New Angles on Fast Calorimeter Shower Simulation

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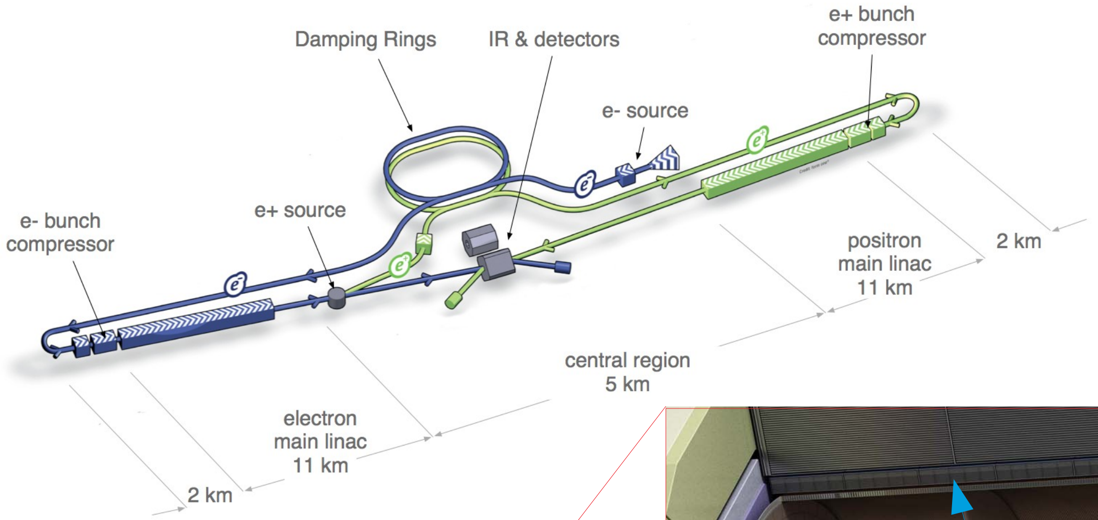
The ILD Concept

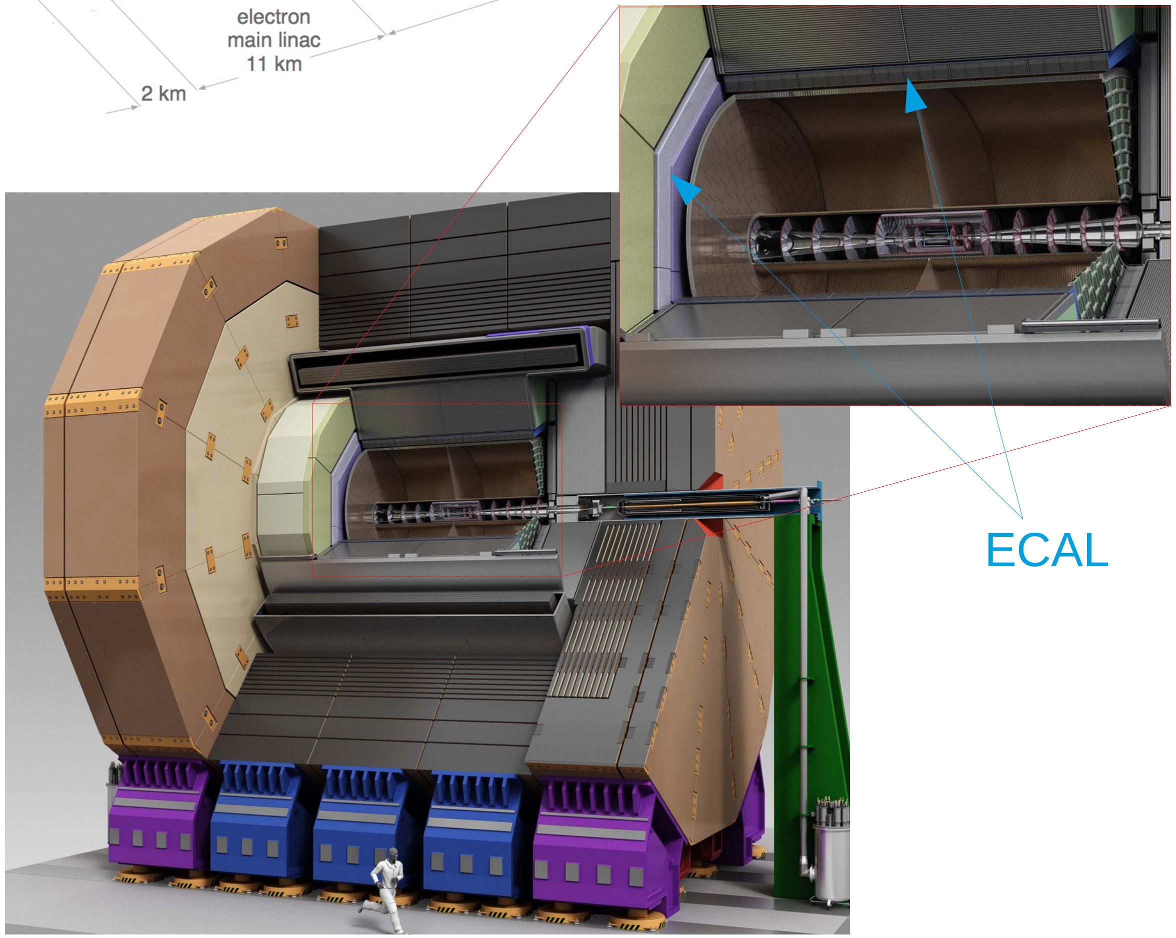
- Context: Future Higgs Factories

- Case Study: International Large Detector (**ILD**) concept for the International Linear Collider (ILC)

