CaloClouds: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation

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EB, S Diefenbacher et al: CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation

EB, F Gaede, et al: CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation

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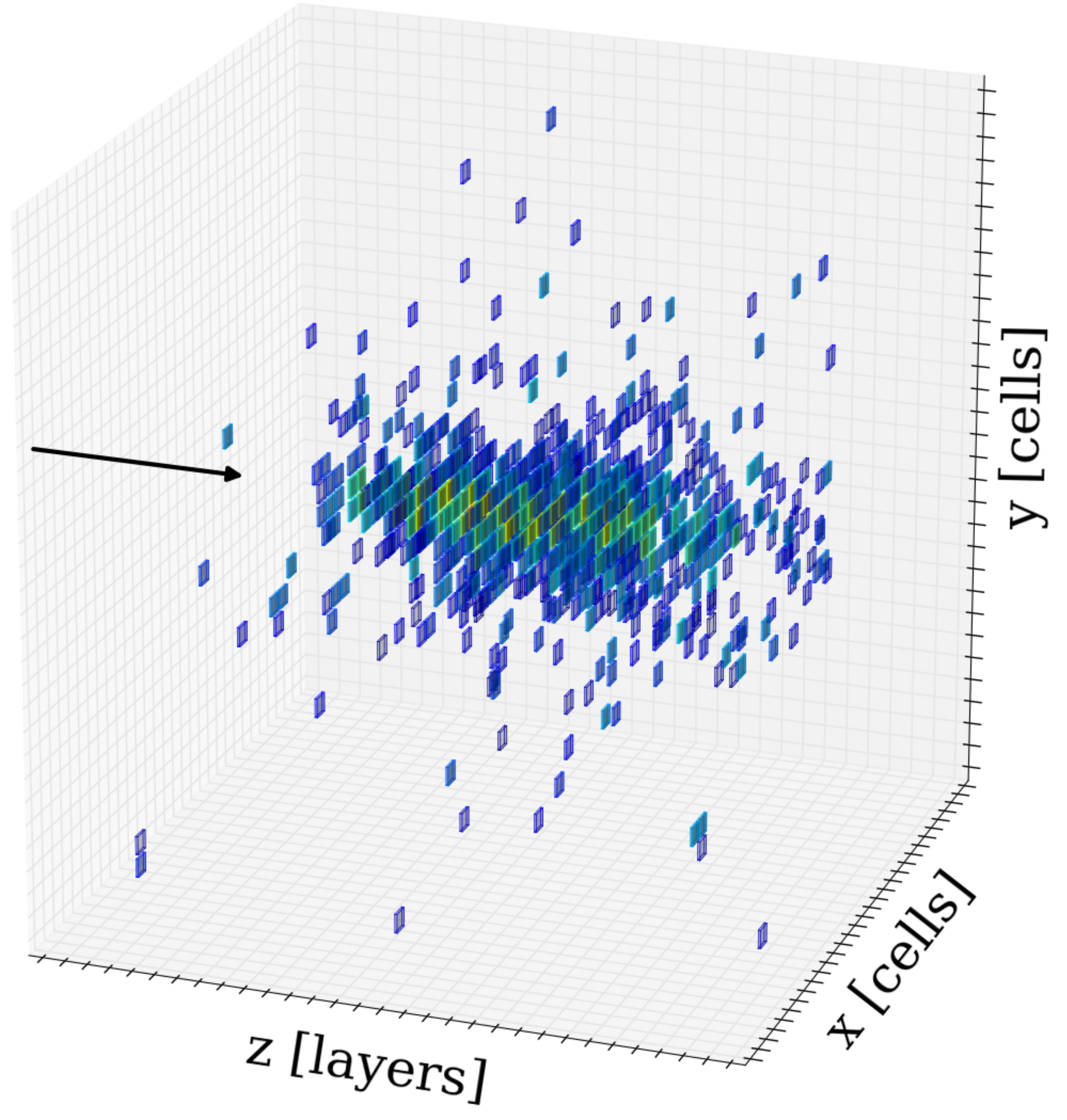
Calorimeter Showers as Point Clouds

- Generative models for calorimeter showers usually applied to fixed geometries, i.e. CNNs for 3D images
  - Calorimeter showers are very sparse (only ~ 4% filled pixels)
- More economically represented as point clouds (variable-length, permutation-invariant sets)
  - Generation of only non-zero points
- Ability to use clustered Geant4 steps with higher granularity than sensor size
  - Allows for cell-geometry independent model
- CaloClouds: Fast & accurate generative model for calorimeter point clouds with $\mathcal{O}(1{,}000)$ points

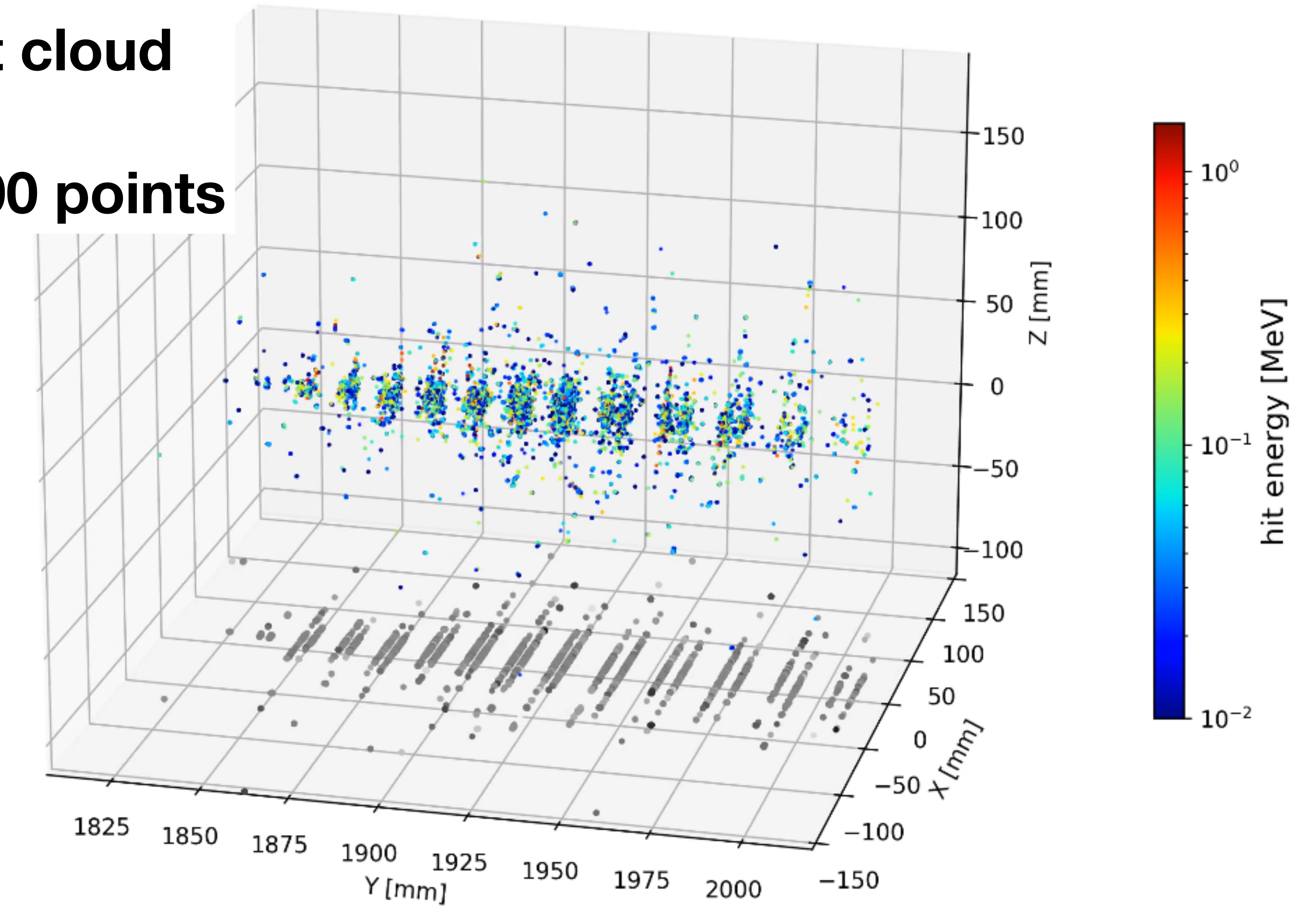
EM shower as 3D image

27,000 pixels (~ 1,000 non-zero)



EM shower as point cloud

~ 40,000 points

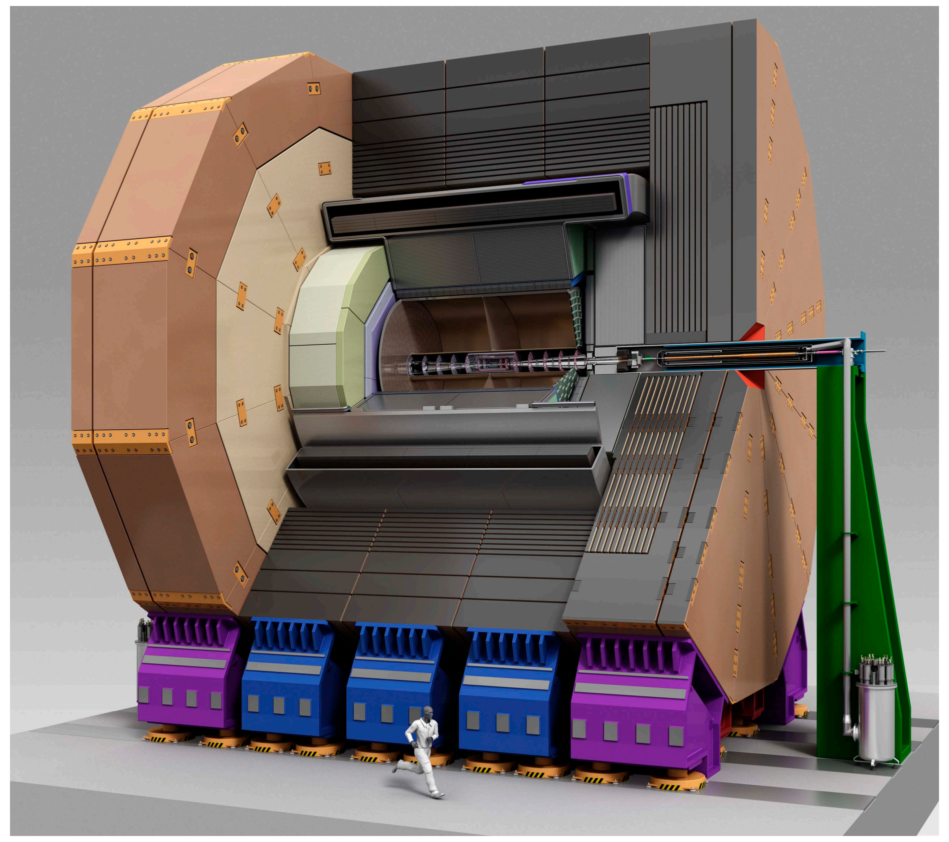


Data Processing

	points / shower	Note
All GEANT4 steps	40 000	Initial output of GEANT4
Clustered GEANT4 steps	6 000	Input/output of CALOCLOUDS
Hits in calorimeter grid	1 500	Calculation of physics observables

