Generation of High-Fidelity and High-Dimensional Calorimeter Showers Using Normalizing Flows

5th Round Table on Deep Learning

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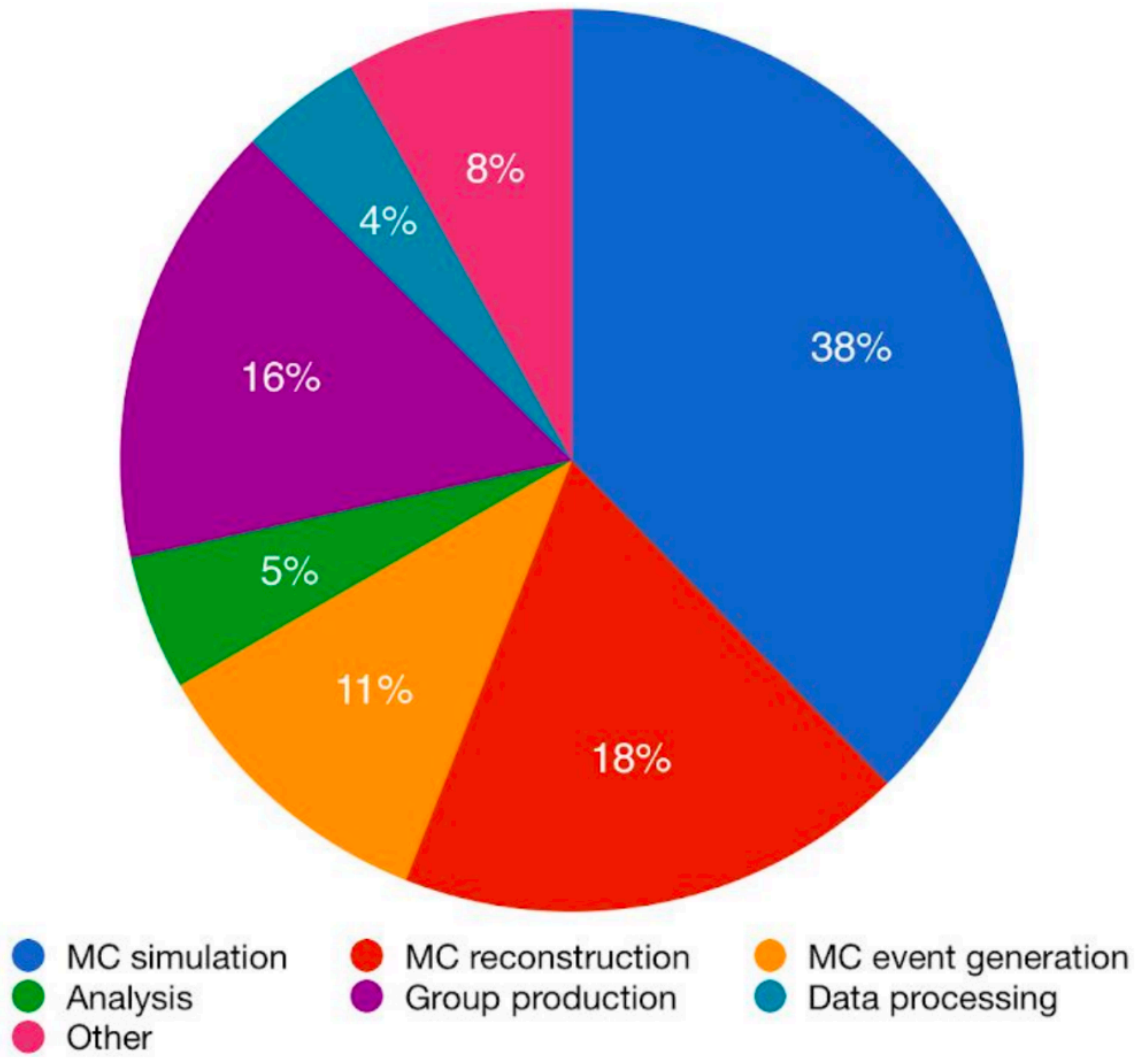
HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

DESY.

Generative Simulation



- MC simulation large part of computing
- Speed up:
  - Train ML model on small dataset
  - Draw majority of samples form ML model

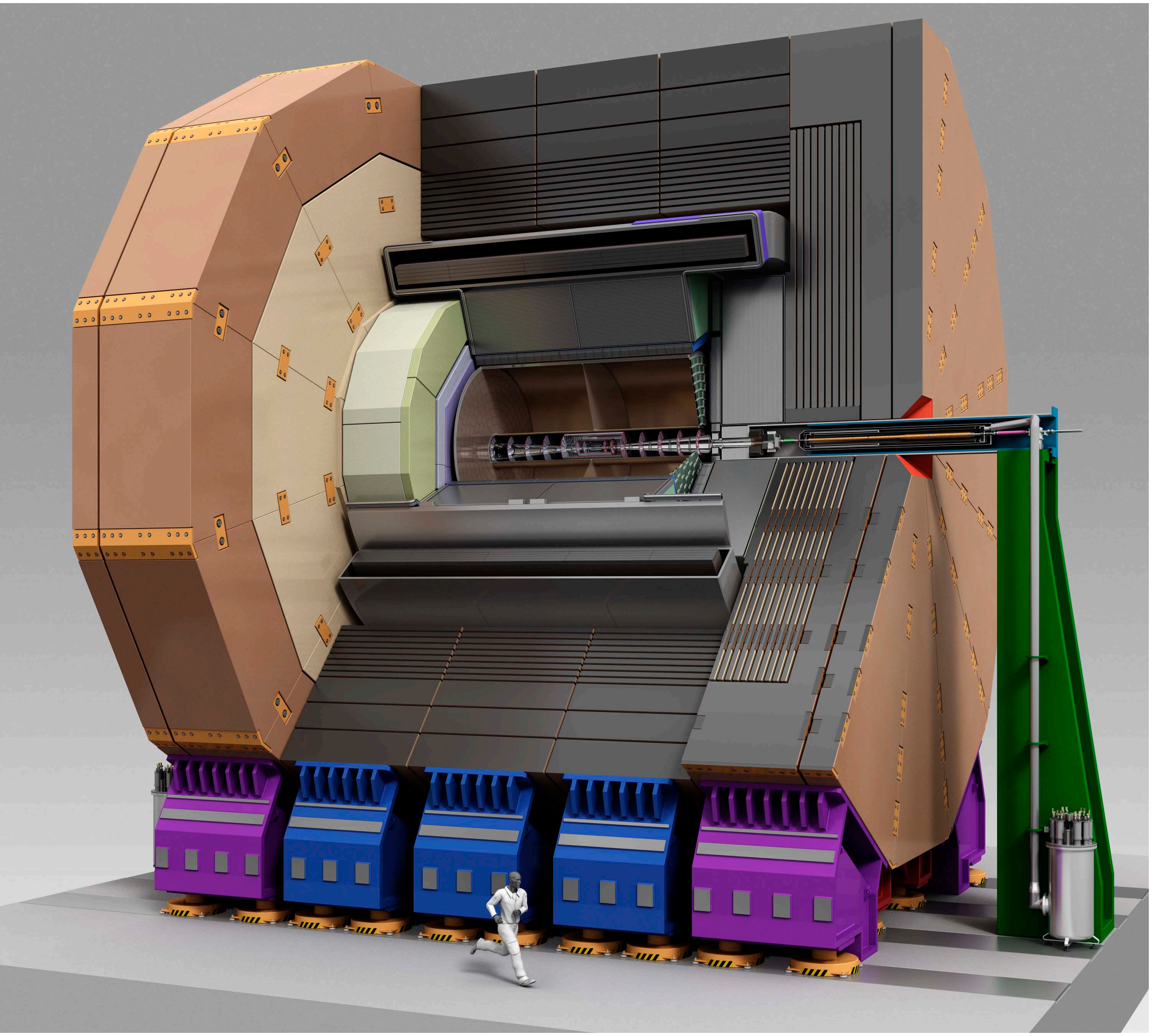
    ➔ Amplify original data set

    ➔ Significantly faster

Catmore et. al. **ATLAS HL-LHC Computing Conceptual Design Report,** CERN-LHCC-2020-015 ; LHCC-G-178

