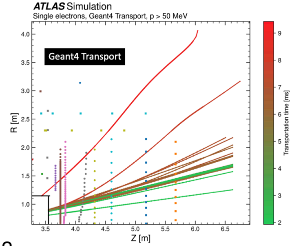
- Beyond ISF: Integration of FastCaloSim within G4VFastSimulationModel
  - Replace ATLAS track transport with Geant4 propagation in simplified geometry: pyGeoSimplify package for simplified geometry inference →repo
- ONNX integration into FastCaloSim → finally!
- Containerisation of FastCaloGAN - allow independence from lxplus architecture and better training on different machines!

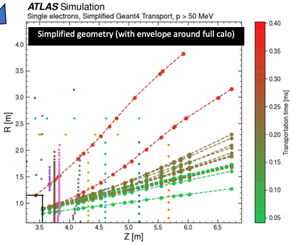
Resource	Details	Testing Situation
INFN-Bologna Cluster	INFN Bologna computing cluster. (Old) nodes w/ CentOS7, CVMFS, HTCondor, no GPUs	Done and successful
OPH Cluster	Cluster of the Open Physics Hub Project of the University of Bologna. Several nodes w/ Rocky Linux 8, SLURM, no CVMFS, no GPUs	Done and successful
INFN-CNAF	INFN-CNAF HPC cluster (close to WLCG INFN-T1) CentOS7 nodes, no CVMFS, SLURM, V100 GPUs	Done and successful

Track Transport: G4 FastSim



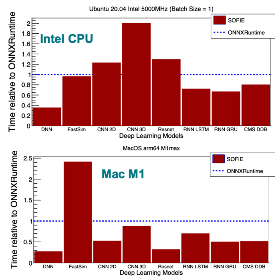


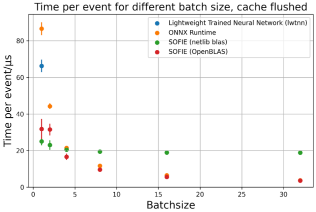




ML Inference: ONNX and Beyond

- GANs for FastCaloSim so far have been trained in LWTNN.
- ONNX: de-facto industry standard → recently implemented into FCS: !68057
- SOFIE: “System for Optimised Fast Inference code Emit”
  - Takes ONNX file and converts into C++ equivalent inference function
  - TMVA-based, minimal dependency: only on BLAS
- Speed-up irrelevant, up to 10x memory reduction allows possibility to expand GAN’s usage.





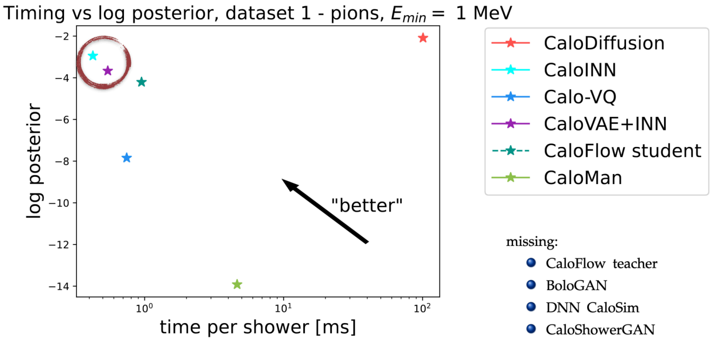
AF3_Workshop_ONNX,SOFIE_CHEP23

Possible Developments

- ML Preprocessor - Parametrised FCS as input to ML models.
- Pre-trained models for extracting subdetector-specific parameters.
- ML inpsired voxelisation scheme : E.g K-mean clustering algorithm, rather than regular voxels.
- More GPU-based implementation for multi-threading in FCSV2.
- Exploring beyond GAN models: CaloChallenge.

Towards Object-based Modelling

- Normalizing flow/diffusion based for photons.
- VAE/INN-based for pions.