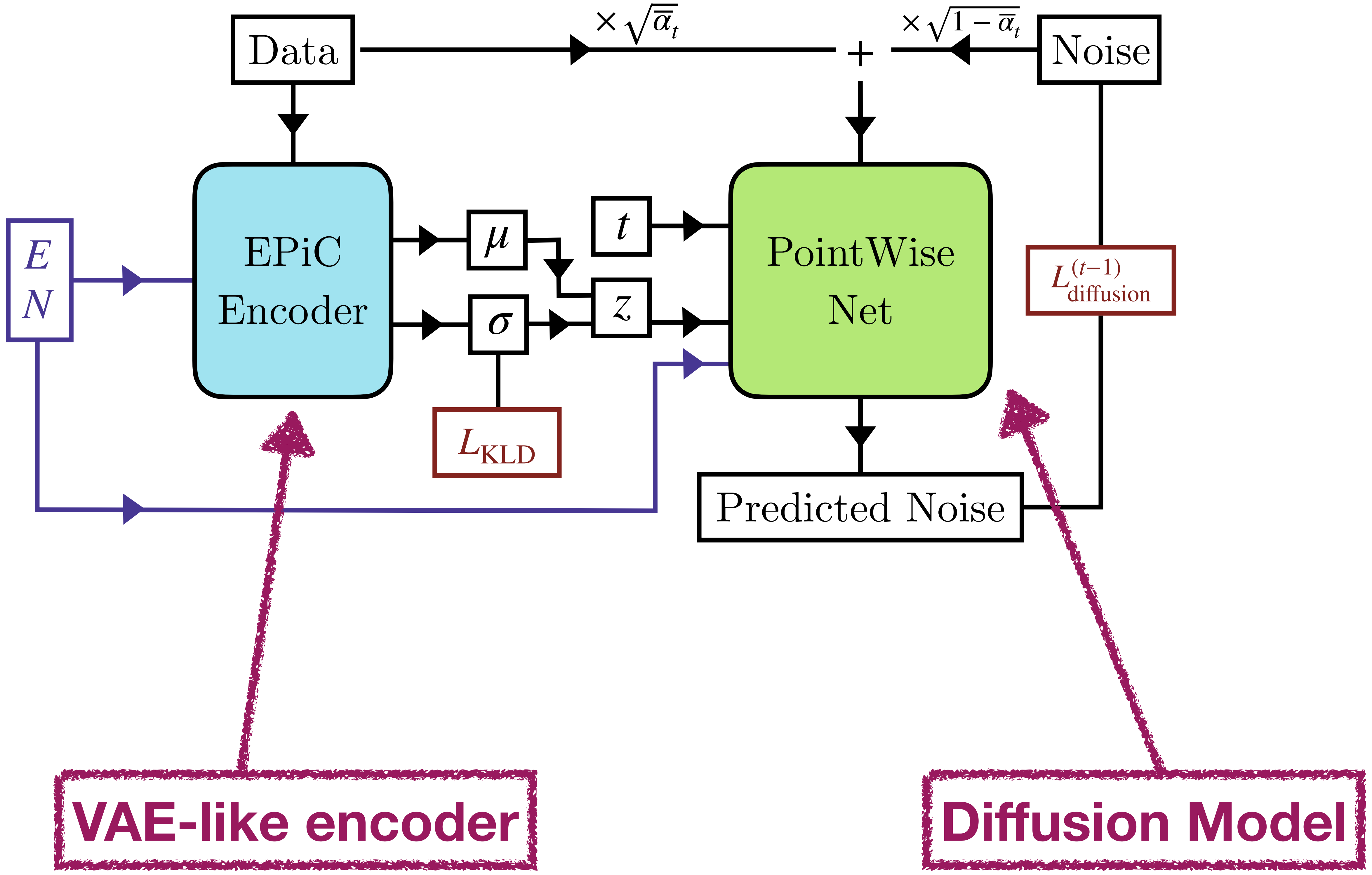
- Photon showers (10-90 GeV) in the electromagnetic calorimeter (ECAL) of the International Large Detector (ILD) at the International Linear Collider (ILC)
- Point clouds of clustered Geant4 steps: 36x higher granularity than cell hits, 7x fewer points than full Geant4 steps
  - Multiple points per cell & geometry independent

International Large Detector (ILD)

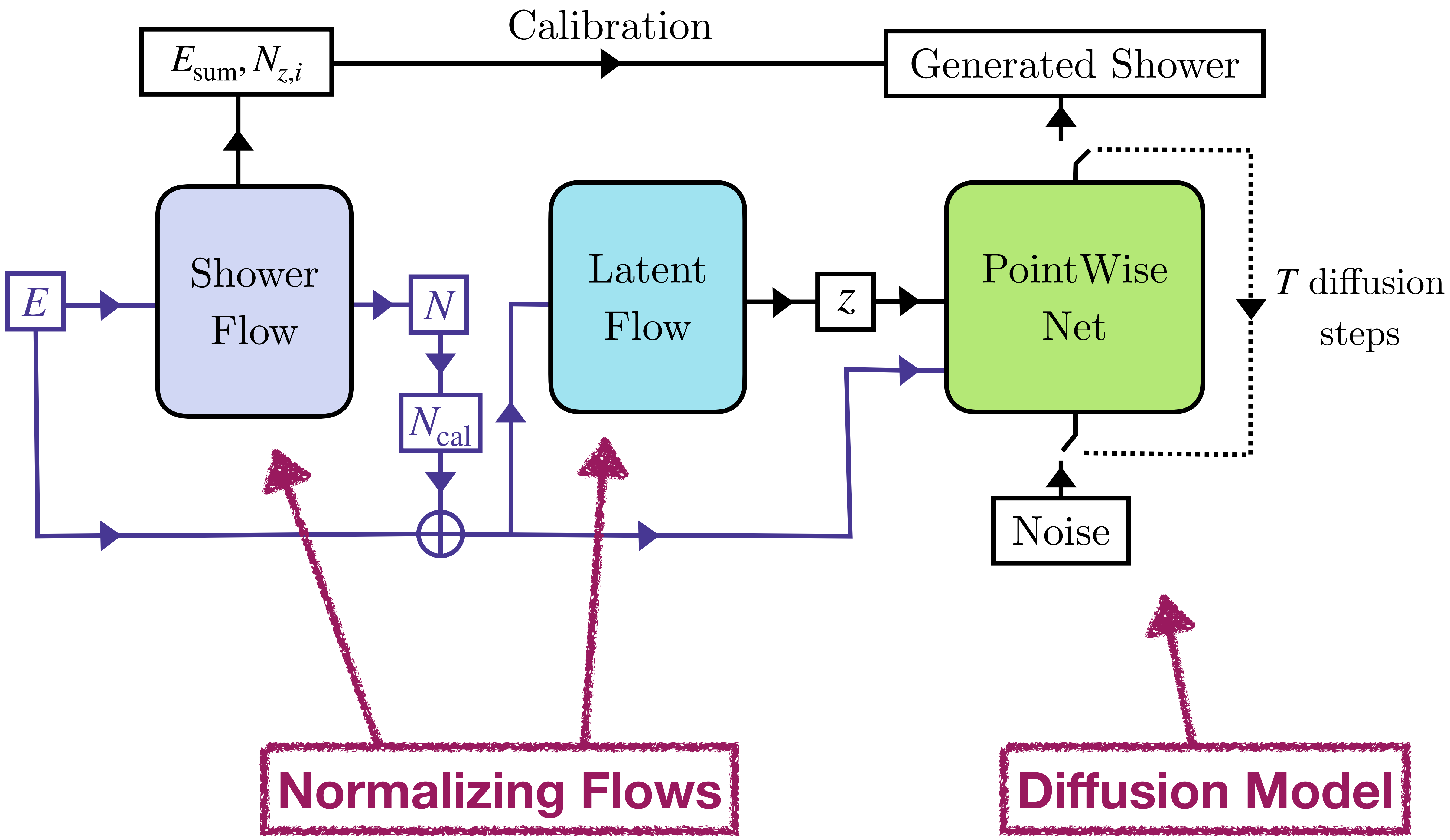


CaloClouds Model

Training



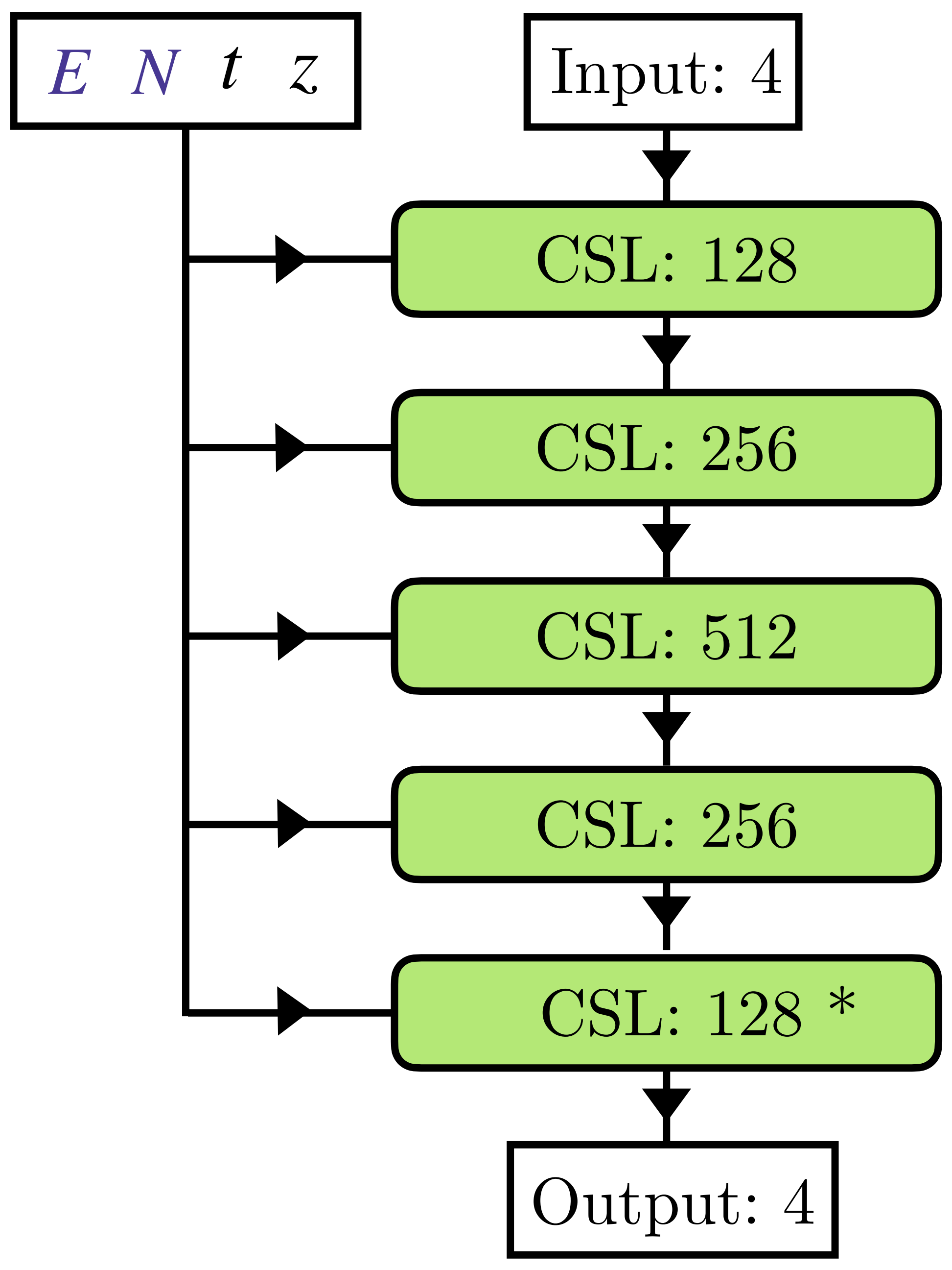
Sampling



Post-diffusion calibration: Number of points per layer, energy per layer, center of gravity in X and Y-direction