Butter et al.: **Amplifying Statistics using Generative Models:** NeurIPS ML4PS 2020, 2008.06545

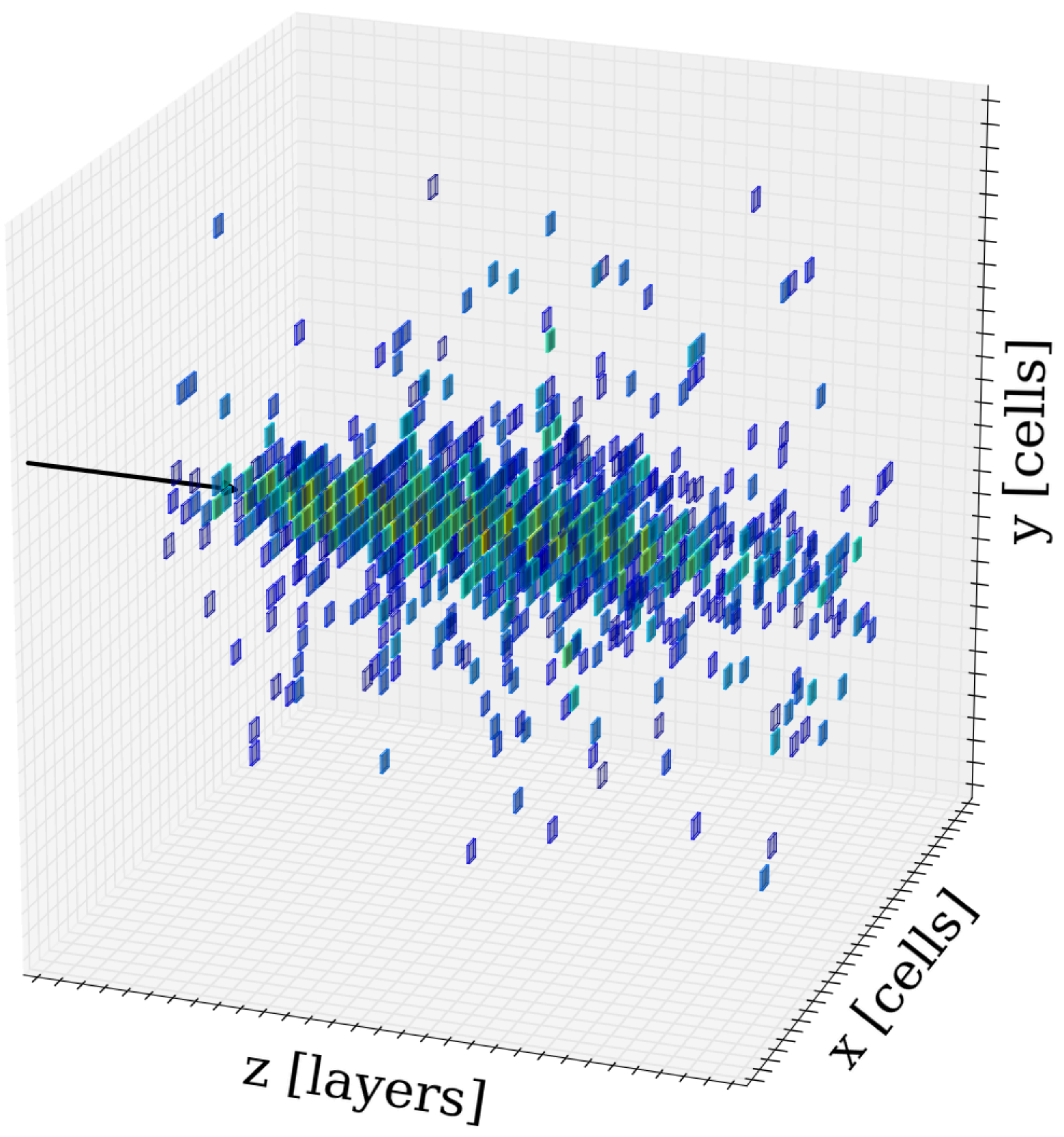
ILD Calorimeters



- International Large Detector
  - Proposed for International Linear Collider
  - Particle Flow optimised
  - Requires highly granular calorimeters
- ILD electromagnetic calorimeter
  - Active silicon, passive tungsten
  - 30 layers, 5mm x 5mm cells

Shower Dataset

Photon shower

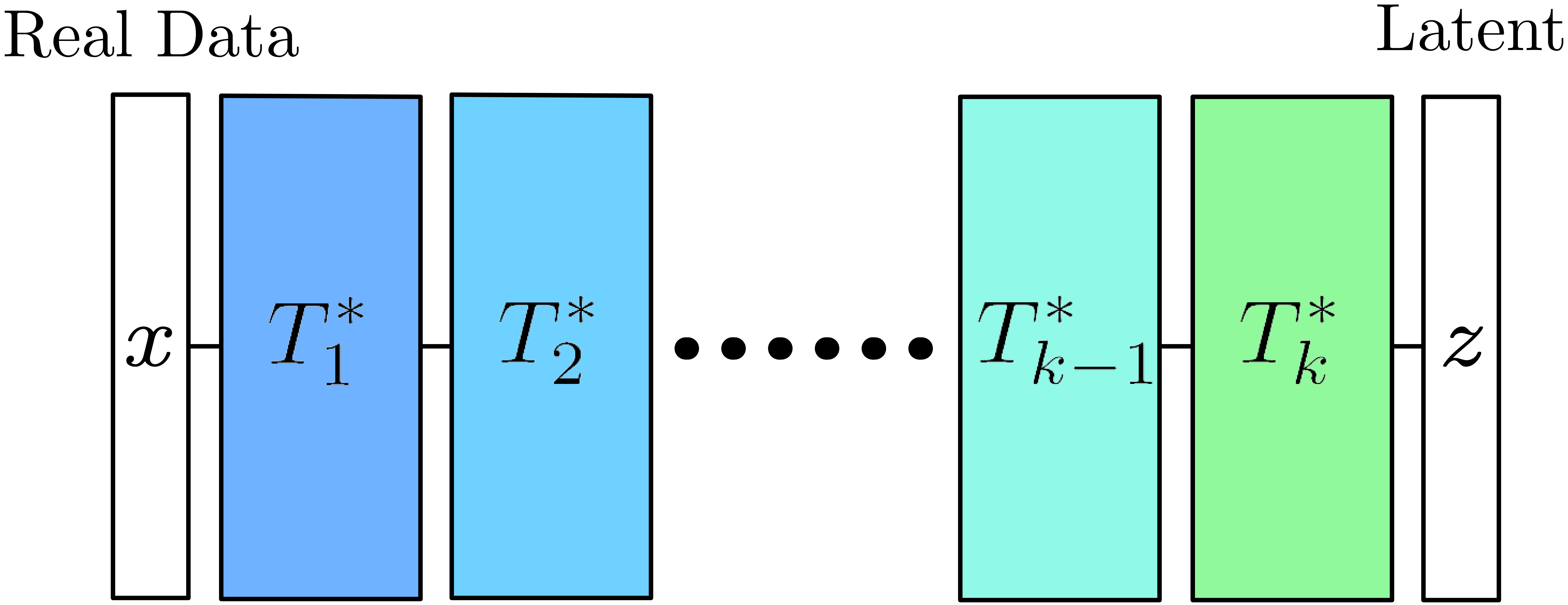


Training data:

- 1 million photon showers in ECAL
- 10 to 100 GeV
- Fixed incident point & angle
- Project to grid
- Originally 30×30×30