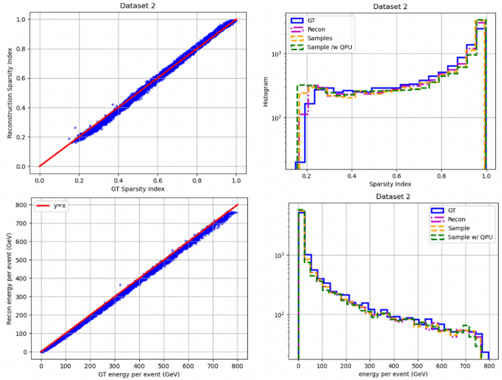
missing:

- CaloFlow teacher
- BoloGAN
- DNN CaloSim
- CaloShowerGAN

QVAE?

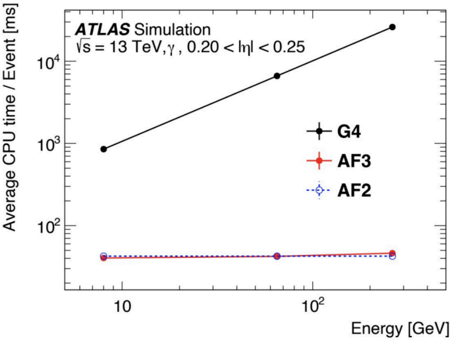
- Possibility of using QPU for fast simulation.
- **12x** faster wall-time (generate 1024 samples) with QPU over GPU.
- Tested in the context of DataSet 2 from CaloChallenge.
- Far-future consideration for quantum-assisted generative model.

	Wall time to generate 1024 samples
Calorimeter Geant4	$\sim 400\ s$
GPU A100	$2.19 \pm 0.14\ s$
QPU	$\sim 0.180\ s$
Decoder	$\sim 0.01\ s$



Summmary

- **AtlFast3 for Run3** - successfully validated, current tag a911, MC23d improves pileup condition.
- **Excellent physics modelling** - good agreement across many physics objects → thanks to comments received from CP groups, more feedback welcome!
- **Speed-up of factor 3x-15x** over full simulation (depending on process/energy range).
- Exciting interplay between machine-learning inspired techniques and physics optimisations → more developments in the pipeline.

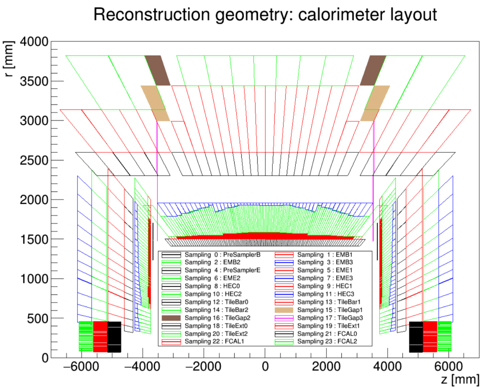


The End

Backup

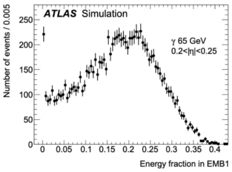
Input Datasets for AF3 modelling

- 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 chraged pions/kaons shower
  - **Proton** samples - for baryonic shower
- Record energy deposit in calo **layers** and **cells**.
- Simulated in grid of η and **incoming momentum**

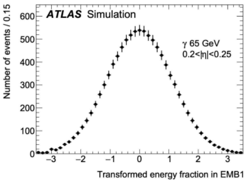


FastCaloSim: Parameterisation

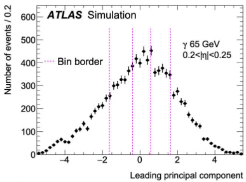
Energy in Each Layer



Transform to Gauss



Apply PCA1

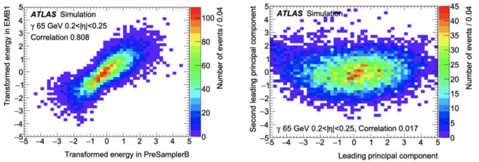


Categorize

Apply PCA2

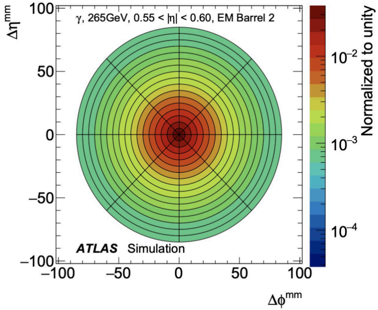
Set of Gaussian distributions

PCA1 Effectiveness



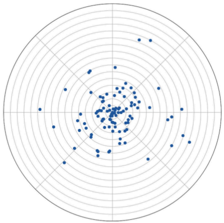
FastCaloSim: Parameterisation

- 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.



