Generative Models for Fast Detector Simulation

— ML4Jets 2022, Rutgers University —

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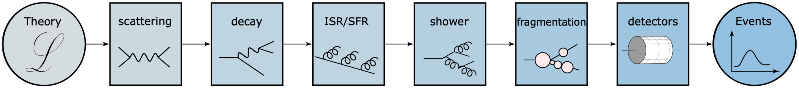
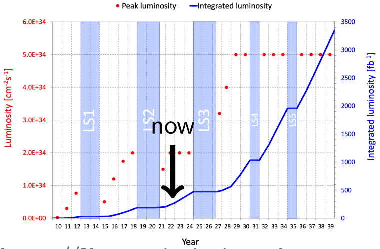
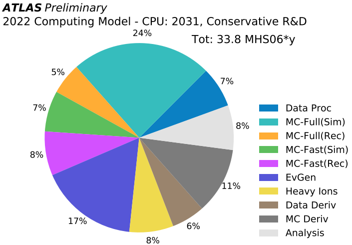
Simulations bridge Theory and Experiment.



Machine Learning and LHC Event Generation, A. Butter et al. [2203.07460]



https://lhc-commissioning.web.cern.ch/schedule/HL-LHC-plots.htm



CERN-LHCC-2022-005

Generative Models sample from intractable distributions.

- The past decade has seen a plethora of new ideas for deep generative models, with incredible results:


https://thispersondoesnotexist.com/, based on T. Karras et al. [1912.04958]

⇒ We have seen the use of GANs, VAEs, Normalizing Flows, Diffusion Models, and their derivates on a variety of datasets in HEP.

Generative Models will be crucial to meet the computing budget.

- FastSimulation is a faster alternative to full (GEANT4-based) simulation, at the expense of fidelity / information.
- Generative Models will drive FastSimulation closer to full simulation:

✓ have more low-level information with higher fidelity

✓ still fast

✓ no energy dependence in generation times

? Are the results statistically limited?

⇒ inductive bias of the models allows to extract some information more.

Butter et al. [2008.06545, Scipost]; Bieringer et al. [2202.07352, JINST]

⇒ combinatorics and symmetries work in our favor.

The first deep generative model for Calorimeter Simulation: CaloGAN.

Paganini, de Oliveira, Nachman [1705.02355, PRL; 1712.10321, PRD]

- Simulating a toy version of the ATLAS ECal: 504 voxels in 3 layers.
- trained on 100k showers of e^+, γ, π^+ with $E_{\text{inc}} \in [1, 100]$ GeV

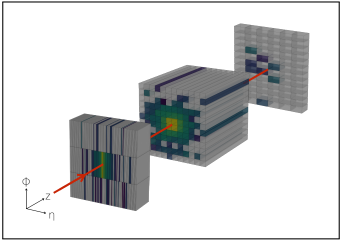
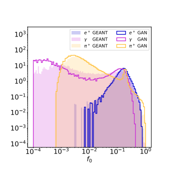
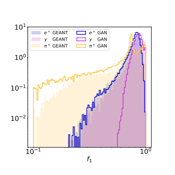
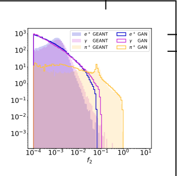


TABLE III: Total expected time (in milliseconds) required to generate a single shower under various algorithm-hardware combinations

Simulator	Hardware	Batch Size	ms/shower
Geant4	CPU	N/A	1772
CaloGAN	CPU	1	13.1
		10	5.11
		128	2.19
		1024	2.03
	GPU	1	14.5
		4	3.68
		128	0.021
		512	0.014
		1024	0.012



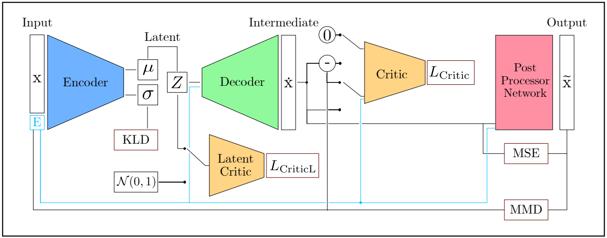


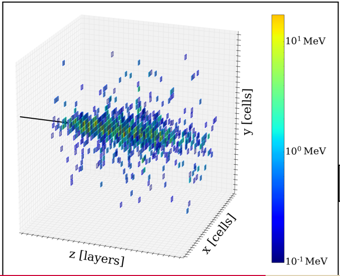


Moving to higher granularity: the BIB-AE

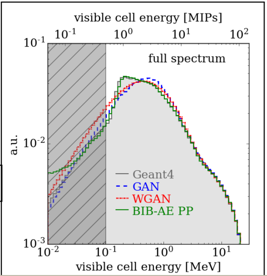
Buhmann et al. [2005.05334, Comput.Softw.Big Sci.], Buhmann et al. [2112.09709, ML:ST]