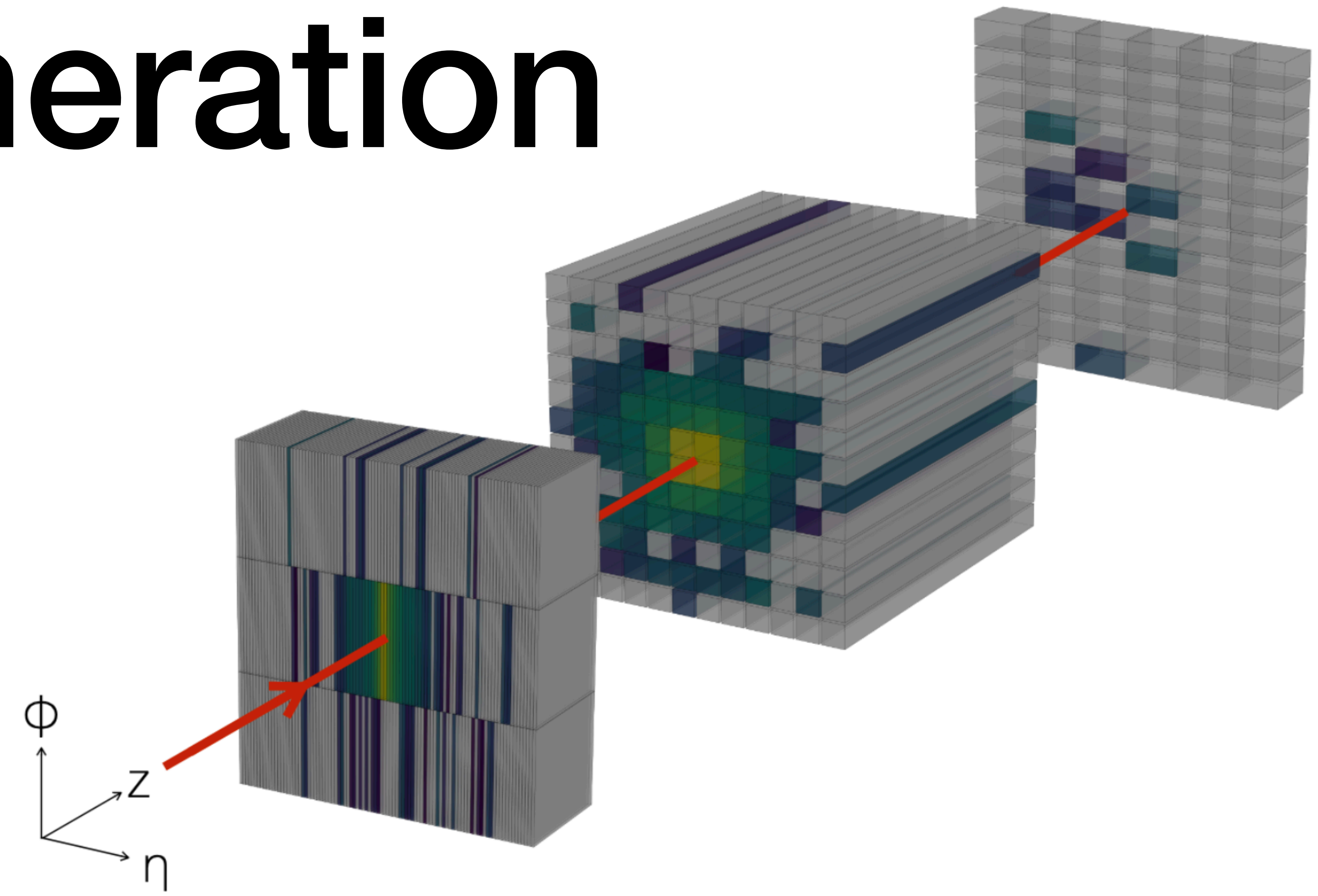
Buhmann et al.: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed** (2020) [2005.05334](https://arxiv.org/abs/2005.05334)

Normalizing Flow



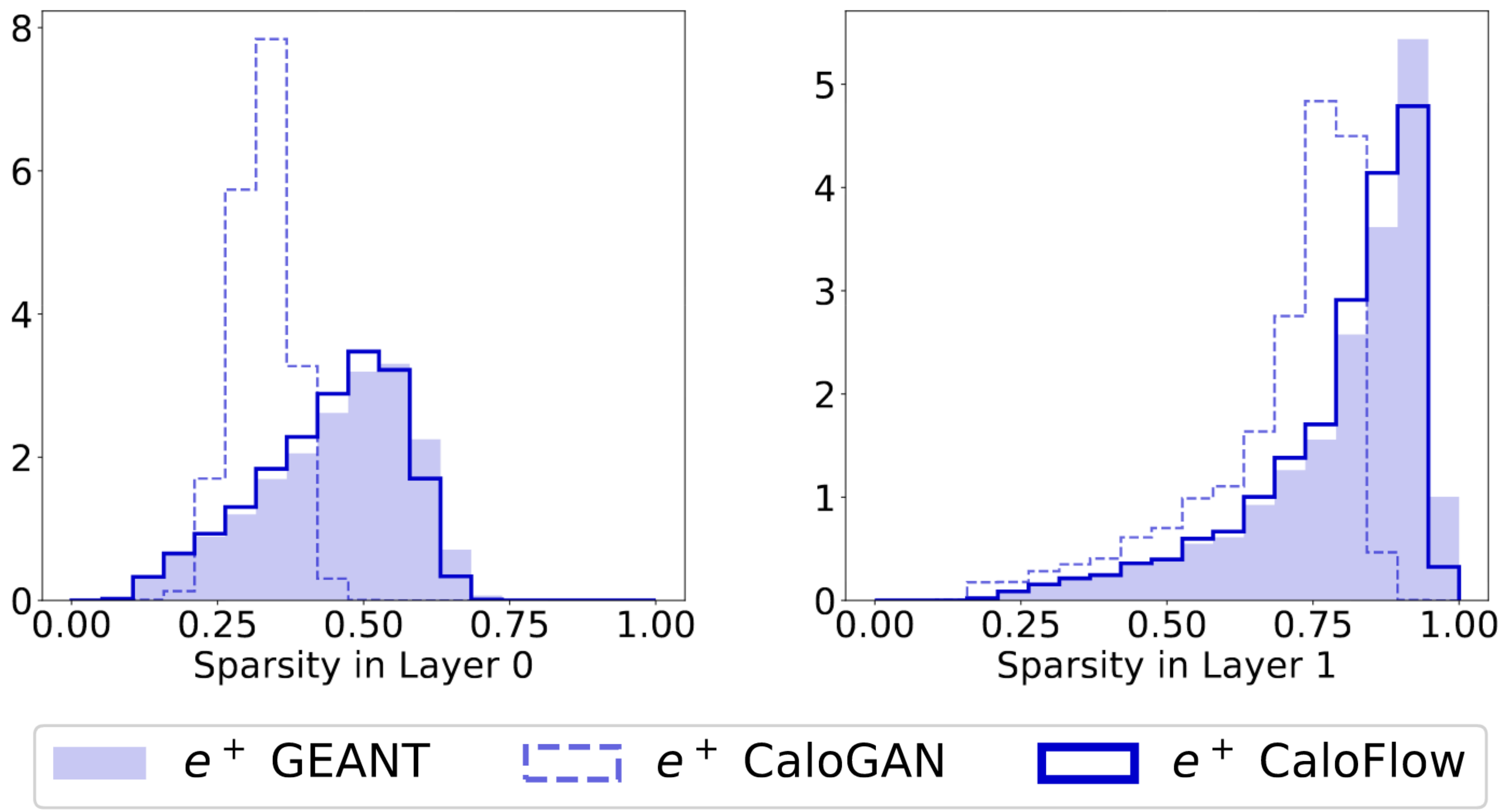
- Invertible neural network, both: (data → latent) and (latent → data)
- Directly minimize log likelihood in (data → latent) direction
- Generate data with (latent → data) direction

Flow Based Generation



- CaloFlow:
  - Demonstration of flows on CaloGAN data set
  - 3 layers, ~500 dimensions total
  - Significant performance increase going from GAN to flow