- Optimized for Particle Flow
  - Reconstruct each individual particle in subdetector
  - Obtain optimal detector resolution

- High granularity calorimeters:
  - Sampling calorimeters
  - **SiW Ecal**: 30 layers, 5x5 mm^2, 2 sampling fractions
  - **FeSci Hcal**: 48 layers, 3x3 cm^2

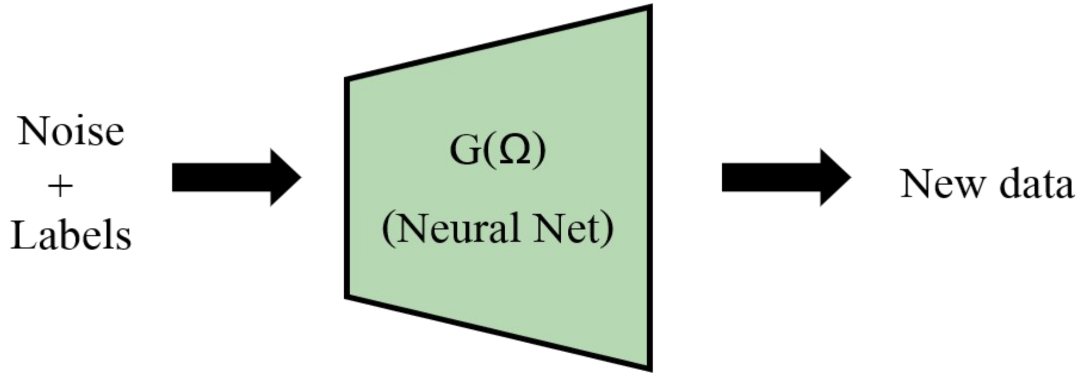


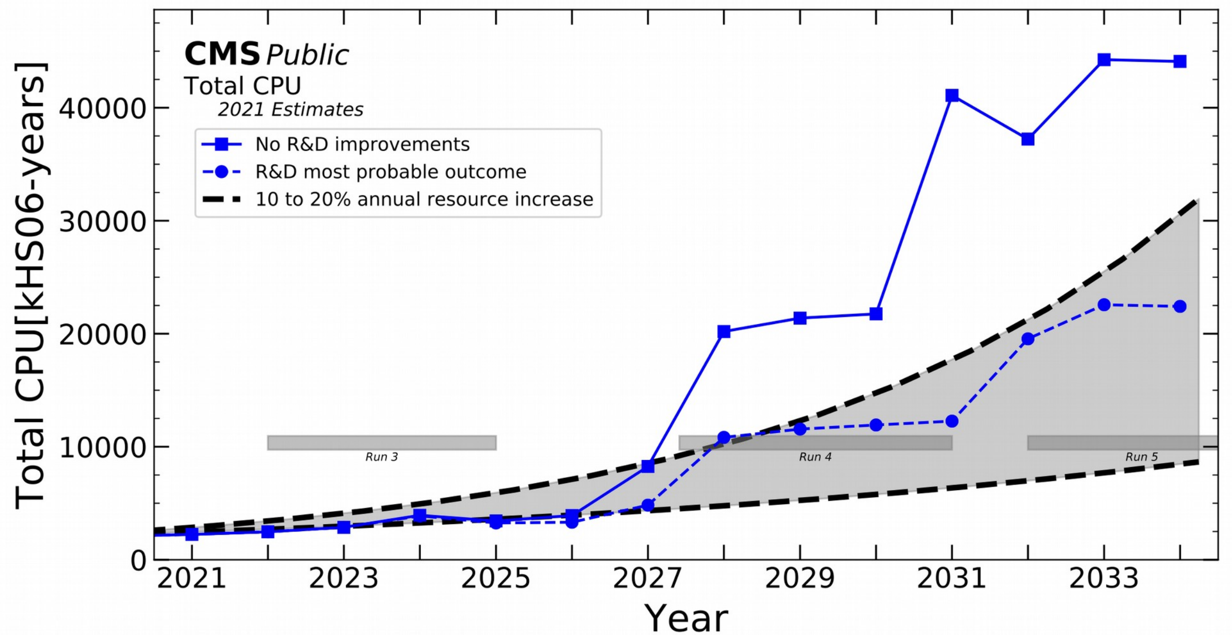


Reducing the Strain on HEP Computing Resources

- **MC simulation (Geant4)** is computationally **expensive**
  - Calorimeters most intensive part of detector simulation

