

```
* *****  
* Welcome to lxplus706.cern.ch, CentOS Linux release 7.9.2009 (Core)  
* Archive of news is available in /etc/motd-archive  
* Reminder: you have agreed to the CERN  
* computing rules, in particular OC5. CERN implements  
* the measures necessary to ensure compliance.  
* https://cern.ch/ComputingRules  
* Puppet environment: production, Roger state: production  
* Foreman hostgroup: lxplus/nodes/login  
* Availability zone: cern-geneva-c  
* LXPLUS Public Login Service - http://lxplusdoc.web.cern.ch/  
* A CentOS based lxplus8.cern.ch is now available  
* A CentOS based lxplus9.cern.ch is  
* Please read LXPLUS Privacy Notice  
* *****
```

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lsetup  
lsetup asetup  
lsetup astyle  
lsetup atlantis  
lsetup client  
lsetup emi  
lsetup <tool1> [ <tool2> ... ] (see  
(or asetup) to setup in Athena rel  
ATLAS style macros  
Atlantis: event display  
Event Index  
EMI: grid middleware user interfac  
job definition and manage  
v: setup tool from cvmfs SFT  
Production and Distributed  
ATLAS Metadata Interface py  
data processing framework  
distributed data management system  
to a full LCG release  
D local proxy cache  
D data access  
tools menu  
static tools menu  
elp  
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ersions of installed software
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Fast Simulation in ATLAS: Overview and Latest Updates

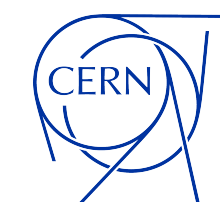
ATLAS Italy Computing Annual Meeting

Federico A.G. Corchia
University of Bologna
and INFN Bologna

Bologna, 16 December 2025

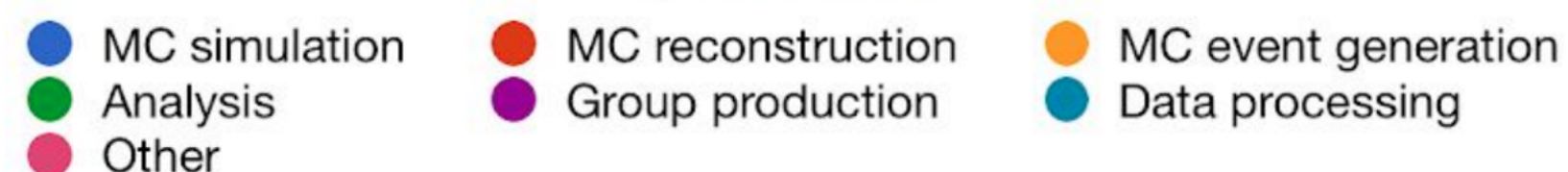
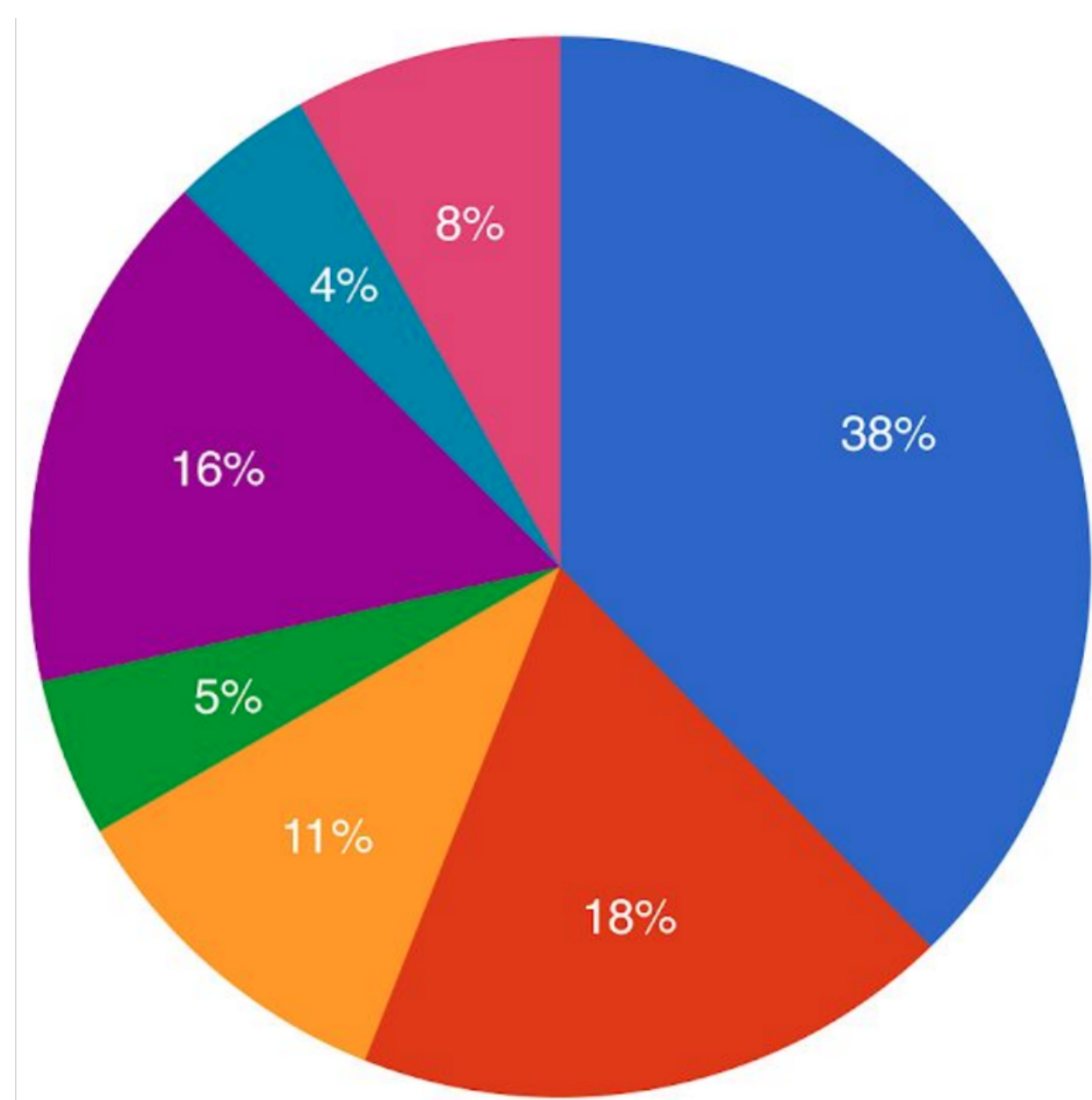


ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA



Introduction

Calorimeter Simulation and Computational Load



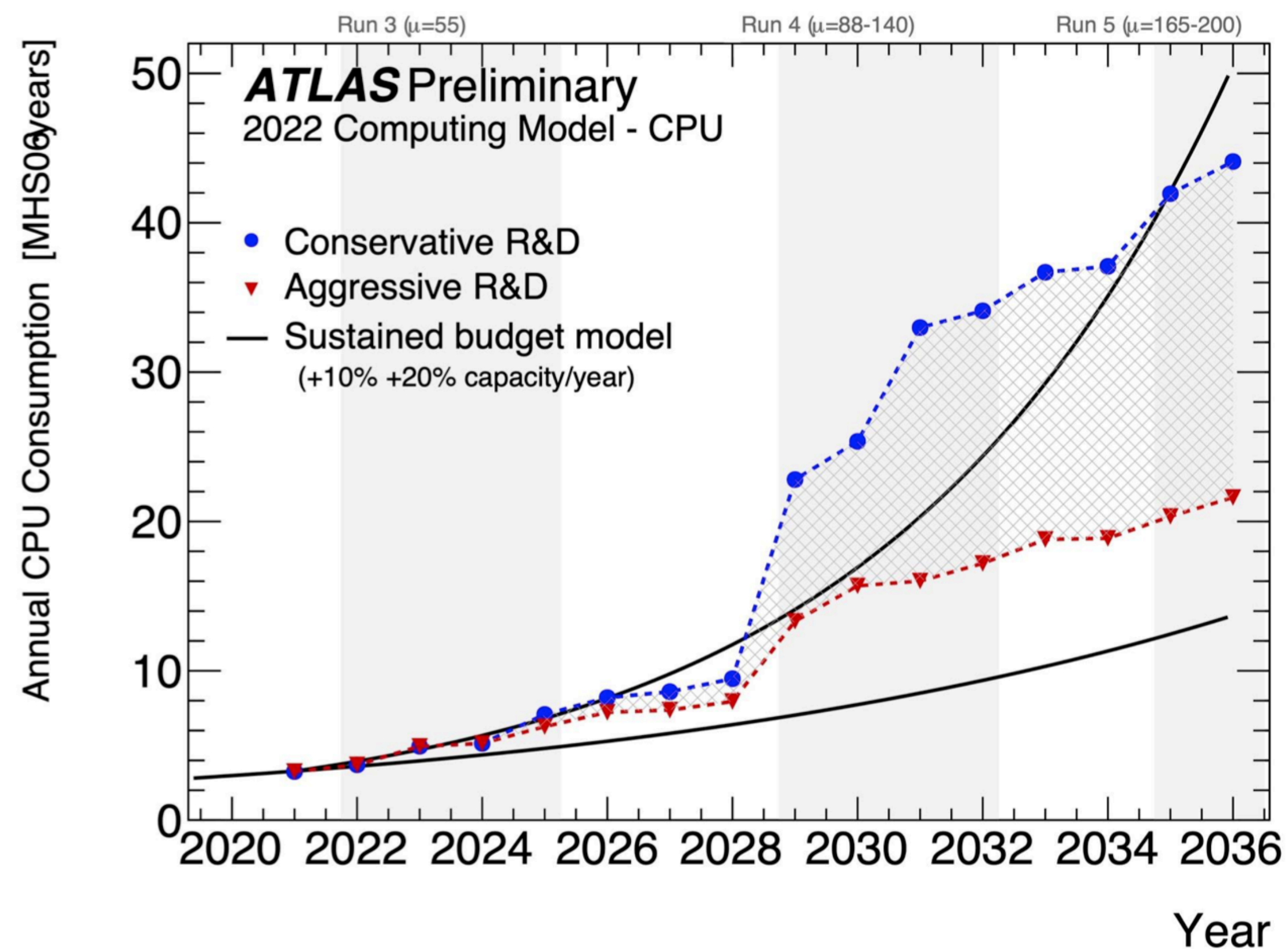
CPU-hours taken by ATLAS activities

The ATLAS Coll., *ATLAS HL-LHC Computing Conceptual Design Report*,
[CERN-LHCC-2020-015](#) (2020)

- MC simulation of detector response is a **major computing challenge** at LHC experiments!
- A **large part** of the resources taken by detector simulation is taken by **calorimeter simulation** (~80% of CPU consumption for $t\bar{t}$ processes).

Introduction

Calorimeter Simulation and Future Computational Load



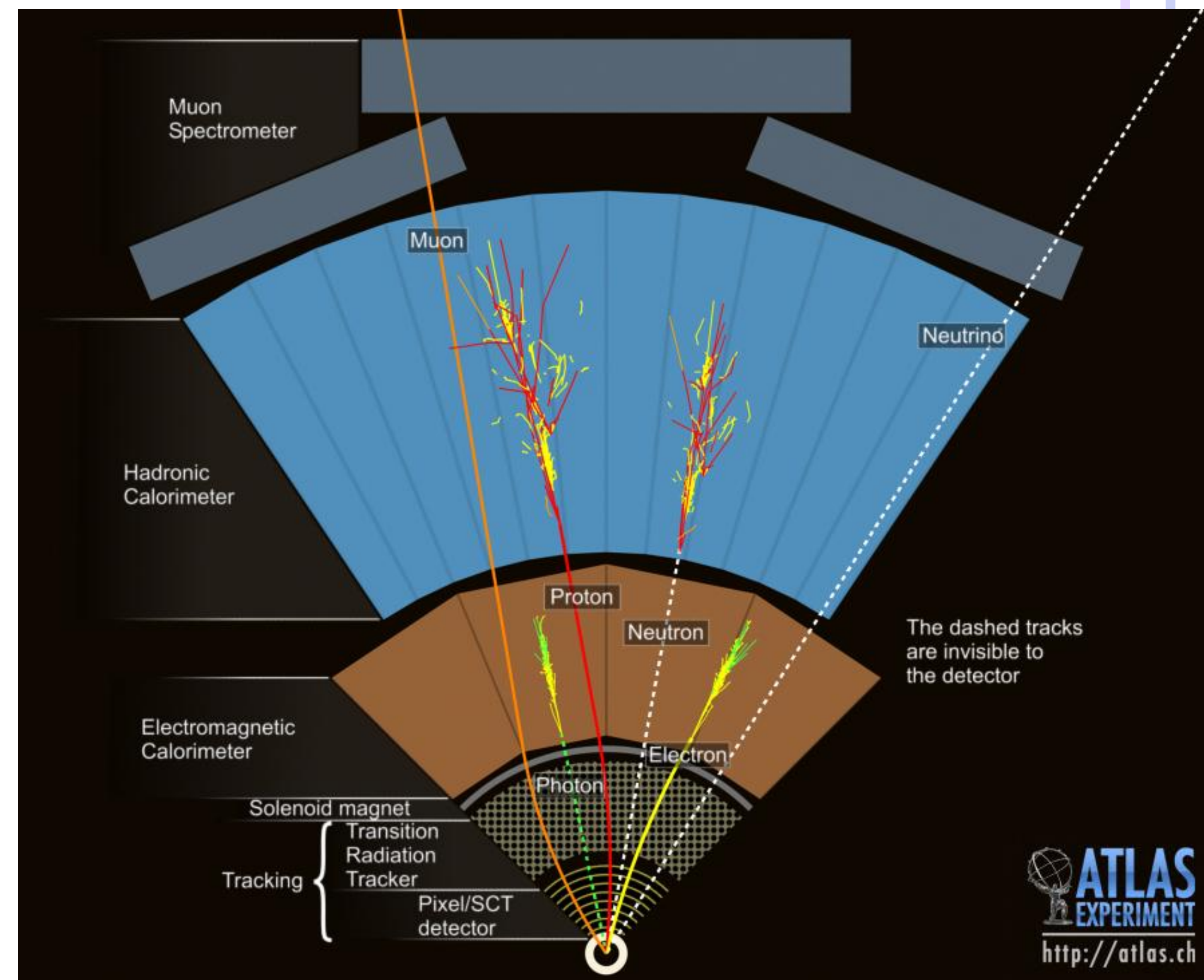
- CPU needs are expected to **increase** during Run 3 and in view of Run 4 → significant R&D required to keep up!
- Solutions needed → **fast simulation!**

