מכון ויצמן למדע

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CaloGraph

Calorimeter simulation via Graph-based diffusion model

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How to represent calorimeter?

2D/3D images	Point Cloud	Graph
↓	↓	↓
Requires additional mappings for non-regular geometries	Need to predict spatial positions and map back to grid	Fits to all geometries Points fixed, edges have physical meaning

How to represent calorimeter?

Our choice

2D/3D images

↓

Requires additional mappings for non-regular geometries

Point Cloud

↓

Need to predict spatial positions and map back to grid

Graph

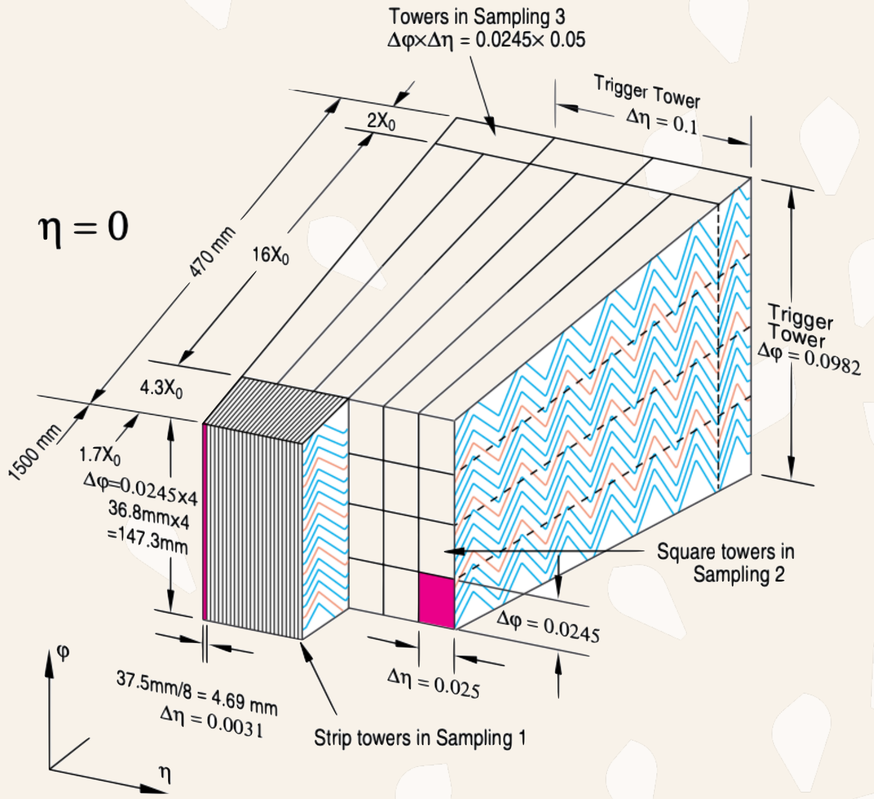
↓

Fits to all geometries

Points fixed, edges have physical meaning

Dataset

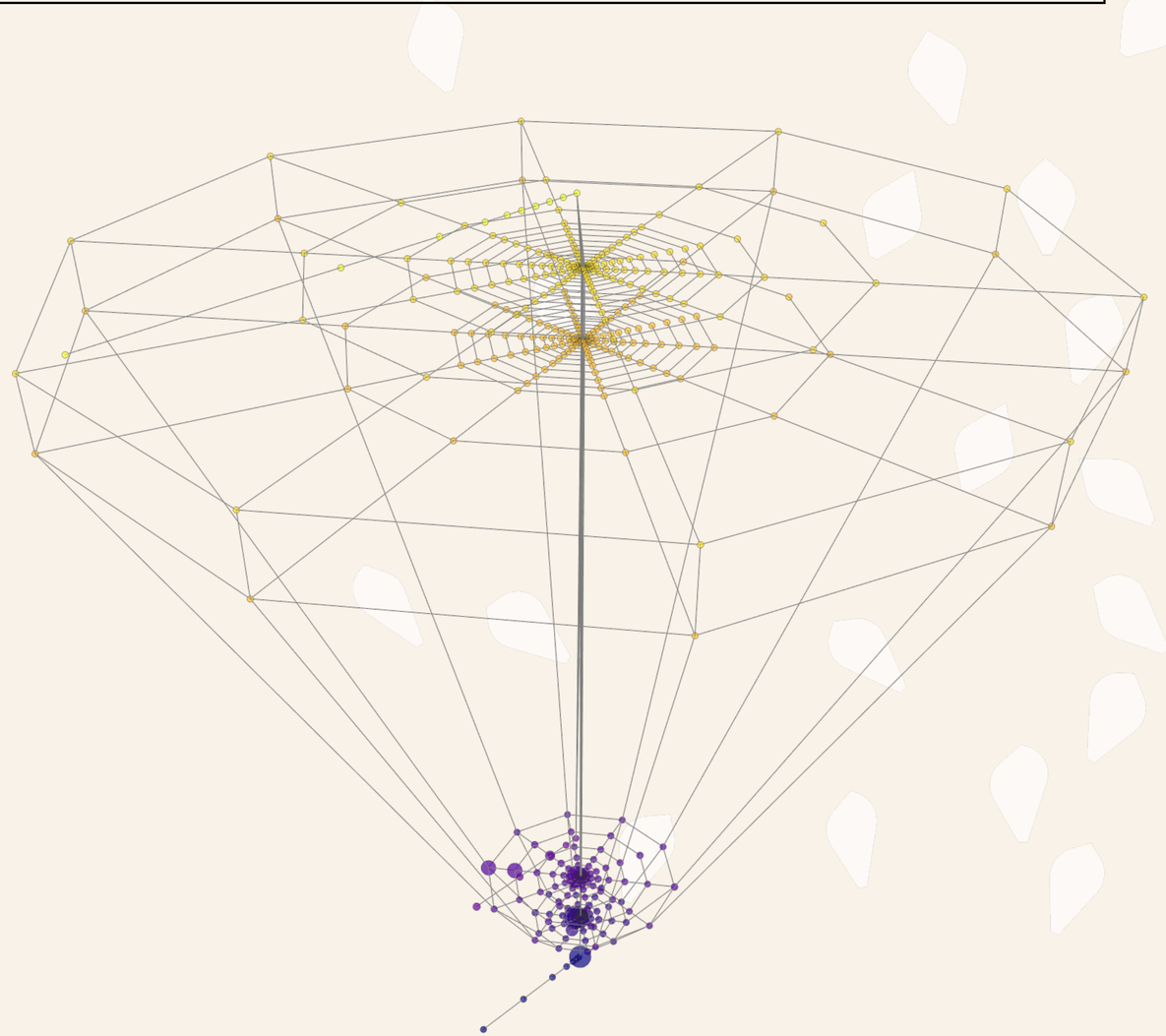
- Dataset 1 from CaloChallenge — ATLAS-like calorimeter
- Pions sample
- 15 discrete incident energies from 256 MeV up to 4 TeV
- Number of radial and angular bins varies from layer to layer, resulting in 533 voxels for pions and non-regular grid.



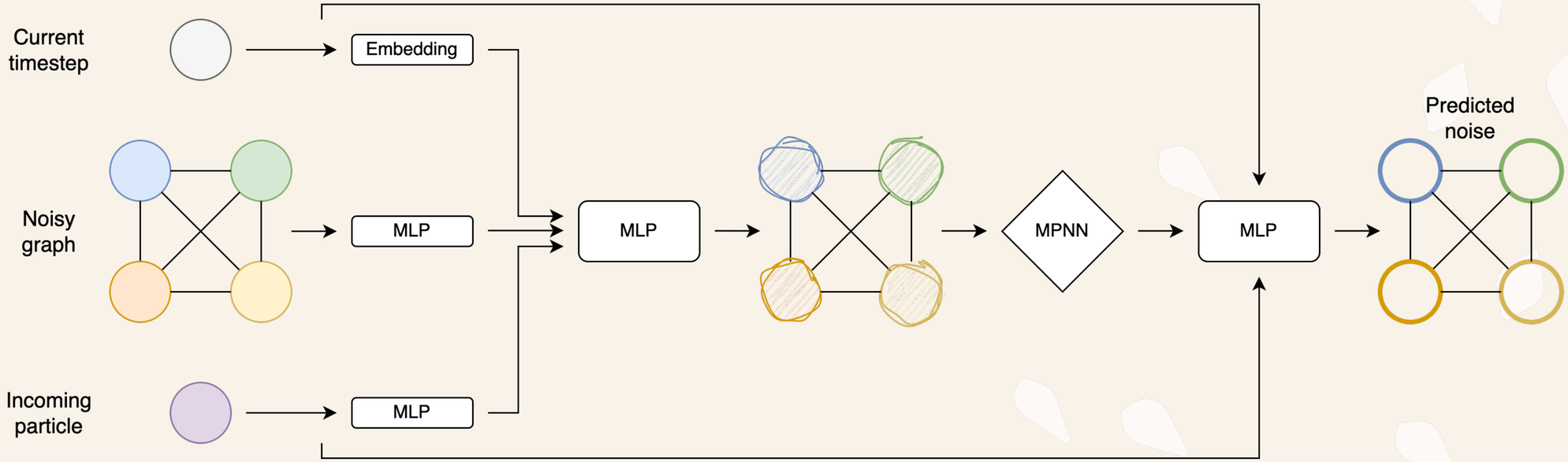
ATL-SOFT-PUB-2020-006

Dataset preprocessing

- Each cell in calorimeter corresponds to graph node, nearest neighbors nodes are connected;
- η, ϕ coordinates are normalized to have zero mean and unit variance;
- Energy preprocessing:
  - Divide by incoming energy
  - Apply logit transform
  - Standardize to zero mean and unit variance