- **Generative models** potentially offer orders of magnitude speed up

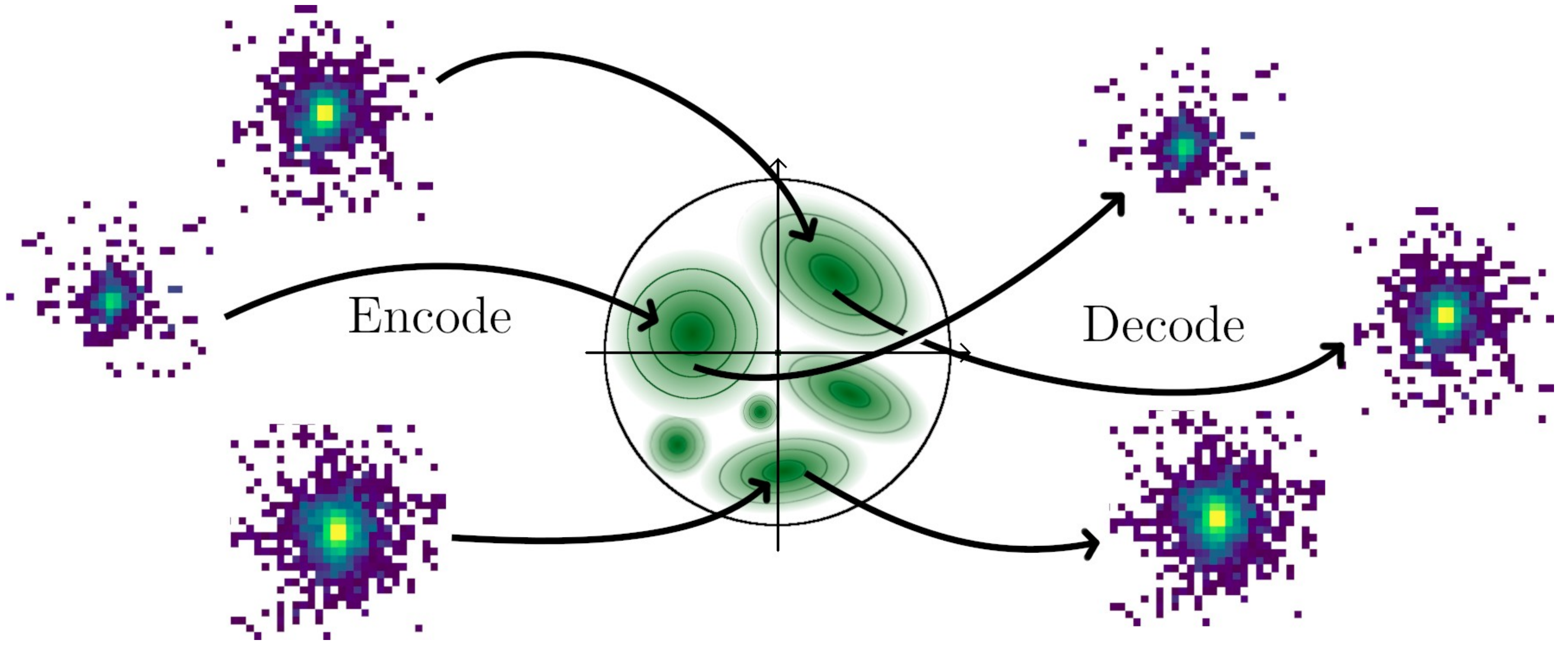




CMS Collaboration, Offline and Computing Public Results (2021), https://twiki.cern.ch/twiki/bin/view/CMSPublic/CMSOfflineComputingResults

Variational Autoencoder (VAE)

- **Encoder-decoder** structure
- Data mapped to regular Gaussians
- Decoder generates samples from **latent space**
- Loss: mean per-pixel difference between input and decoded shower



