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ATLAS dataset & models

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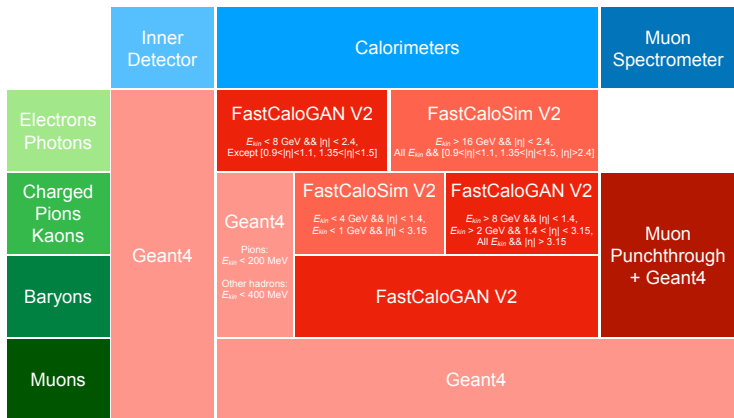
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Structure

- 1 Introduction
- 2 New Dataset
- 3 Machine Learning models
- 4 Performance evaluation

Introduction

AtIFast3



Currently ATLAS uses [AtIFast3](#), a fast calorimeter simulation framework, that employs a mixture of classical parametric simulations (FCSV2) and generative adversarial networks (FastCaloGAN). So far, generative ML models were rarely usable for electromagnetic particles.

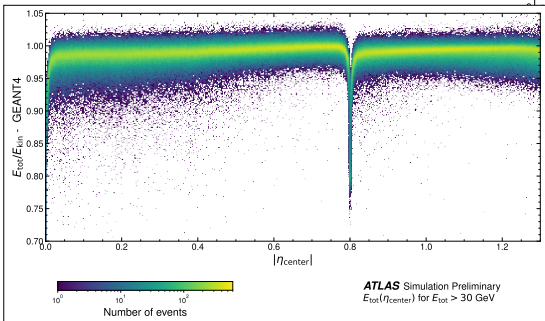
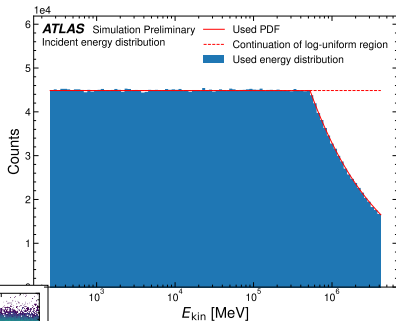
New Dataset

Motivation

- Following the CaloChallenge, ATLAS decided to improve the current AtlFast3 simulation by using more modern ML approaches.
- To transfer the results to the ATLAS calorimeter, a proper training dataset was necessary. The FastCaloGAN voxelization itself never underwent a rigorous optimization and introducing visible artifacts in the fast simulation.

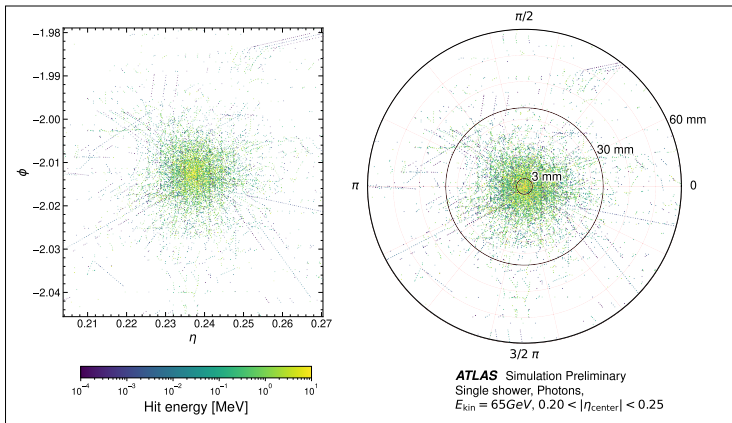
New dataset

- Created 4.05 M new single photon GEANT4 events.
- No calorimeter noise and pileup.
- Photon kinetic energy $256 \text{ MeV} < E_{\text{kin}} < 4.2 \text{ TeV}$.
- Shower center $|\eta_{\text{center}}| < 1.35$.