The ATLAS Coll., *ATLAS Software and Computing HL-LHC Roadmap*,
[CERN-LHCC-2022-005](#) (2022)

AtlFast3

The ATLAS Fast Simulation Tool

- **Fast simulation tools:** able to simulate calorimeter response faster than the (“traditional”) full process simulation tool Geant4 but keeping high accuracy.
- **AtlFast3:** the fast simulation tool developed by ATLAS.
 - Introduced for Run 2 and further improved for Run 3. Already in production for Run 3.
 - It replaces the slow propagation and interactions of incident particles inside the calorimeter volume with the direct generation of energy deposits based on an underlying parametrisation.
 - Uses a simplified geometry of the calorimeter cells to simplify its complex and non-homogeneous structure.



cds.cern.ch/record/1096081

AtlFast3

Components

- Employs two fast simulation approaches:
 - **FastCaloSim V2**: **parametric** approach for shower development;
 - **FastCaloGAN V2**: based on **Generative Adversarial Networks (GANs)**.
- AtlFast3 runs fast simulation through one of the two approaches, depending on which one **returns the best simulation** (i.e. the most accurate with respect to Geant4) for the type of the particle initiating the shower, its energy and η .

Geant4 still used to simulate all particles in the Inner Detector, low energy hadrons in the calorimeters and muons.

Muon Punchthrough (the spray of particles into the Muon Spectrometer resulting from late interacting high-energy hadrons) is modelled with a tool based on DNNs.

	Inner Detector	Calorimeters		Muon Spectrometer	
Electrons Photons	Geant4	FastCaloGAN V2 $E_{kin} < 8 \text{ GeV} \ \&\& \ \eta < 2.4,$ Except $[0.9 < \eta < 1.1, 1.35 < \eta < 1.5]$	FastCaloSim V2 $E_{kin} > 16 \text{ GeV} \ \&\& \ \eta < 2.4,$ All $E_{kin} \ \&\& \ [0.9 < \eta < 1.1, 1.35 < \eta < 1.5, \eta > 2.4]$		
Charged Pions Kaons		Geant4 Pions: $E_{kin} < 200 \text{ MeV}$ Other hadrons: $E_{kin} < 400 \text{ MeV}$	FastCaloSim V2 $E_{kin} < 4 \text{ GeV} \ \&\& \ \eta < 1.4,$ $E_{kin} < 1 \text{ GeV} \ \&\& \ \eta < 3.15$	FastCaloGAN V2 $E_{kin} > 8 \text{ GeV} \ \&\& \ \eta < 1.4,$ $E_{kin} > 2 \text{ GeV} \ \&\& \ 1.4 < \eta < 3.15,$ All $E_{kin} \ \&\& \ \eta > 3.15$	Muon Punchthrough + Geant4
Baryons		FastCaloGAN V2			
Muons		Geant4			

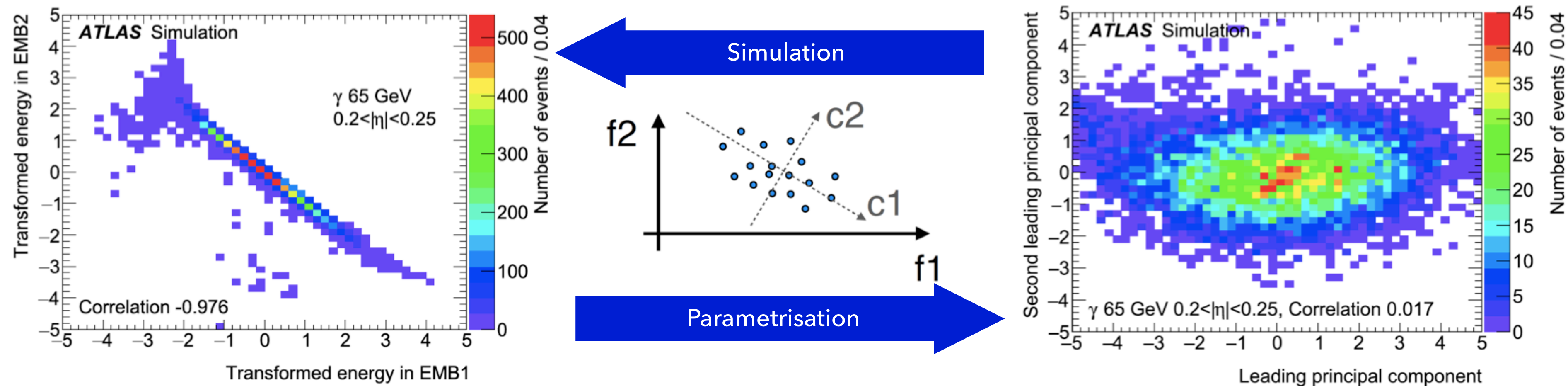
The ATLAS Coll., *Software and computing for Run 3 of the ATLAS experiment at the LHC*,
Eur. Phys. J. C **85**, 234 (2025)

AtFast3

FastCaloSim V2

- **Parametrised** modelling using Geant4 single photon, electron and charged pion samples in 17 logarithmically spaced energy bins from 64 MeV to 4 TeV and 100 linearly spaced bins in $|\eta|$ from 0 to 5.
- **Separate** parametrisation of longitudinal and lateral shower development:
 - **Energy in layers** decorrelated through Principal Component Analysis (PCA);
 - **Average lateral energy distribution** parametrised as 2D probability functions.

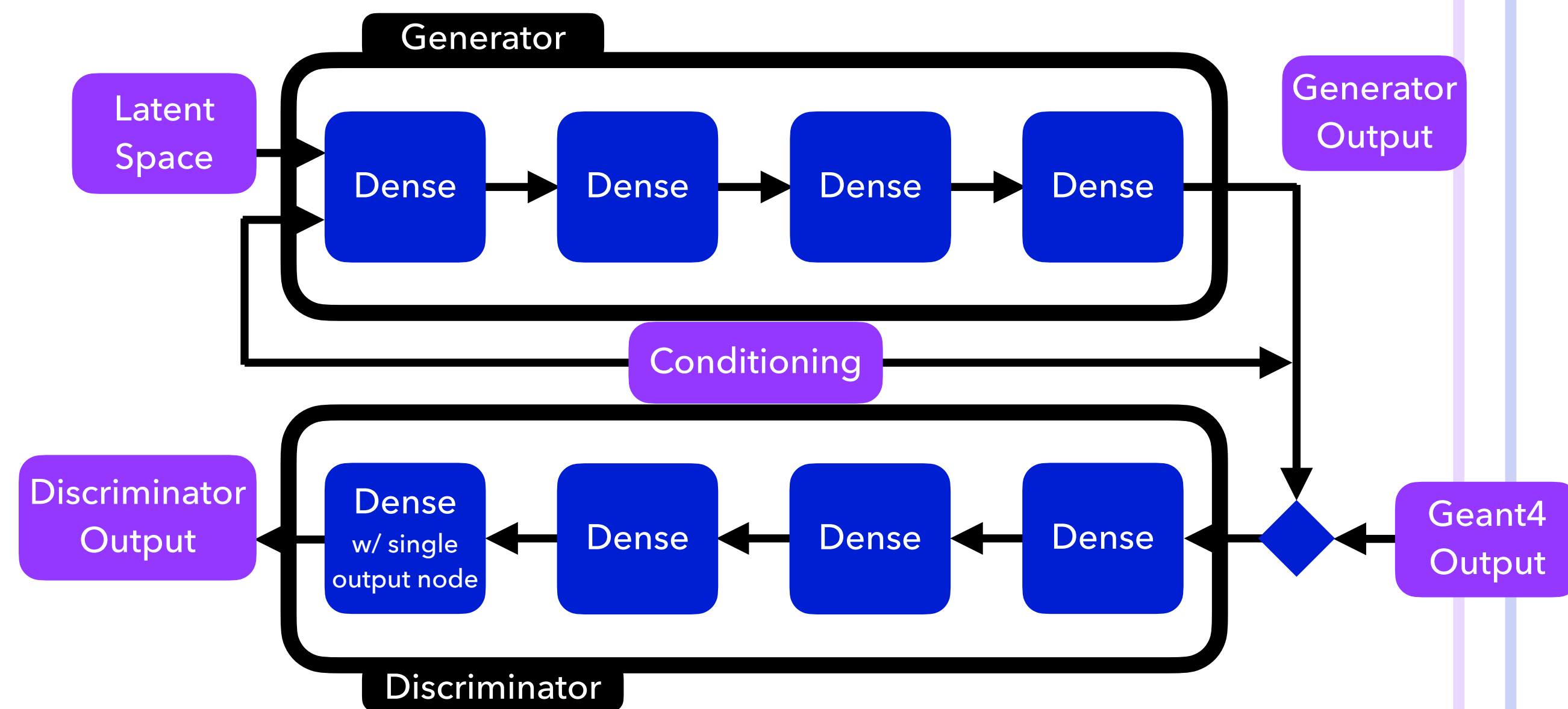
ATLAS Coll., *AtFast3: The Next Generation of Fast Simulation in ATLAS*,
Comput Softw Big Sci **6**, 7 (2022)



AtlFast3

FastCaloGAN V2

- Based on **Wasserstein GANs** with gradient penalty
I. Gulrajani, F. Ahmed, M. Arjovsky, V. Dumoulin and A. Courville,
Improved Training of Wasserstein GANs, [arXiv:1704.00028](https://arxiv.org/abs/1704.00028) [cs.LG]
(2017)
- **Simultaneous training of two neural networks** (i.e. the typical GAN structure):
 - **Generator**: aims to generate sample the most similar to Geant4 datasets;
 - **Discriminator**: aims to distinguish Geant4 samples from the ones produced by the generator.
- When reached an **equilibrium** between the two, the generator is ready to simulate!
- Trained on e^- , γ , p , π^\pm as incident particles on each of the 100 bins in $|\eta|$, with conditioning on truth momentum. Calorimeter hits grouped into *voxels* (= 3D bins).
- Already **widely used** in AtlFast3!