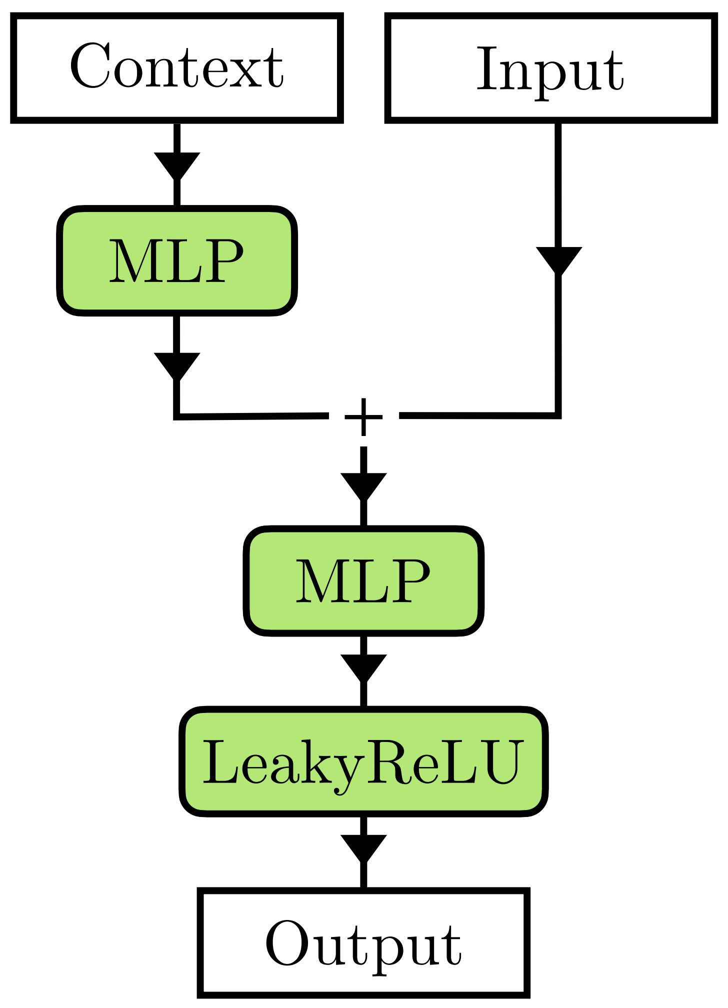
Equivariant Point Cloud (EPiC) layers from:
EB, G Kasieczka, J Thaler:
EPiC-GAN: Equivariant Point Cloud Generation for Particle Jets

Diffusion Architecture

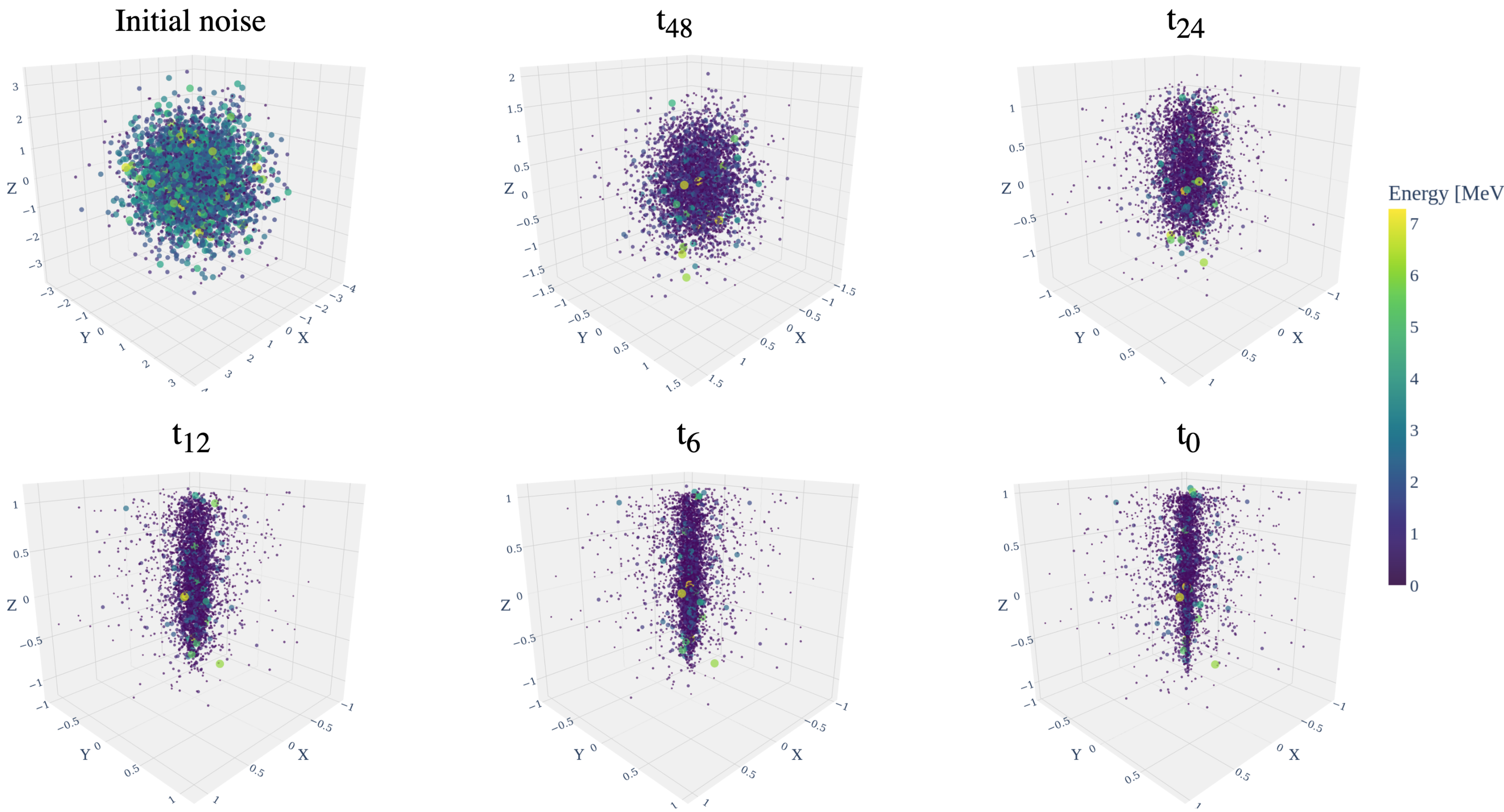


[x,y,z,E]

Concat Squash Linear (CSL) Layer



Reverse diffusion process (100 steps)



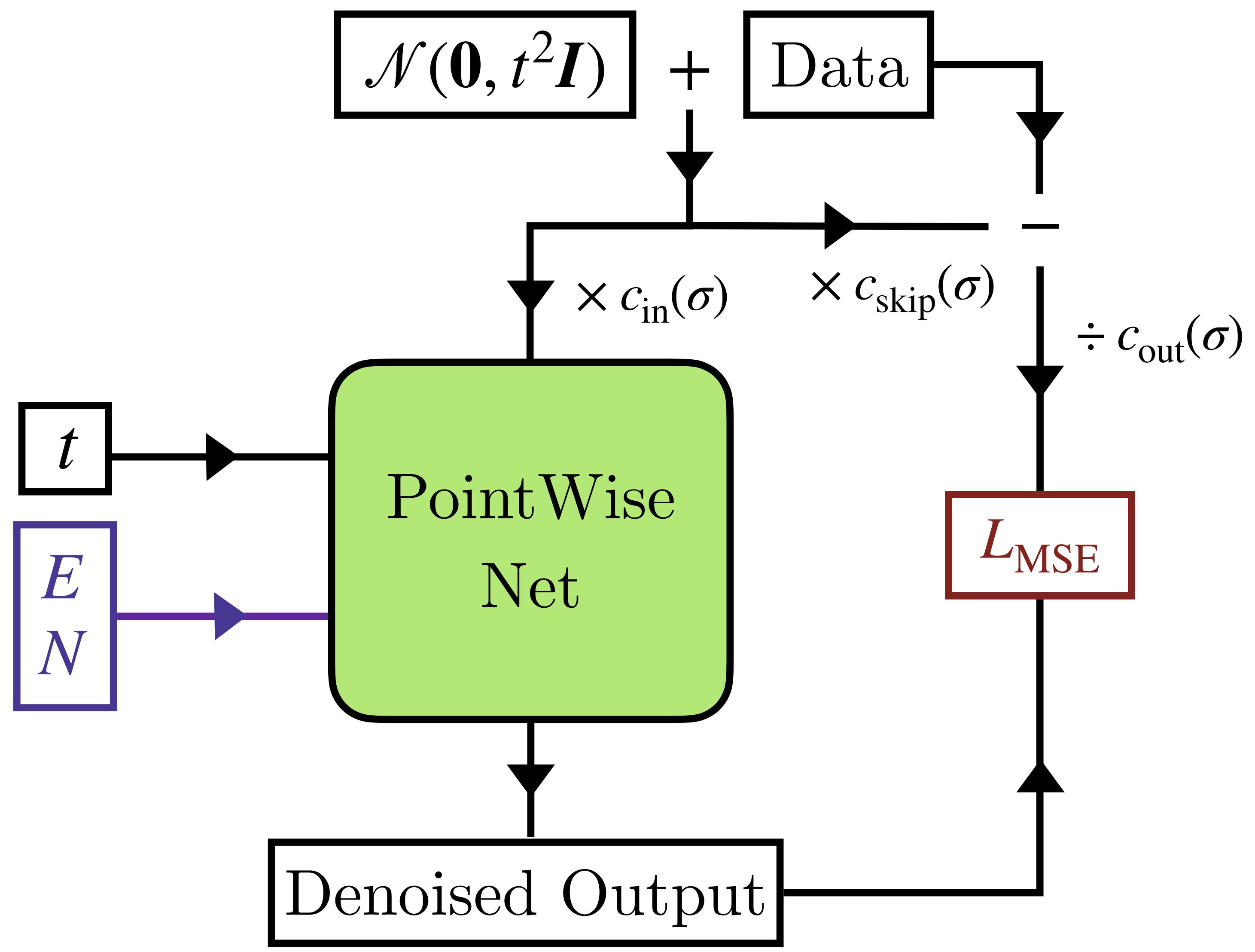
- Weight sharing across all points
- Each point independently sampled
- No interaction between points → very fast sampling

Architecture from:
S Luo, W Hu: Diffusion Probabilistic Models for 3D Point Cloud Generation

