Generating Accurate Showers in Highly Granular Calorimeters Using Normalizing Flows

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May 11, 2023

Detector Simulation

- monte carlo (MC) necessary to compare theory and measurements
- detector simulation most expensive part of simulation chain
- computational requirements expected to exceed available resources soon

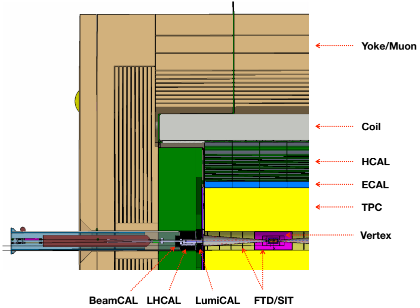
  → need for speeding up detector simulation
- generative neuronal networks learn distributions and can sample from them
- work flow:
  - simulate small amounts of data using slow monte carlo
  - train generative model on these data
  - draw large amounts of data from fast ML models

International Large Detector (ILD)

- proposed detector for the ILC
- has two sampling calorimeters
- electromagnetic calorimeter
  - 30 layers, 5mm x 5mm cells
- hadronic calorimeter
  - 48 layers, 30mm x 30mm cells

dataset[1]:

- photon showers in ECAL
- 30x30x30 voxels



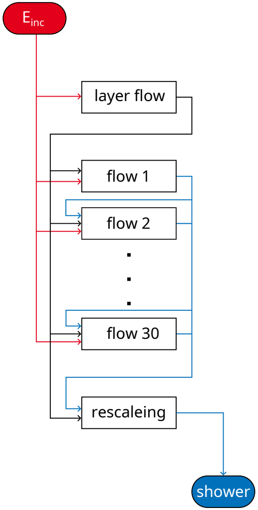
graphics taken from "ILD: Design Report"[2]

[1] Erik Buhmann et al. *Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed*. 2021. arXiv: 2005.05334.

[2] ILD Concept Group. *International Large Detector: Interim Design Report*. 2020. arXiv: 2003.01116.

Architecture

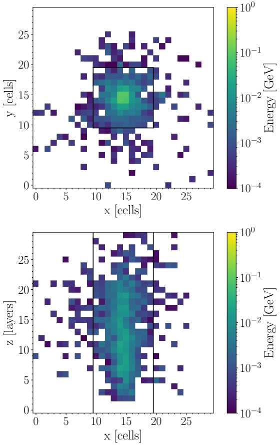
- based on CaloFlow[3] and L2L Flow[4]
- one layer flow
  - learns distribution of layer energies
  - conditioned on incident energy
- 30 multiple flows
  - learn shower shape in layer
  - conditioned on
    - incident energy
    - layer energy
    - privies layers
  - summary network reduces cardinality
- generation
  - sample layer energies using layer flow
  - sample shower shape using multiple flows
  - rescale voxel energies



[3] Claudius Krause and David Shih. *CaloFlow: Fast and Accurate Generation of Calorimeter Showers with Normalizing Flows*. 2021. arXiv: 2106.05285.

[4] Sascha Diefenbacher et al. *L2LFlows: Generating High-Fidelity 3D Calorimeter Images*. 2023. arXiv: 2302.11594.

Upscaling

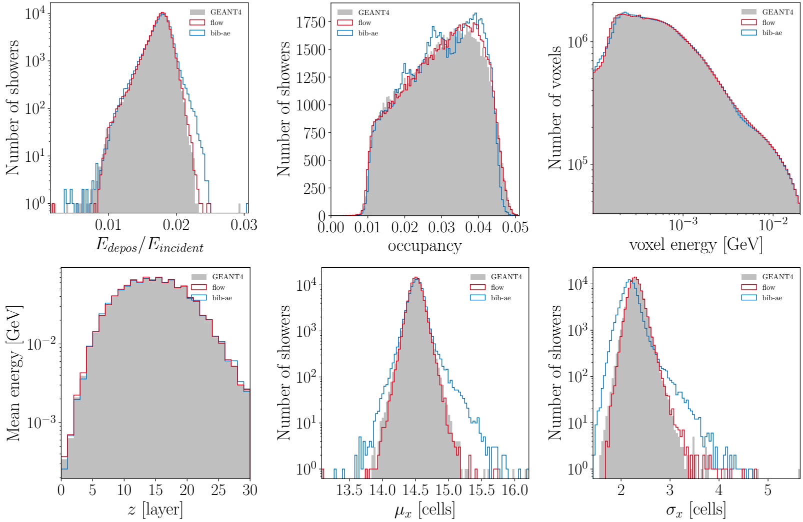


photon shower

- scaling up to 30x30x30 voxels
- switch to convolution flows
  - using multi scale architecture like in Glow[5]
  - faster generation
  - less weights
  - more accurate showers
- improve training
  - apply gradient clipping
  - add LR scheduler
- features in energy spectrum are smeared out
  → apply element with function to get them back

[5] Diederik P. Kingma and Prafulla Dhariwal. *Glow: Generative Flow with Invertible 1x1 Convolutions*. 2018. arXiv: 1807.03039.