- Bounded Information Bottleneck Autoencoder: a VAE + GAN hybrid
- photon showers at $30 \times 30 \times 30$, pion showers at $25 \times 25 \times 48$ voxels





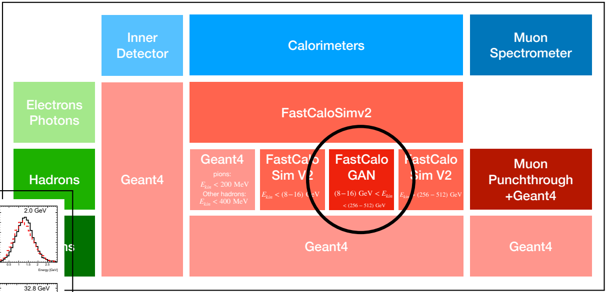
⇒ see Sascha's talk!

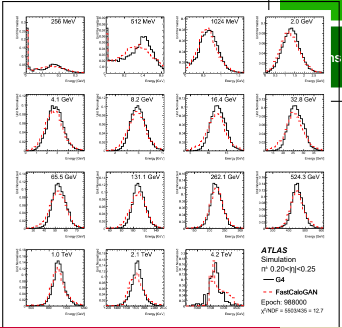


Generative Models in ATLAS: AtlFast3

ATLAS Collaboration [2109.02551, Comput Softw Big Sci]

- WGAN for hadronic showers inside ATLAS.
- Model needs to be light enough to handle large detectors.



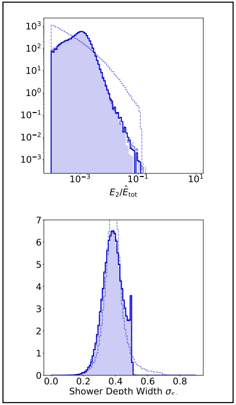


⇒ see Michele's talk!

Normalizing Flows improve the fidelity.

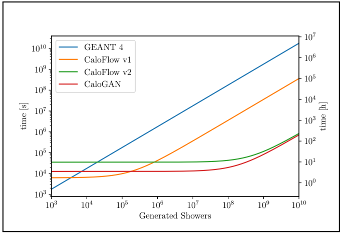
CK, D. Shih [2106.05285, 2110.11377]

- Uses CaloGAN dataset
- First generative model to fool a classifier.
- Does not scale well to higher dimensions.
- Good generation times with teacher-student-training or CL-based flow.



AUC	DNN based classifier			
	GEANT4 vs. CALOGAN	GEANT4 vs. (teacher) CALOFLOW v1	GEANT4 vs. (student) CALOFLOW v2	GEANT4 vs. CL-based flow
e^+	1.000(0)	0.859(10)	0.786(7)	0.638
γ	1.000(0)	0.756(48)	0.758(14)	0.631
π^+	1.000(0)	0.649(3)	0.729(2)	0.705

Work in progress with F. Ernst, L. Favaro, T. Plehn, D. Shih

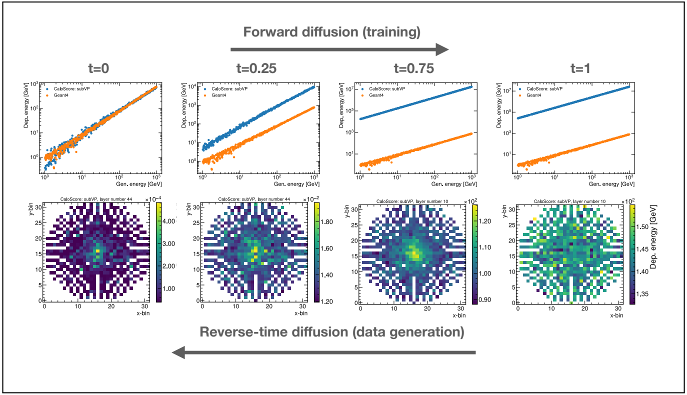


$\Rightarrow$ see Ian's talk!

Score-based Diffusion Models are the newest Player.