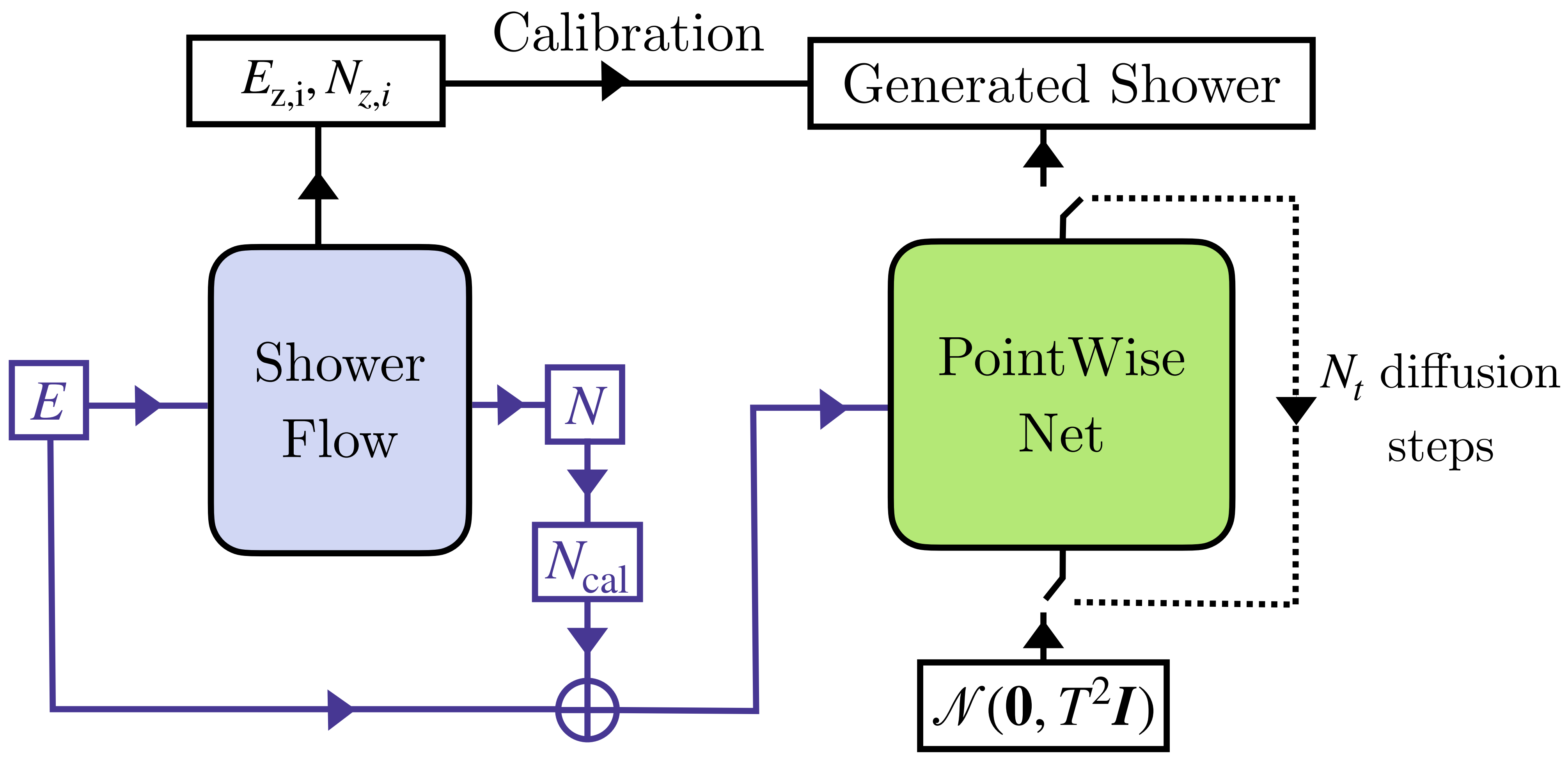
CaloClouds & CaloClouds II

- CaloClouds diffusion model based on discrete-time Denoising Diffusion Probabilistic Models (DDPM) [1]
  - Number of diffusion steps: training = sampling
    - Here: 100 denoising steps
- CaloClouds II diffusion model based on a continuous-time diffusion model [2]
  - Allows for a variety of stochastic and ordinary differential equation solvers (ODE / SDE solvers)
  - Fewer & variable number of steps during sampling
    - Here: Heun ODE solver with 25 model evaluations
  - Allows for distillation into a consistency model [3]
    - Here: Consistency model for single-shot generation
- CaloClouds II: No latent space (no encoder & latent flow)

Training (CaloClouds II)



Sampling (CaloClouds II)

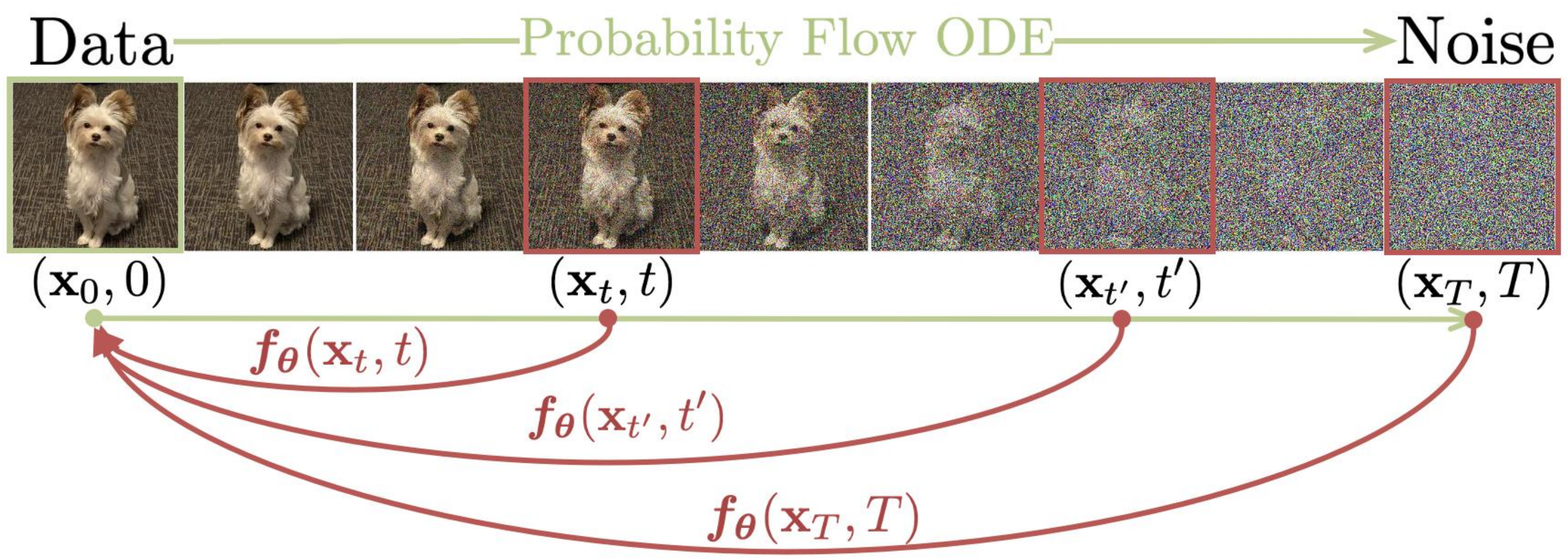


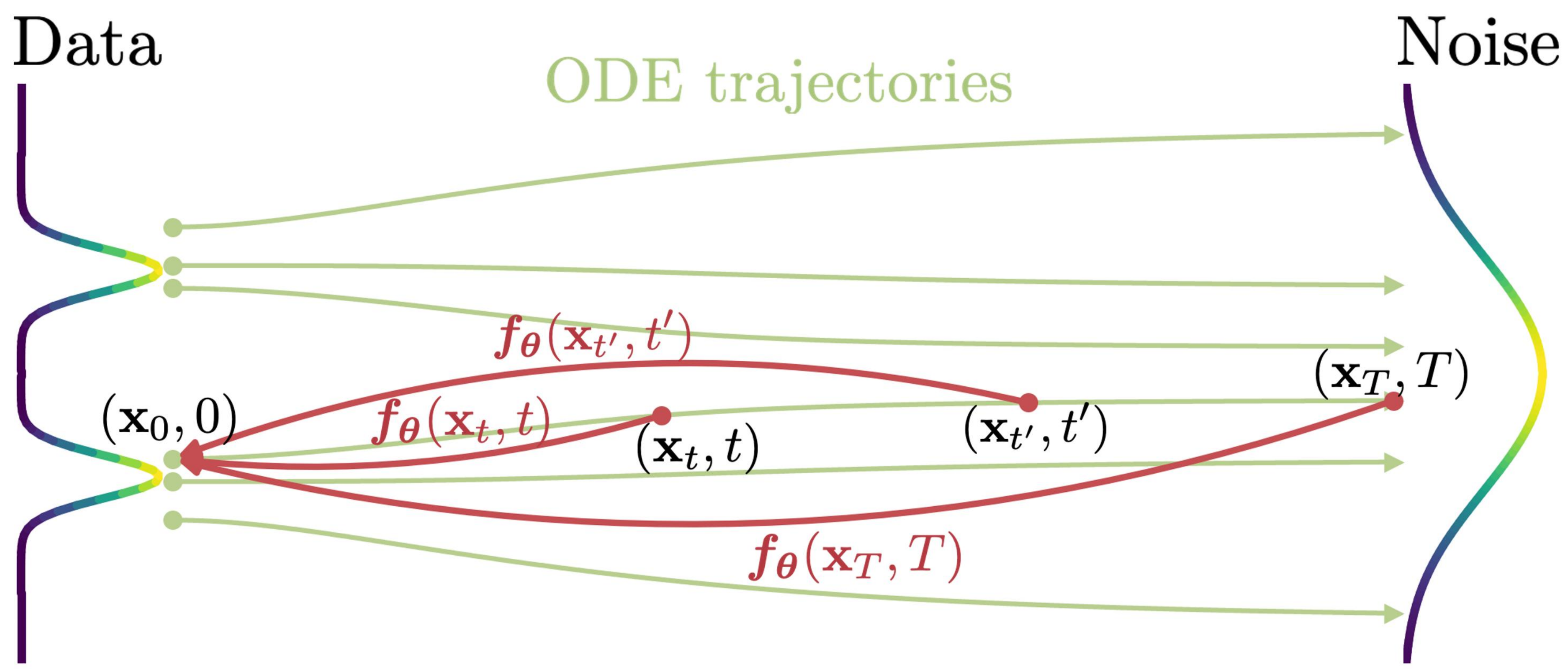
[1] J Ho et al.: Denoising Diffusion Probabilistic Models

[2] T. Karras et al: Elucidating the Design Space of Diffusion-Based Generative Models