CaloGraph



- Trained embedding of cell layers
- Positional embedding of time
- 0.8M parameters
- 4 MPNN iterations
- Sampling with PNDM sampler

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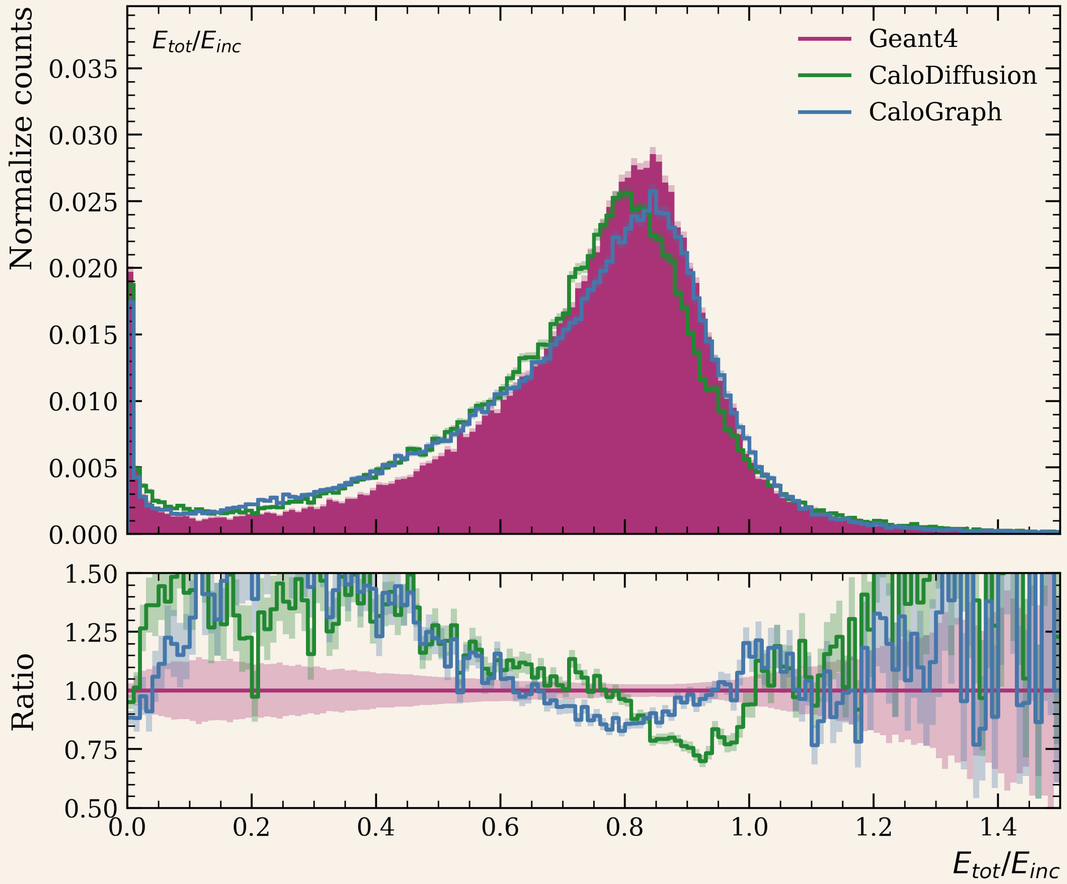
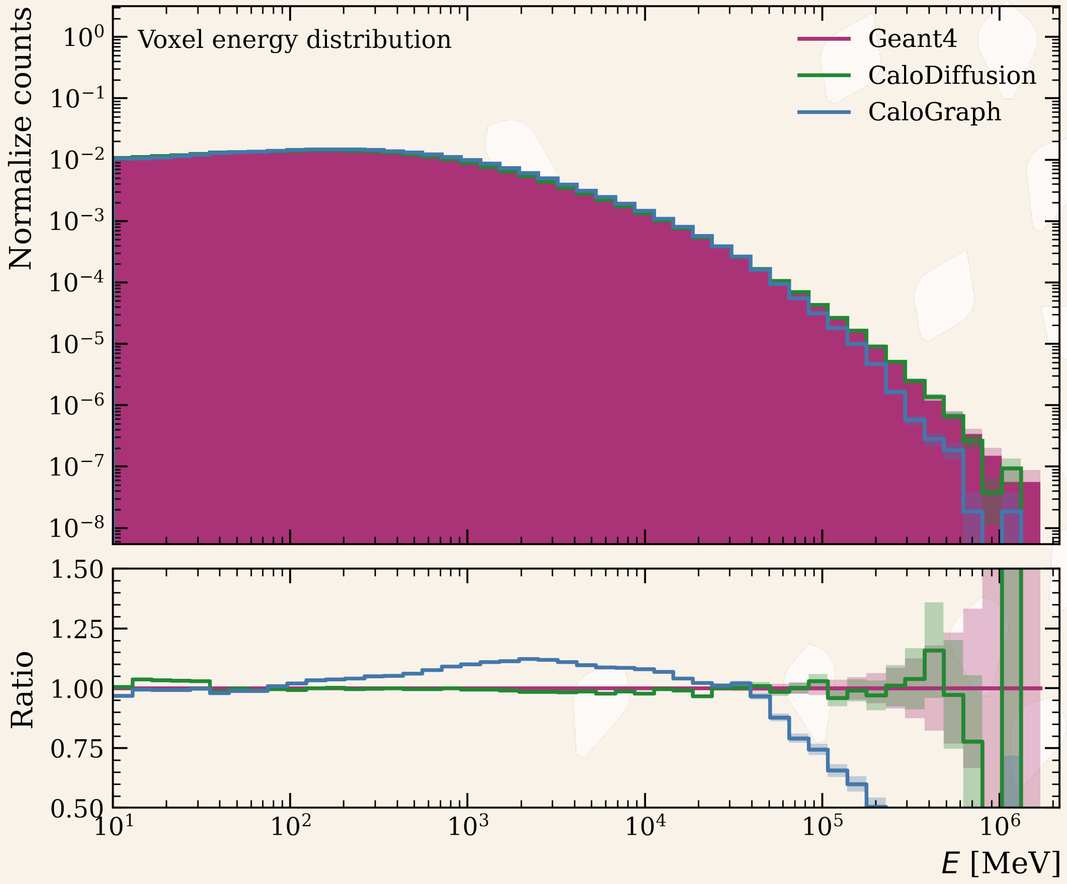
Results: Overall plots





O. Amram, K. Pedro: Denoising diffusion models with geometry adaptation for high fidelity calorimeter simulation (arXiv:2308.03876)