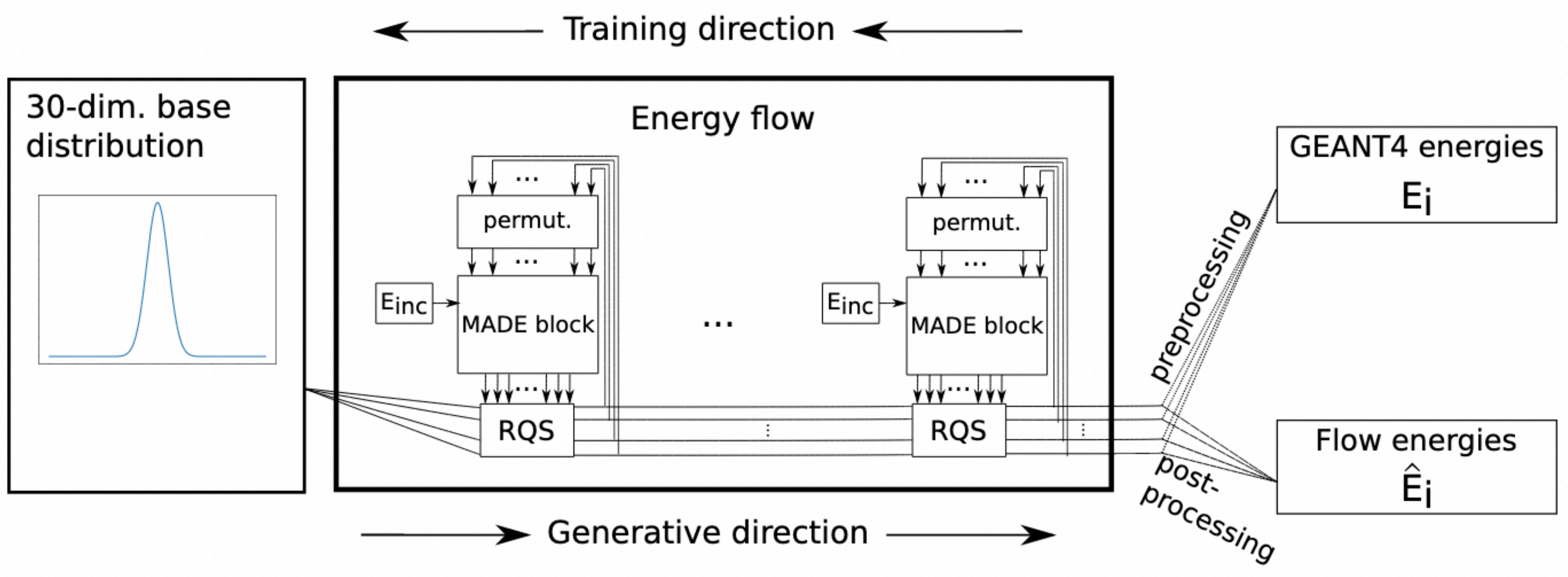
➔ Test on ILD ECAL data set

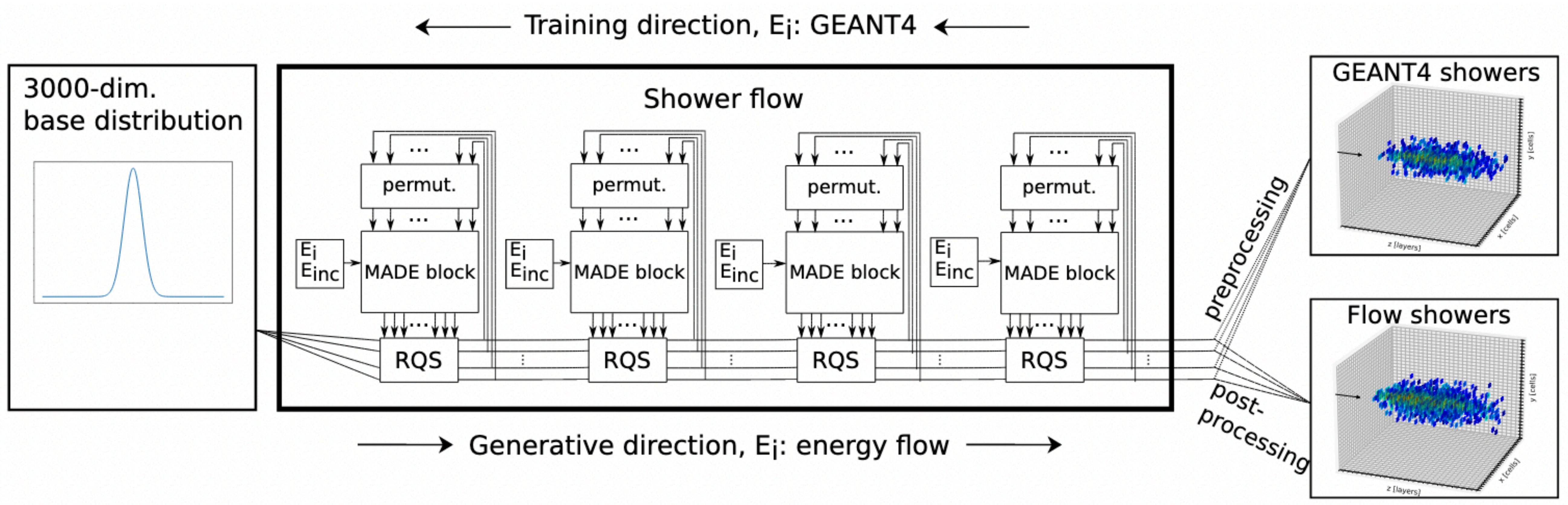


Krause et. al. **CaloFlow: Fast and Accurate Generation of Calorimeter Showers with Normalizing Flows:** (2021) [2106.05285](https://arxiv.org/abs/2106.05285)

Flow-Based Generation

- Two step generation approach:
  - "Layer flow" learns deposited energies per layer
  - "Shower flow" learns energy depositions per ECal cell





- Shower flow conditioned on layer flow output
- Additionally: Generated showers re-scaled using layer flow