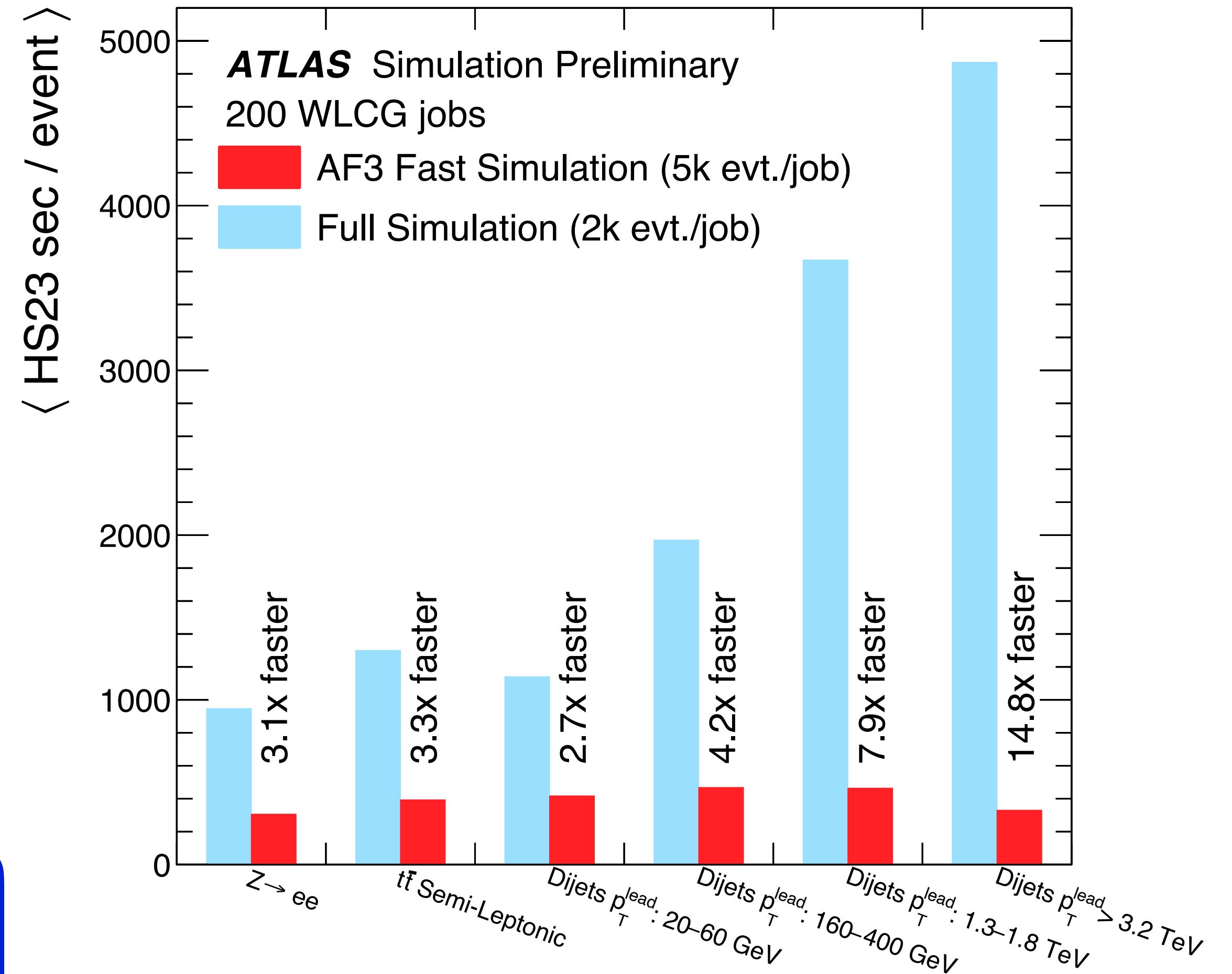


AtlFast3

Computing Performance

- **3** (for $Z \rightarrow ee$ events) to **15** (for high- p_T dijet events) **times faster** than Geant4 (simulation of the ATLAS detector for Run 3 for 2023 data taking)!
- Only needing on average **20% of CPU** with respect to Geant4!

Simulation time in AtlFast3 dominated by full simulation of the Inner Detector.



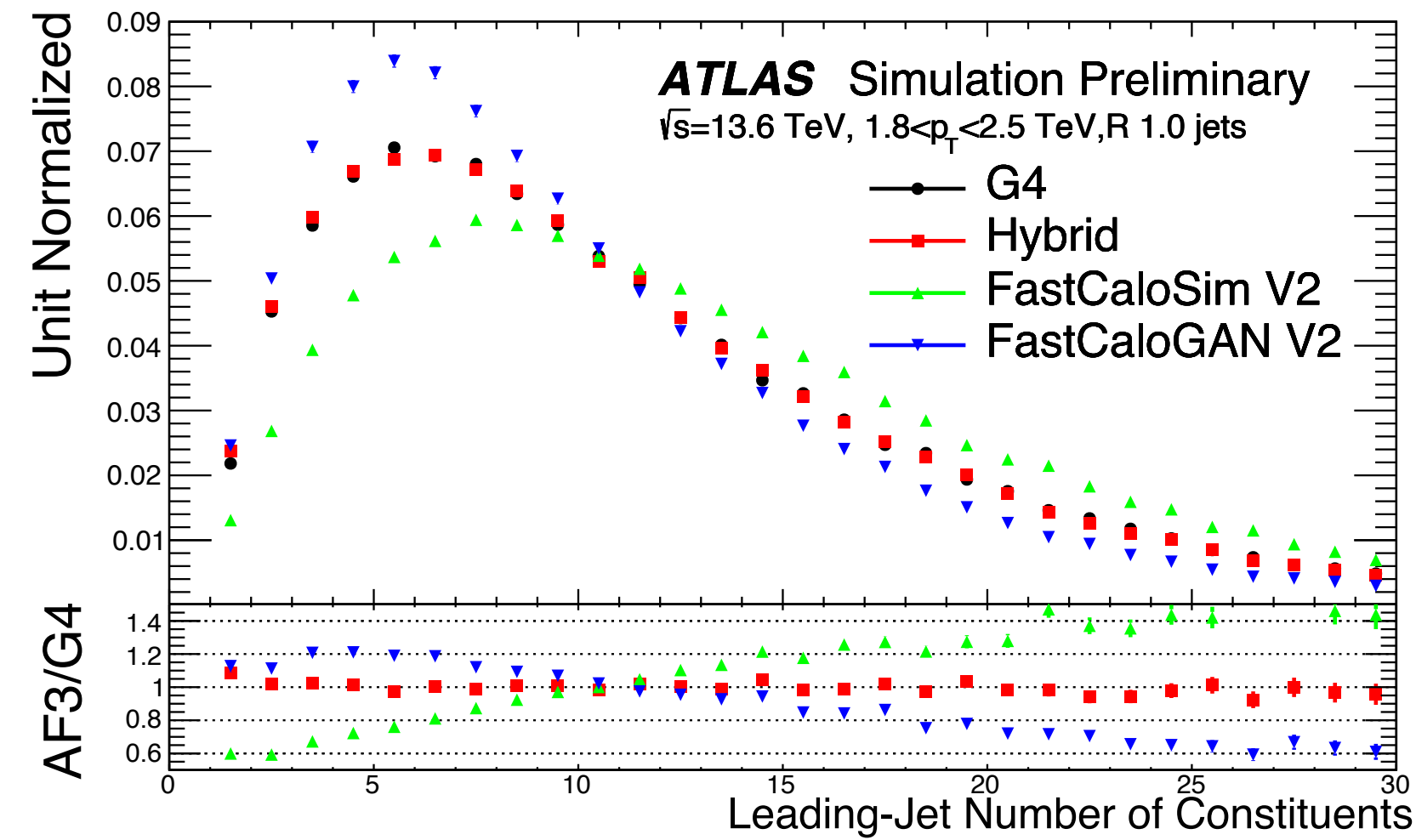
ATLAS-SIM-2023-005

AtFast3

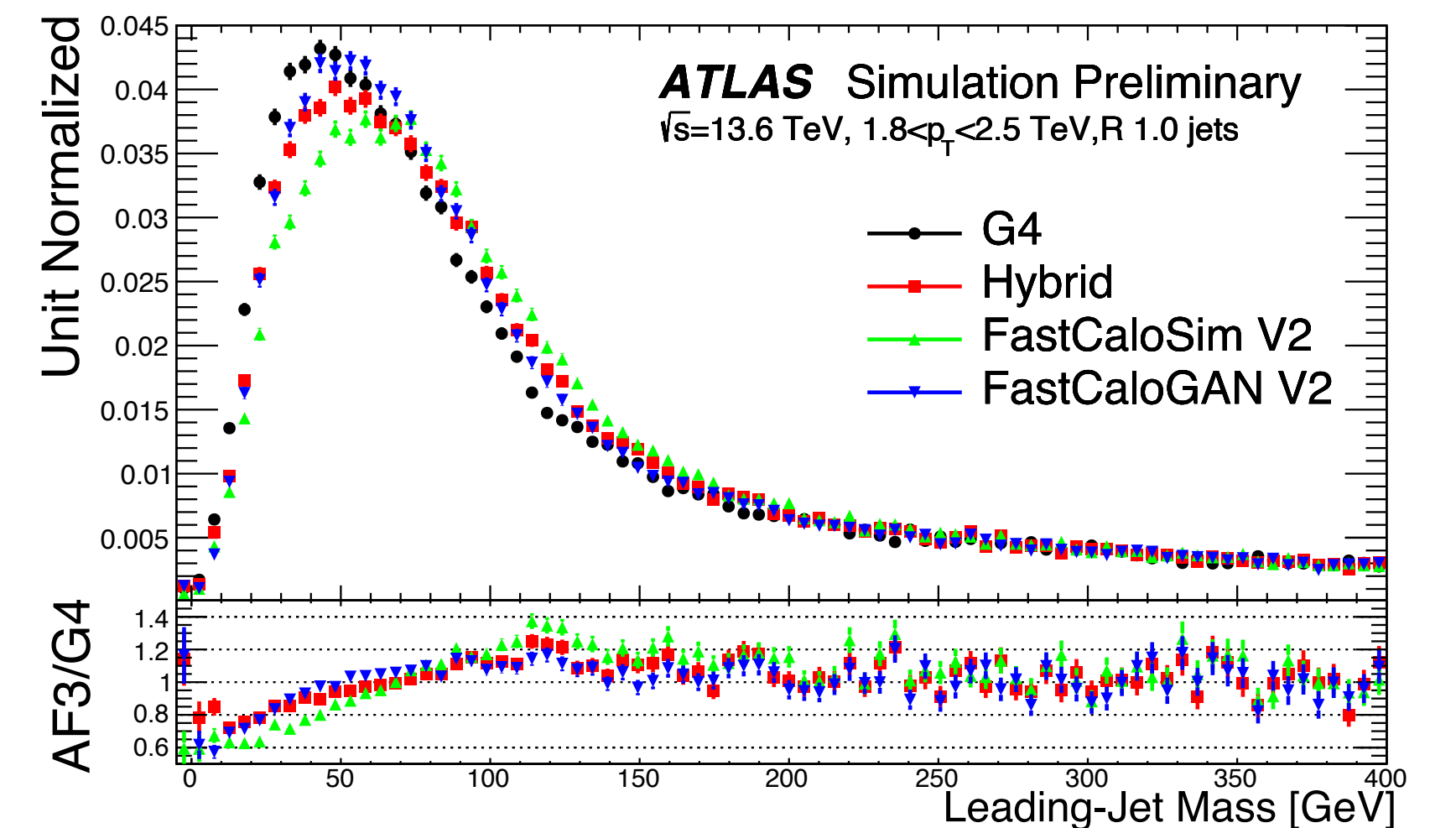
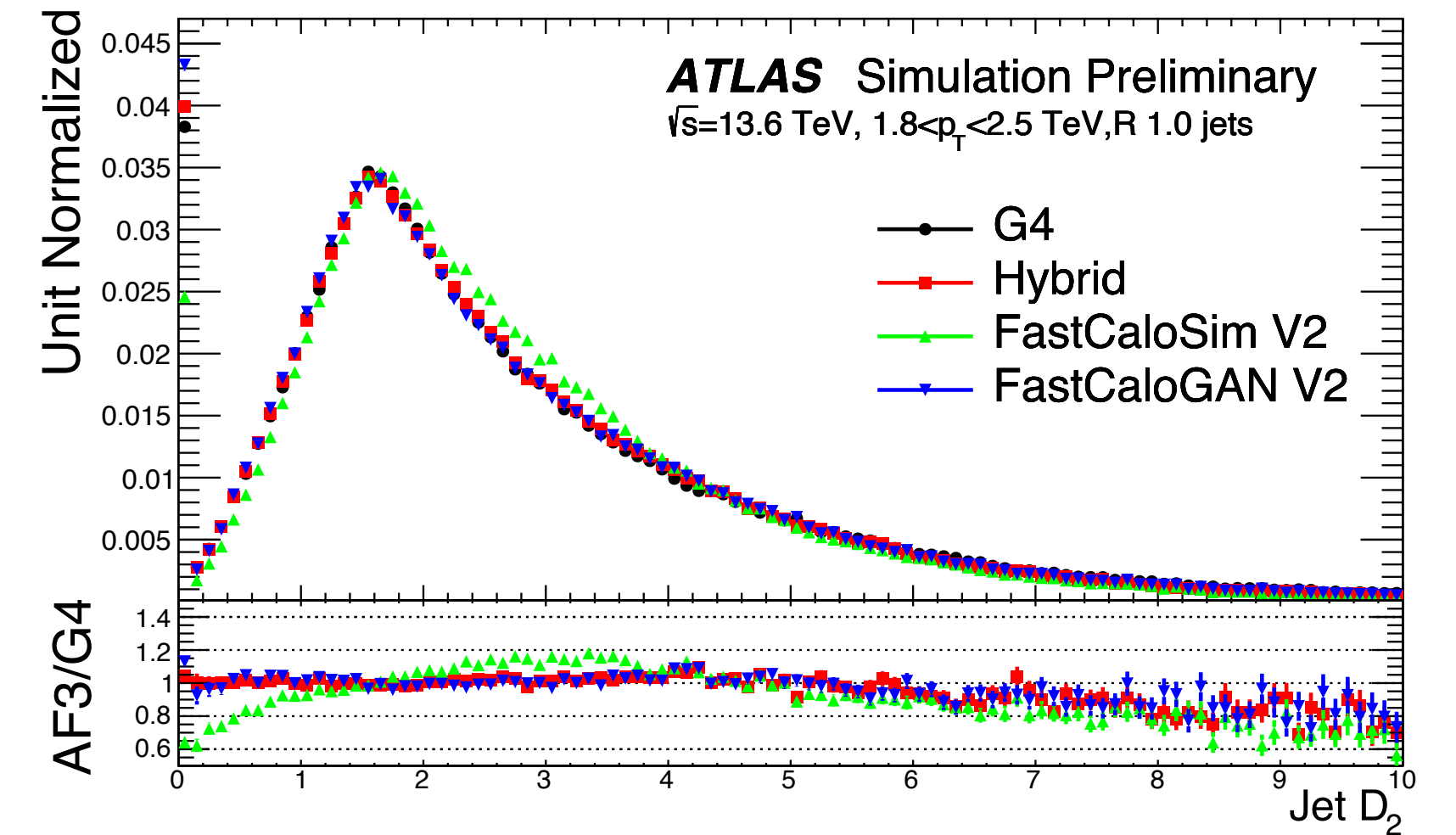
Physics Performance