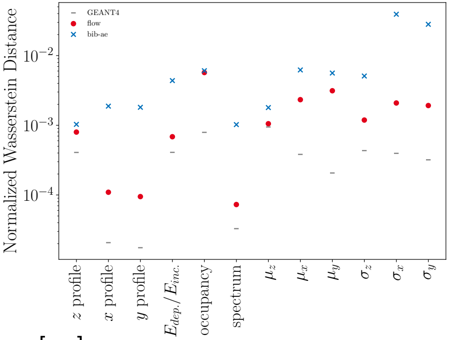
Preliminary Results



Metrics & Timing

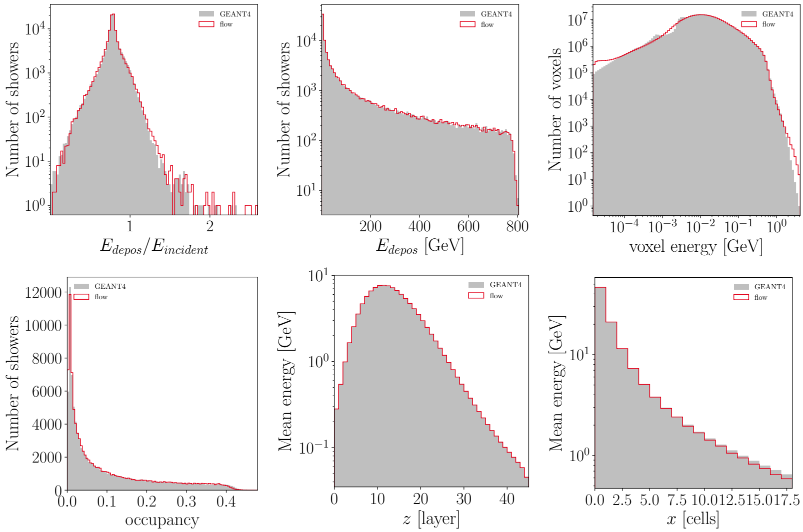
High Level Classifier:
(10 features)

	AUC	Acc	JSD
flow	0.68	0.62	0.08
bib-ae	0.90	0.81	0.43



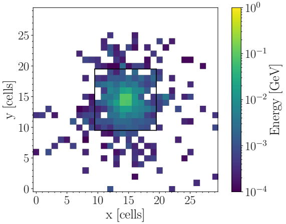
Simulator	Hardware	Batch size	time [ms]
GEANT4	CPU	1	4081.53
BIB-AE	CPU	1	102.25
Flow	CPU	1	1746.61
BIB-AE	GPU	1000	0.25
Flow	GPU	1000	3.39

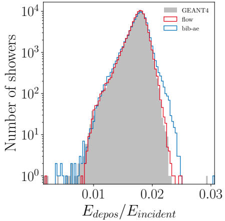
Calo Challenge



Summary

- ML generators fast alternative to MC simulations
- the ILD has highly granular calorimeter
  $\rightarrow$ hard to learn
- convolutional flows scale well with input dimensions
- flows can generate highly accurate showers

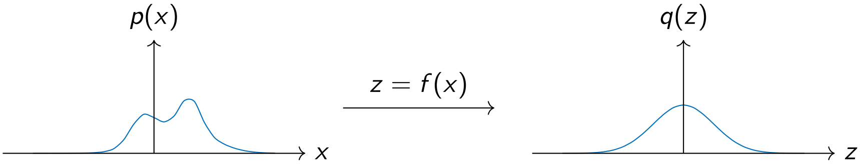




Normalizing Flows

- diffeomorphism between physics space and latent space
- transform physics space distribution into a simple prior distribution
- change of variables formula allows for physics space density estimation
- training: minimize negative log-likelihood
- generation: sample from latent distribution and apply inverse of function

$$p(x) = q(f(x))\,|J(x)| \qquad \mathcal{L} = -\log q(f(x)) - \log|J(x)|$$



Timing

Simulator	Hardware	Batch size	time [ms]	Speedup
GEANT4	CPU	1	4081.53 ± 169.92	×1.0
BIB-AE	CPU	1	102.25 ± 0.64	×40.0
		10	37.81 ± 0.13	×108.0
		100	48.51 ± 0.01	×84.1
		1000	48.19 ± 0.01	×84.7
Flow	CPU	1	1746.61 ± 64.50	x2.3
		10	392.61 ± 0.34	x10.4
		100	228.86 ± 7.09	x17.8
		1000	275.55 ± 3.01	x14.8
BIB-AE	GPU	1	74.22 ± 3.18	×42.5
		1000	0.249 ± 0.002	×16326.1
Flow	GPU	1	2471.07 ± 70.20	x1.7
		1000	3.39 ± 0.09	×1202.3