[3] Y Song et al: Consistency Models

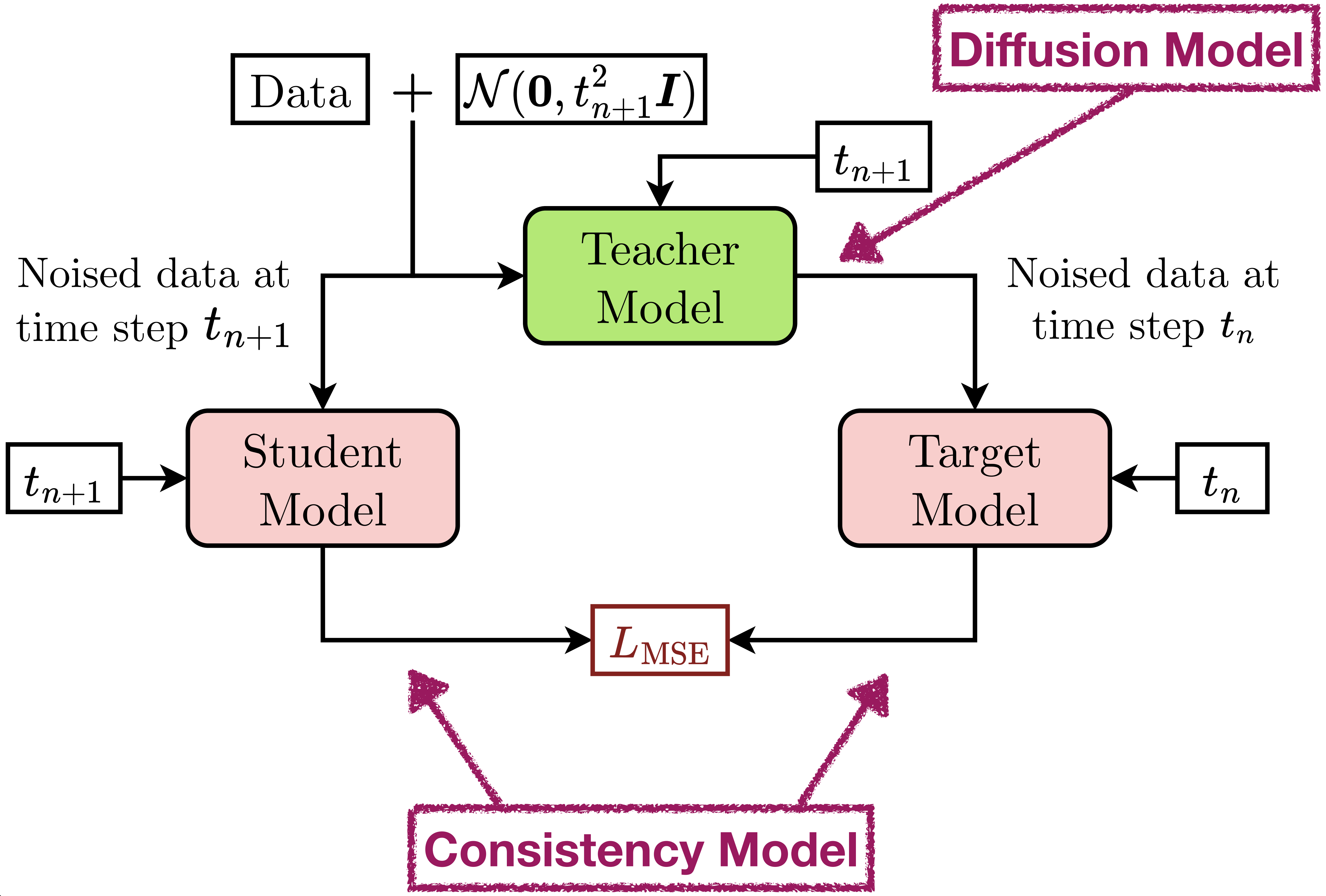
Consistency Models





- Consistency Models trainable standalone or distilled from a diffusion model
- Allow for single-step & multi-step generation

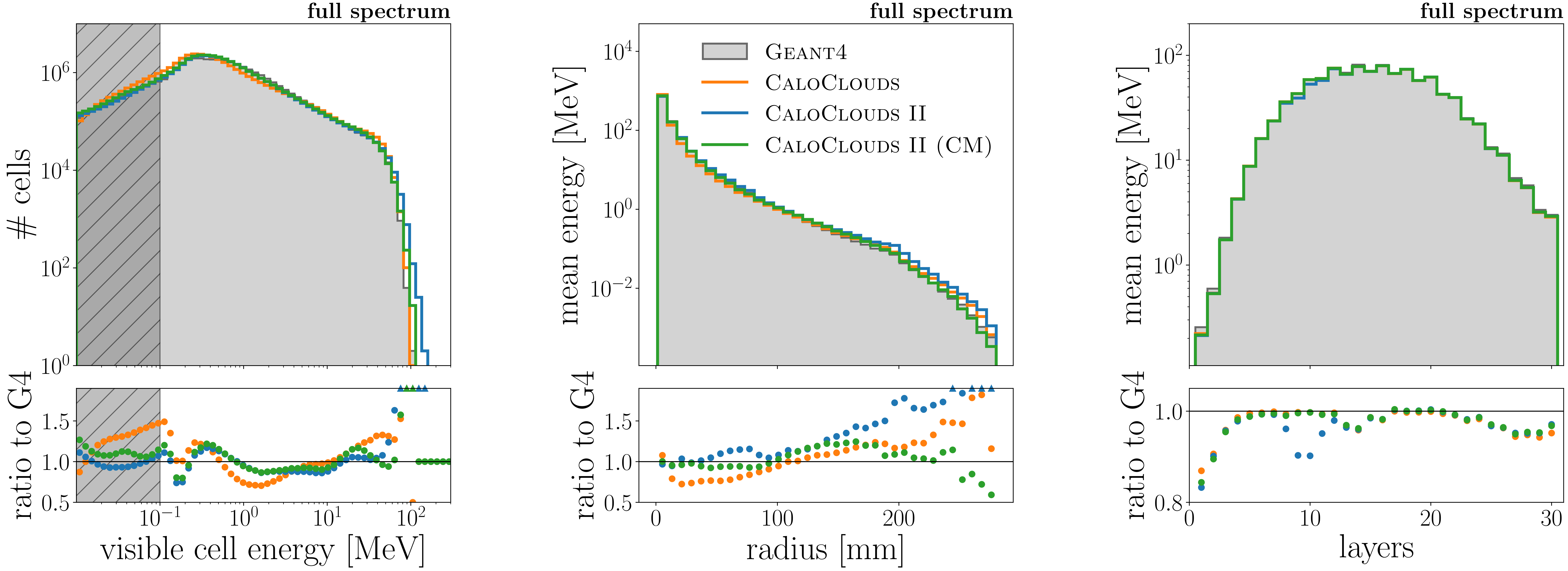
Consistency distillation:



Student model: updated via gradient descent
Target model: updated via weight average

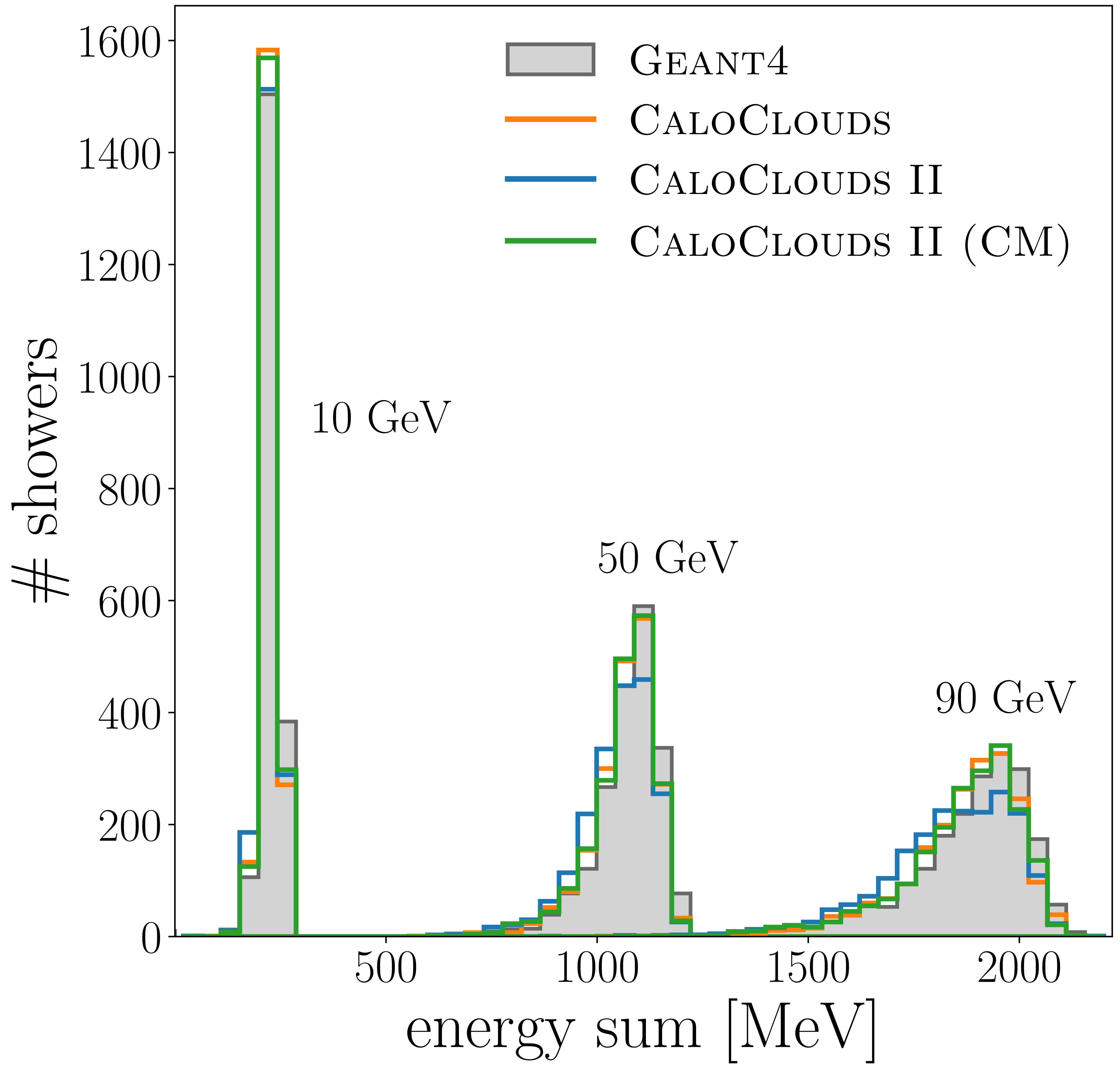
Y Song et al: Consistency Models

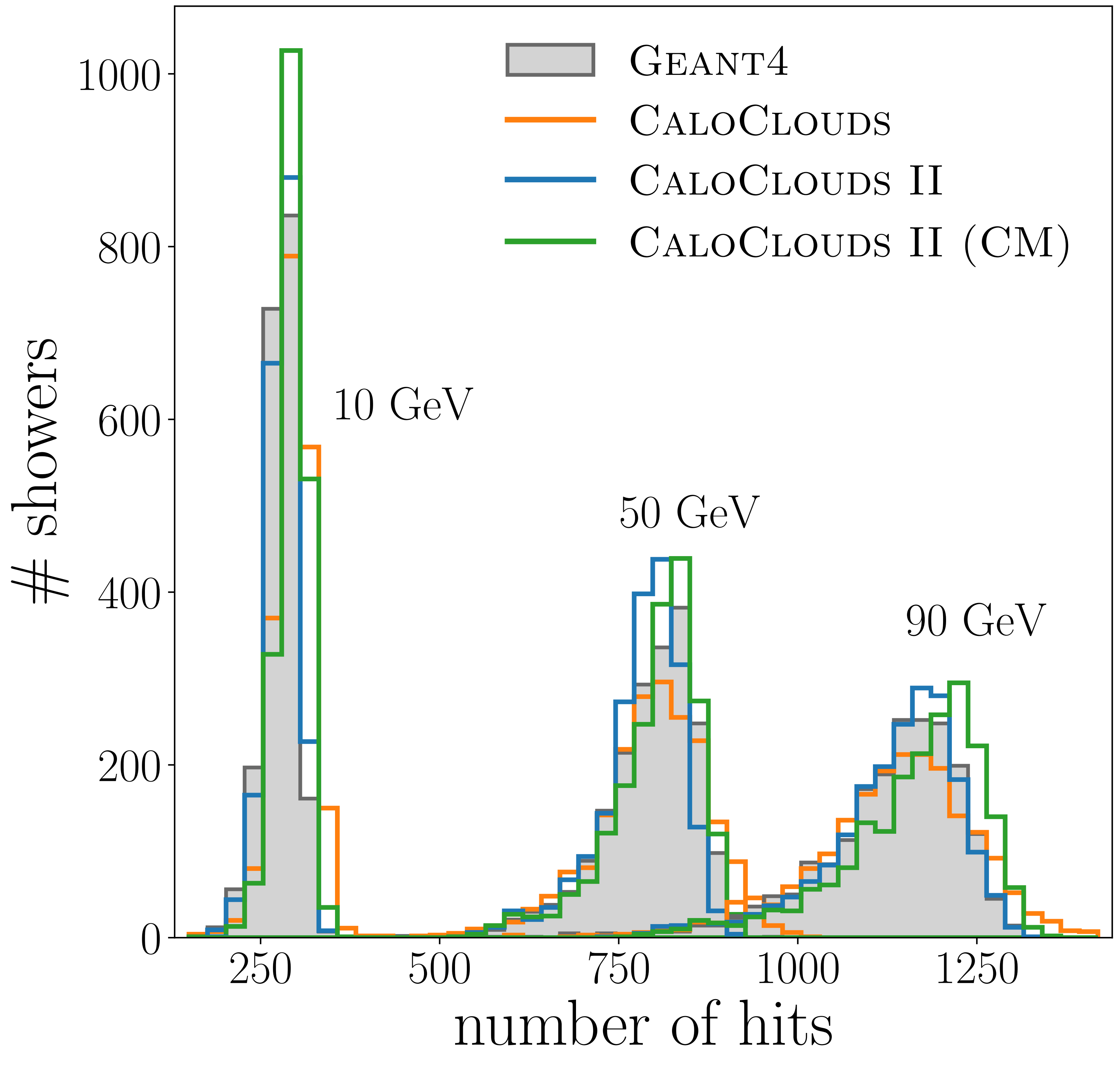
Results: 10-90 GeV Photons



- All evaluations with point cloud showers projected to regular cell geometry
- Hit energy spectrum, radial energy profile, and longitudinal energy profile well modeled by all three CaloClouds variants (40,000 showers each)
- CaloClouds II models improve the radial energy profile