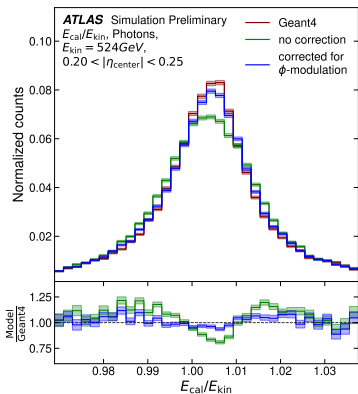
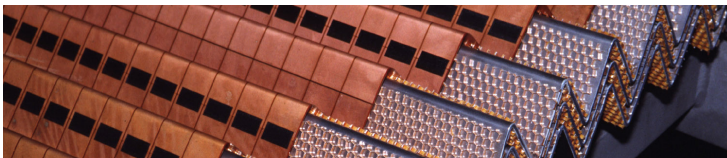
- Critical property: energy response $E_{\text{tot}}/E_{\text{kin}}$, the total deposited energy per event normalized by the kinetic energy of the photon E_{kin} .

Used voxelization for an example shower



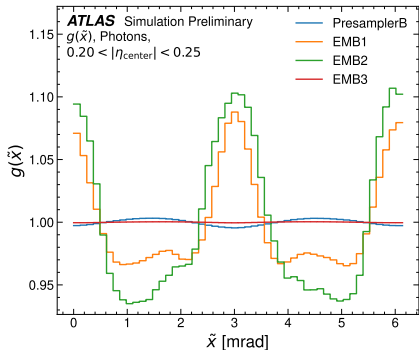
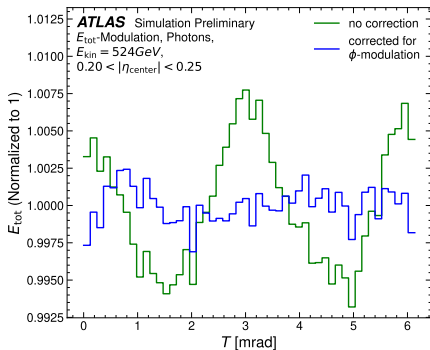
- The dashed red lines indicate the non-uniform voxelization.
- This non-regular voxelization with 382 and a regular voxelization with 1680 voxels, with different use-cases, were performed.
- The publication of these two datasets is approved and we are waiting for CERN OpenData to merge the files into their database.

ϕ -Modulation



- The accordion structure of the ATLAS calorimeter introduces absorber-periodic fluctuations in the calibrated energy response $E_{\text{cal}}/E_{\text{kin}}$.
- By randomly shifting the shower wrt. its original ϕ -position this random modulation is increasing the width of the observed calibrated energy (green curve) compared to GEANT4 (brown curve).
- In the new dataset, this modulation was corrected for as a pre-processing step (blue curve).

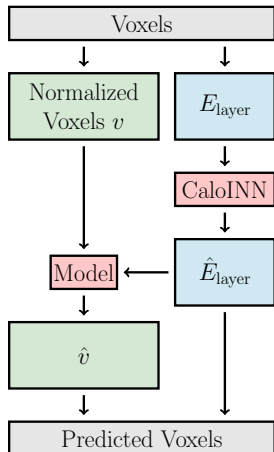
ϕ -modulation



- We minimized the fluctuation of $E_{\text{tot}}(T)$, where T is the distance of the shower center from its corresponding cell center.
- The optimization was performed by fitting a correction curve $g(\tilde{x})$ on hit level, where \tilde{x} is the distance of each hit from its corresponding cell center.