All plots here from
ATLAS-SIM-2023-004

- For most observables used in Physics analyses, AtFast3 and Geant4 **agree within a few %**.
- AtFast3 can be used **for almost every analysis** (either signal or background).
- Aggressive 2022 computing model (plot in slide 3) assumes that **90%** of all simulation **is fast simulation** in Run 4 (remaining 10% is full simulation input samples used for training) → need of **more precise AtFast3!**



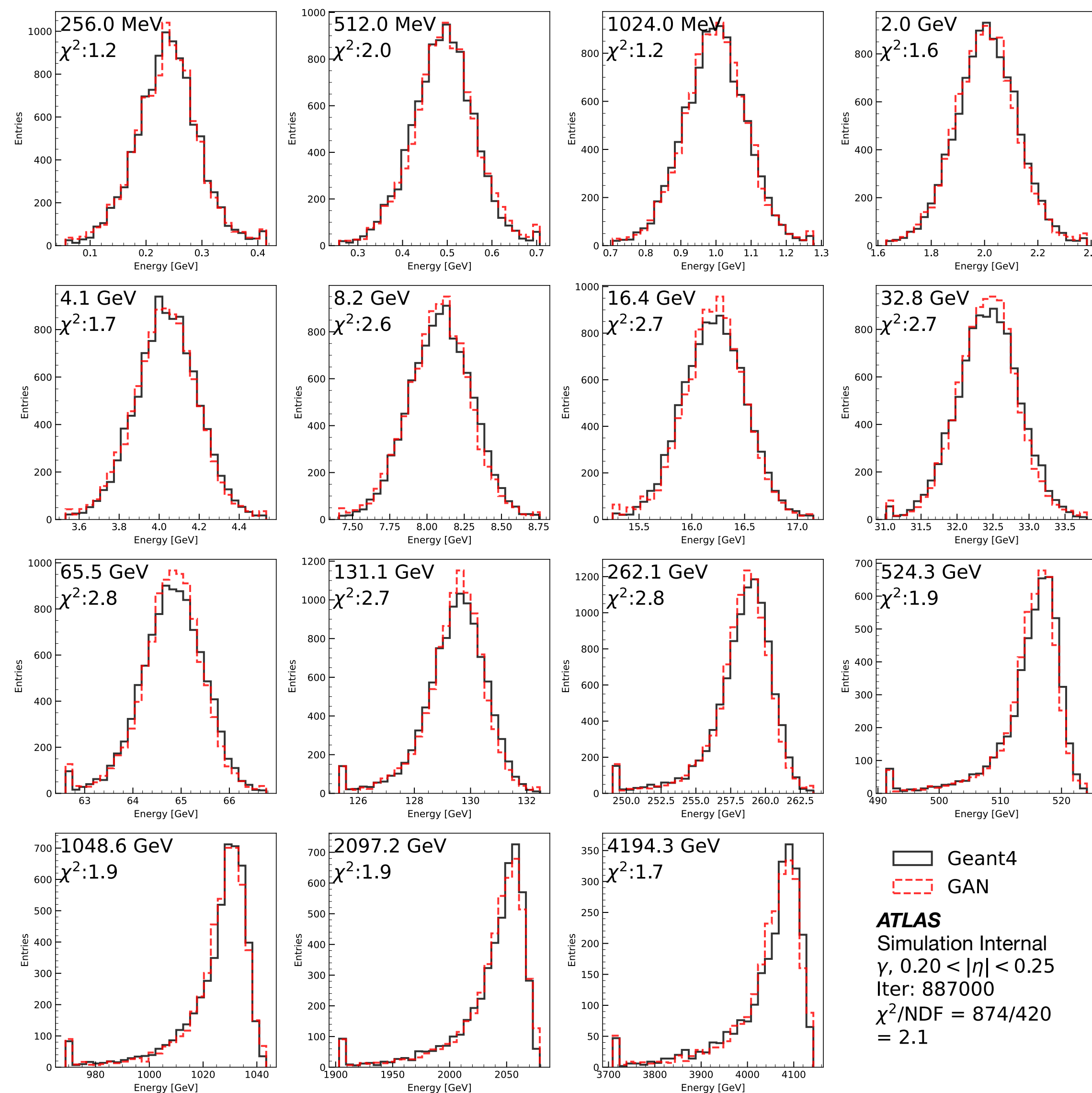
Hybrid = usage of FastCaloSim V2 or FastCaloGAN V2 depending on particle type, energy and η as per diagram in slide 5 (instead of just one of them for all cases)



New ML Models

Improved FastCaloGAN V2

- FastCaloGAN V2 has been **further improved**:
 - Generator featuring incident energy skip connections;
 - Explicit learning of layer energies and total energy;
 - Individual, disconnected linear output layers, corresponding to different calorimeter layers;
 - Also tested replacing FastCaloGAN components with **transformer blocks** (first prototype developed, needs optimisation).
- However, GANs have trouble modelling properly **shower shapes** for photons!



New ML Models

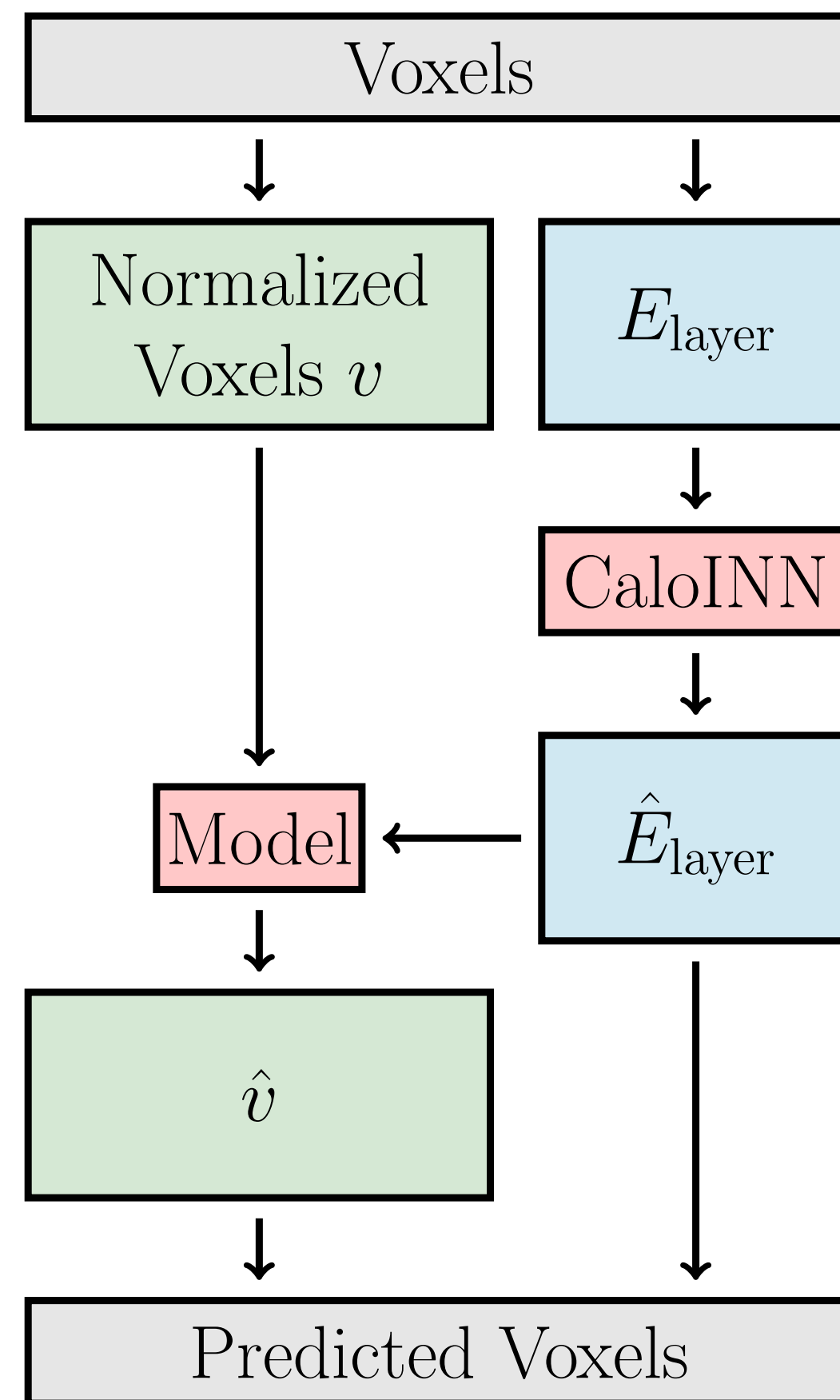
Considerations from the CaloChallenge

- Recently, the **CaloChallenge**, a community challenge to investigate the usage of generative ML models for fast calorimeter simulation, concluded with a community paper Claudius Krause et al., *CaloChallenge 2022: a community challenge for fast calorimeter simulation*, Rep. Prog. Phys. 88 116201 (2025)
- The “winner” models for photons were (continuous) **normalising flows, diffusion models and vision transformers**. They are potential **more expressive** alternatives to GANs, whose trouble when dealing with shower shapes is confirmed also by this paper!
 - Let's apply these conclusions!

New ML Models

Normalising Flows for Photon Simulation

Normalising Flow: transformation of simple probability distribution into a more complex distribution by a sequence of invertible and differentiable mappings.



ATL-SOFT-PUB-2025-003

- Split training into **two stages**:
 - **Layer energies**: learnt with **CaloINN (normalising flow)**;
 - **Shower shapes**: normalising flow trained with 2 approaches:
 - **CaloCFM** (Conditional Flow Matching. Using small, irregular dataset - see next slide);
 - **CaloDiT-2** (diffusion transformer. Using larger, regular dataset - see next slide).
- In both cases, just 2 separate models were needed to cover the 27 η slices.
- Models trained on $|\eta_{\text{centre}}| < 0.7$ and $0.7 \leq |\eta_{\text{centre}}| < 1.35$, respectively. Implementing successful η -conditioning.

New ML Models

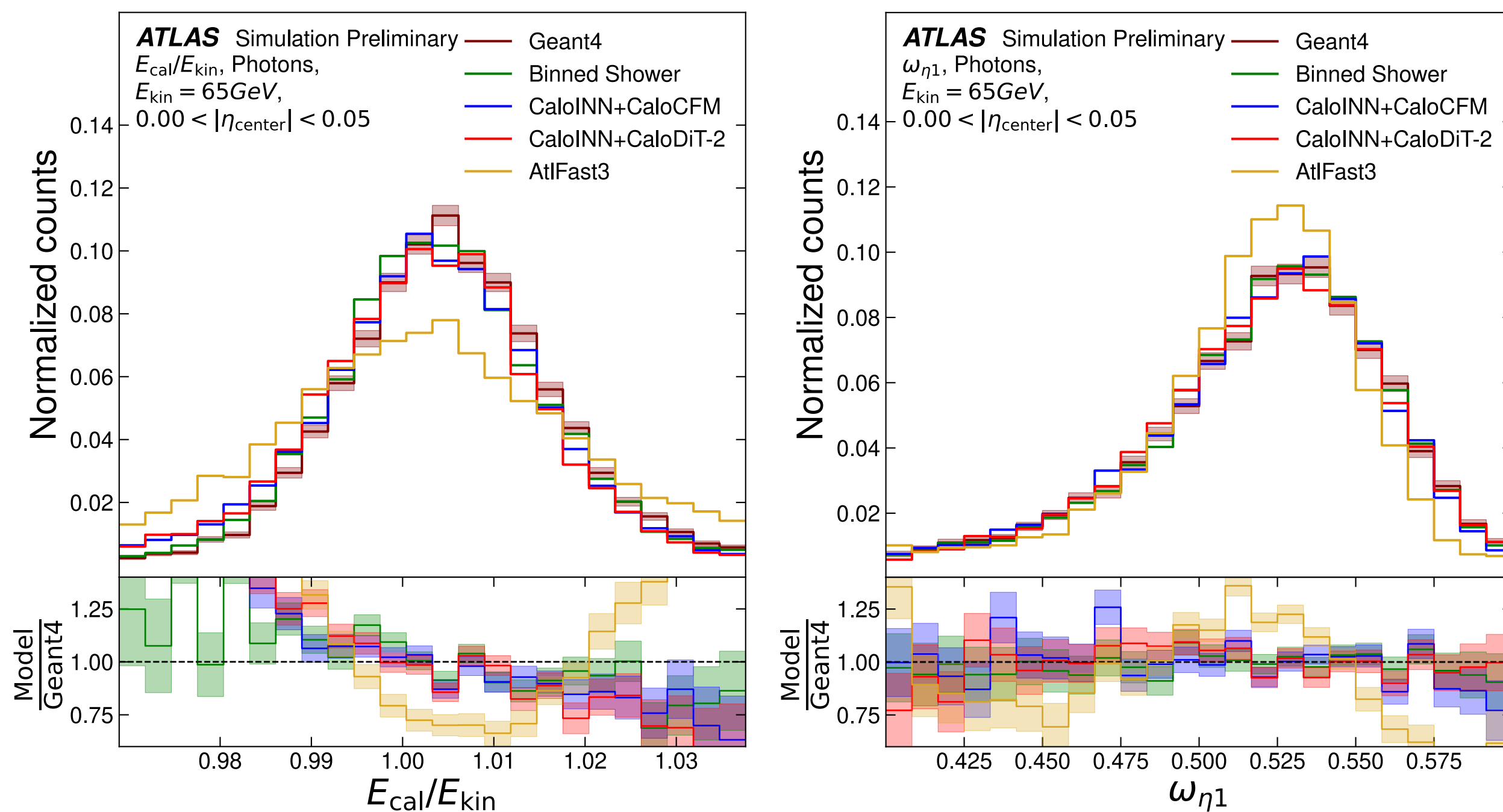
Improved Voxelisation and Dataset for Photons