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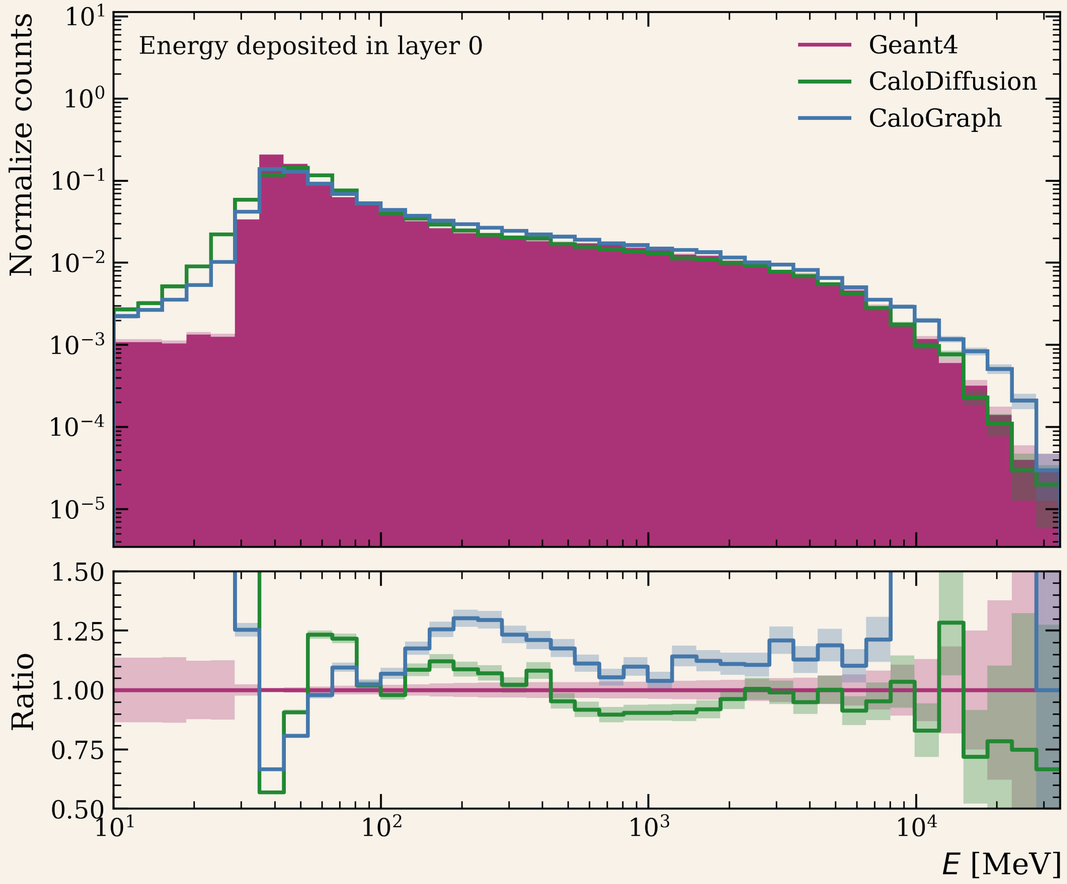
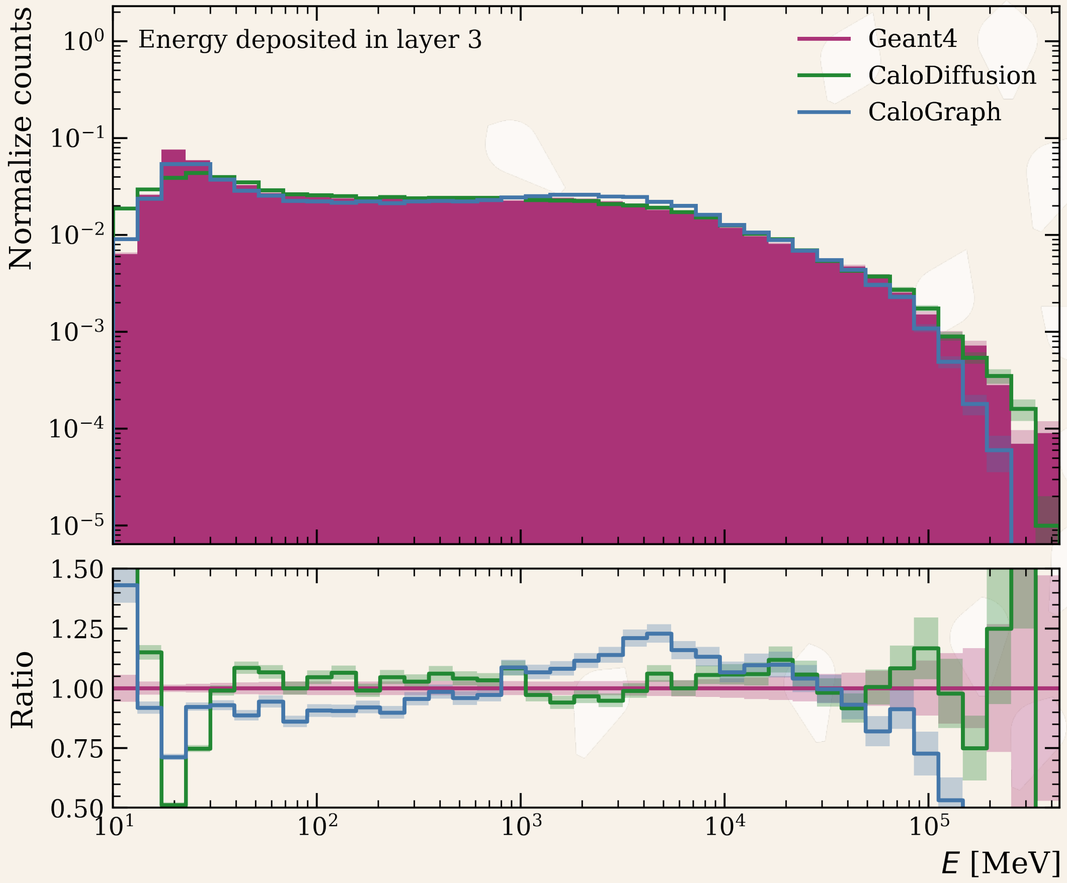
Results: Energy per layer





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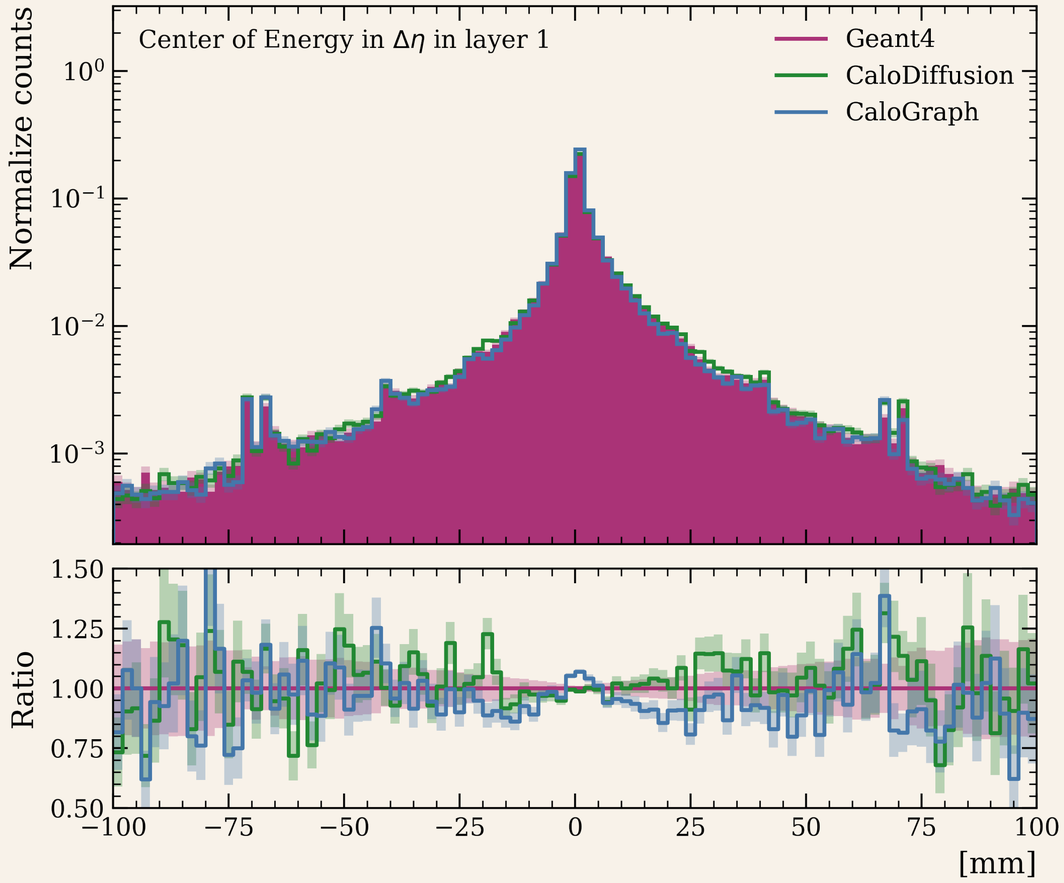
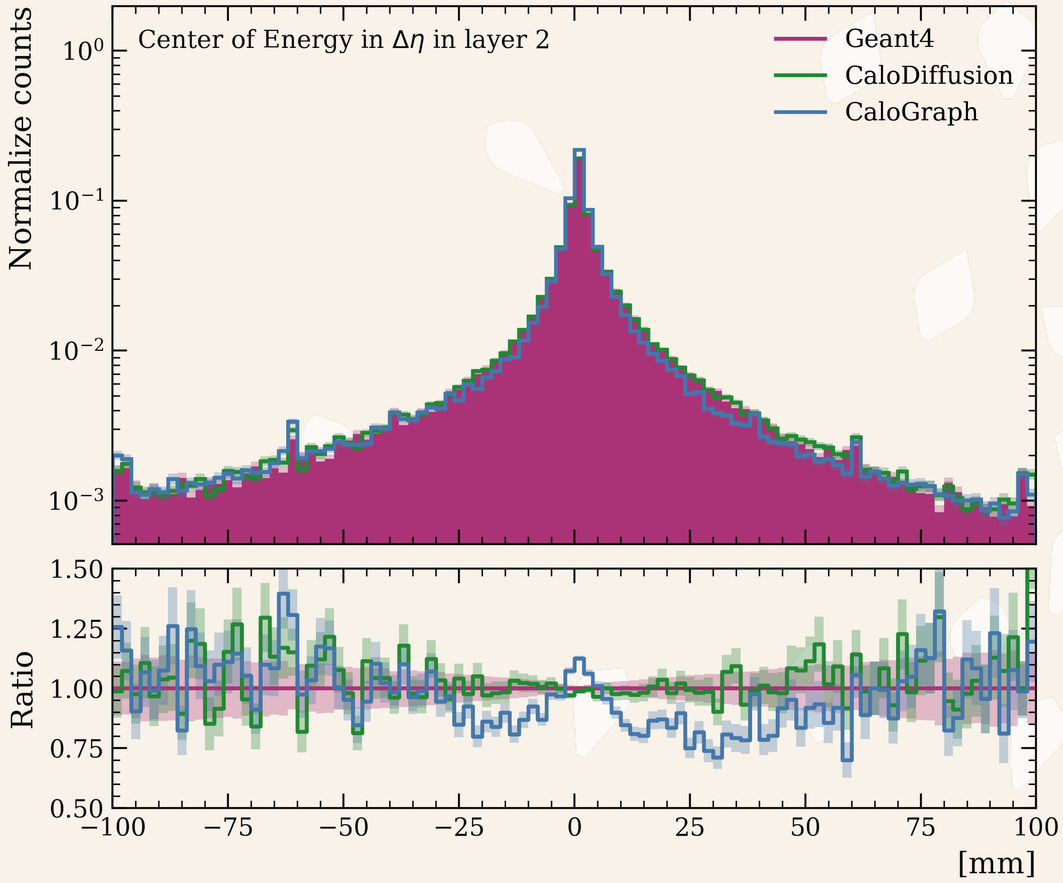
Results: Center of Energy in $\Delta\eta$