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

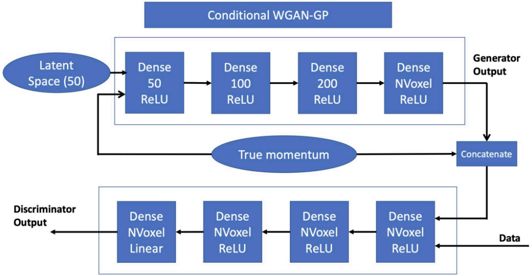
$$N_{hits}^{layer} \sim Poisson\left(\frac{1}{\sigma_E^2}\right)$$

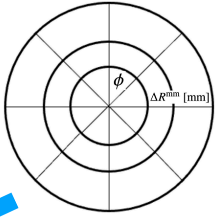


$$E_{hit} = E_{layer}/N_{hits}$$

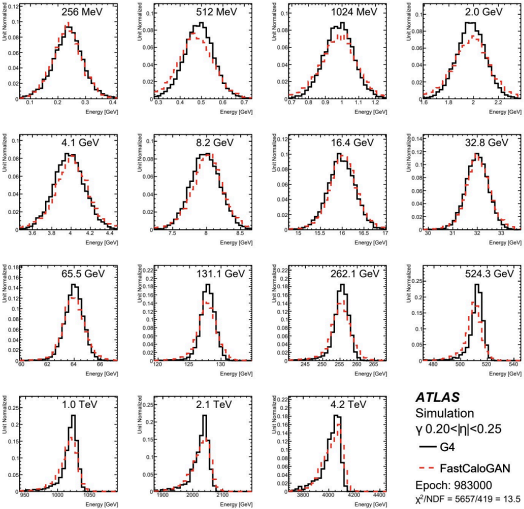
FastCaloGAN: GAN Setup

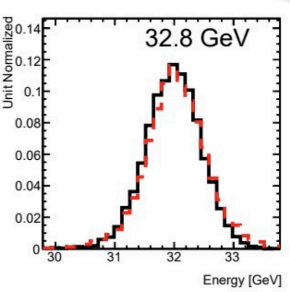
- **Generative Adversarial Network (GAN)** using **TensorFlow2** to generate showers
- Incorporates longitudinal and lateral modelling, and correlations
- Calorimeter deposits are **voxelized** in ΔR and η
- One GAN is trained with gradient penalty for each region, inclusive in truth momentum





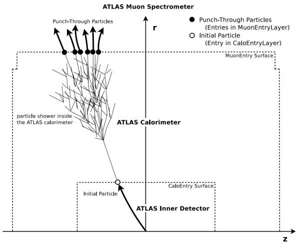
FastCaloGAN: Best Epoch

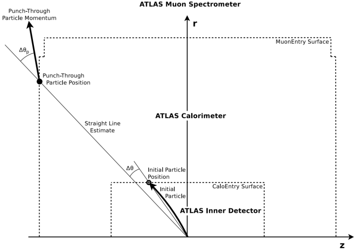




FastCaloSim: Muon Punchthrough

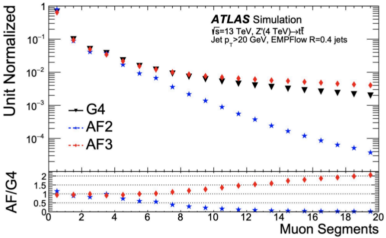
- The punch-through particles are **parametrized by their dependence in energy and direction:** E, $\Delta\theta$ $\Delta\phi$, $\Delta\theta_p$ **and** $\Delta\phi_p$
- **NN classifier** to estimate probability to produce punch-through particle of various types
- **Principal Component Analysis (PCA)** is run on FullG4 input samples to decorrelate the dependence.
- Simulate kinematics of secondary punch-through particles by sampling parametrization (inverse PCA).