Machine learning models

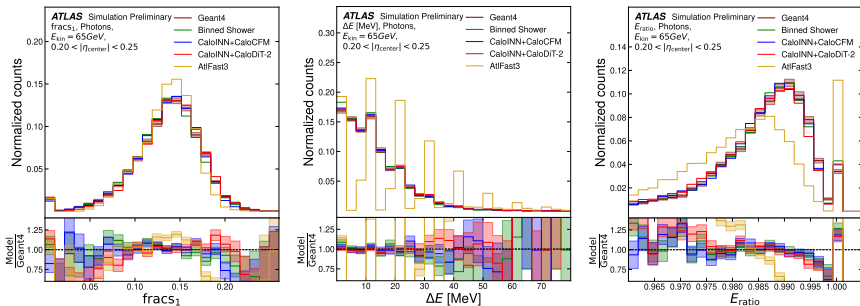
ML setup



- Use a 2-stage training like [CaloFlow](#).
- As energy model the [CaloINN](#) is used.
- As shape models a continuous normalizing flow, trained via conditional flow matching, (CaloCFM) was developed.
- We also trained a diffusion transformer in collaboration with EP-SFT. Peter McKeown is going to talk about the CaloDiT-2 in more detail in the [next talk](#).
- The fully connected CaloCFM, conceptually inspired by [CaloDREAM](#), is trained on the non-regular dataset.
- The models were trained on $|\eta_{\text{center}}| < 0.7$ and $0.7 \leq |\eta_{\text{center}}| < 1.35$, respectively. Implementing successful η -conditioning.

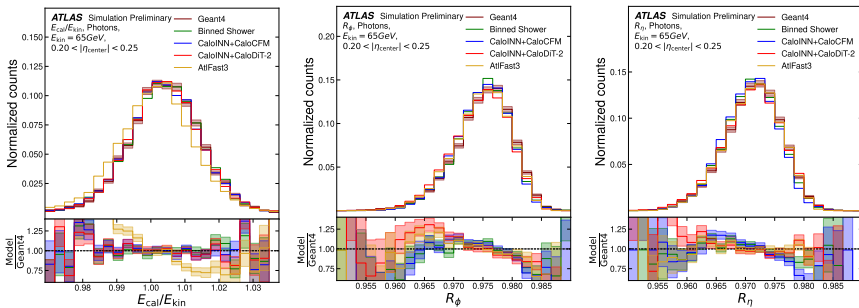
Performance evaluation

Reconstructed shower shapes for $E_{\text{kin}} \sim 65 \text{ GeV}$, $|\eta| \sim 0.2$



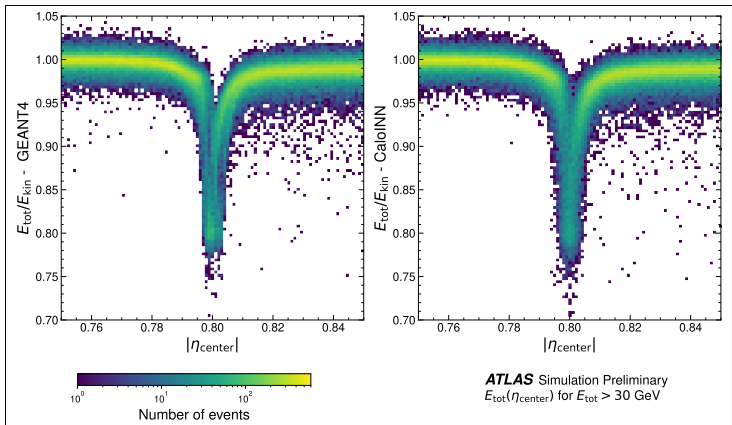
- Depicted: some reconstructed shower shapes sensitive to the high granular first electromagnetic barrel layer - definitions on slide 22.
- The binned shower, using directly the non-regular binning, and the CFM agree (mostly) within the expected Poissonian error with the G4 baseline.
- clear improvement over the currently used AtIFast3.

Reconstructed shower shapes for $E_{\text{kin}} \sim 65 \text{ GeV}$, $|\eta| \sim 0.2$



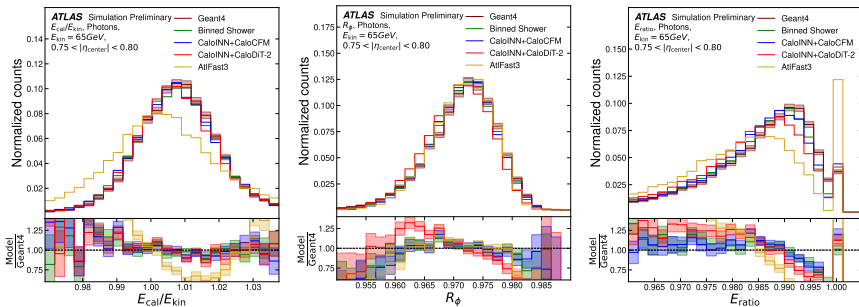
- Depicted: some reconstructed shower shapes sensitive to the calibrated energy and the second electromagnetic barrel layer, which contains the dominant part of the shower energy - definitions on slide 22.
- As before agreement with the G4 baseline.
- AtlFast3 calibrated energy response $E_{\text{cal}}/E_{\text{kin}}$ difference due to not perfectly matched reconstruction versions.