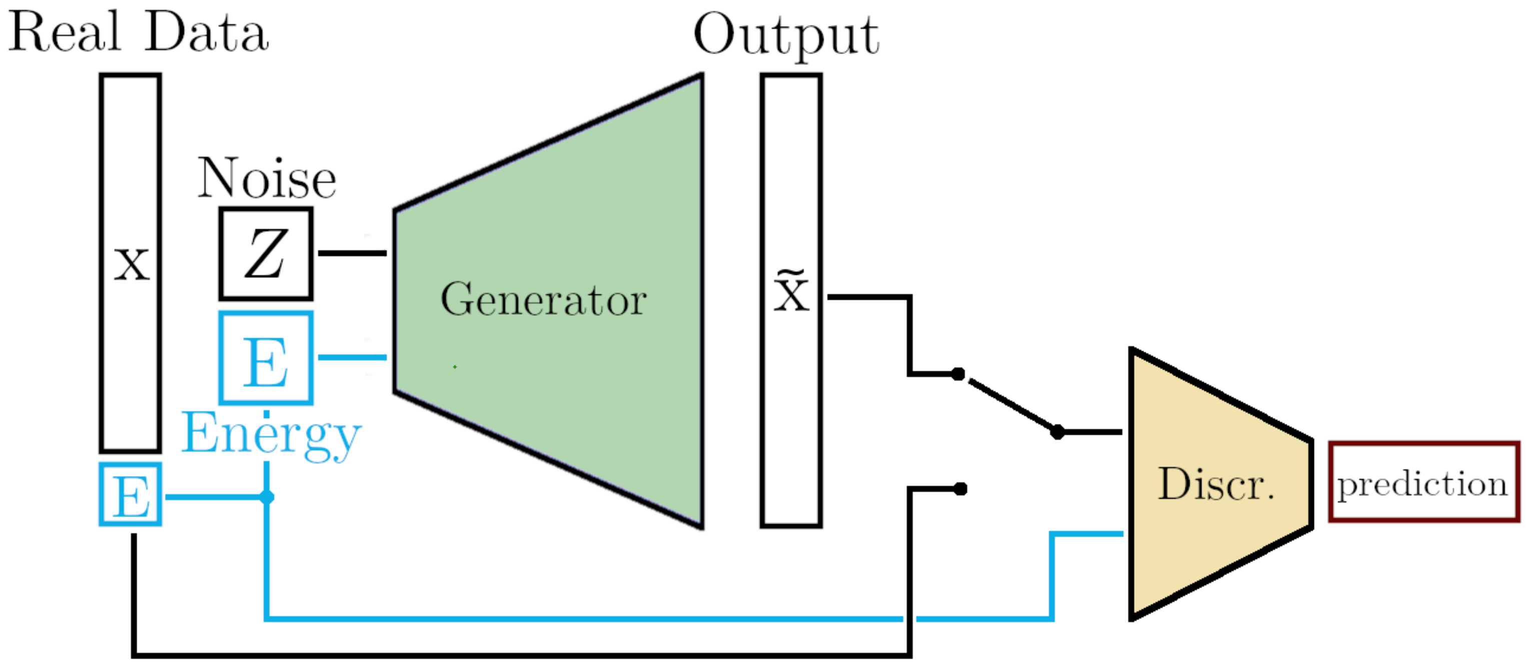
✓ Easier to train

X Less expressive

D.P. Kingma, M. Welling. Auto-encoding Variational Bayes (2014), arXiv:1312.6114

Generative Adversarial Network (GAN)

- **Generator**: tries to generate fake data that fools discriminator
- **Discriminator**: tries to distinguish real data from fake
- Loss: **adversarial** feedback from discriminator
- Ideally: fake samples from generator can't be distinguished by discriminator



✗ Hard to train

✓ Can be rather expressive

Ian Goodfellow et. al., Generative Adversarial Nets (2014), [arXiv:1406.2661]

Architectures: BIB-AE

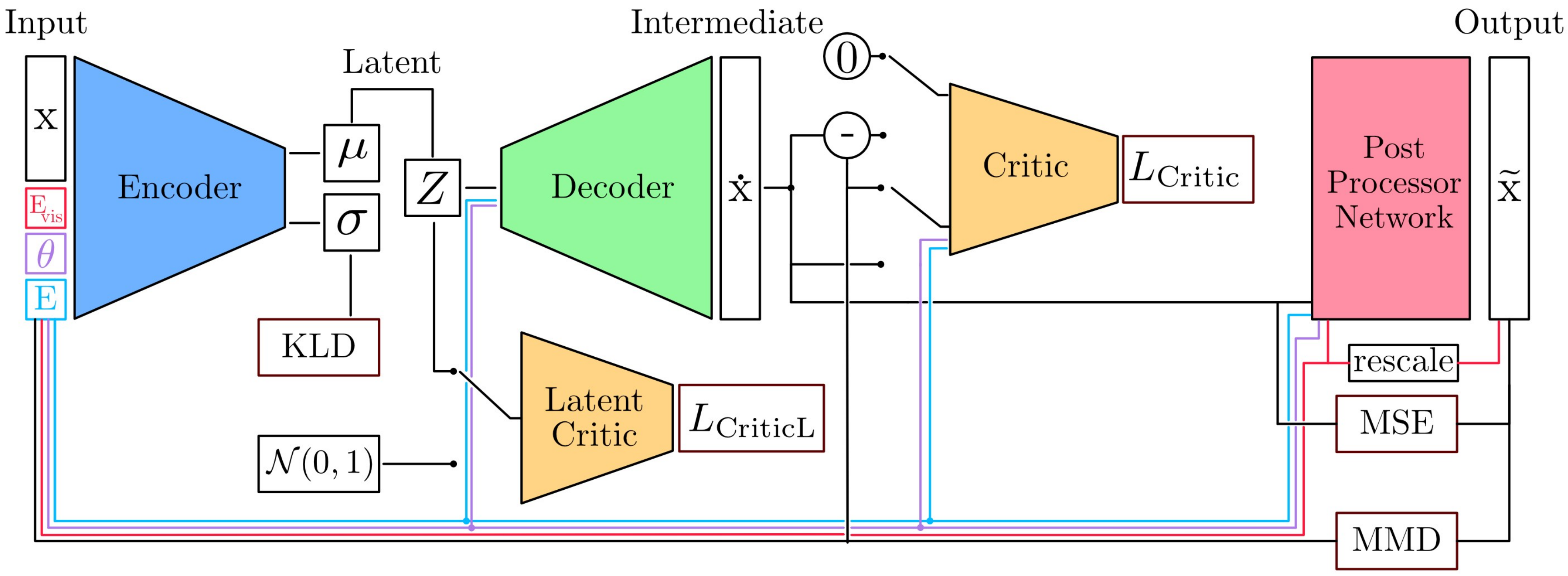
Voloshynovskiy et. al: Information bottleneck through variational glasses, arXiv:1912.00830 (2019)