Number of Parameters

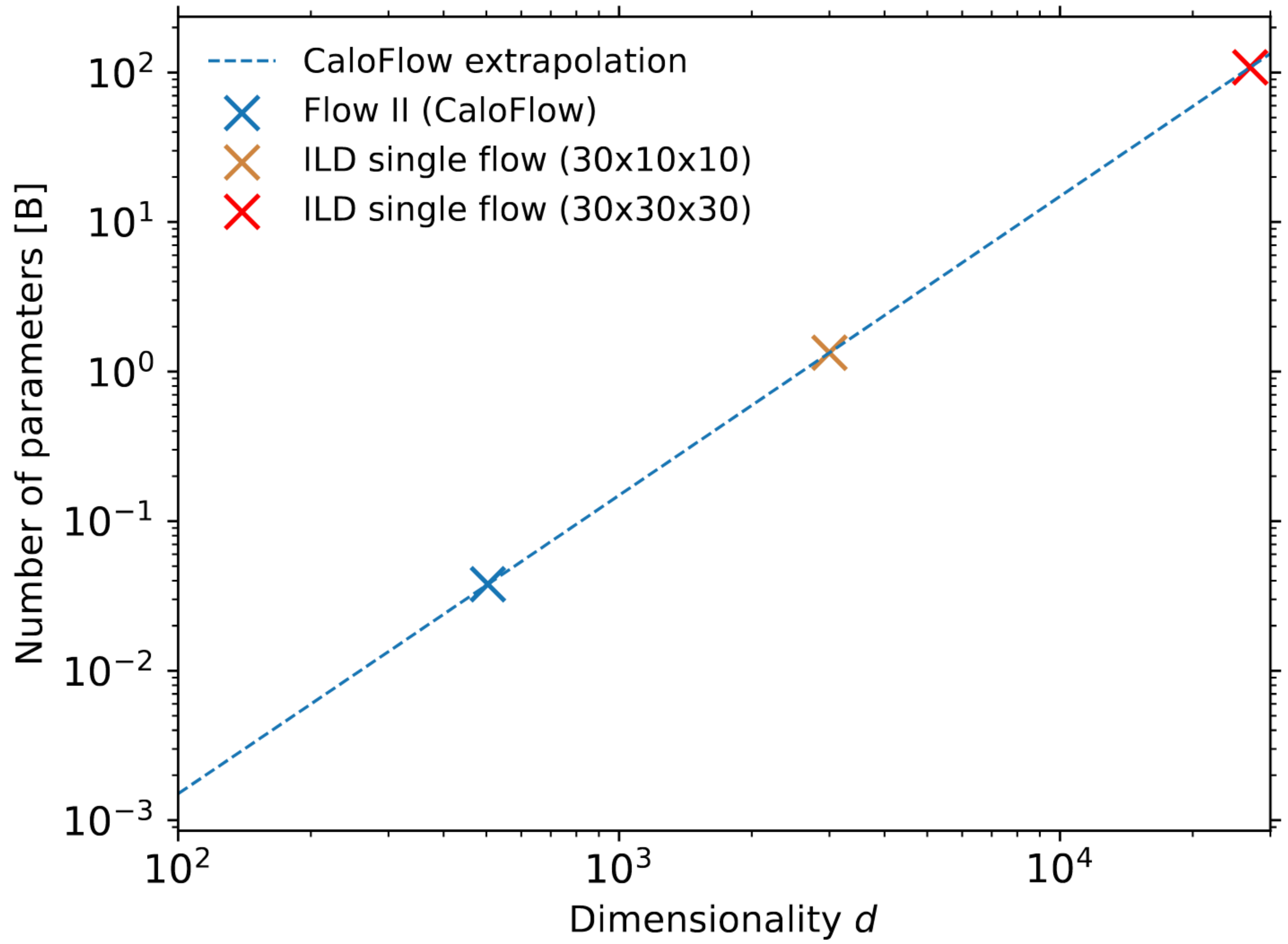
- Shower flow on 30x30x30 too large

➡ Focus in central 10x10x30 region

- O(1,000,000,000) parameters
- Still too large for single flow

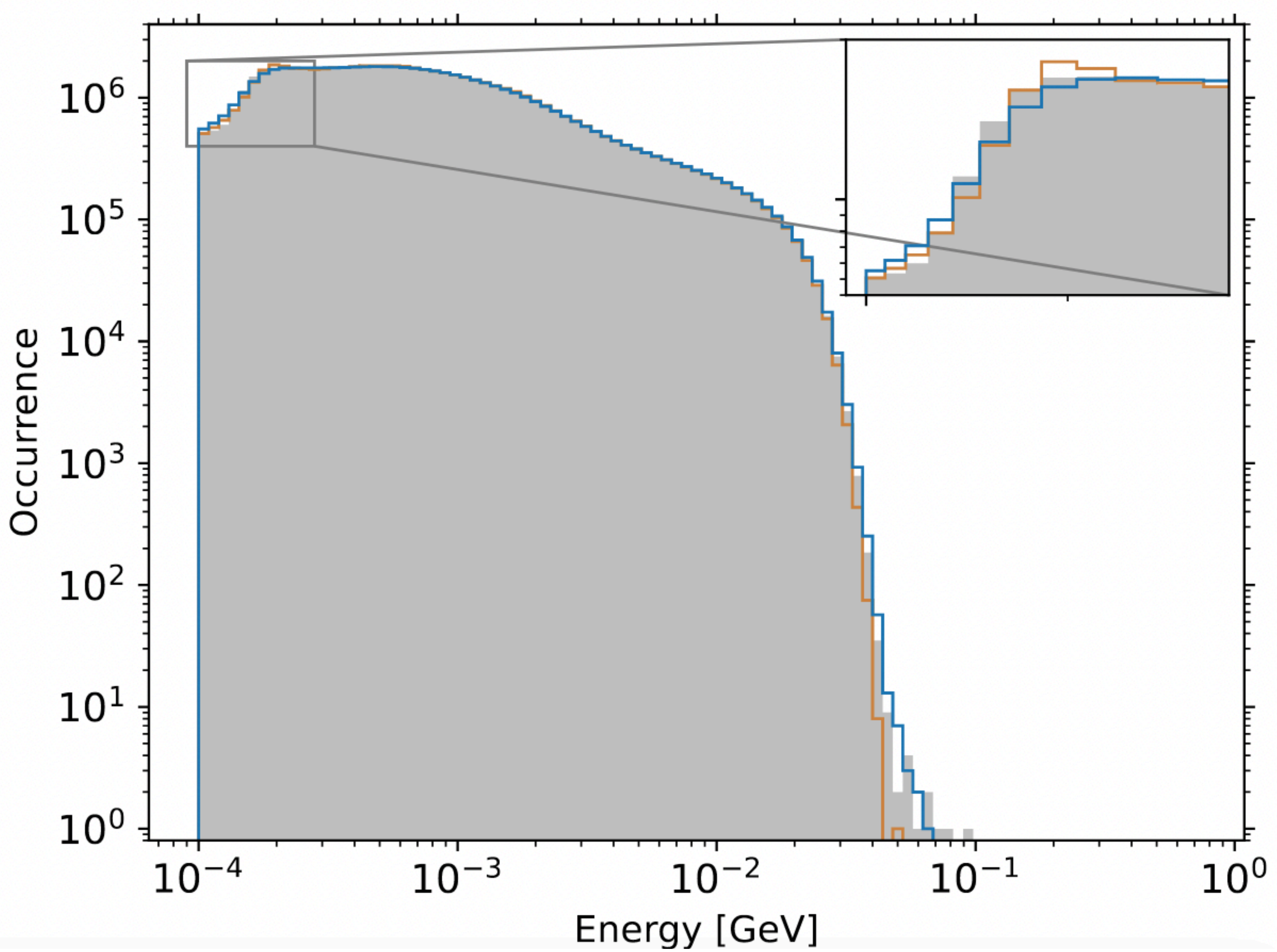
➡ Multiple flows:

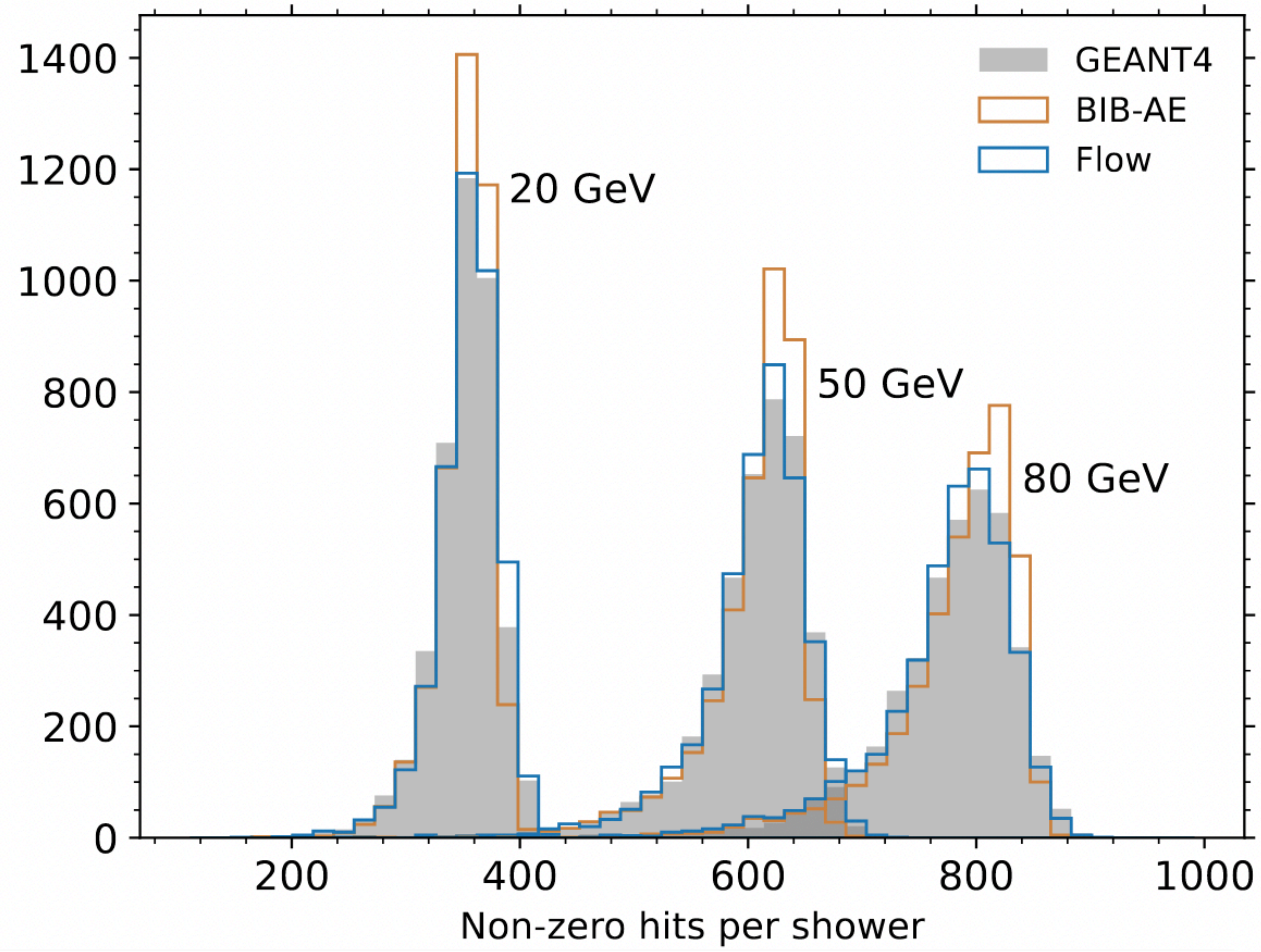
  - Each flow conditioned on previous 5 layers
  - Reduced overall model size