Results: Single Incident Energies





- Total visible energy & number of cell hits for single incident energies well modelled by all three CaloClouds variants (2,000 showers each)
- Number of hits better modeled by the CaloClouds II variants
- Expecting further improvements with wider energy range during training

Results: Metrics & Classifier

Simulator	$W_1^{N_{\text{hits}}}$ $(\times 10^{-3})$	$W_1^{E_{\text{vis}}/E_{\text{inc}}}$ $(\times 10^{-3})$	$W_1^{E_{\text{cell}}}$ $(\times 10^{-3})$	$W_1^{E_{\text{long}}}$ $(\times 10^{-3})$	$W_1^{E_{\text{radial}}}$ $(\times 10^{-3})$	$W_1^{m_{1,X}}$ $(\times 10^{-3})$	$W_1^{m_{1,Y}}$ $(\times 10^{-3})$	$W_1^{m_{1,Z}}$ $(\times 10^{-3})$
Geant4	0.7 ± 0.2	0.8 ± 0.2	0.9 ± 0.4	0.7 ± 0.8	0.7 ± 0.1	0.9 ± 0.1	1.1 ± 0.3	0.9 ± 0.3
CaloClouds	**2.5 ± 0.3**	11.4 ± 0.4	15.9 ± 0.7	**2.0 ± 1.3**	38.8 ± 1.4	4.0 ± 0.4	8.7 ± 0.3	1.4 ± 0.5
CaloClouds II	3.6 ± 0.5	26.4 ± 0.4	**15.3 ± 0.6**	3.7 ± 1.6	11.6 ± 1.5	**2.4 ± 0.4**	**7.6 ± 0.2**	3.9 ± 0.4
CaloClouds II (CM)	6.1 ± 0.7	**9.8 ± 0.5**	16.0 ± 0.7	**2.0 ± 1.4**	**8.3 ± 1.9**	3.0 ± 0.4	9.5 ± 0.6	**1.2 ± 0.5**

- Evaluation metrics based on 1-Wasserstein distance [1]
- Similar performance between all three CaloClouds versions
- High-level classifier “metric”: CaloClouds II better than CaloClouds

High-level fully connected classifier:

Simulator	AUC
CaloClouds	0.999 ± 0.001
CaloClouds II	0.928 ± 0.001
CaloClouds II (CM)	**0.923 ± 0.001**

[1] R Kansal, et al: Particle Cloud Generation with Message Passing Generative Adversarial Networks

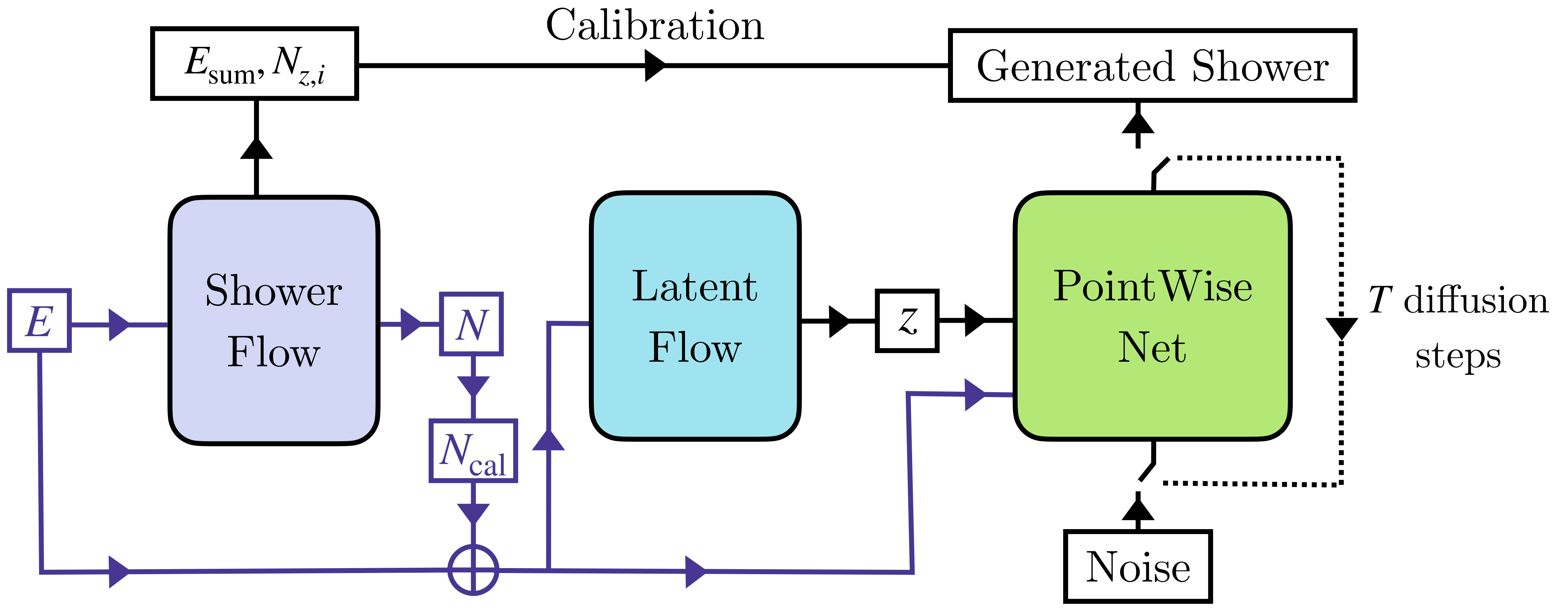
Sampling Speed-Up (CPU & GPU)

Hardware	Simulator	NFE	Batch Size	Time / Shower [ms]	Speed-up
CPU (Intel Xeon CPU E5-2640)	GEANT4			3914.80 ± 74.09	$\times 1$
	CALOCLOUDS	100	1	3146.71 ± 31.66	$\times 1.2$
	CALOCLOUDS II	25	1	651.68 ± 4.21	$\times 6.0$
	CALOCLOUDS II (CM)	1	1	84.35 ± 0.22	$\times 46$ ← !
GPU (NVIDIA A100 40 GB)	CALOCLOUDS	100	64	24.91 ± 0.72	$\times 157$
	CALOCLOUDS II	25	64	6.12 ± 0.13	$\times 640$
	CALOCLOUDS II (CM)	1	64	2.09 ± 0.13	$\times 1873$

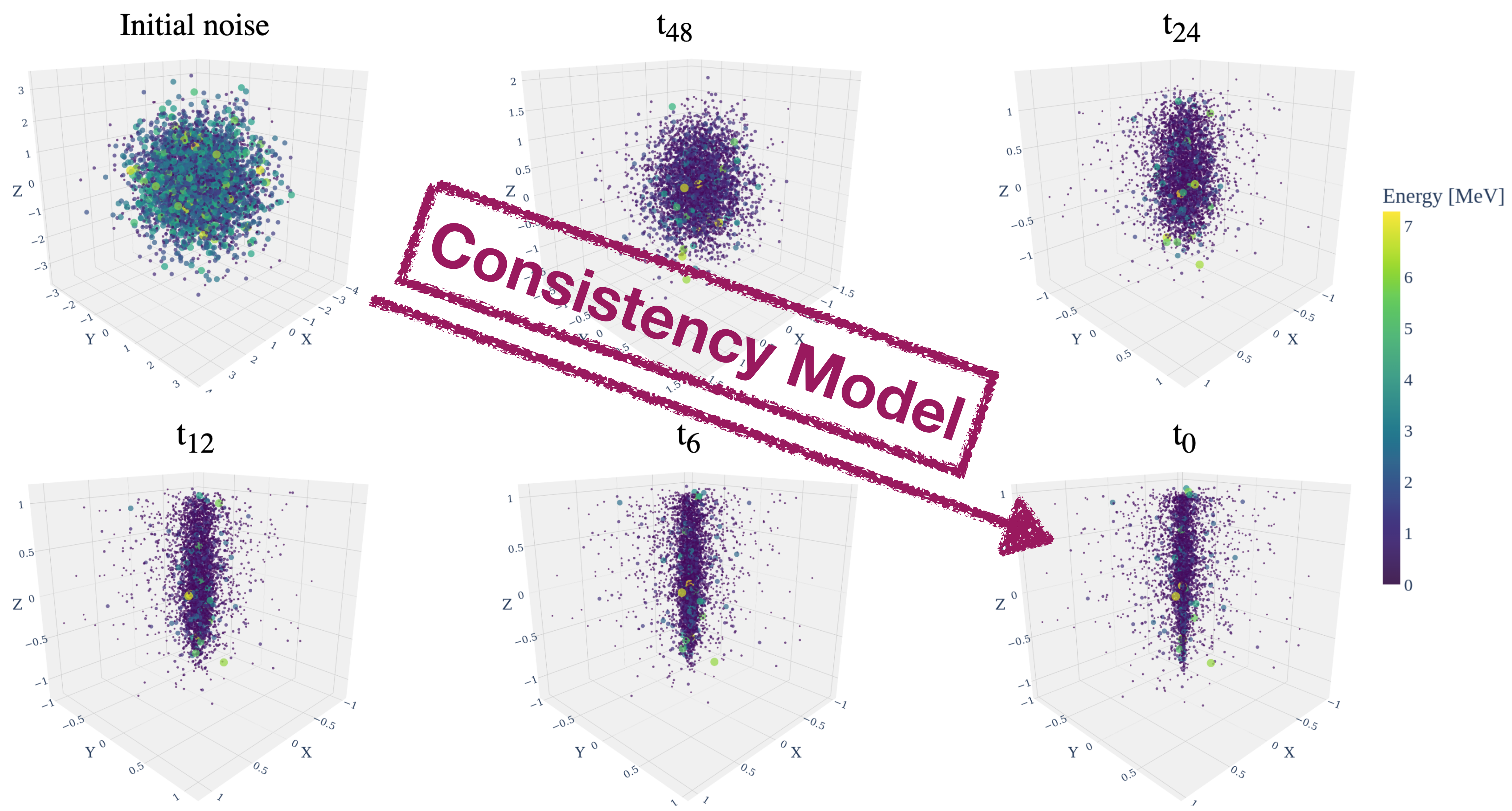
- Speed-up scales with the number of function evaluations (NFE)
- Largest speed-up for CaloClouds II (CM), even on CPU
- CPUs more widely available than GPUs, cheaper, and current simulation chain optimised on CPUs

Summary

- CaloClouds: First model to generate high-fidelity calorimeter showers as point clouds with $\mathcal{O}(1{,}000)$ points
- Clustered Geant4 steps allow for a cell-geometry-independent model
- Continuous-time diffusion allows for 4x fewer diffusion steps than discrete-time diffusion without loss in fidelity
- Distillation into a consistency model allows for single-shot generation
    - 46x faster generation than Geant4 on CPU
- First consistency model for calorimeter shower generation