Buhmann et. al: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed**, CSBS 5, 13 (2021)

Buhmann et. al., **Hadrons, Better, Faster, Stronger**, MLST 3 025014, (2022)

Bounded-Information Bottleneck Autoencoder (BIB-AE)

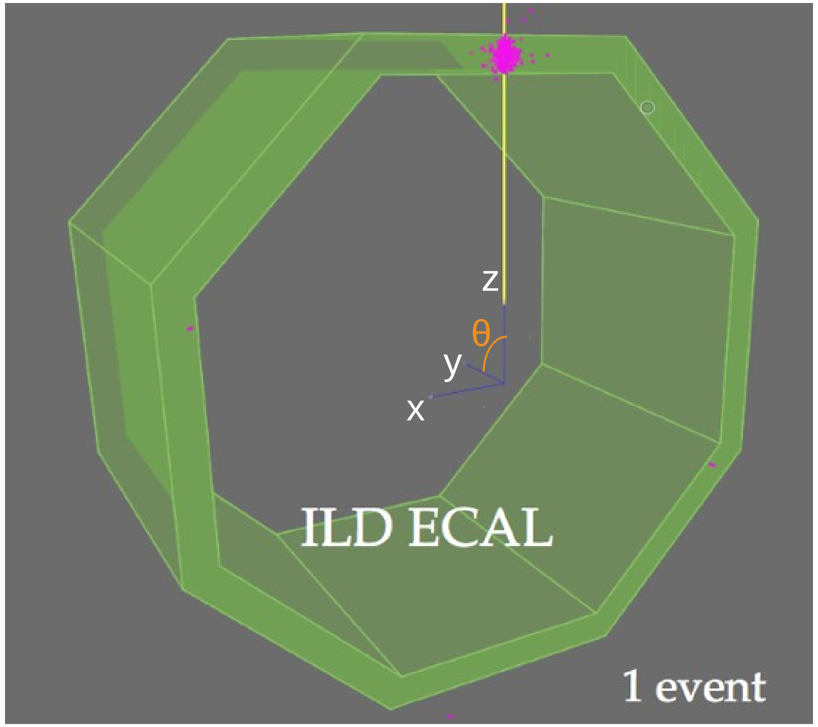
- **Unifies** features of both **GANs** and **VAEs**
- **Post-Processor** network: Improve per-pixel energies; second training