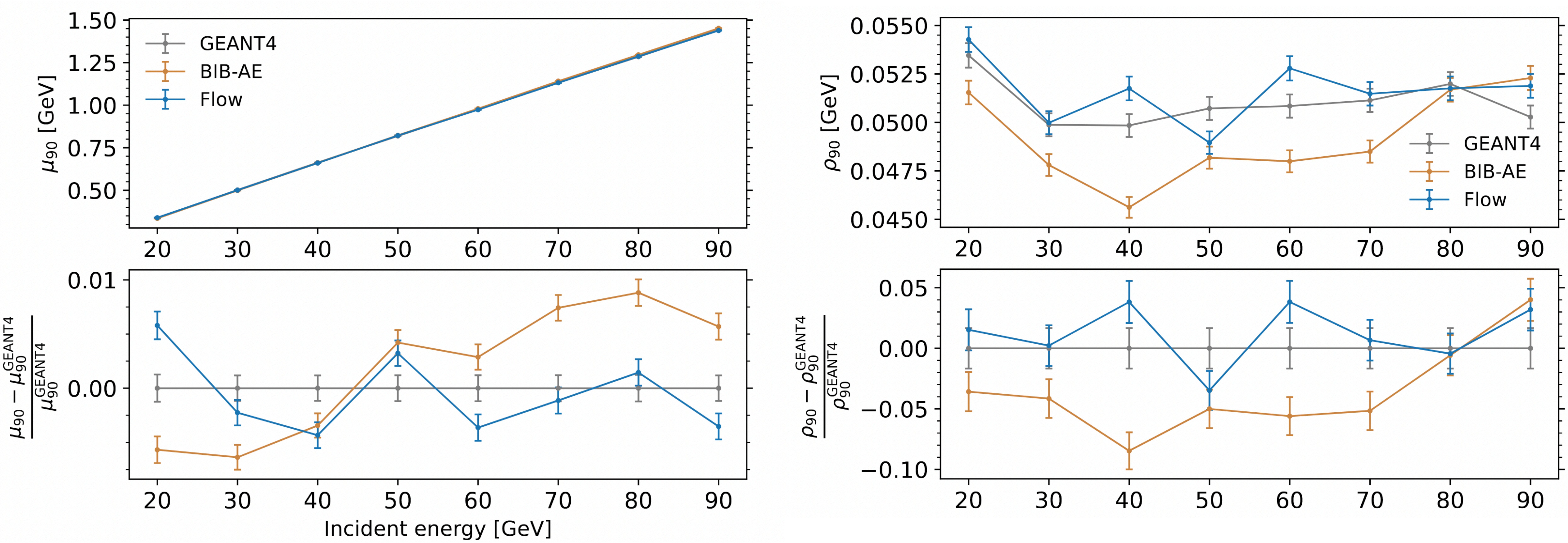
Flow i	Context features	Context shape
0	$E_0,\ E_{\text{inc}}$	$[N,\ 2]$
1	$I_0,\ E_1,\ E_{\text{inc}}$	$[N,\ 102]$
2	$I_1,\ I_0,\ E_2,\ E_{\text{inc}}$	$[N,\ 202]$
3	$I_2,\ I_1,\ I_0,\ E_3,\ E_{\text{inc}}$	$[N,\ 302]$
4	$I_3,\ I_2,\ I_1,\ I_0,\ E_4,\ E_{\text{inc}}$	$[N,\ 402]$
≥ 5	$I_{i-1},\ I_{i-2},\ I_{i-3},\ I_{i-4},\ I_{i-5},\ E_i,\ E_{\text{inc}}$	$[N,\ 502]$

Cell Spectrum and Number of Hits





Visible Energy Sum (Mean and Width)



Compute Times

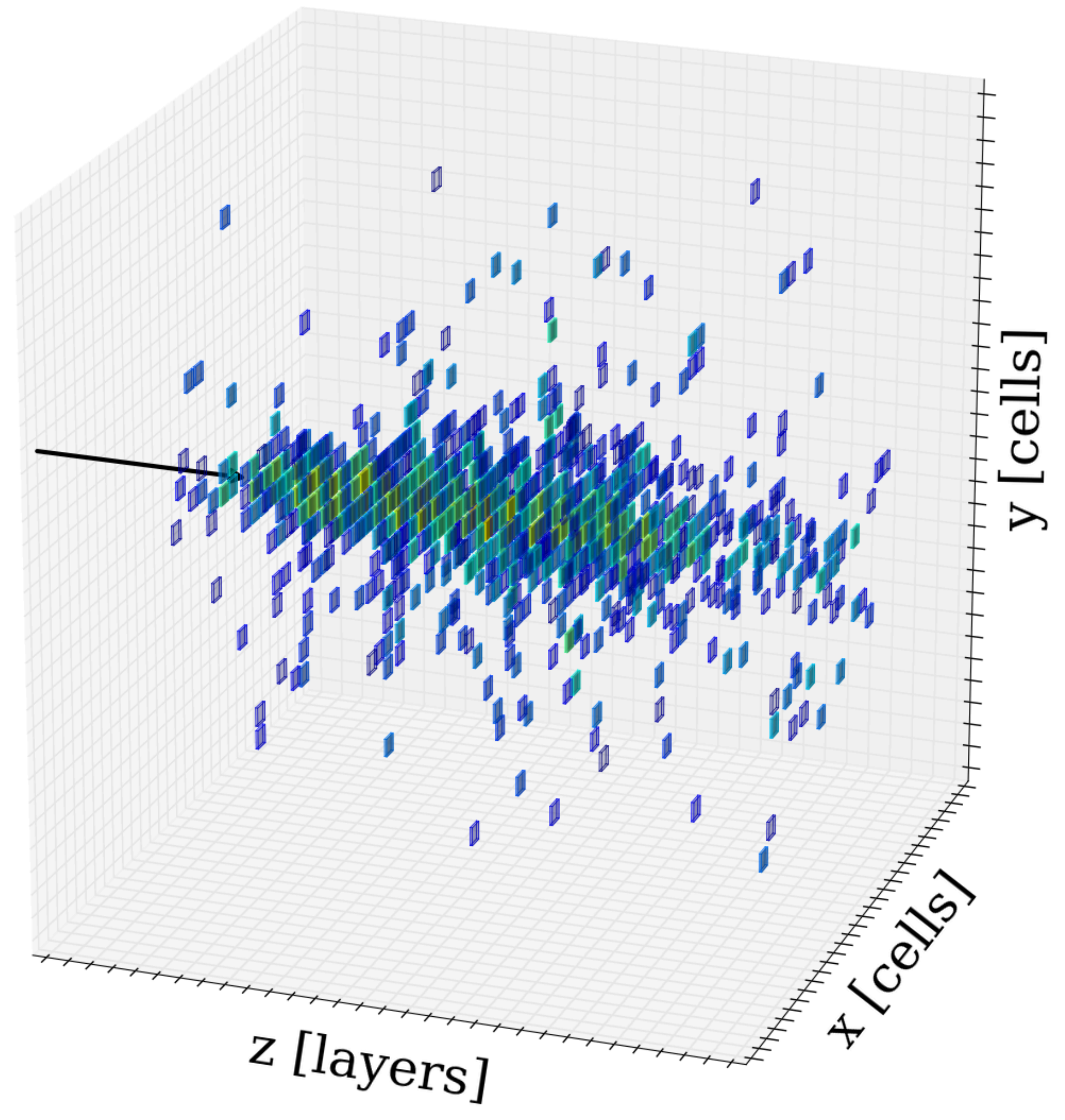
Simulator	Hardware	Photons 10x10	Speedup
GEANT4	CPU	4082±170 ms	-
BIB-AE	CPU	37.81±0.13 ms	x108
Flow	CPU	2066±31 ms	x2
BIB-AE	GPU	0.23±0.01 ms	x17745
Flow	GPU	12.51±0.01 ms	x326