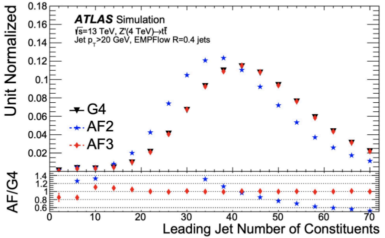




Result: Physics Modelling

- **FCSv2** – Improved correlation and shower depth modelling from V1.
- **FCSv2** – Improved lateral modelling and correlations
- **FastCaloGAN** – Better correlations, and sub structure modelling.
- **MuonPunchThrough** – Modelling of fake muons, improved modelling, added more particle types including kaons.





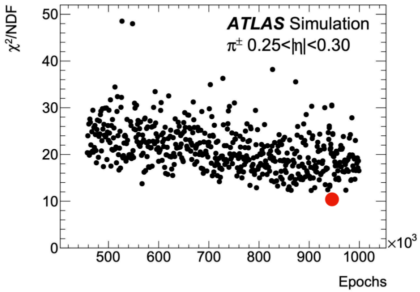
FastCaloGAN: GAN Training

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



FastCaloSim - Energy Interpolation

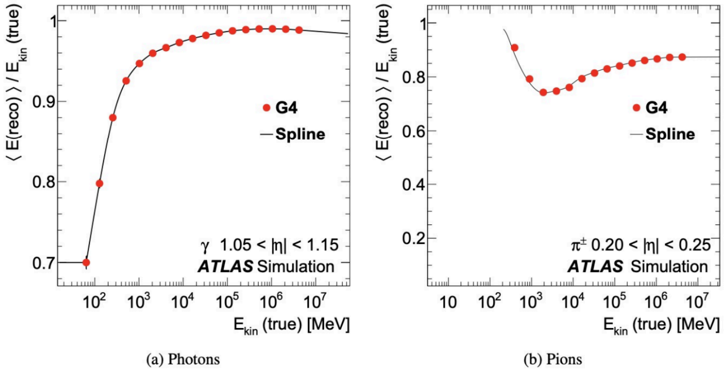
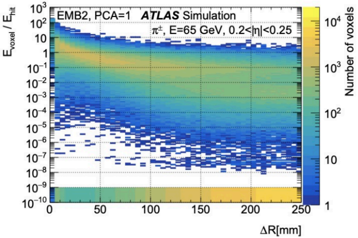
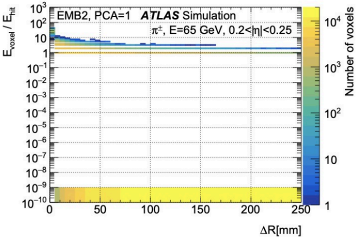


Figure 22: Energy response, defined as the ratio of the reconstructed energy in the calorimeter cells to the kinetic energy of the particle, for (a) photons in $1.05 < |\eta| < 1.10$ and (b) pions in $0.20 < |\eta| < 0.25$. The red dotted points represent the response derived at discrete energies, using 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.

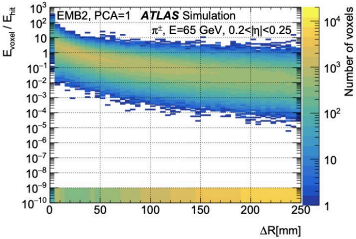
FastCaloSim - Weighted Hits

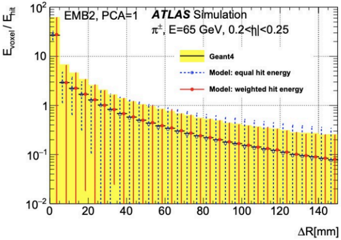


(a) GEANT4



(b) Model: equal hit energy





$Z'(4TeV) \rightarrow tt$