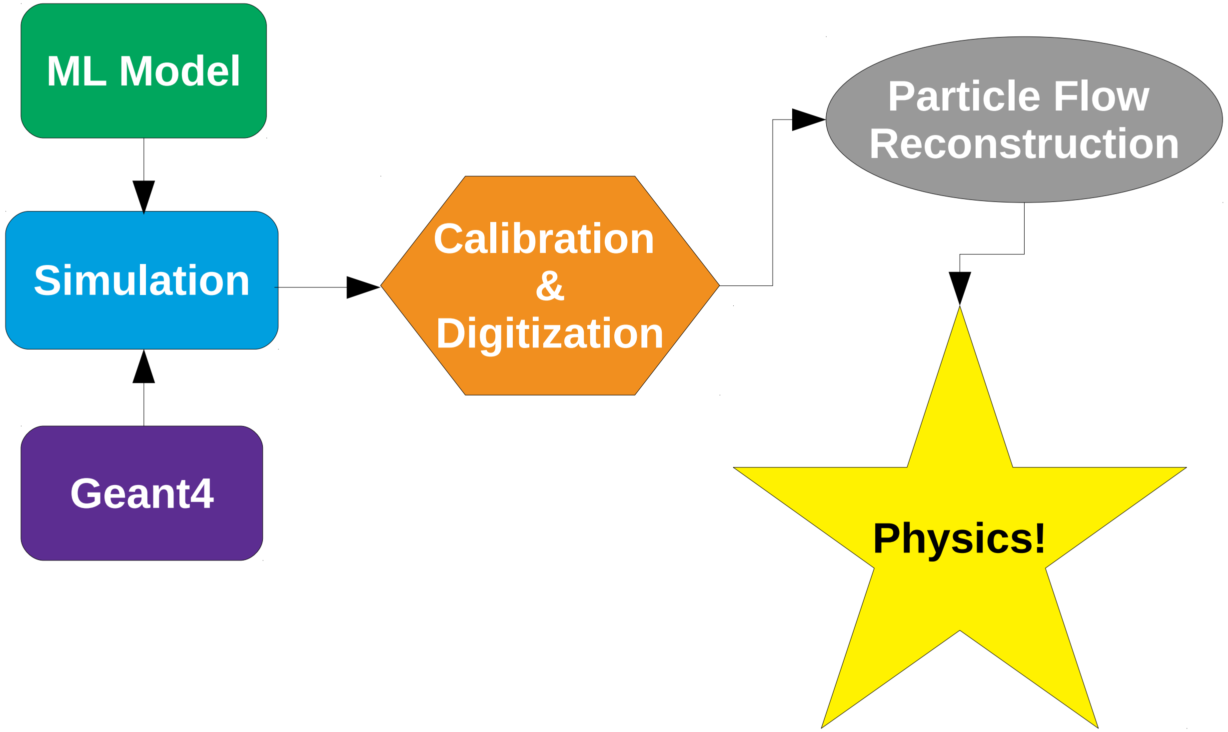


$$L_{BIB-AE} = KLD + L_{CriticL} + L_{Critic}$$

$$L_{Post} = MMD + MSE$$

The New Angles





Multi-Parameter Conditioning

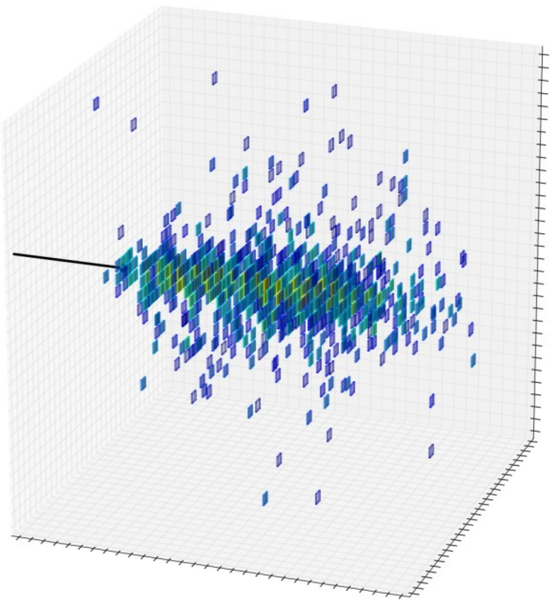
- **Simultaneous conditioning** on multiple parameters crucial for a general simulation tool
  - Start with **photons**
  - Vary incident **energy and angle**

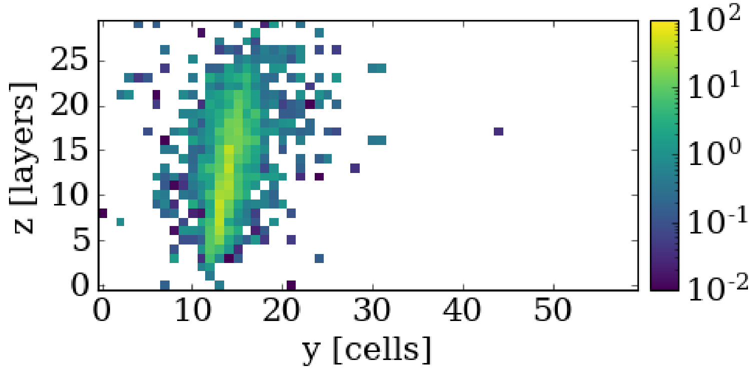
Study effects of reconstruction- Pandora PFA

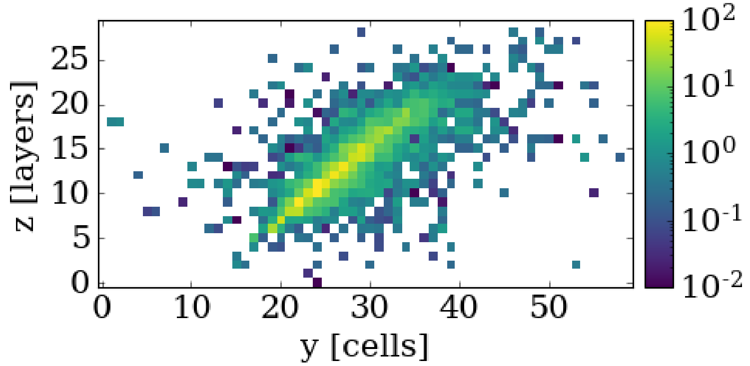
- Ultimate goal is **physics performance** after **reconstruction**
- Want our models to **maintain performance** after reconstruction
  - **Compare observables** before and after