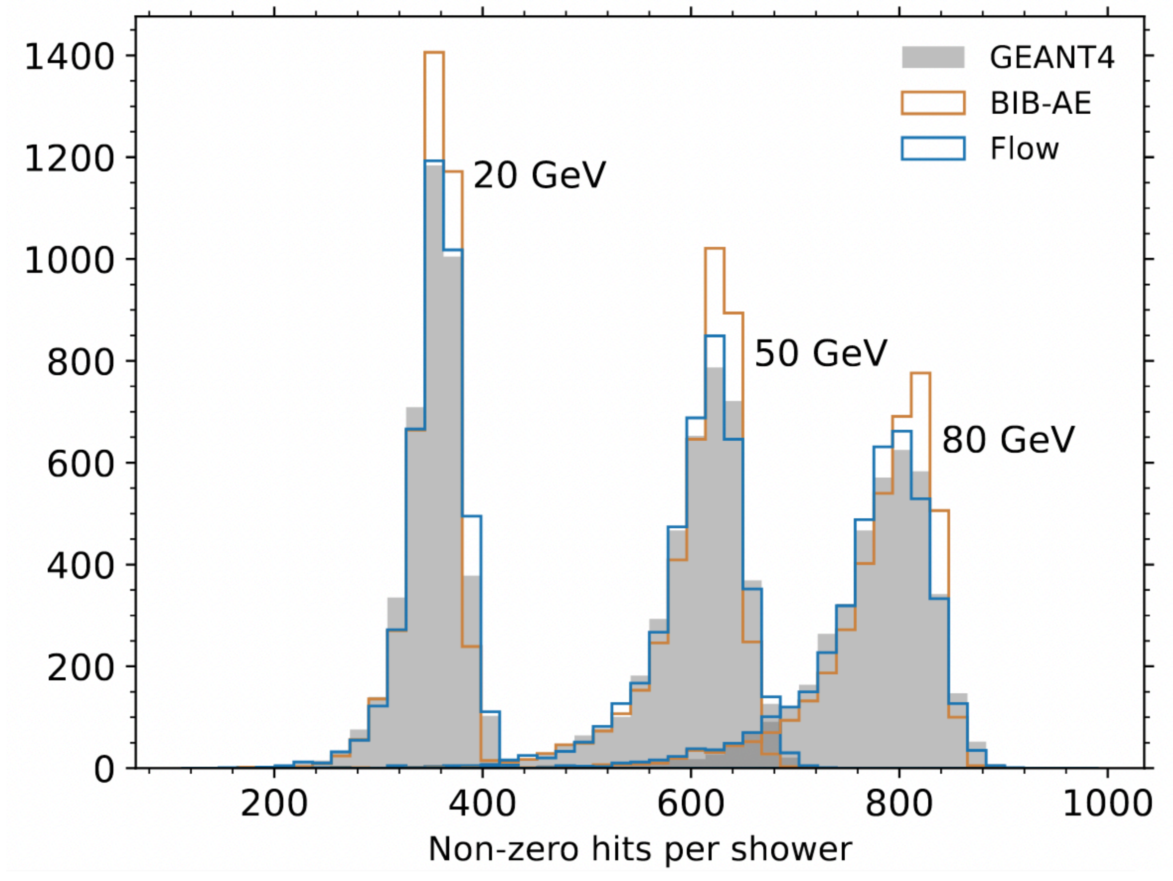
Times for fastest evaluation batch sizes, GPU times have to be normalised by cost

- MAF setup used in flow slow for generation
- Teacher-student IAF setup can lead to speedup, work in progress

Conclusion

- Generative calorimeter simulation:
  - Flow based models provide increased accuracy on smaller scale data
  - Generation slow for far, improvement work in process
  - Extension to full size data set under way