V. Mikuni and B. Nachman [2206.11898]

- Optimization task comparable to Flow-based optimization.
- Are able to handle higher-dimensional dataset.



⇒ see Vini's talk!

We need a systematic comparison of available methods!

- We have a rapidly evolving field: need a survey of current approaches on a common dataset!

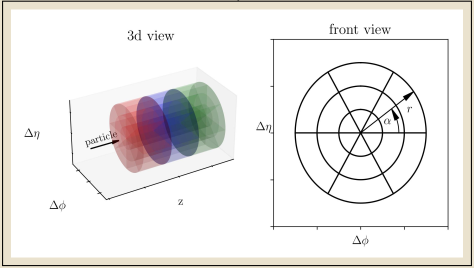
$\Rightarrow$ Make a challenge out of it!

- A challenge compares a variety of models on the same dataset.
- The datasets will also be benchmarks in the future, once new models become available.
- A challenge also collects ideas and approaches for preprocessing etc.
- Previous challenges on top tagging and anomaly detection were very successful.

Introducing: Fast Calorimeter Simulation Challenge 2022

`https://calochallenge.github.io/homepage/`
#calochallenge channel in the ML4Jets Slack workspace

- We provide 3 datasets that differ in size/complexity ("easy" $\rightarrow$ "medium" $\rightarrow$ "hard").



$\Rightarrow$ The main task:

$\boxed{\text{Develop a model that samples from } p(\text{shower}|E_{\text{incident}})}$

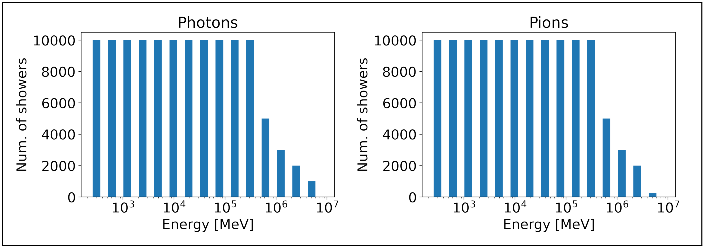
(for the dataset(s) you like.)

Dataset 1: "easy"

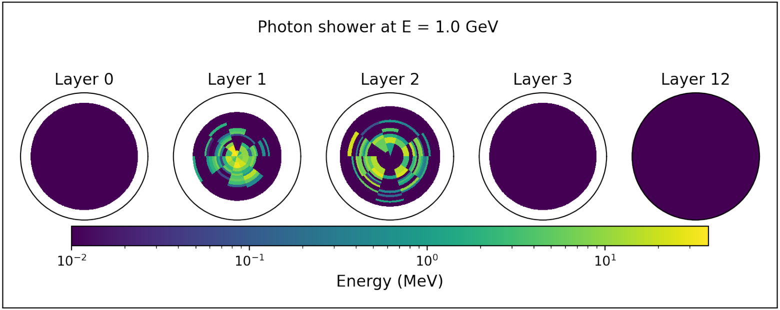
- Based on the ATLAS geometry in the η-range [0.2, 0.25].
- Comes in 2 "flavors": photons and charged pions.
- Was used to train the FastCaloGAN of AtlFast3.

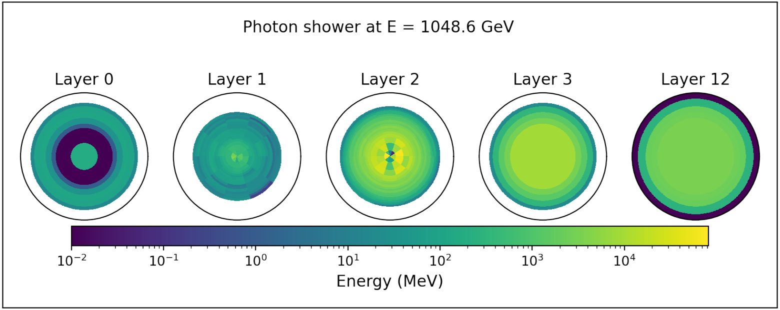
  AtlFast3: 2109.02551; FastCaloGAN: ATL-SOFT-PUB-2020-006

	Number of voxels	N_z	N_α	N_r
γ	368	5	[1, 10, 10, 1, 1]	[8, 16, 19, 5, 5]
π^+	533	7	[1, 10, 10, 1, 10, 10, 1]	[8, 10, 10, 5, 15, 16, 10]