- New datasets with **improved voxelisation** for photons to reduce bias (an “optimal” smaller one with irregular binning - 382 voxels - and a larger one with regular binning - 1680 voxels).
 - 27 η bins, with 150k events each - 4.05M events in total;
 - Covered kinematics: $|\eta_{\text{centre}}| < 1.35$ $256 \text{ MeV} \leq E \leq 4.2 \text{ TeV}$.
- 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 with respect to its original φ -position this random **φ -modulation is increasing the width of the observed calibrated energy** compared to Geant4.
 - In the new dataset, this modulation is **corrected** for as a pre-processing step. Eases later generative model training.

New ML Models

Physics Performance

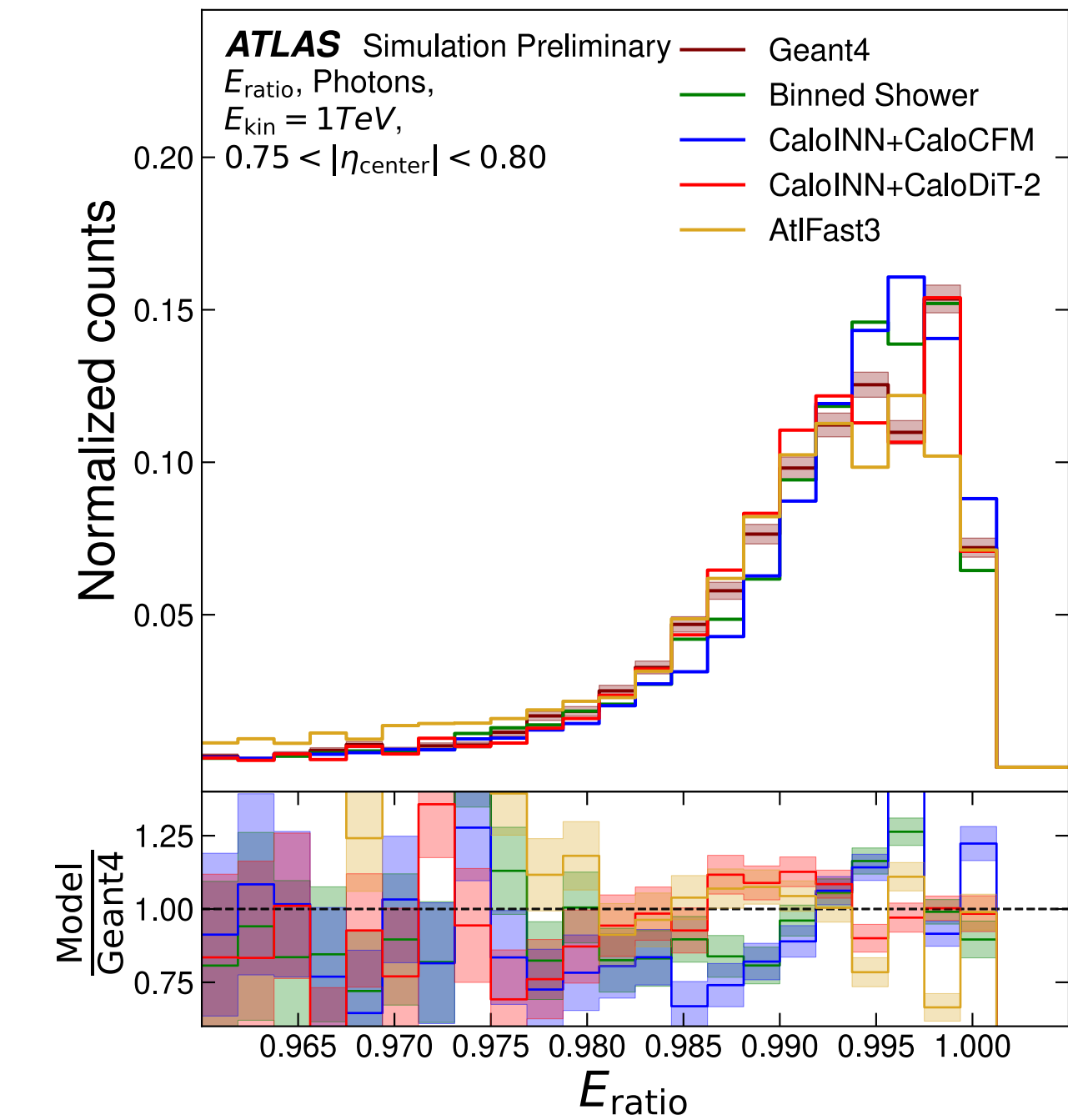
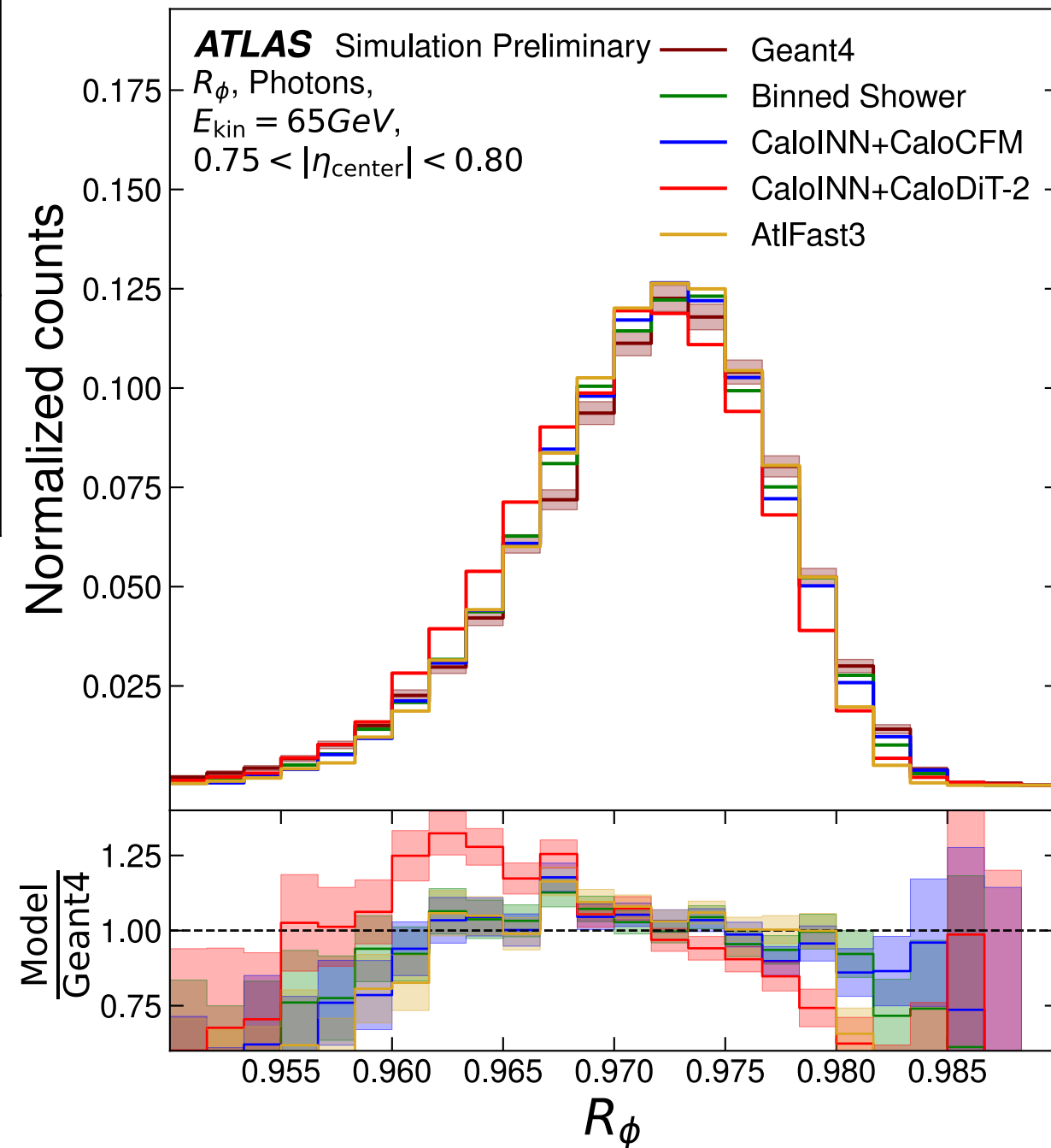
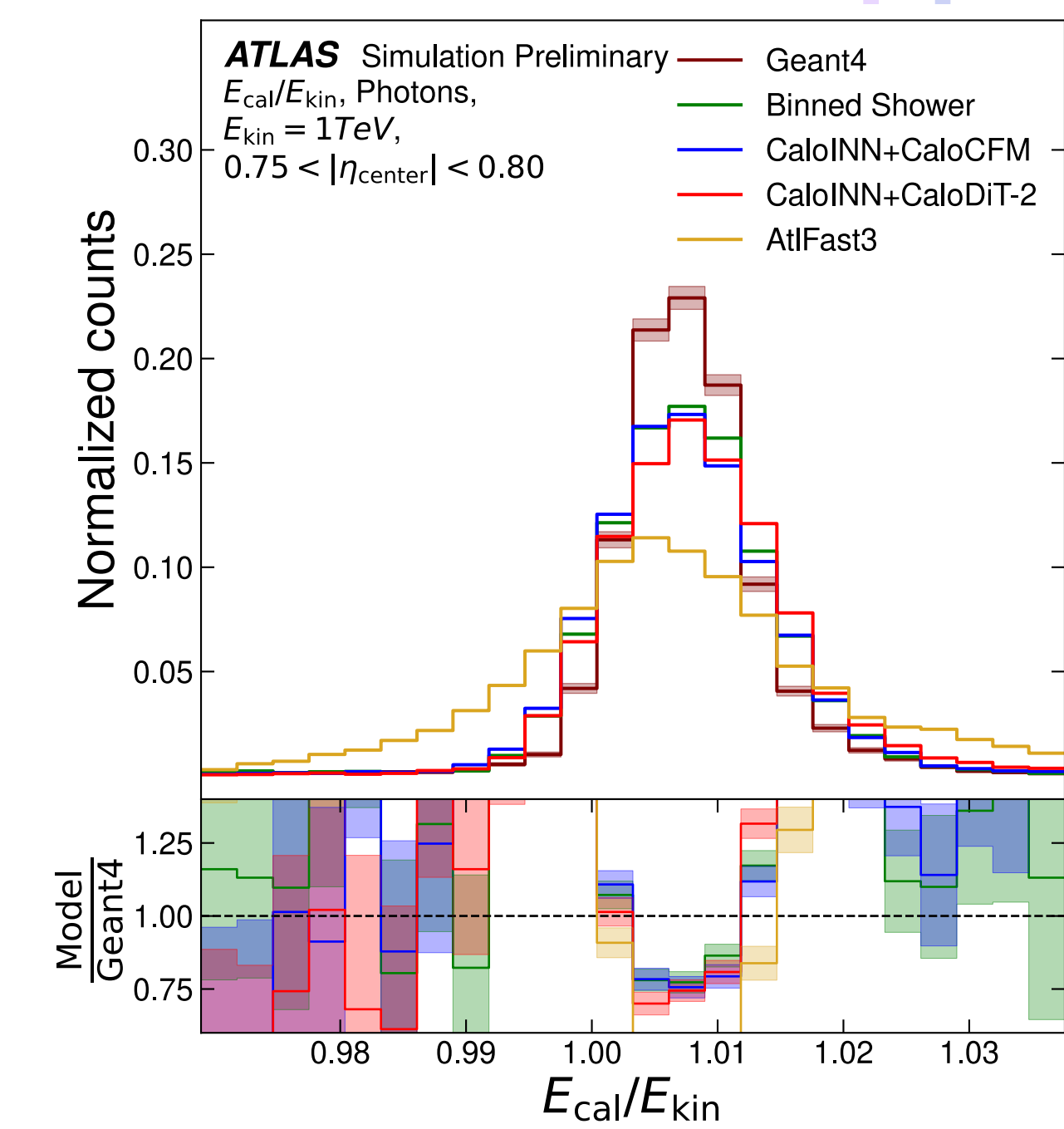
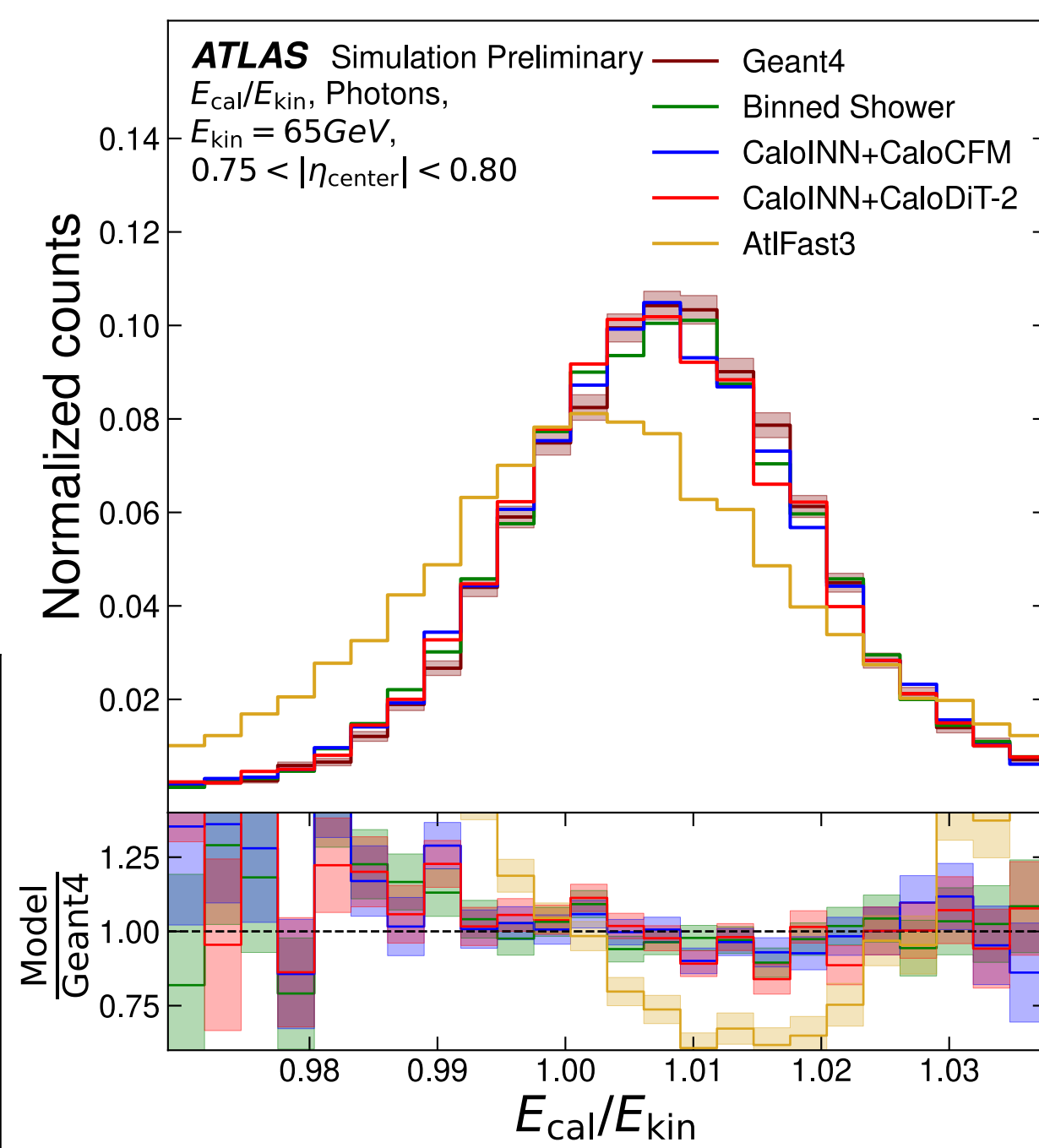
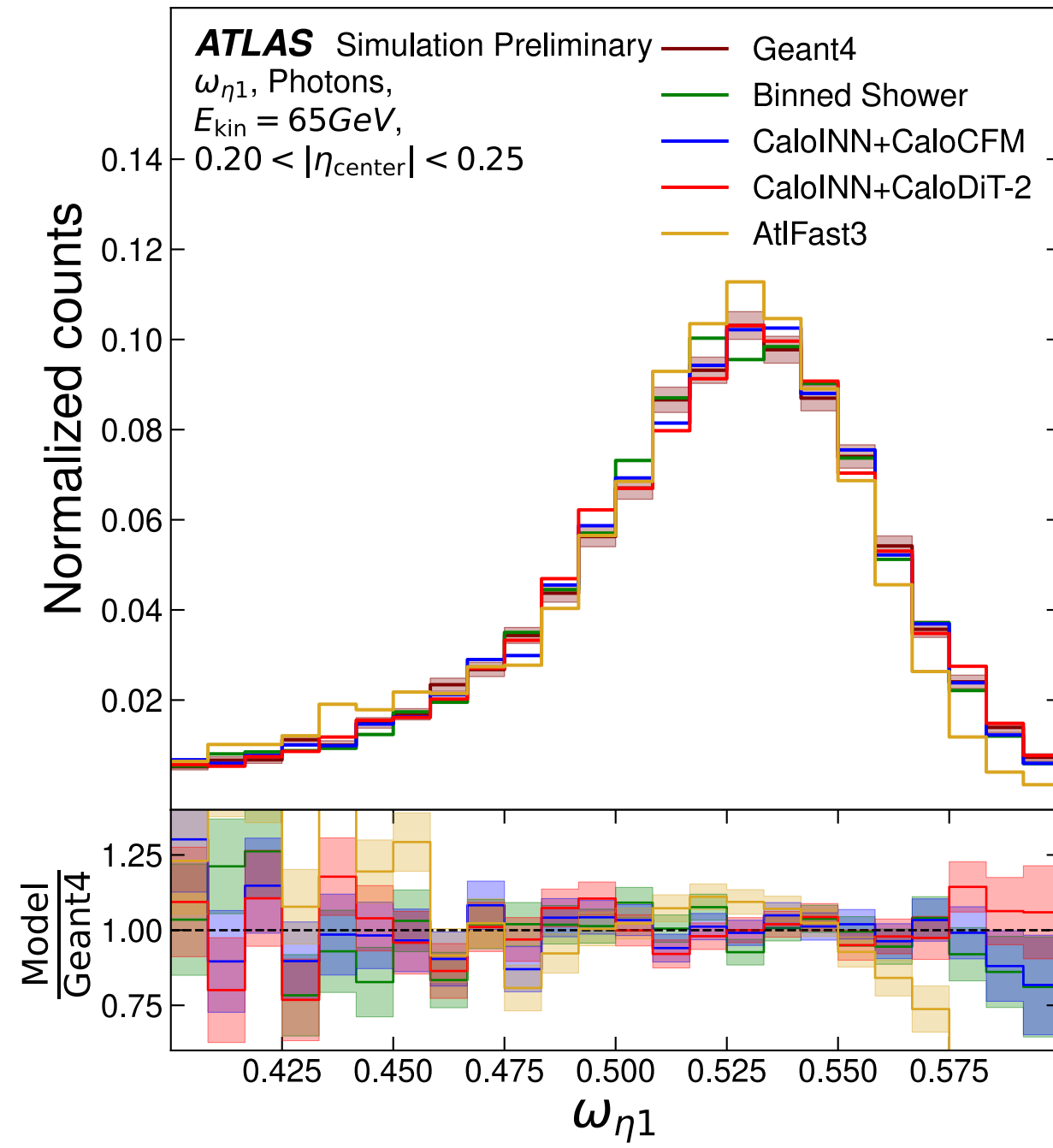
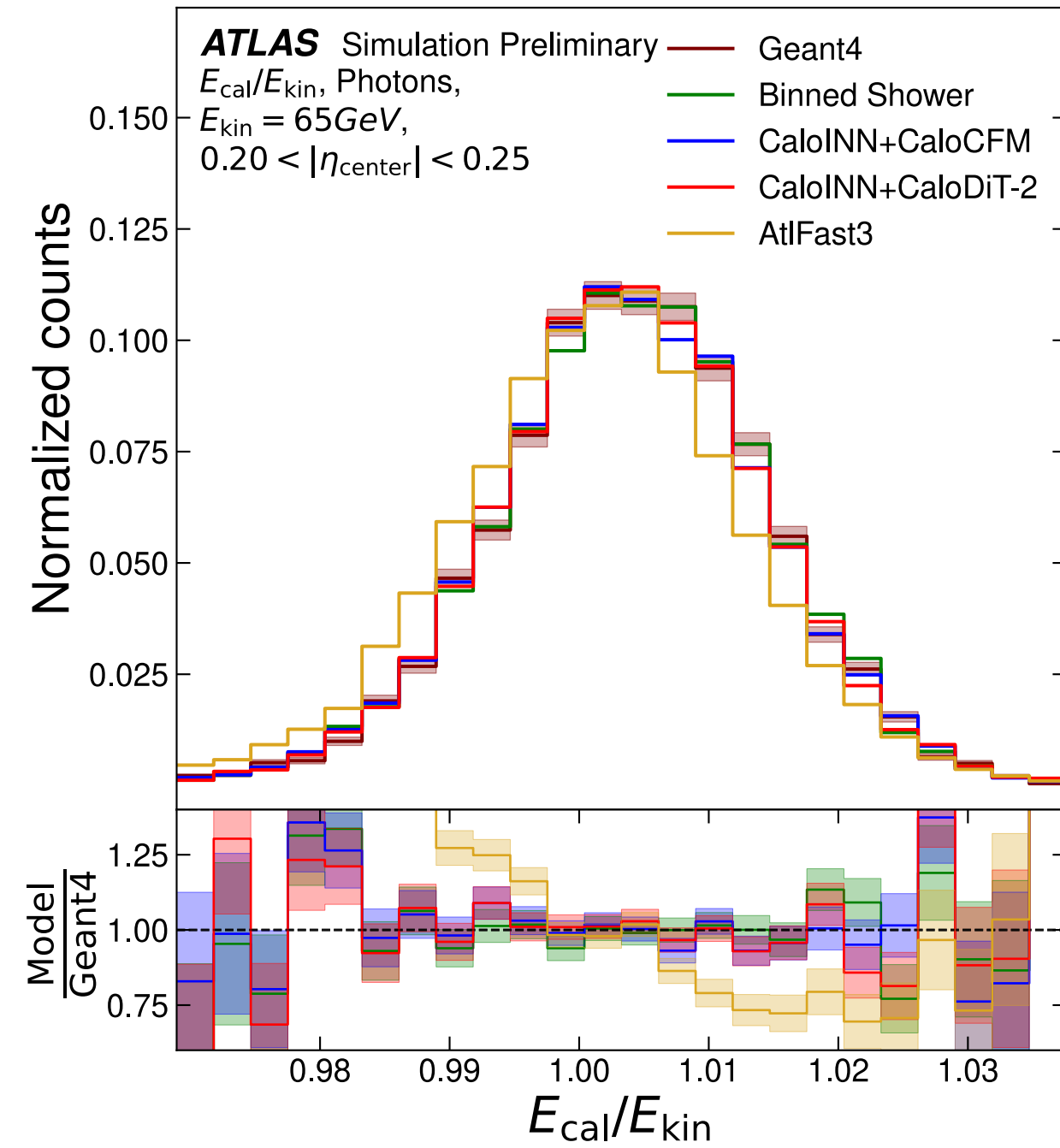
ATL-SOFT-PUB-2025-003



- Broadly, observed **strong improvements** over current AtIFast3.
- More noticeable **deviations** relative to Geant4 **observed for higher energies and in more difficult transition region** ($0.75 < |\eta| < 0.80$), anyway an **improvement** relative to current AtIFast3.