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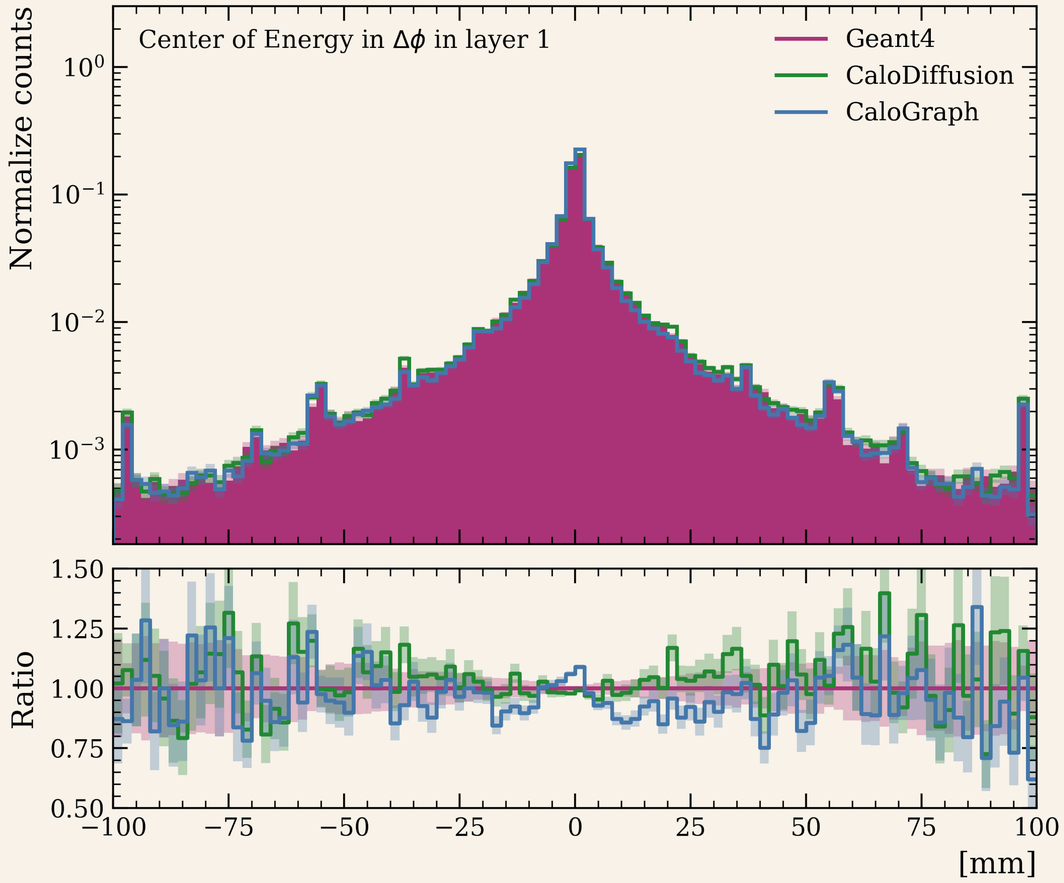
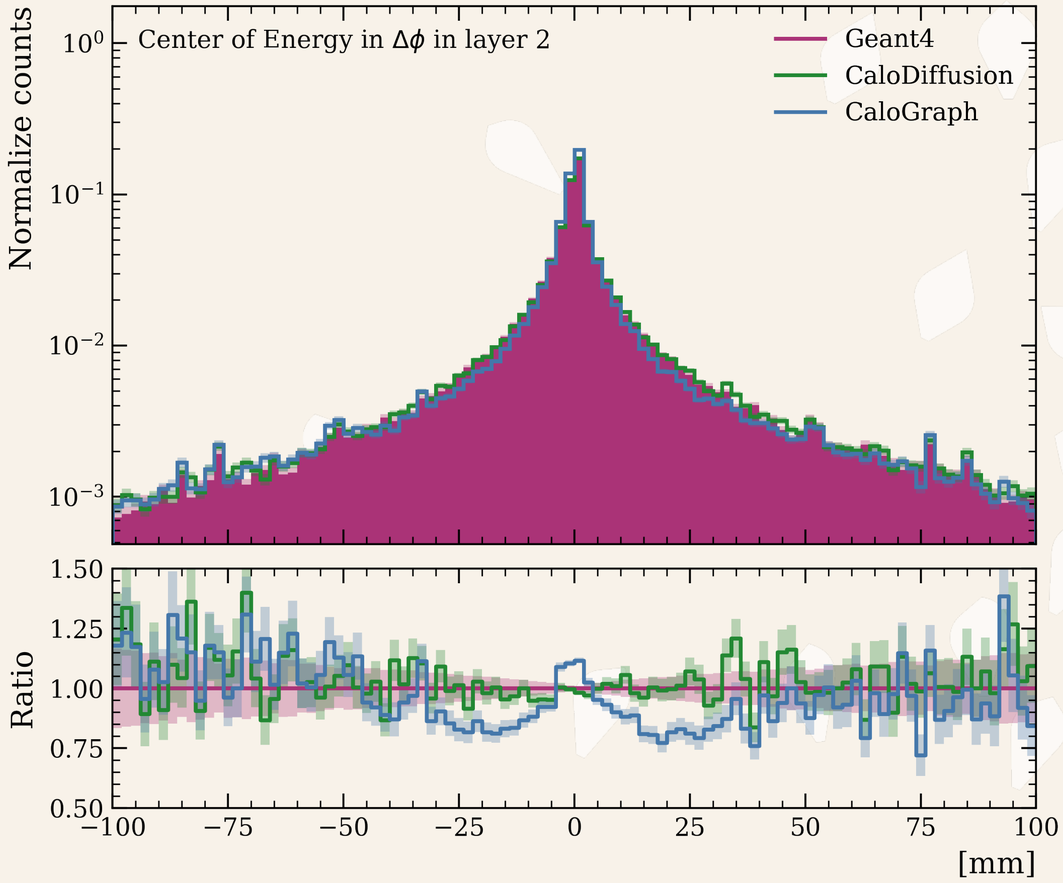
Results: Center of Energy in $\Delta\phi$





