

CLUSTER OF EXCELLENCE QUANTUM UNIVERSE





Higher Resolution and Angular Conditioning for Normalizing-Flow-based Generation of Calorimeter Showers

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November 5, 2024 ML4Jets 2024

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Detector Simulation

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



1 CMS Offline Software and Computing. CMS Phase-2 Computing Model: Update Document. 2022. URL: https://cds.cern.ch/record/2815292

International Large Detector (ILD)

- proposed detector for the International Linear Collider ILC
- has two sampling calorimeters
- electromagnetic calorimeter (ECAL)
 - 30 layers, 5mm × 5mm cells
- hadronic calorimeter (HCAL)
 - 48 layers, 30mm × 30mm cells
- dataset:
 - photon showers in ECAL
 - uniform distribution of incident energies

 $1~{\rm GeV} \le {\it E}_{\rm inc} \le 127~{\rm GeV}$



²Erik Buhmann et al. Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed. 2021. arXiv: 2005.05334
 ³ILD Concept Group. International Large Detector: Interim Design Report. 2020. arXiv: 2003.01116

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Data Representation of Showers

Fixed Grid

- 3D array filled with energy values
- entries correspond to calorimeter cells
- allows for convolutional networks
- needs bounding box

Point Clouds

- variable-length, permutation-invariant sets
- only c.a. 4% of cells are non-zero
- more economically represented
- only generation of non-zero points



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Convolutional L2LFlows⁴



- learns distribution of layer energies
- conditioned on incident energy
- masked autoregressive flow⁵
- ▶ 30 causal flows
 - learn shower shape in layer
 - conditioned on
 - incident energy
 - layer energy
 - previous layers
 - ▶ Glow-like⁶ architecture with U-Nets





⁴ Thorsten Buss et al. Convolutional L2LFlows: generating accurate showers in highly granular calorimeters using convolutional normalizing flows. 2024. arXiv: 2405.20407 ⁵ Mathieu Germain et al. MADE: Masked Autoencoder for Distribution Estimation. 2015. arXiv: 1502.03509

⁶Diederik P. Kingma and Prafulla Dhariwal. Glow: Generative Flow with Invertible 1x1 Convolutions. 2018. arXiv: 1807.03039

Integration into Full Simulation

Geometry Dependensy

- training on single incident point
 - $\rightarrow\,$ decrease in performance when shifted
- solution⁷:
 - training with 9× higher granularity (90 × 90 × 30)
 - removing detector irregularities Thur. A.K.

Angular Conditioning

- training on single incident angle
- solution⁸:
 - conditioning on incident angle

Integration

- 1. Pytorch model Thur. P.M.
- 2. export to Torchscript and load from C++ $% \left({{{C_{{\rm{C}}}}} \right) = {{C_{{\rm{C}}}}} \right)$
- 3. integrate into simulation chain using DDFastShowerML

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⁷Erik Buhmann et al. CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation. 2023. arXiv: 2309.05704

⁸Sascha Diefenbacher et al. New angles on fast calorimeter shower simulation. 2023. arXiv: 2303.18150

Results with Box Cut



- evaluation at same incident point
- evaluated with 30x30 cell box cut

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Normalizing-Flow-based Generation of Calorimeter Showers

good agreement with data

Shifting the Showers



- shift the showers in the calorimeter
- still apply 30x30 box cut

 need to train L2LFlows with nine times higher granularity

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No Box Cut



- shift the showers in the calorimeter
- no box cut applied

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Angular Conditioning



- L2LFlows: good agreement within bounding box
- CaloClouds: not restricted to bounding box

Di-Photon Separation

Can the detector separate two photons?



using ILD reconstruction software

possible due to Integration into full simulation

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Speedup over GEANT4

		Simulator	Batch size	time [ms]	speed up
		GEANT4	1	3915	×1.0
	comparison of generation times	CaloClouds II		652	×6.0
 hardware: Intel[®] Xeon[®] E5-2640 		CaloClouds (cm))	84	×46.6
		L2LFlows		1203	x3.3
► #thr	eads: 1	L2LFlows (x9)		3713	×1.1
on G	^D U speed up	L2LFlows	100	371	×10.6
of \times	50 to $\times 1800$	L2LFlows (x9)		2453	×1.6

timing on single CPU thread

Summary

General

- higher granularity allows for shifting of showers
- angular conditioning allows for varying incident angles

L2LFlows

very higher fidelity generation of shower core

CaloClouds

- no bounding box necessary
- very fast inference

Integration

- allows for more involved studies
- running reconstruction software on generated data

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