New ML Models

Physics Performance (cont'd)

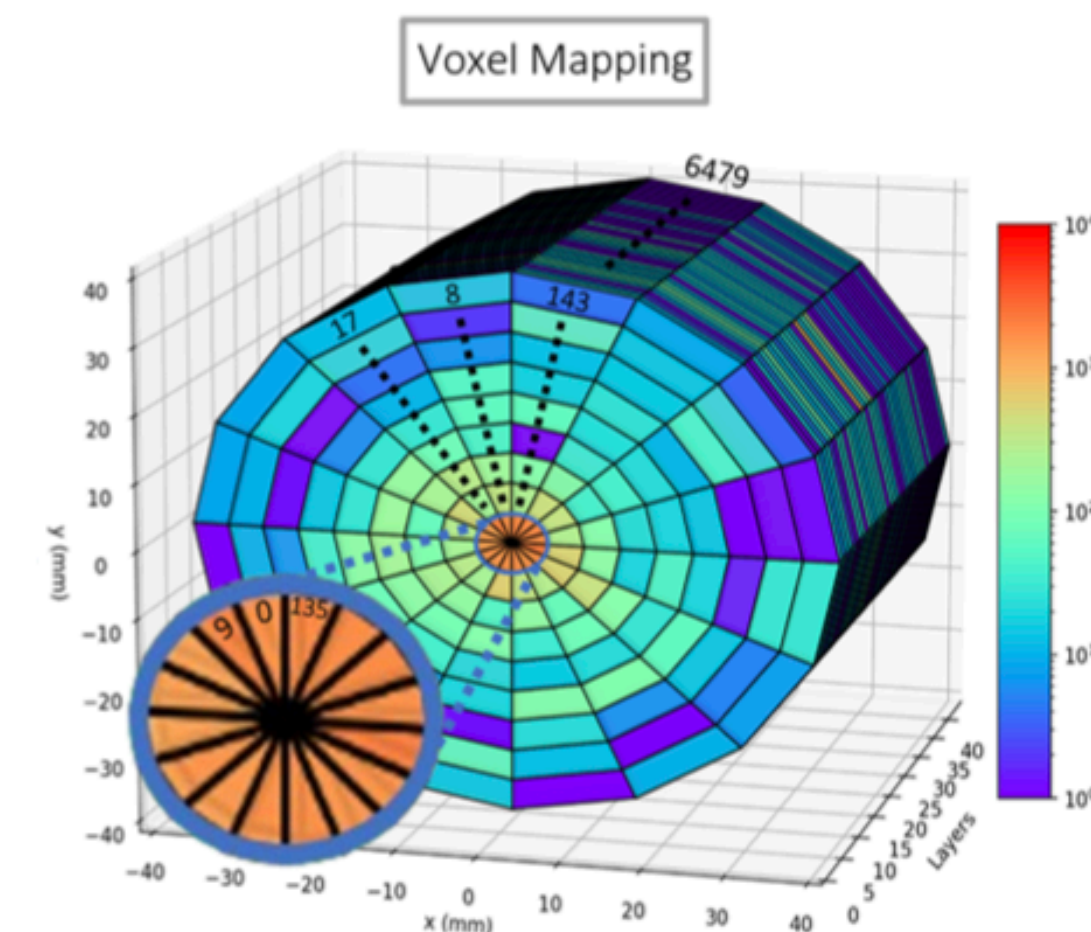
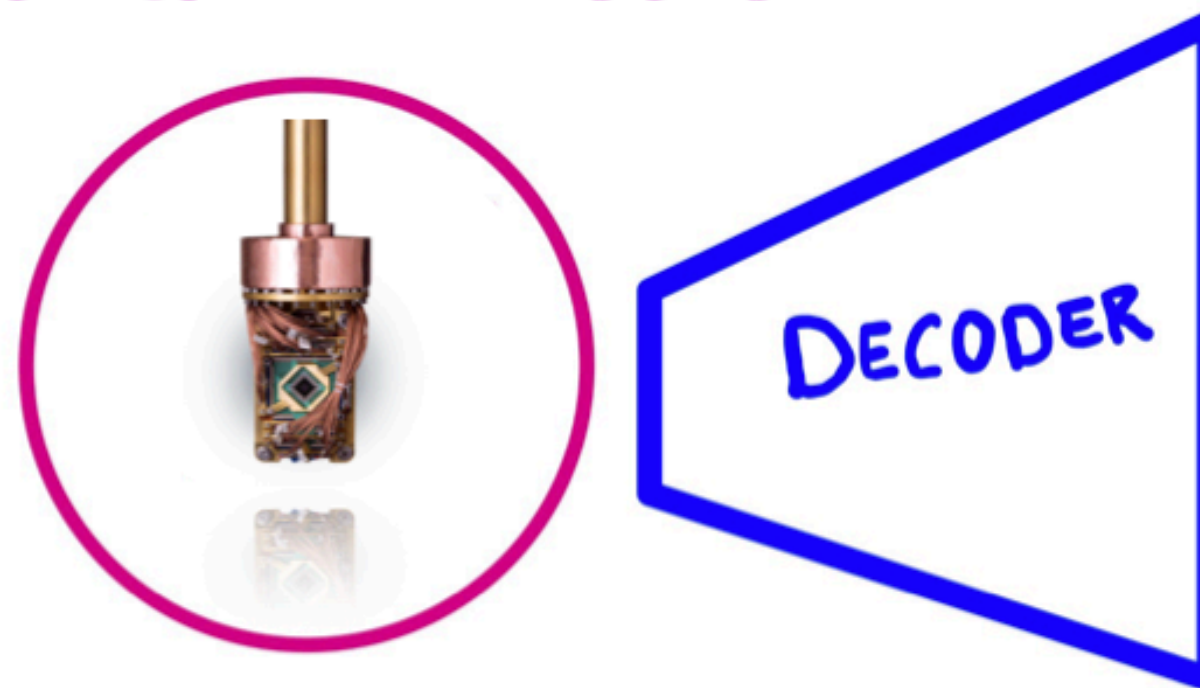


All plots here from
[ATL-SOFT-PUB-2025-003](https://arxiv.org/abs/2503.14111)

CaloQVAE

Basics on QVAE and Architecture

Quantum Annealer



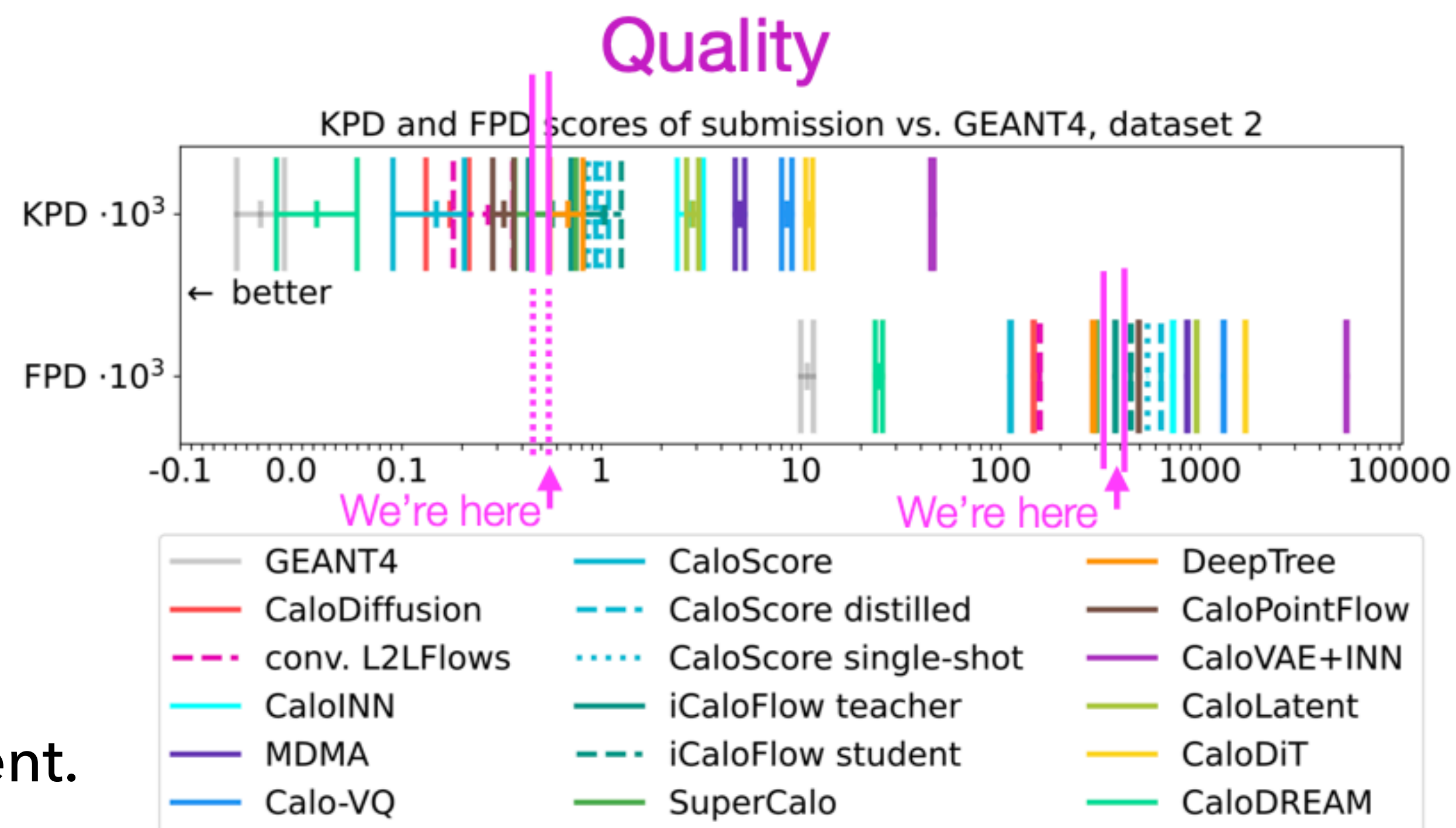
- **Quantum**-assisted Generative Model for particle-calorimeter interactions.
- **Conditioned quantum annealer as a prior** in a deep generative model to generate particle-calorimeter showers (instead of having a Gaussian multivariate distribution as a prior, as in typical VAEs).
- *Zephyr* topology. Conditioning on incident energy of the event (currently; possible to use more variables); a function encodes the condition into a qubit array.
- Rank-3 tensors and 3D convolutions to operate in the cylinder calorimeter geometry.

CaloQVAE

Performance

- $\sim 10^3$ to 10^6 times faster than Geant4!
(tested on the CaloChallenge dataset)
- **Energy-competitive** to well-competing models!
- Work in progress for further improvement.