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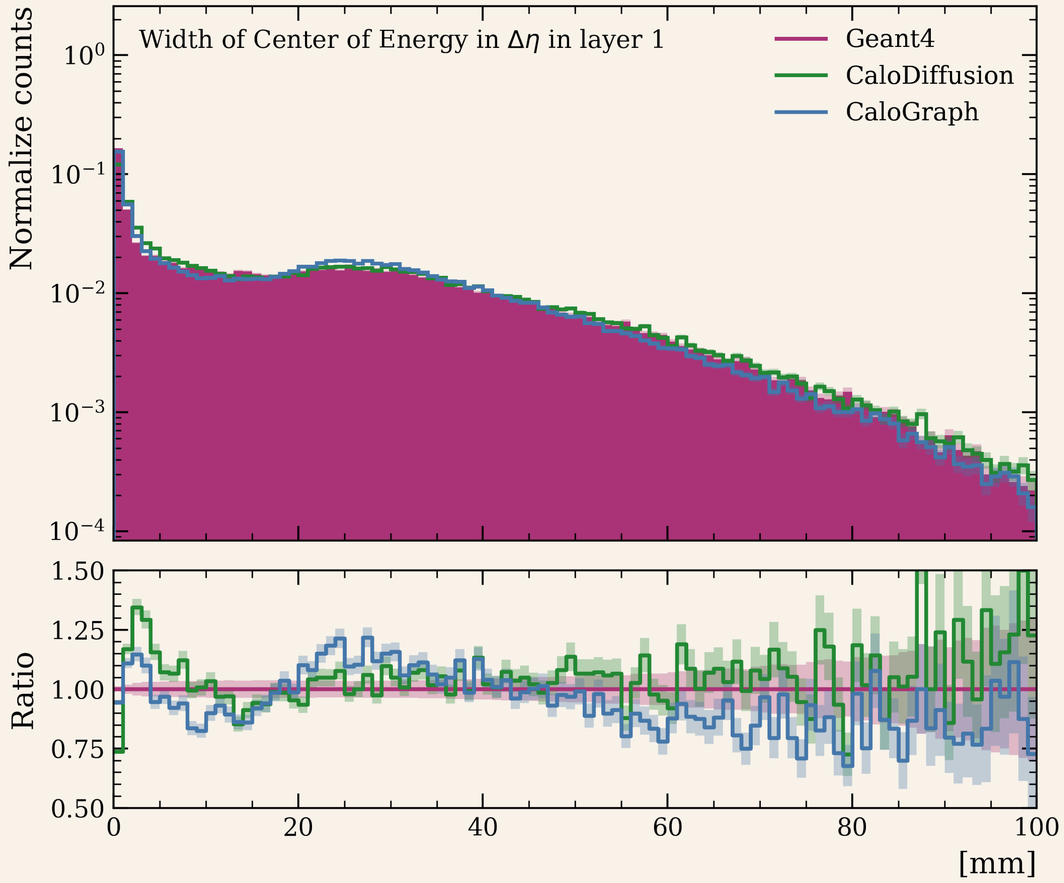
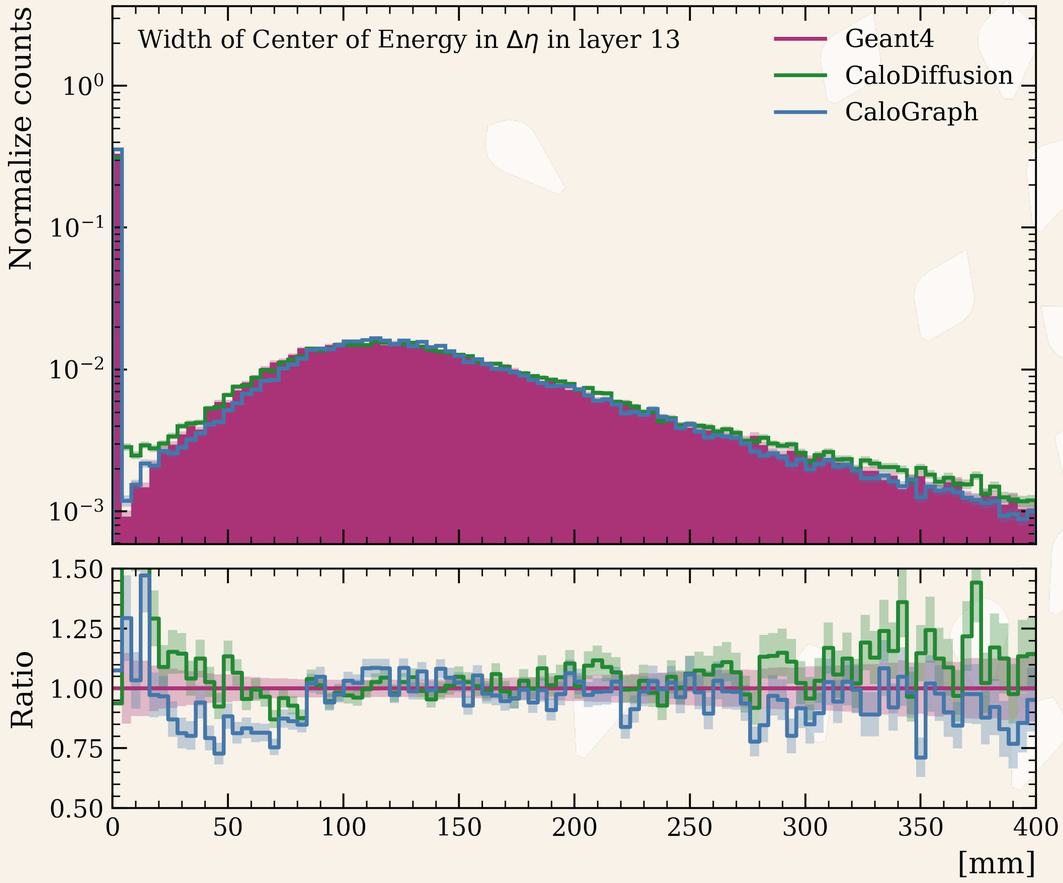
Results: Width of Center of Energy in $\Delta\eta$





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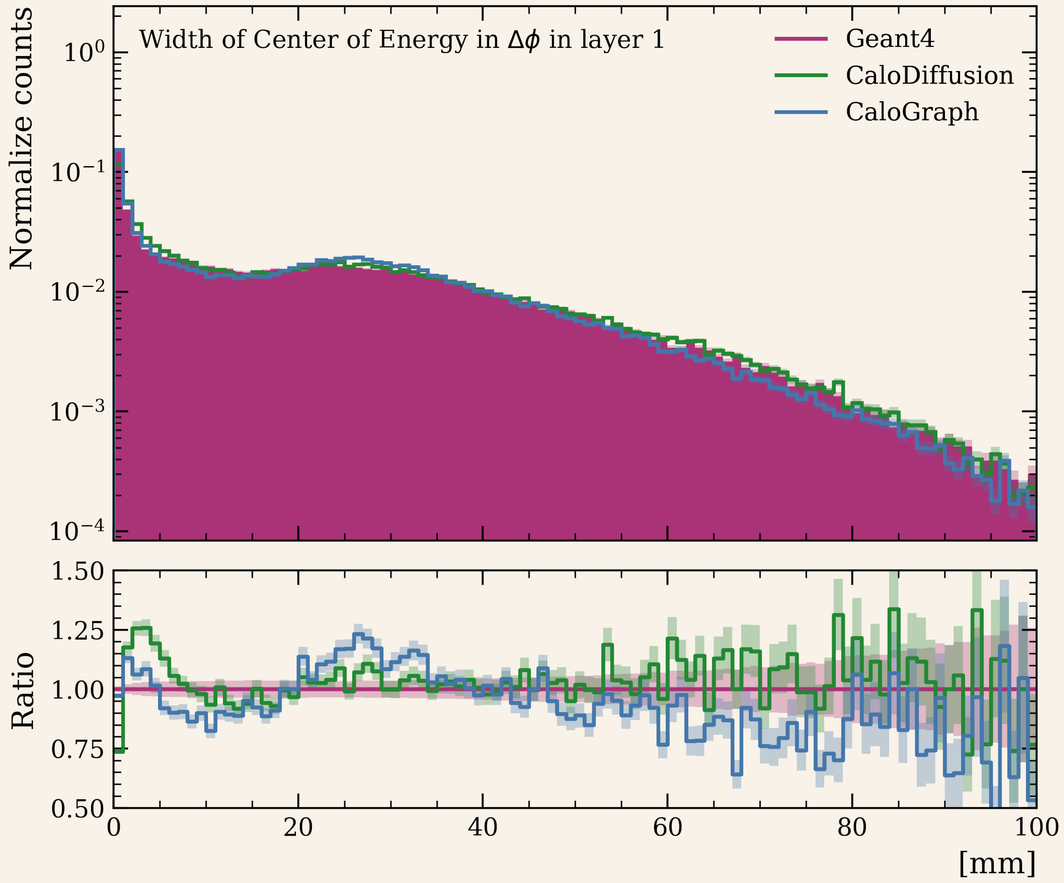
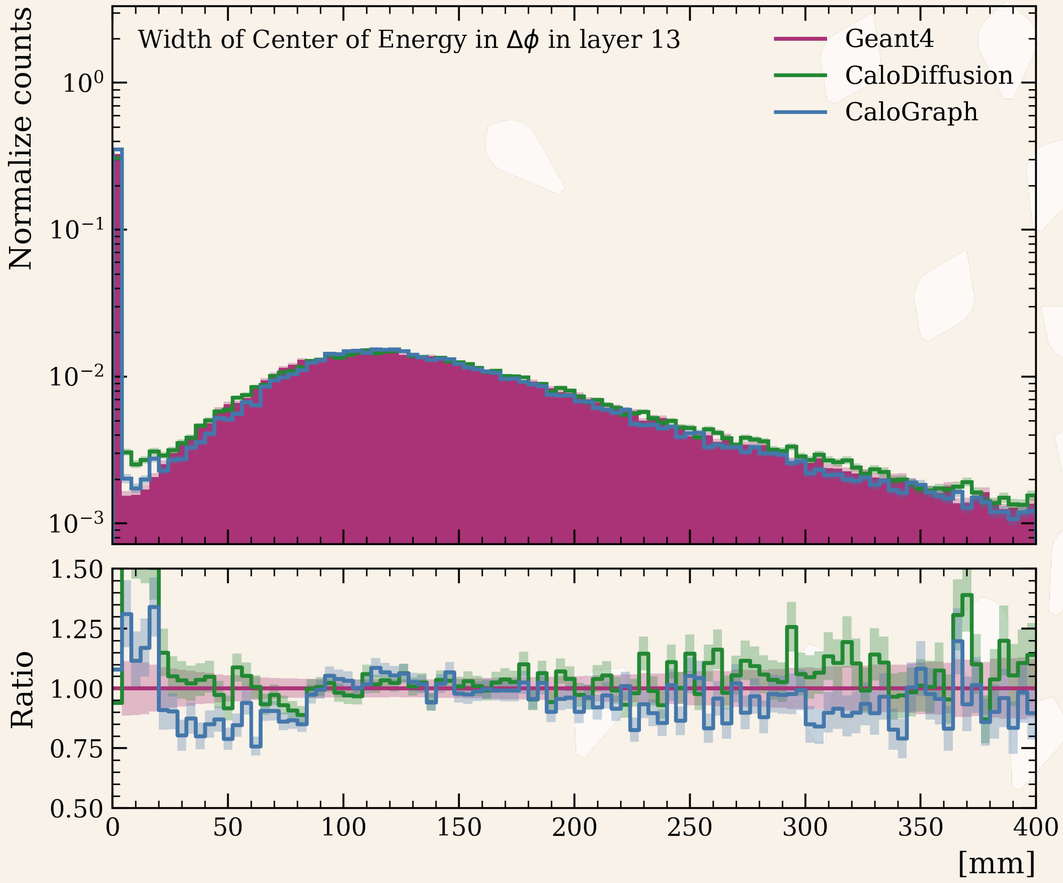
Results: Width of Center of Energy in $\Delta\phi$