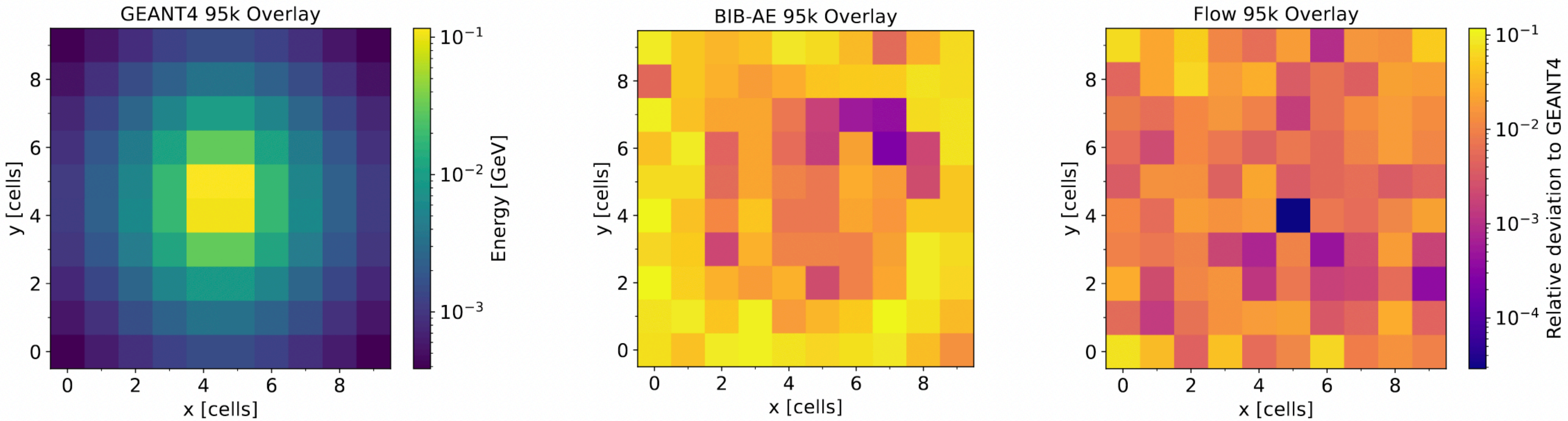
Thank you

Classifier Performance

/	BIB-AE	Multiple flows
Classifier AUC	0.9912 ± 0.0018	0.8399 ± 0.0036

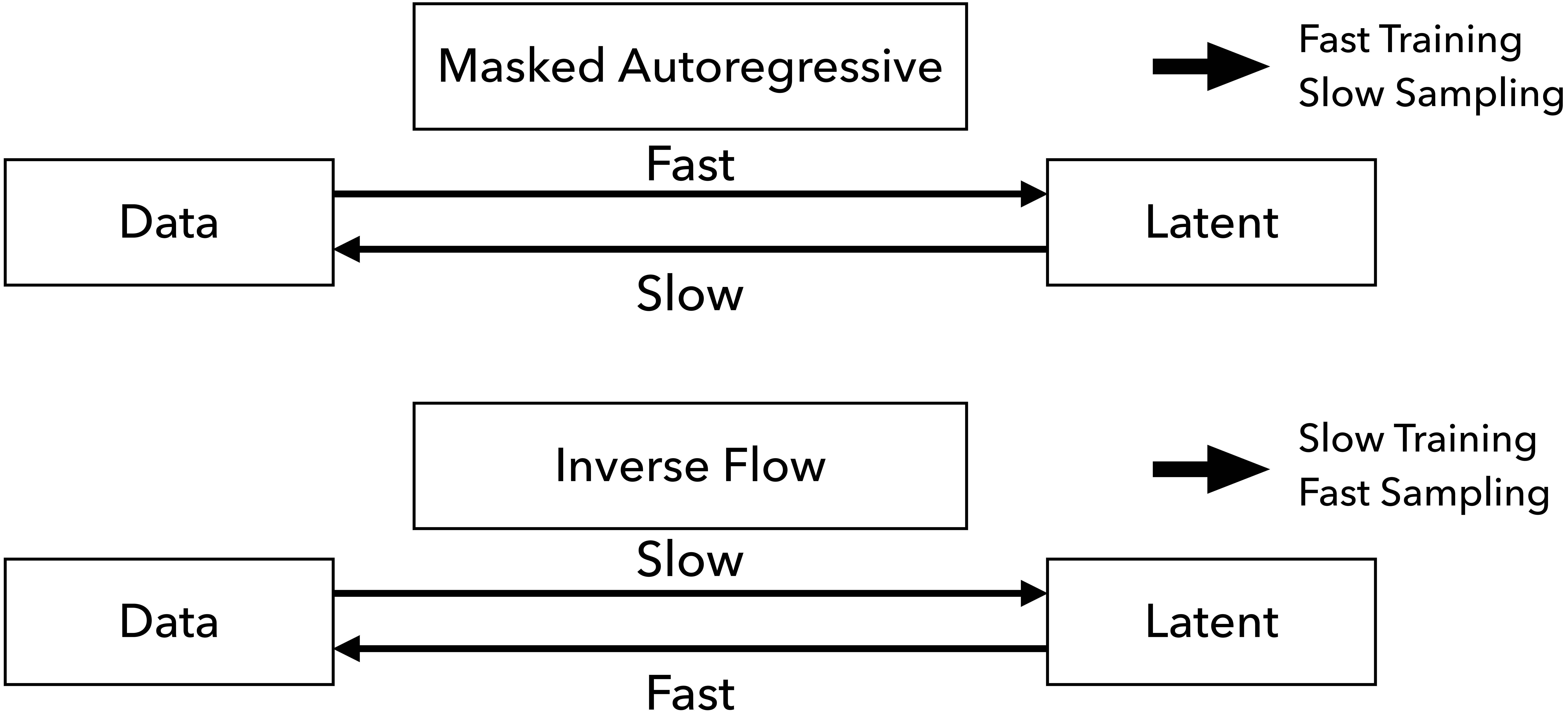
- Classifier trained to distinguish GEANT4 from generated showers
- 5 trainings used to estimate uncertainty
- Both methods imperfect
- BIB-AE may have tells/artefacts resulting in perfect classification
- Flow performs better

Shower Overlay

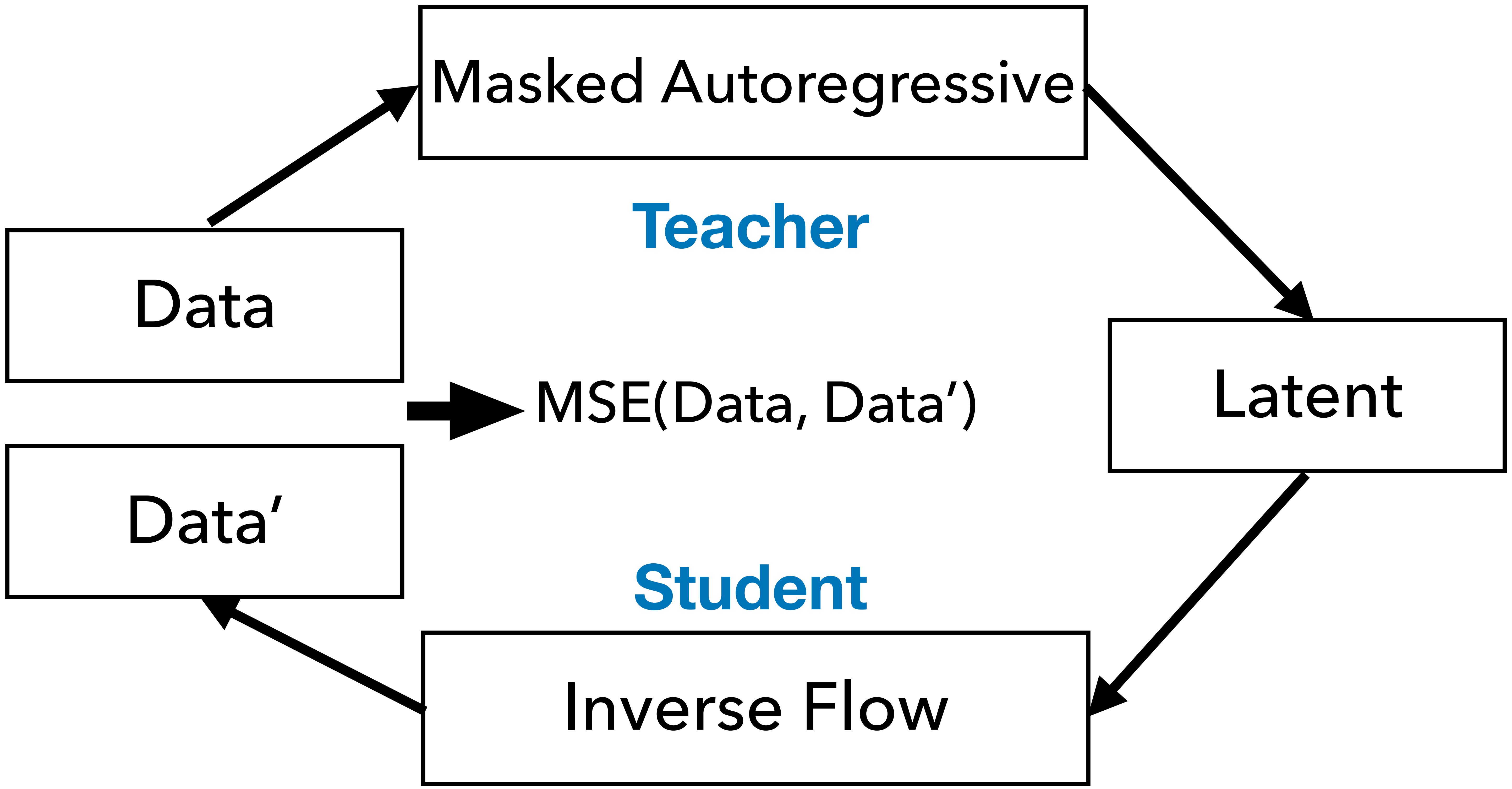


- Compare multiple flow approach to BIB-AE re-trained on 10x10x30 data set
- Overlay of flow showers has better agreement with GEANT4

MAF vs IF


Masked Autoregressive
Fast Training
Slow Sampling
Fast
Data
Latent
Slow
Inverse Flow
Slow Training
Fast Sampling
Slow
Data
Latent
Fast

Teacher-Student Paradigm



- CaloFlow II method:
- Train teacher MAF
  - Fast training times
- Train student IF
  - Only needs inverse evaluation in training
  - Fast training
  - Fast sampling

Krause et. al. **CaloFlow II: Even Faster and Still Accurate Generation of Calorimeter Showers with Normalizing Flows:** 2110.11377