Reverse diffusion process (100 steps)



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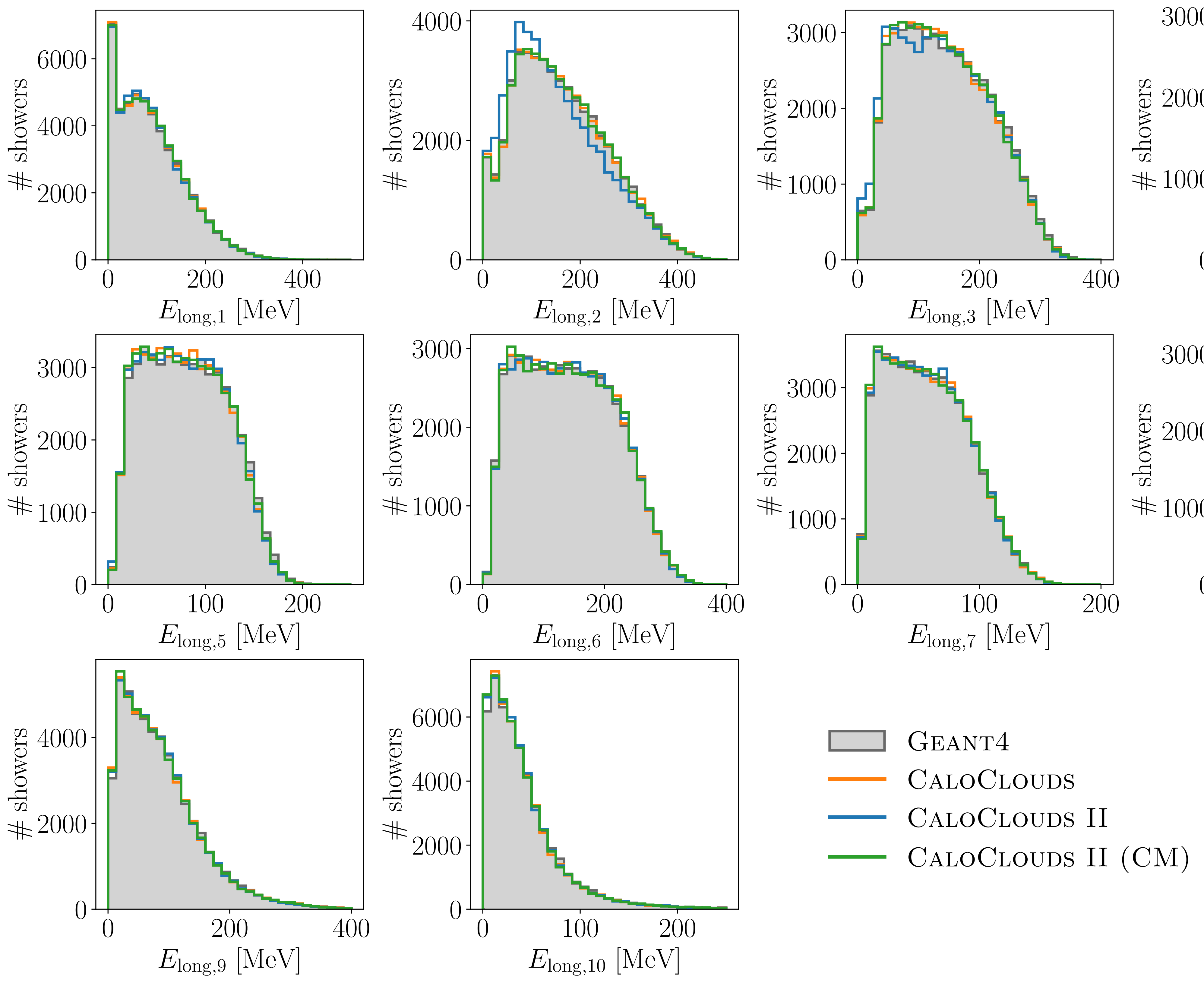
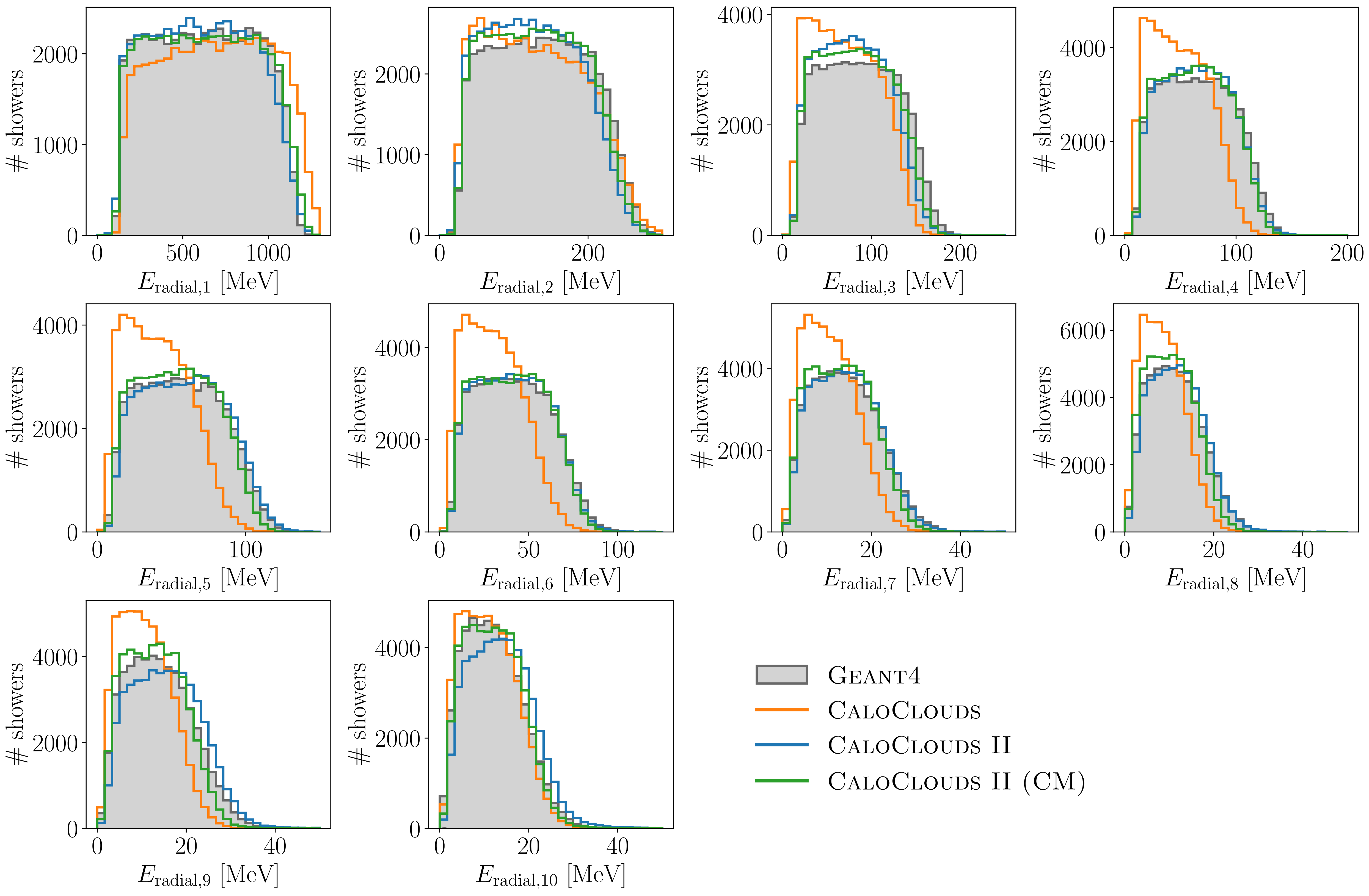
Bonus slides

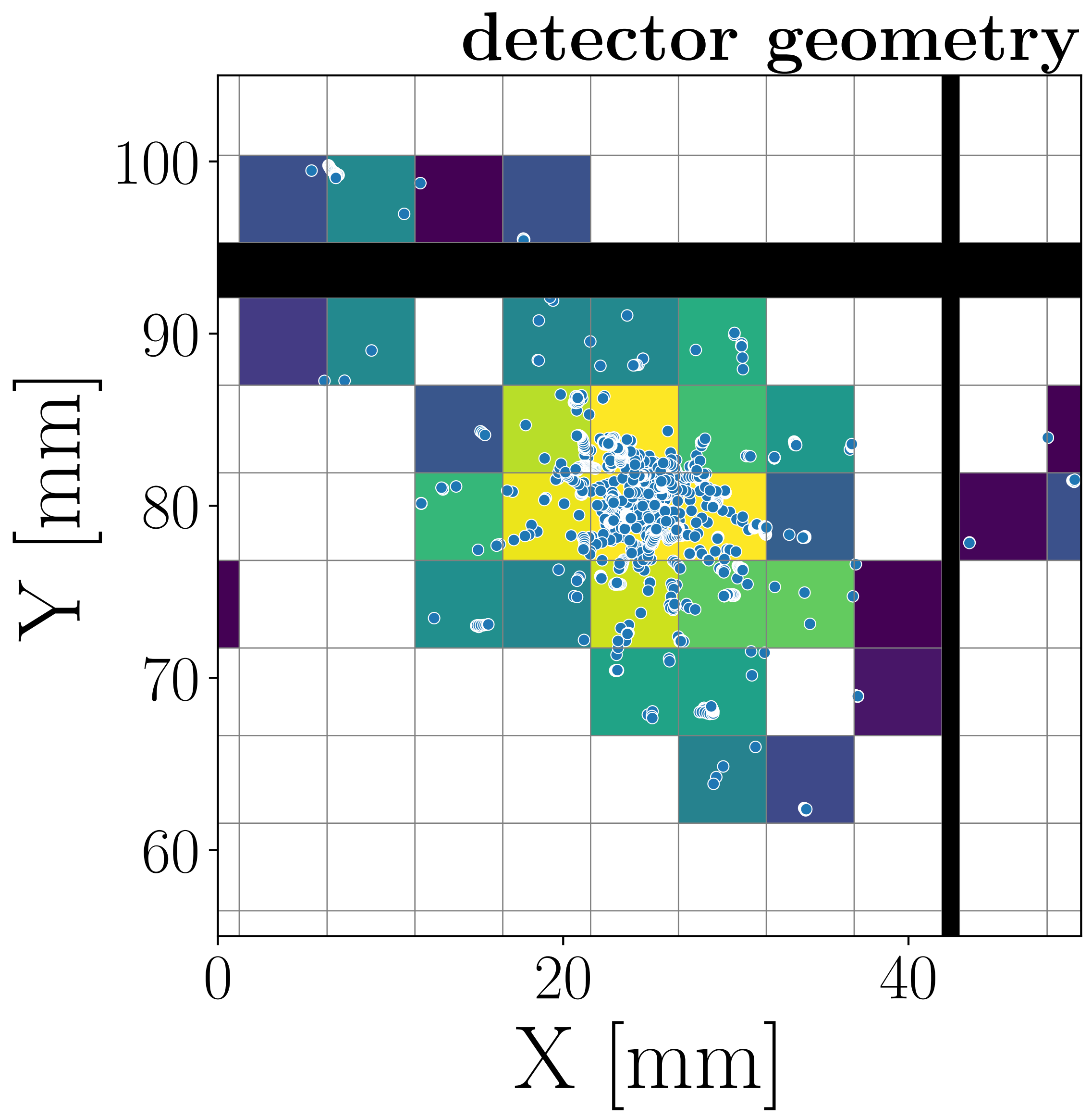
Longitudinal and Radial Profile Regions (10 each)