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Results: Quantitive performance

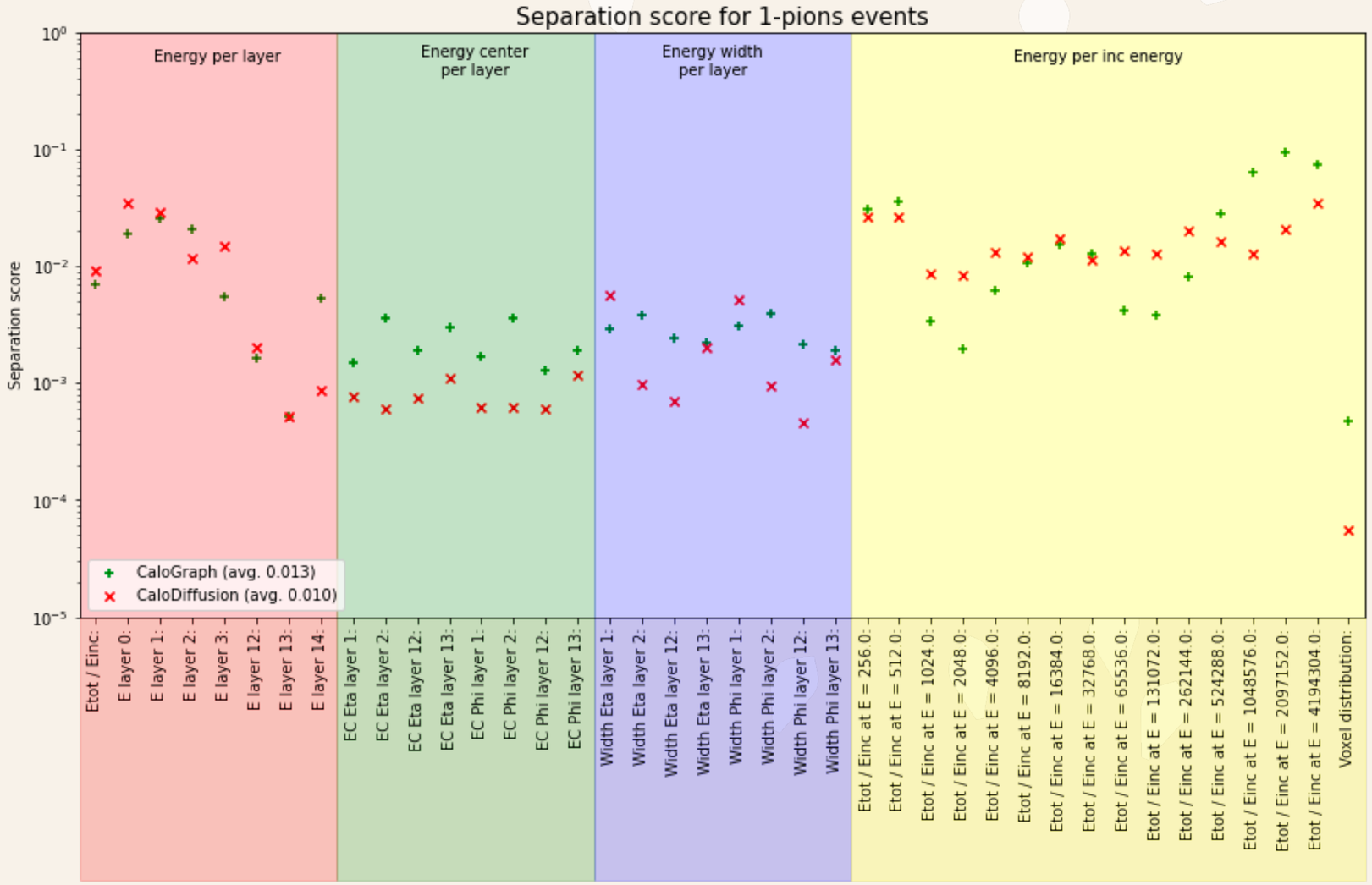
$$\langle S^2 \rangle = \frac{1}{2} \sum_{i=1}^{n_{bins}} \frac{(h_{1,i} - h_{2,i})^2}{h_{1,i} + h_{2,i}}$$

Classifier AUC metric

Model	Classifier low	Classifier high
CaloGraph	0.79	0.71
CaloDiffusion	<u>0.66</u>	0.71

Timing on GPU (batch size 1500)

Model	Time/Shower [s]
CaloGraph	<u>0.02</u>
CaloDiffusion	0.08



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Summary

- CaloGraph shows comparable performance with other diffusion models;
- Naturally works with non-regular geometries, doesn't require additional mapping;
- 4 times speed-up compared to CaloDiffusion
- Not very suitable for very high granularity — can be solved with Nilotpal's SR (https://indi.to/DJxmn)