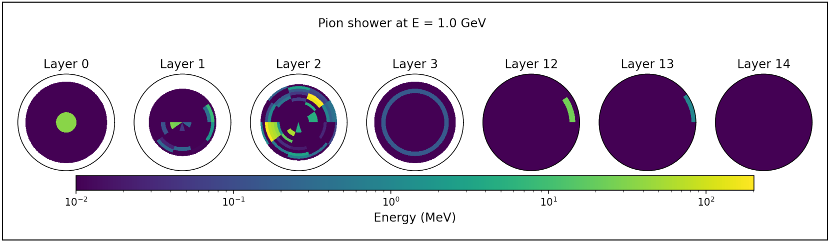


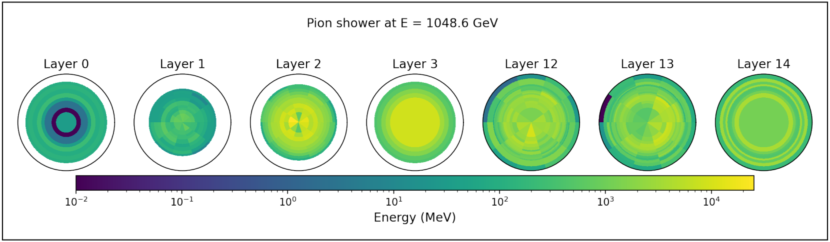
Dataset 1: "easy" Photon Showers





Dataset 1: “easy” Pion Showers

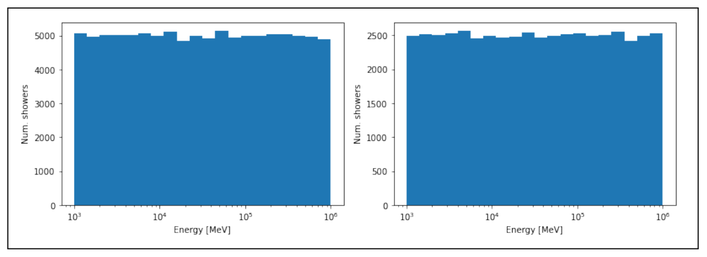




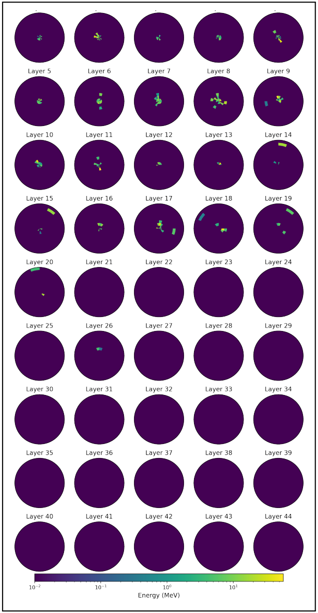
Dataset 2: "medium" and Dataset 3: "hard"

- Both consider electron showers in same geometry, but have different voxelization.
- Use detector made of alternating active (silicon) and passive (tungsten) layers based on the par04 GEANT4 example.

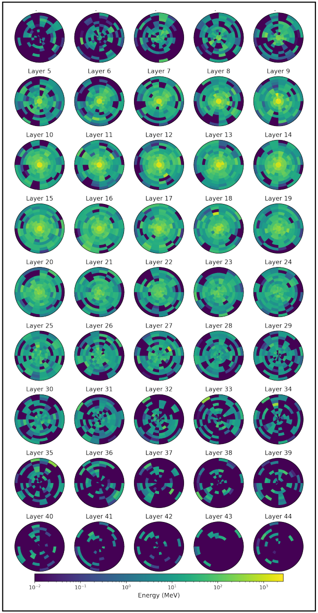
Dataset	Particle	Number of voxels	N_z	N_α	N_r
2	e^-	6480	45	16	9
3	e^-	40500	45	50	18