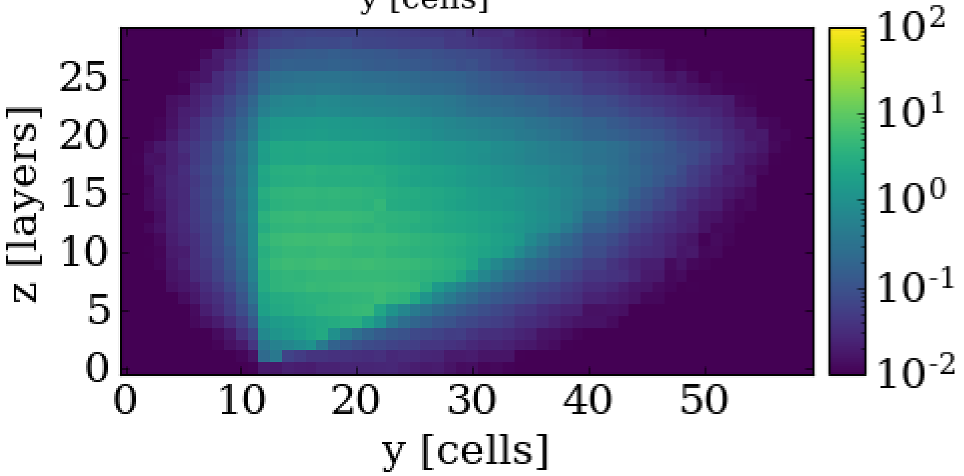
Training data

- 500,000 **photons** with fixed incident point
- Vary **energy**: **10-100 GeV**
- Vary **polar angle** in one direction: **90°-30°**
- Project to regular grid
  - Shape (30,60,30) (x,y,z)





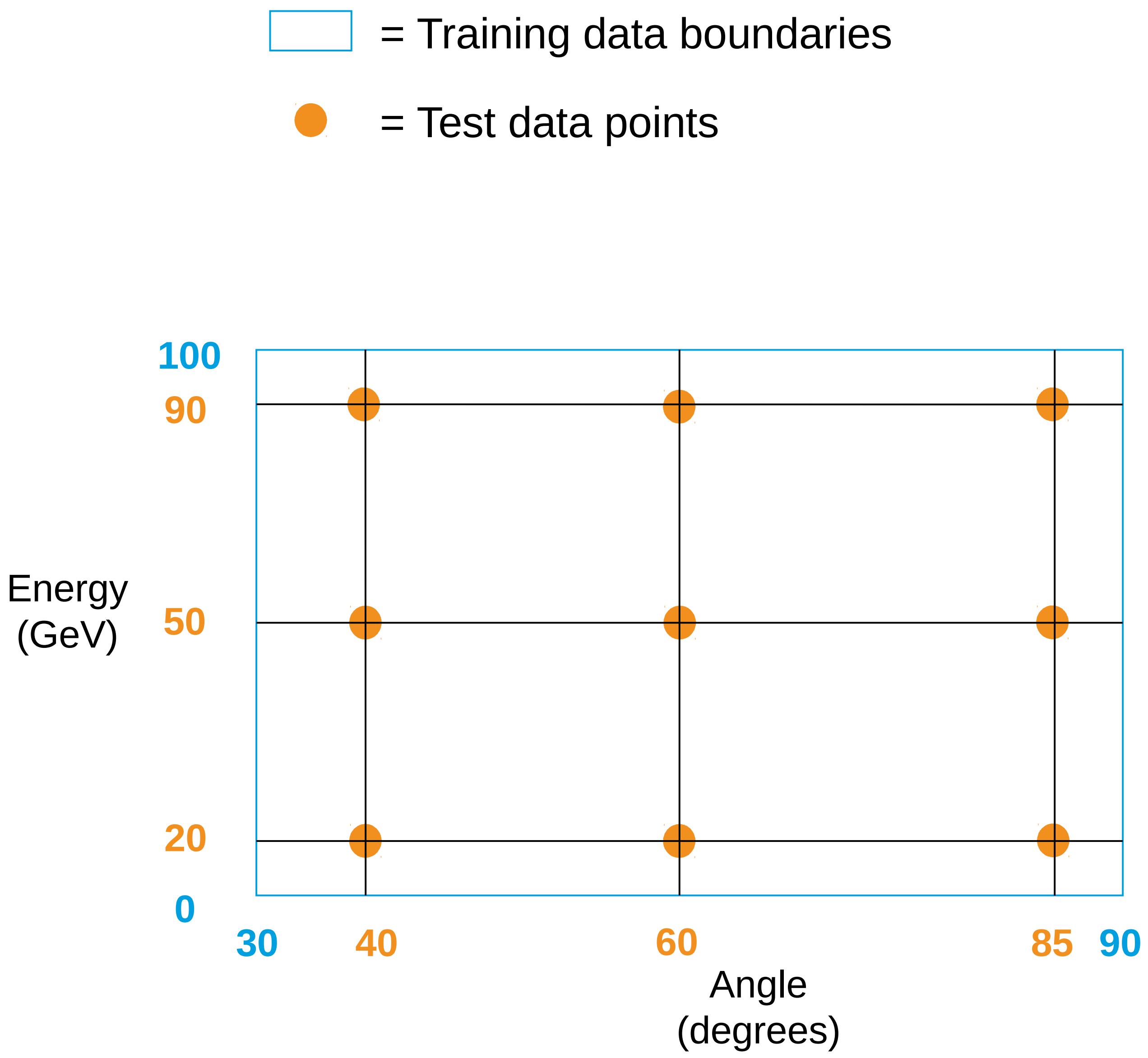




Test data

- Choose **fixed combinations** of energies and angles
- **9 points** in the phase space in total
- Avoid phase space boundaries