Backup

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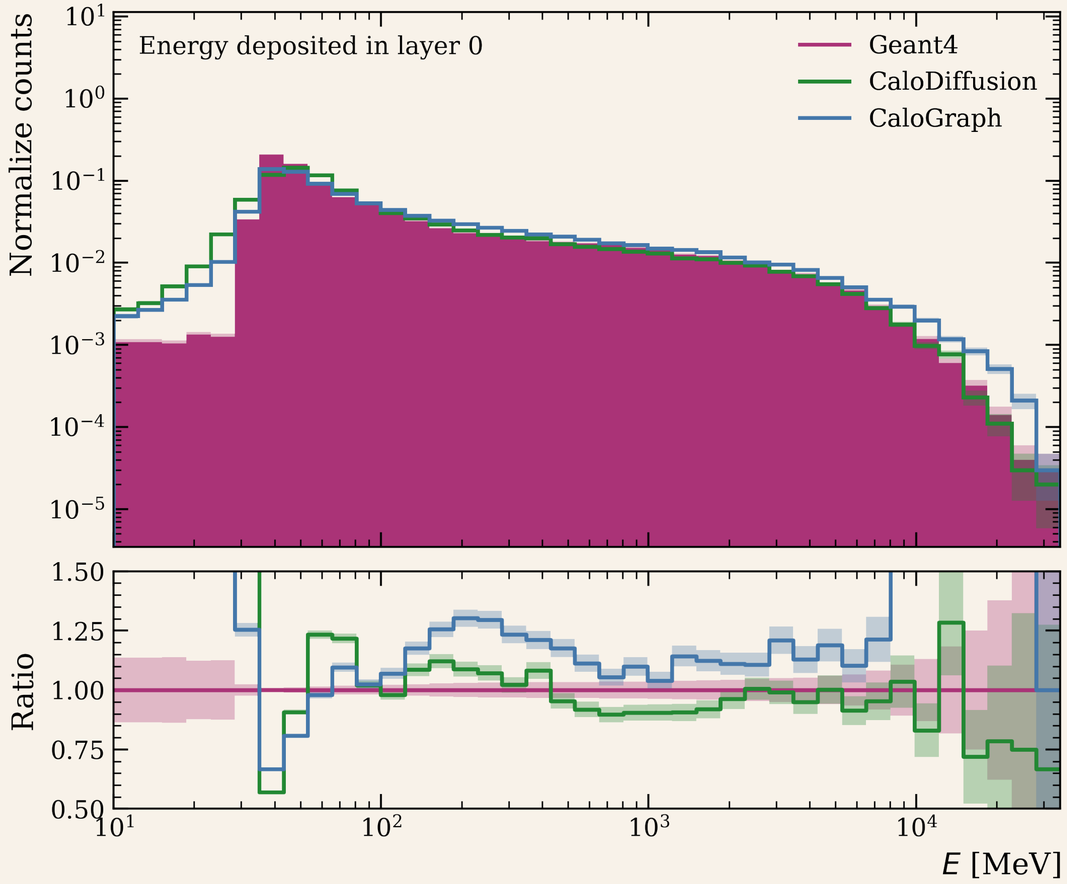
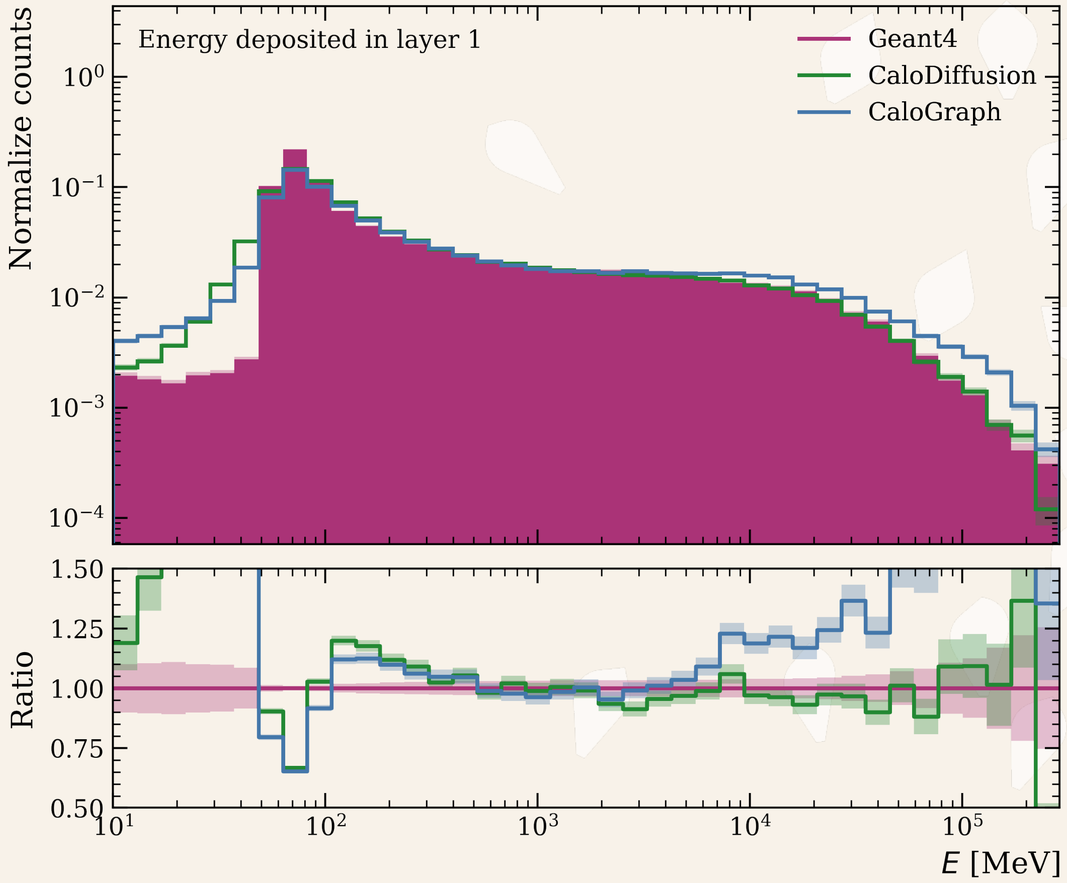
Results: Energy per layer





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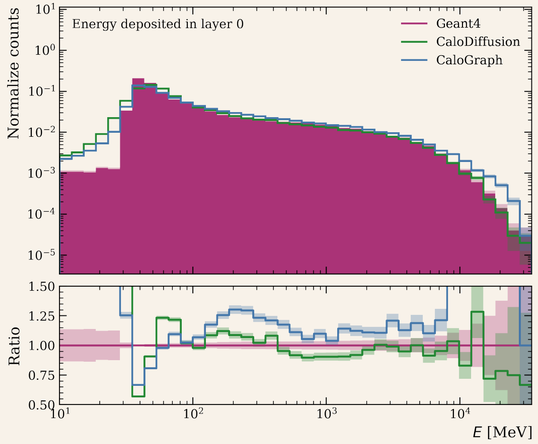
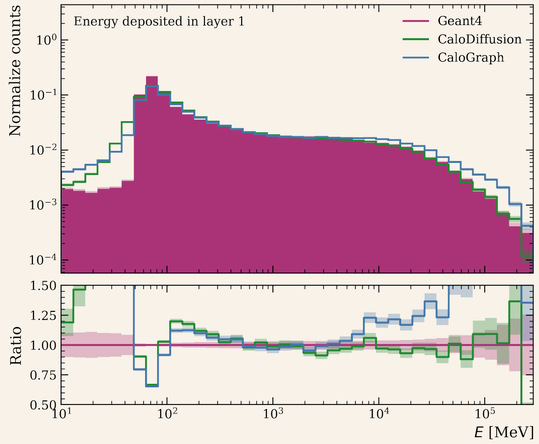
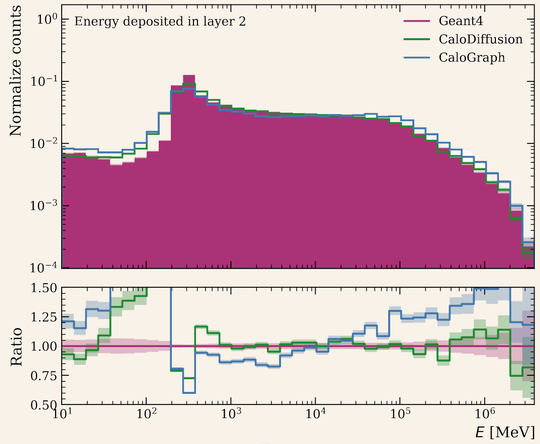
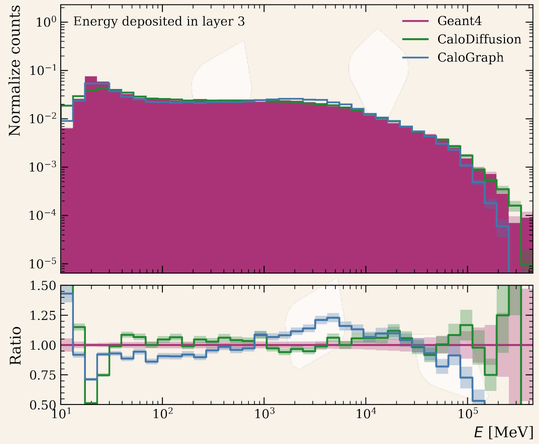
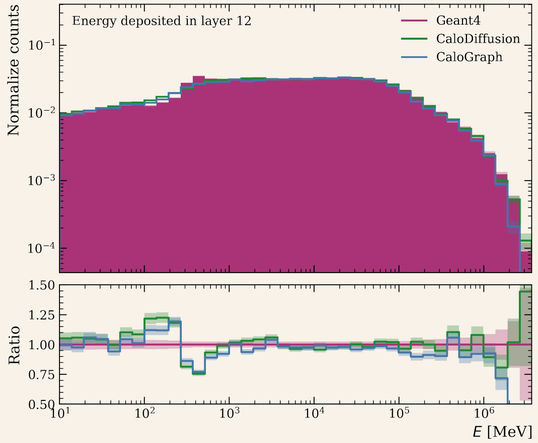
Results: Energy per layer