Raw total energy for $|\eta| \sim 0.8$



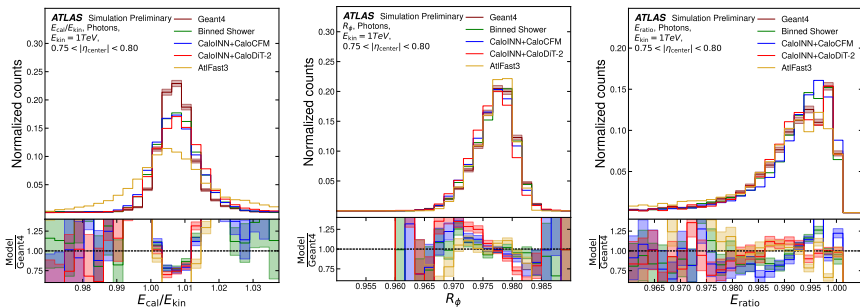
- Depicted: CaloINN prediction of the energy response $E_{\text{tot}}/E_{\text{kin}}$.
- Highly accurate energy modeling, even in the difficult region $|\eta_{\text{center}}| \sim 0.8$ (transition point of calorimeter structure).

Reconstructed shower shapes for $E_{\text{kin}} \sim 65 \text{ GeV}$, $|\eta| \sim 0.8$



- Depicted: some reconstructed shower shapes for the “difficult” region $|\eta_{\text{center}}| \sim 0.8$ - definitions on slide 22.
- Strong improvements over AtI Fast3 due to η -conditioning.

Reconstructed shower shapes for $E_{\text{kin}} \sim 1 \text{ TeV}$, $|\eta| \sim 0.8$



- Depicted: some reconstructed shower shapes for the “difficult” region $|\eta_{\text{center}}| \sim 0.8$ at higher energies as worst case example - definitions on slide 22.
- E_{cal} -problems more pronounced due to smaller width. Small ϕ -modulation problems visible.
- E_{ratio} shows small deviations for the non-regular binning. Currently, they are not considered problematic.

Conclusion

- A new calorimeter shower dataset, featuring two different voxelizations, was created and is expected to be published in the near future.
- Using these datasets, directly, the GEANT4 sim of EM particles in the ATLAS calorimeter can be reproduced with little to no artifacts.
- The dataset itself can be learned and reproduced by current state-of-the-art ML models with high accuracy.

Questions?

Backup

Shower Shape definitions

Definition of the investigated shower shapes. E_{ijk} denotes the energy sum of the $j \times k$ cells within layer i , within a $j \times k$ rectangle around the cell with the highest energy. j corresponds to the η -direction and k to the ϕ -direction.

Observable	Description
E_{cal}	The calibrated energy response
ΔE	Difference between the second 3-cell-wide energy maximum in EMB1 and the cell with the lowest energy that corresponds to either the first or second maximum
E_{ratio}	Ratio between A, the difference between the brightest cell in EMB1 and the second 3-cell-wide energy maximum in EMB1, and B, the sum of these two values
frac_{s1}	$\frac{E_{117} - E_{113}}{E_{113}}$ - Ratio of the outer shower to the inner shower in EMB1
R_{ϕ}	$\frac{E_{237}}{E_{277}}$ - Ratio, describing the energy decay in ϕ -direction in EMB2
R_{η}	$\frac{E_{233}}{E_{237}}$ - Ratio, describing the energy decay in η -direction in EMB2

Benchmarks

	CaloCFM (small/large)	CaloDiT-2
# Params	3.3 M / 6.1 M	2.1 M
Memory (MB)	75 / 176	59
Time / Photon (ms)	4.87 ± 0.05 / 9.62 ± 0.05	12.75 ± 0.05

Some preliminary benchmarks on the new generative models. The large CaloCFM was used for $0.7 \leq |\eta_{\text{center}}| < 1.35$, to better capture the strong η -dependence. The smaller model was not performing much worse and might be an alternative in case of memory or runtime constraints. The measurement was performed on an AMD EPYC 9654 CPU using a batch size of one. The CaloINN is included in the timing and memory measurements of both models.