Dataset 2: “medium” Electron Showers

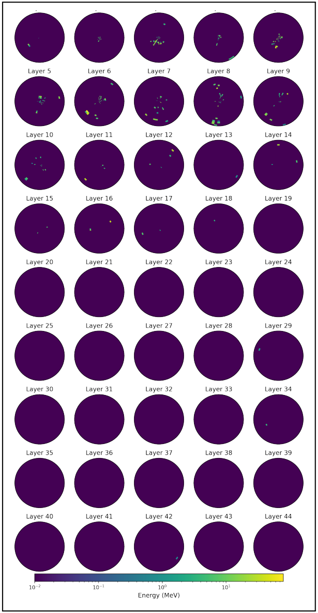


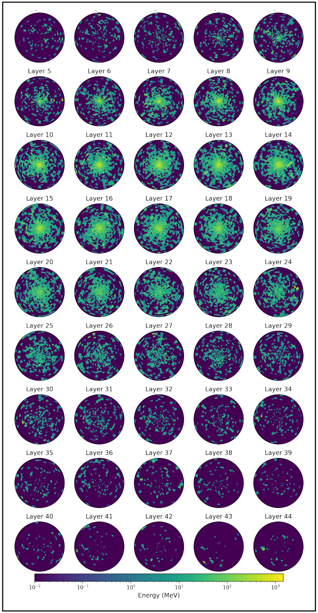
$E_{\mathrm{inc}} = 3.8$ GeV



$E_{\mathrm{inc}} = 545.1$ GeV

Dataset 3: “hard” Electron Showers





$E_{\text{inc}} = 3.1$ GeV

$E_{\text{inc}} = 913.4$ GeV

Evaluating the Models

The surrogates should be fast, light, and faithful!

⇒ There is no single metric, so we don't expect to see a single winner!

⇒ see Raghav's talk yesterday!

We will be looking at:

⇒ Sampling time, (training time, memory usage)

⇒ high-level features:
layer energies E_i, center of energy in η, ϕ, and their widths

- histograms
- histogram separation power: $\langle S^2 \rangle = \frac{1}{2} \sum_{i=1}^{n_{\text{bins}}} \frac{(h_{1,i} - h_{2,i})^2}{h_{1,i} + h_{2,i}}$

  Diefenbacher et al. 2009.03796
- A binary classifier to distinguish samples from GEANT4.

⇒ A binary classifier to distinguish samples from GEANT4, based on voxel information.

⇒ Fréchet Gaussian distance (FGD), other metrics tbd ???

Looking Ahead

14:00	**Introduction to Generative Models for Fast Detector Simulation** *Multipurpose Room (aka Livingston Hall), Rutgers University*	*Dr Claudius Krause* 14:00 - 14:25
	AtlFast3, the new ATLAS fast simulation tool *Multipurpose Room (aka Livingston Hall), Rutgers University*	*Michele Faucci Giannelli* 14:25 - 14:45
	CaloFlow for CaloChallenge *Multipurpose Room (aka Livingston Hall), Rutgers University*	*Ian Pang et al.* 14:45 - 15:05
15:00	**Score-based Generative Models for Calorimeter Shower Simulation** *Multipurpose Room (aka Livingston Hall), Rutgers University*	*Vinicius Massami Mikuni* 15:05 - 15:25
	CaloMan: Fast generation of calorimeter showers with density estimation on learned manifolds *Multipurpose Room (aka Livingston Hall), Rutgers University*	*Jesse Cresswell* 15:25 - 15:45
	Coffee *Multipurpose Room (aka Livingston Hall), Rutgers University*	15:45 - 16:15
16:00	**Generative Models for Fast Simulation of Electromagnetic and Hadronic Showers in Highly Granular Calorimeters** *Sascha Daniel Diefenbacher*	
	Fast calorimeter simulation with VQVAE *Multipurpose Room (aka Livingston Hall), Rutgers University*	*Chase Owen Shimmin* 16:35 - 16:55
17:00	**IEA-GAN: Intra-Event Aware GAN with Relational Reasoning for the Fast Detector Simulation** *Multipurpose Room (aka Livingston Hall), Rutgers University*	*Hosein Hashemi et al.* 16:55 - 17:15
	Discussion *Multipurpose Room (aka Livingston Hall), Rutgers University*	17:15 - 17:45

- We will announce the deadline for contributions.
- We plan a dedicated meeting to discuss results.
- There will be a final, summary write-up.

Generative Models for Fast Detector Simulation

- We expect 25$\times$ more LHC data in the future.
- Understanding everything based on 1st principles suffers from computational bottlenecks, especially in Detector Simulation.

$\Rightarrow$ These can be tackled with Generative Models.

- We have seen many different architectures being tested and used.
- It's time to bring these models into deployment, i.e. part of FastSimulation.

Introducing: The Fast Calorimeter Simulation Challenge 2022

- It surveys the field for state-of-the-art generative models.
- It provides benchmark datasets for (future) R&D.

$\Rightarrow$ https://calochallenge.github.io/homepage/