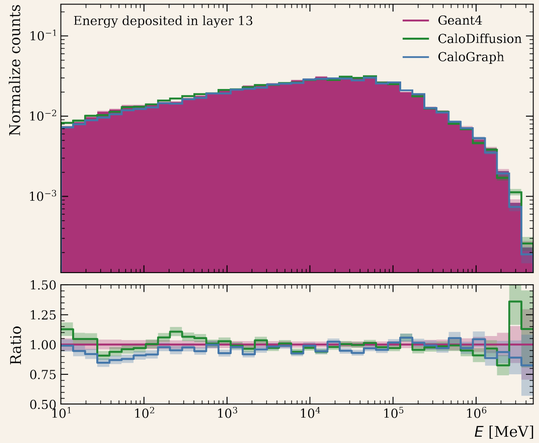


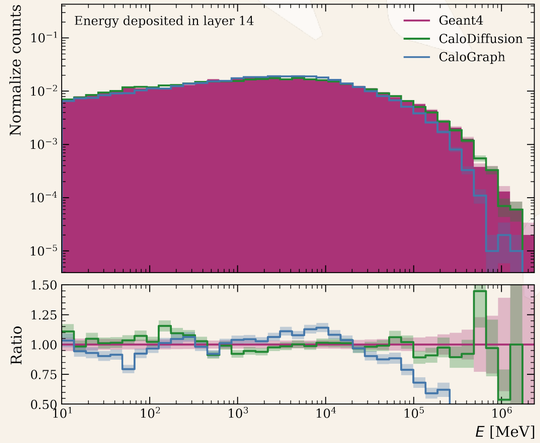












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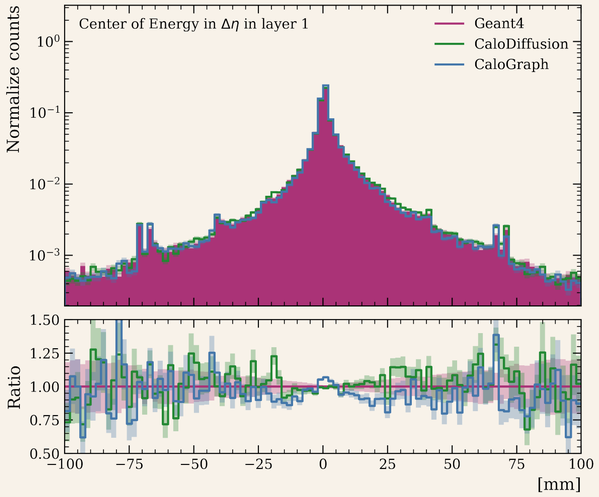
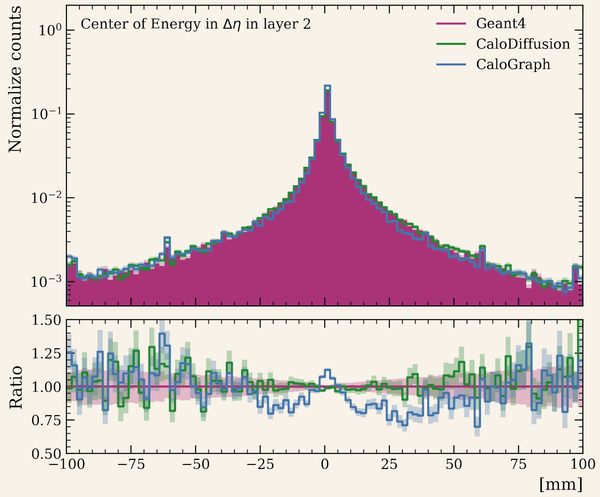
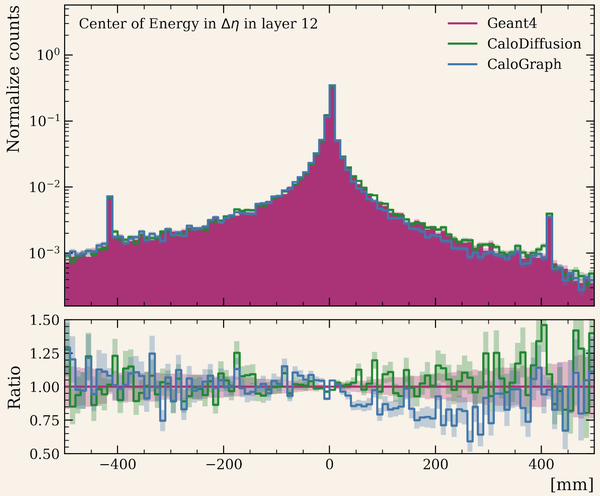
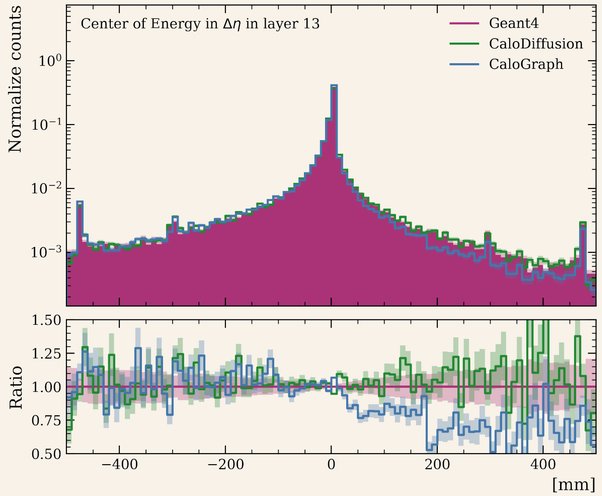
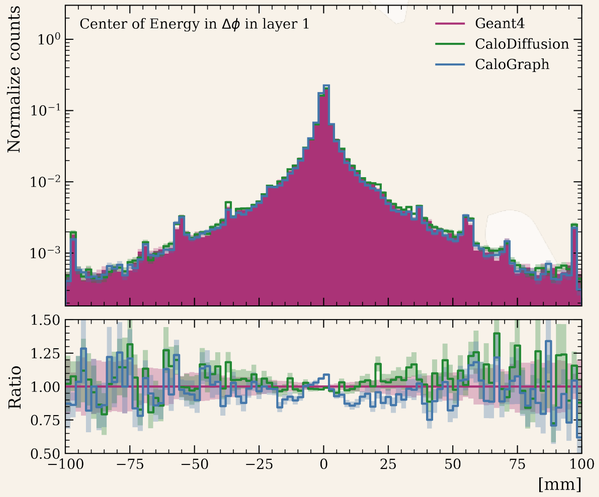
Results: Center of Energy in $\Delta\eta/\Delta\phi$

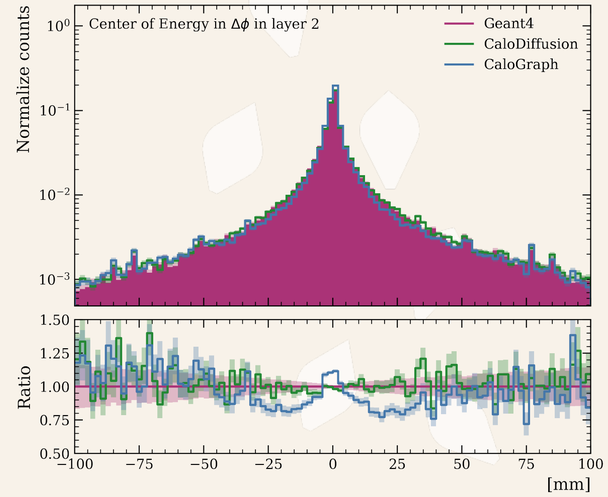


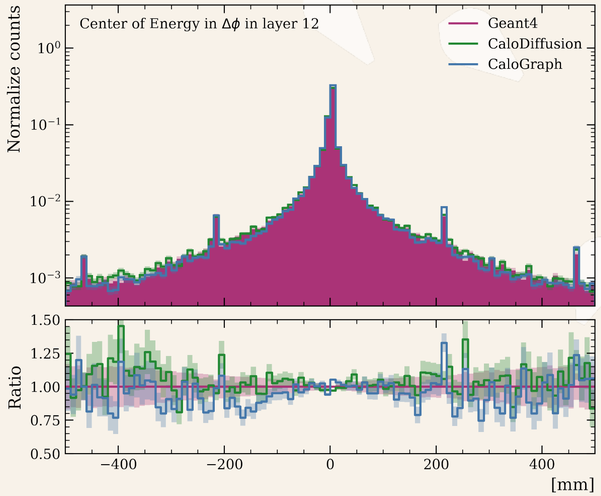


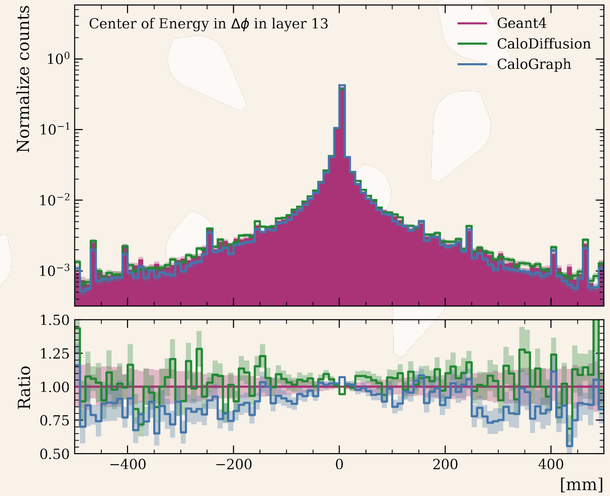












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Results: Width of Center of Energy in $\Delta\eta/\Delta\phi$