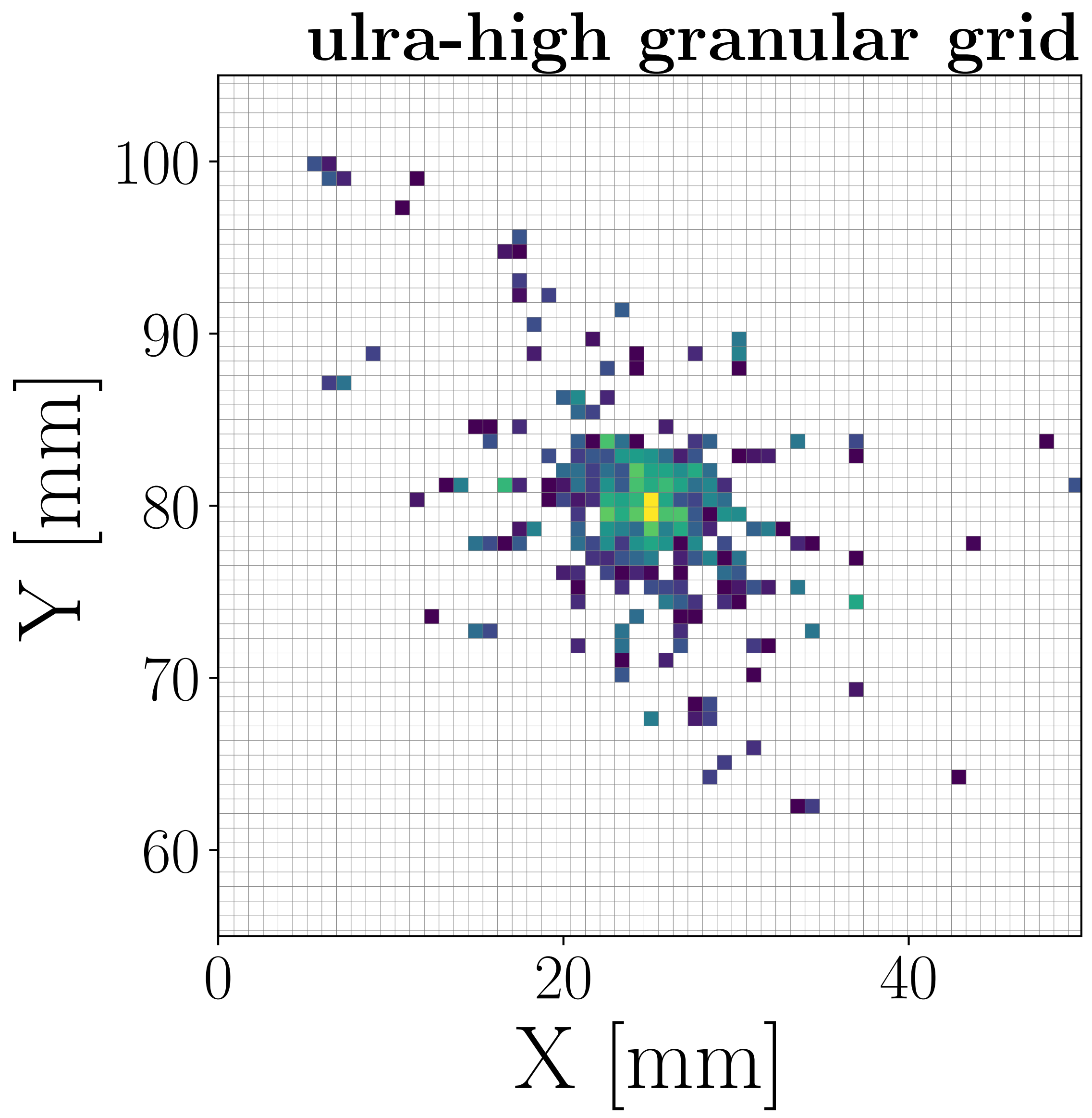


Ultra-high granular grid

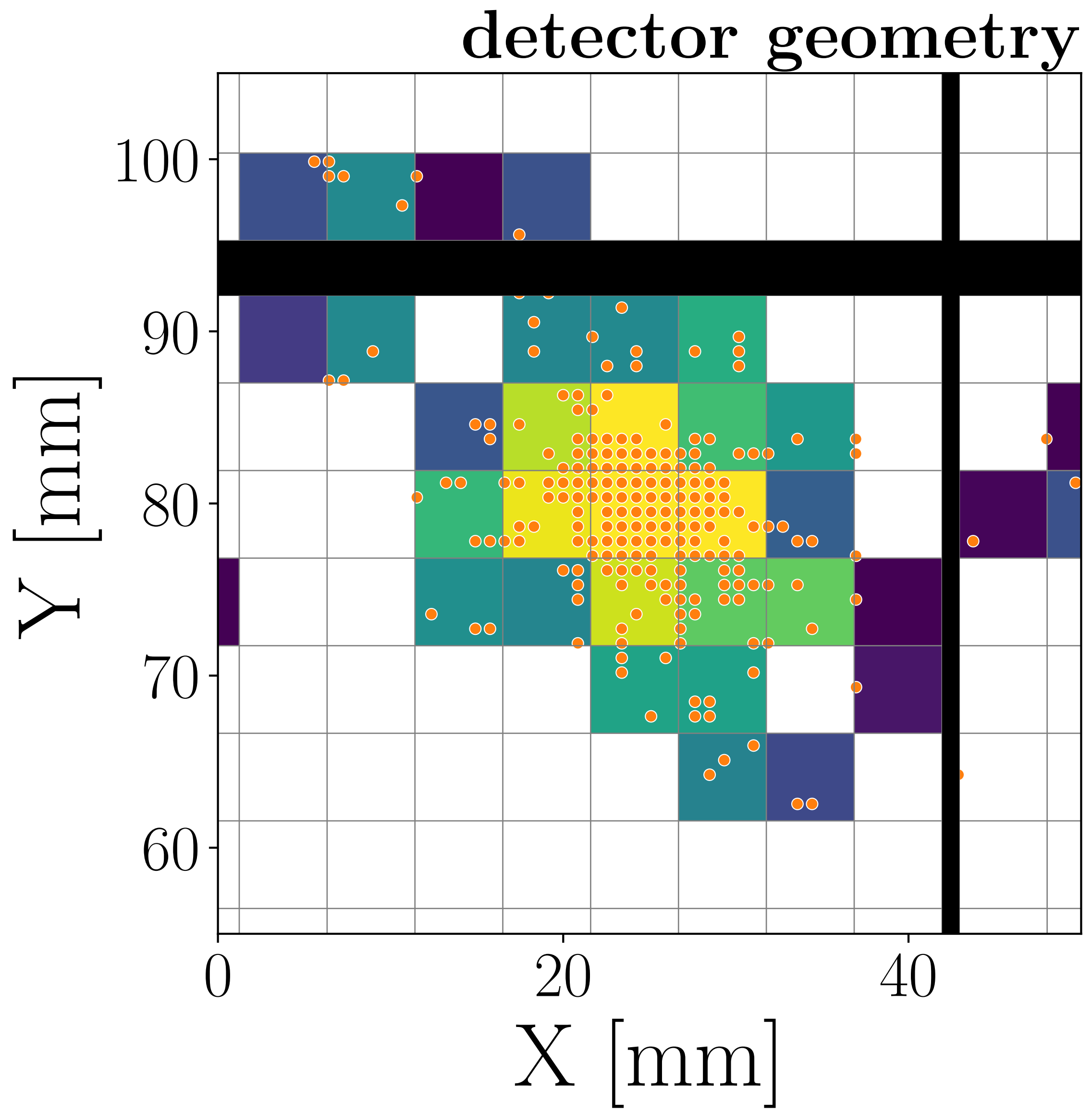
Geant4 steps —> Sensor hits



Steps clustered in ultra-high grid

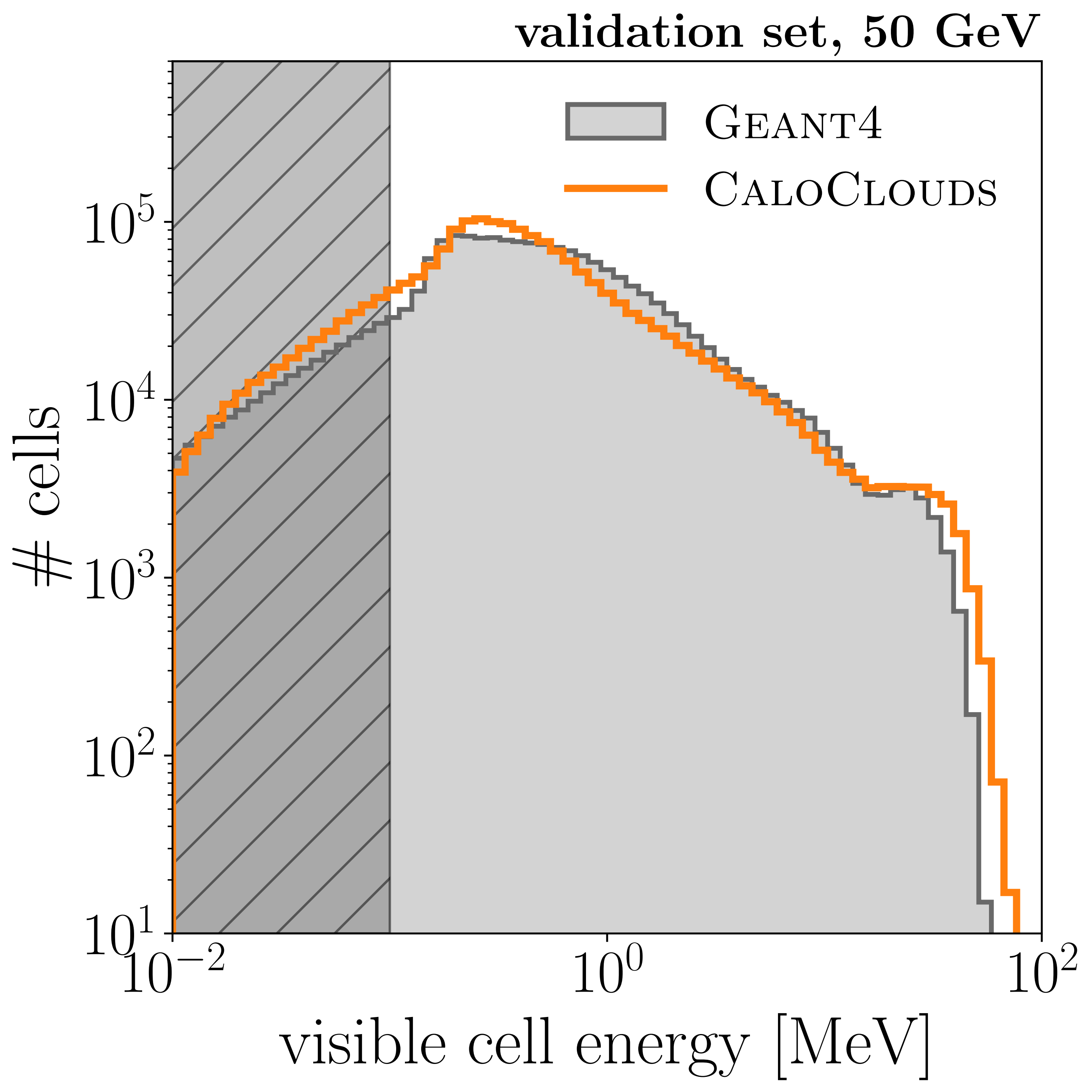


Ultra-high hits —> Sensor hits



Shower translation

Same position as training set



Shifted position