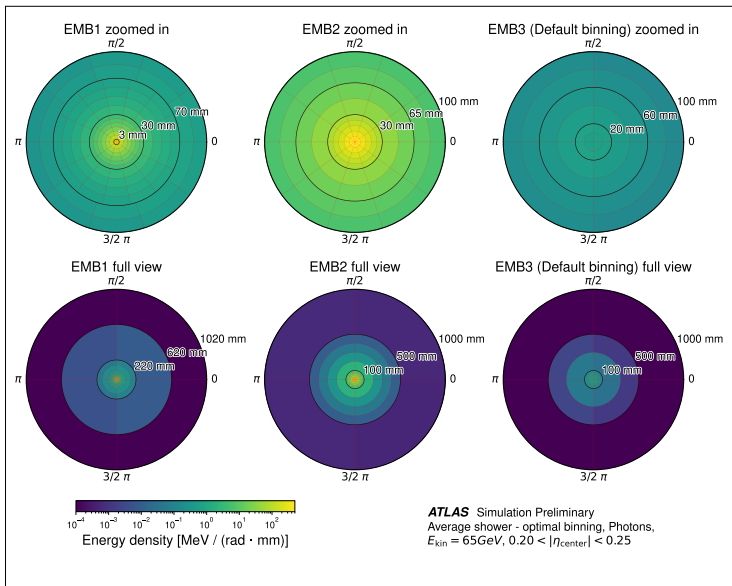
Non-regular voxelization

Ring [mm]	EMB1		Ring [mm]	EMB2	
	n_α	$\Delta r[\text{mm}]$		n_α	$\Delta r[\text{mm}]$
0 – 3	4	1.0	0 – 30	10	6.0
3 – 30	10	4.5			
30 – 70	14	10.0	30 – 100	10	17.5
70 – 100	10	15.0			
100 – 220	4	60.0	100 – 500	4	100.0
220 – 1020	4	400.0			
			500 – 1000	4	500.0

Non-regular voxelization

Ring [mm]	Default	
	n_α	Δr [mm]
0 – 20	4	10.0
20 – 100	4	20.0
100 – 500	4	200.0
500 – 1000	4	500.0

Non-regular voxelization - Voxelized average shower

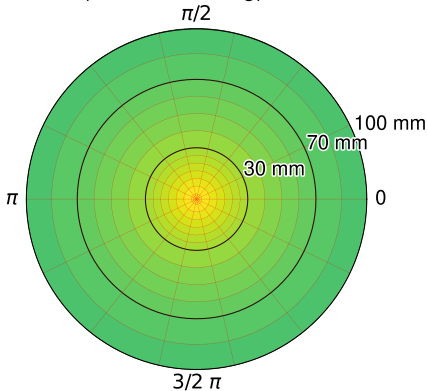


Regular voxelization

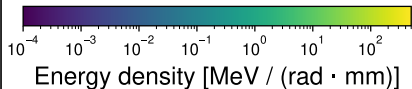
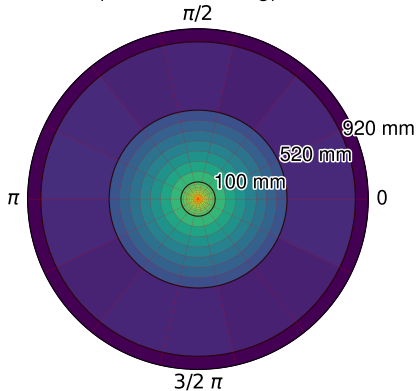
Ring [mm]	Default	
	n_α	Δr [mm]
0 – 3	14	1.0
3 – 30	14	4.5
30 – 70	14	10.0
70 – 100	14	15.0
100 – 520	14	60.0
520 – 1320	14	400.0

Regular voxelization - Voxelized average shower

EMB2 (Default binning) zoomed in



EMB2 (Default binning) full view



ATLAS Simulation Preliminary
Average shower - regular binning, Photons,
 $E_{\text{kin}} = 65\text{GeV}$, $0.20 < |\eta_{\text{center}}| < 0.25$