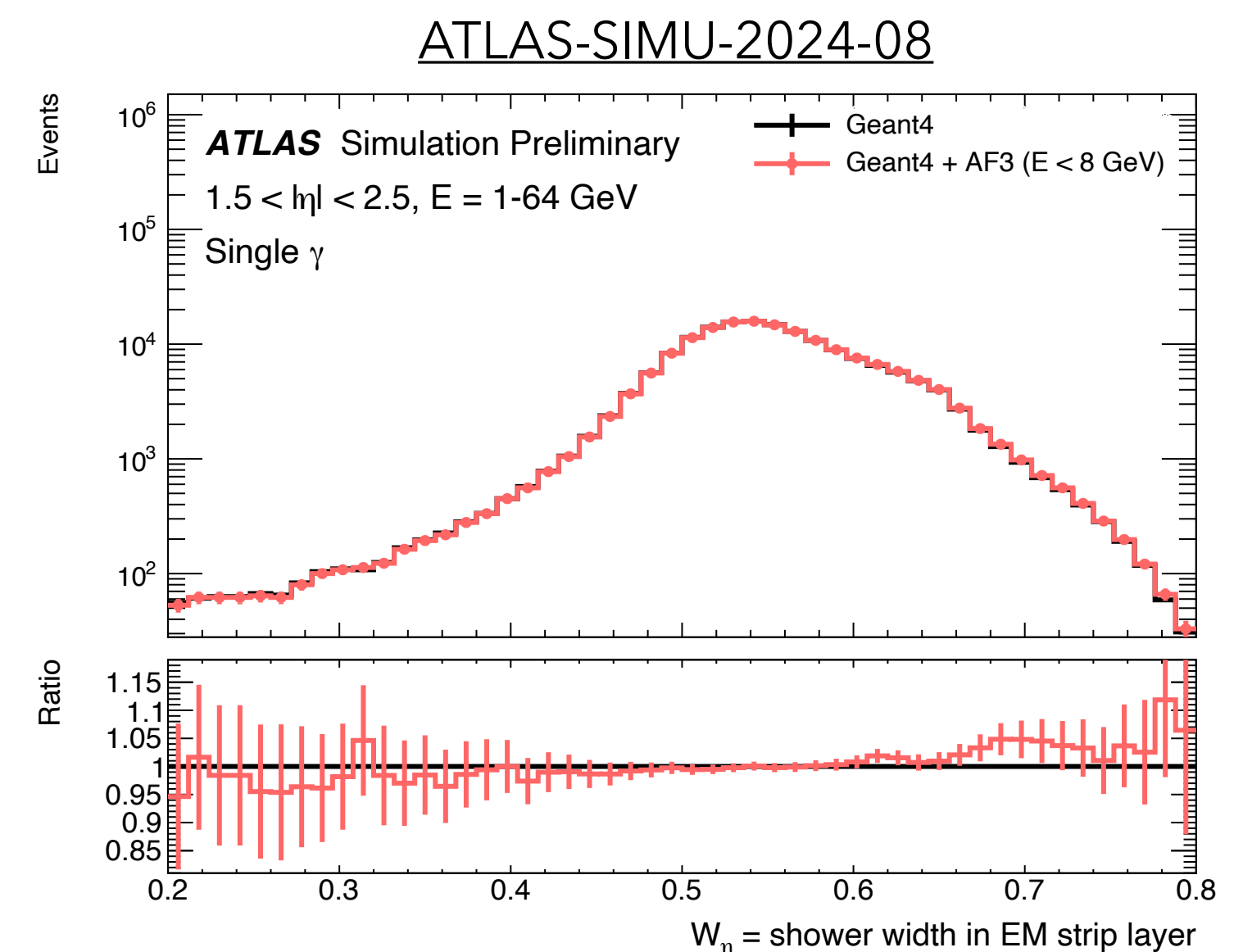
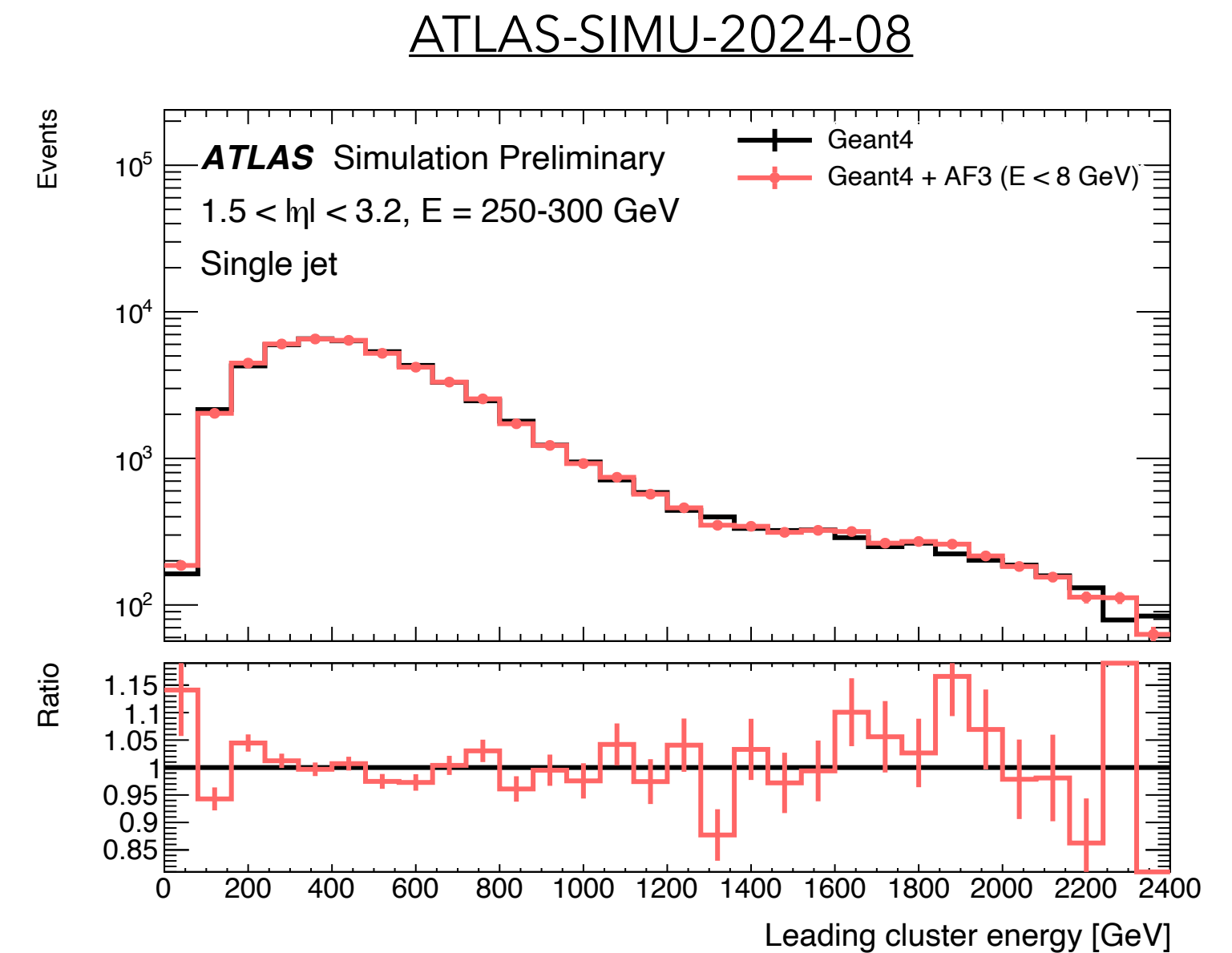
CaloQVAE results overlaid over plot from
C. Krause et al., *CaloChallenge 2022: A
Community Challenge for Fast Calorimeter
Simulation*, Rep. Prog. Phys. **88** 116201
(2025)



Other Studies

AtlFast3 in EMEC for Low e/γ

- e/γ in EMEC still one of the **biggest contributors** to the total steps-per-event → **Use AtlFast3** to handle **low energy e/γ in the EMEC for the full simulation workflow!**
 - Similar to Frozen Showers in ATLAS forward calorimeter for low energy $e/\gamma/\nu$.
 - Find energy/ η region where outputs do not differ with respect to full Geant4.
- Particles with $E < 8$ GeV, $1.5 < |\eta| < 2.5$ provide **~10% speed-up** in this region compared to full Geant4.



Other Studies

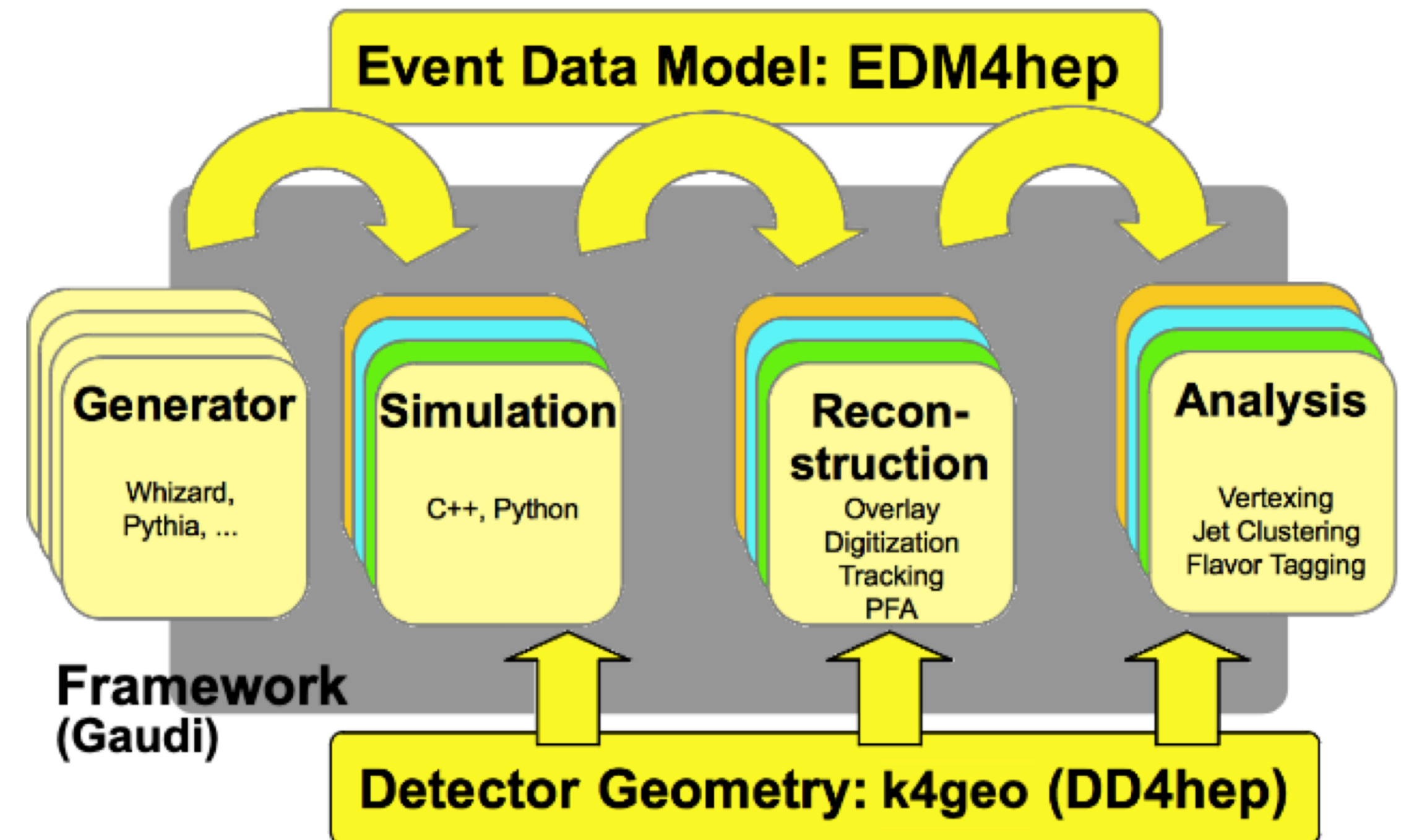
Experiment Independent AtlFast3

- AtlFast3 implemented using the Integrated Simulation Framework (ISF) within Athena. Significant code complexity of this setup → ISF and thus AtlFast3 **hard to maintain**.
 - Solution: Make AtlFast3 **independent** from ISF and turn AtlFast3 into a **Geant4 fast simulation model** = able to be invoked directly from Geant4 (= non-ATLAS-specific) thanks to its built-in fast simulation model interface → Fully **experiment-independent** library for fast calorimeter simulation (also useful for FCC!).
- **ODD** = Open Data Detector, **prototype for next-gen** HL-LHC-like detectors (and also useful for FCC!).
 - To make **AtlFast3 available for this and other detectors**, we're working on a Key4hep compatibility.
- **Key4hep** = particle physics software framework designed to be **detector independent**, aiming to contain the **full pipeline** (simulation, tracking, reconstruction...).
 - Has DD4hep = Geant4 wrapper → **can include AtlFast3!**

Other Studies

Experiment Independent AtlFast3 (cont'd)

- Created initial robust **implementation** of AtlFast3 as Geant4 fast simulation model in the Key4hep environment as demonstrator for the ODD.
- The ODD has **700x** the cells we use for ATLAS! → this implementation adopts various strategies to handle this.
- Fast simulation transport can be run in full ODD geometry → **results as expected**.
- New version adding Muon Punchthrough currently undergoing PhysVal.



Key4hep contains the full pipeline (sim, tracking, reco...).
AtlFast3 should be inserted into this!

Other Studies

Jet Performance and Magnetic Field Effects

- Work investigating causes of **mis-modelling of jet observables** with AtlFast3.
 - Pion modelling certainly involved.
- Investigation of **magnetic field effects** in fast simulation.
 - Studied shower shapes for single electrons from $Z \rightarrow e^+e^-$.
 - No significant difference found in any shower shape.

Conclusions

- The **AtFast3** fast simulation tool is able, thanks to its combination of FastCaloSim V2 and FastCaloGAN V2, to provide **great improvement in computing performance** for simulation. **Physics performance shows good agreement** with Geant4, but computing requirements for Run 4 **need further precision!**
- **Combination of CaloINN and CaloCFM/CaloDiT-2** for photons, trained on **new voxelisations** reducing bias → **improved physics modelling** with respect to current AtFast3 configuration!

Conclusions *(cont'd)*

- The Fast Simulation Group is also doing many other investigations:
 - Investigation on the potential of **quantum computing** (CaloQVAE), AtlFast3 in EMEC for low e/γ , implementation in Key4hep, studies on jet mis-modelling and magnetic field effects...
- All this work is providing and will provide **relevant benefit** to ATLAS analyses!

```
* *****  
* Welcome to lxplus706.cern.ch, CentOS Linux release 7.9.2009 (Core)  
* Archive of news is available in /etc/motd-archive  
* Reminder: you have agreed to the CERN  
* computing rules, in particular OC5. CERN implements  
* the measures necessary to ensure compliance.  
* https://cern.ch/ComputingRules  
* Puppet environment: production, Roger state: production  
* Foreman hostgroup: lxplus/nodes/login  
* Availability zone: cern-geneva-c  
* LXPLUS Public Login Service - http://lxplusdoc.web.cern.ch/  
* A CentOS based lxplus8.cern.ch is now available  
* A CentOS based lxplus9.cern.ch is  
* Please read LXPLUS Privacy Notice  
* *****
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```
lsetup  
lsetup as2 (or asetup) to setup in Athena release  
lsetup astyle ATLAS style macros  
lsetup atlantis Atlantis: event display  
lsetup client Event Index  
lsetup emi EMI: grid middleware user interface  
: job definition and management  
v: setup tool from cvmfs SFT  
: production and Distributed  
: ATLAS Metadata Interface python  
data processing framework  
distributed data management system  
to a full LCG release  
D local proxy cache  
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Backup

Backup

Shower Shapes Definitions

ATL-SOFT-PUB-2025-003

Table 4: 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_{raw}	The raw sum over all cell energies
E_{cal}	The calibrated cluster energy
f_1	Energy reconstructed in the first layer, divided by the full reconstructed energy
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
$\omega_{\eta 1}$	η -width of the shower in EMB1, calculated by using the brightest cell in EMB1 and its 3 nearest cells within positive and negative η direction, respectively
$\text{frac}s_1$	$\frac{E_{117} - E_{113}}{E_{113}}$ - 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