- Investigate how well generative model learns **key physics** properties of showers:
  - Visible energy sum
  - Number of hits and Hit energy spectrum
  - Shower profiles
  - Angular response

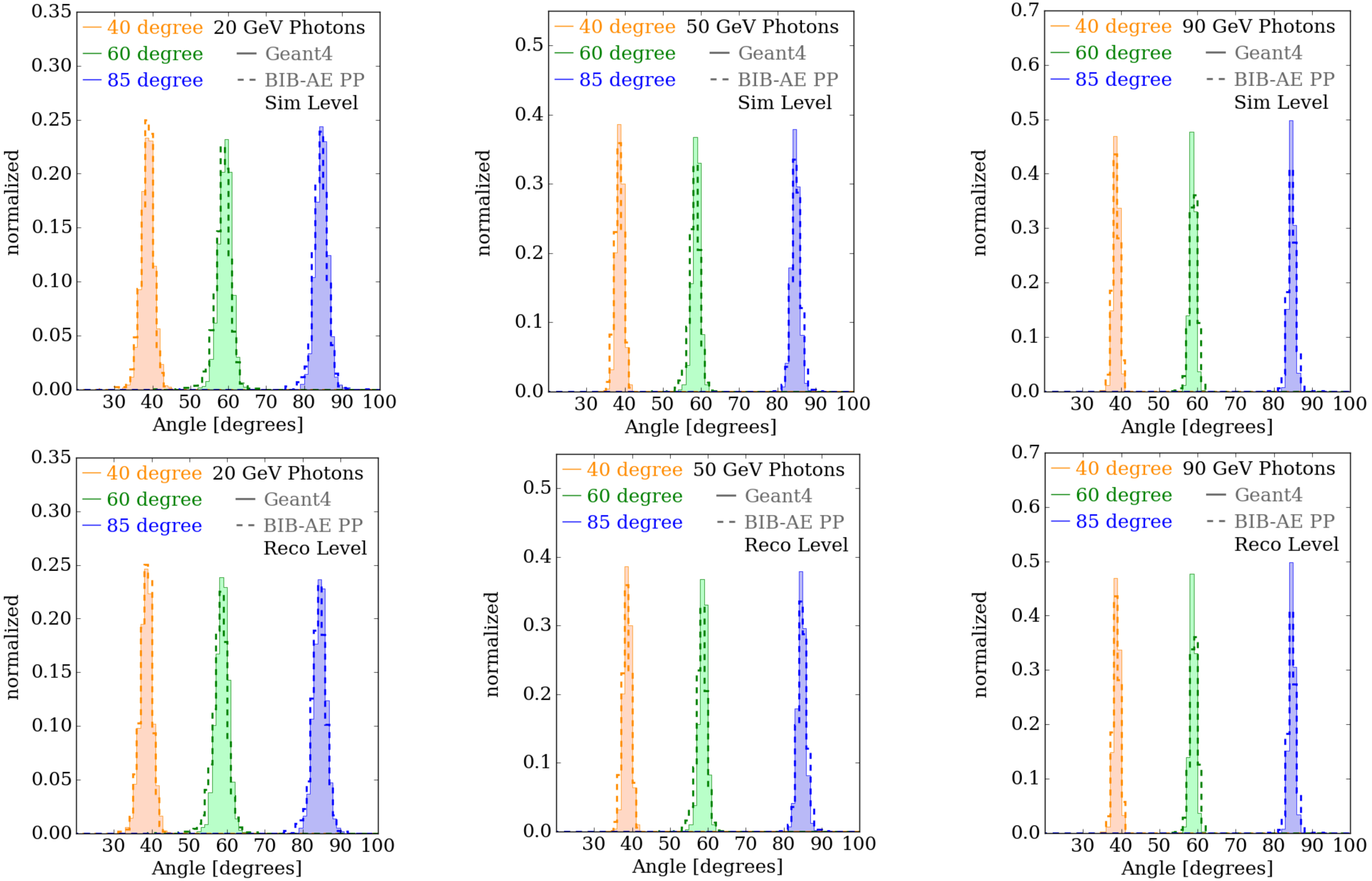


Results: Angular resolution- Sim vs Reco

20 GeV | 50 GeV | 90 GeV

Sim Level

Reco Level

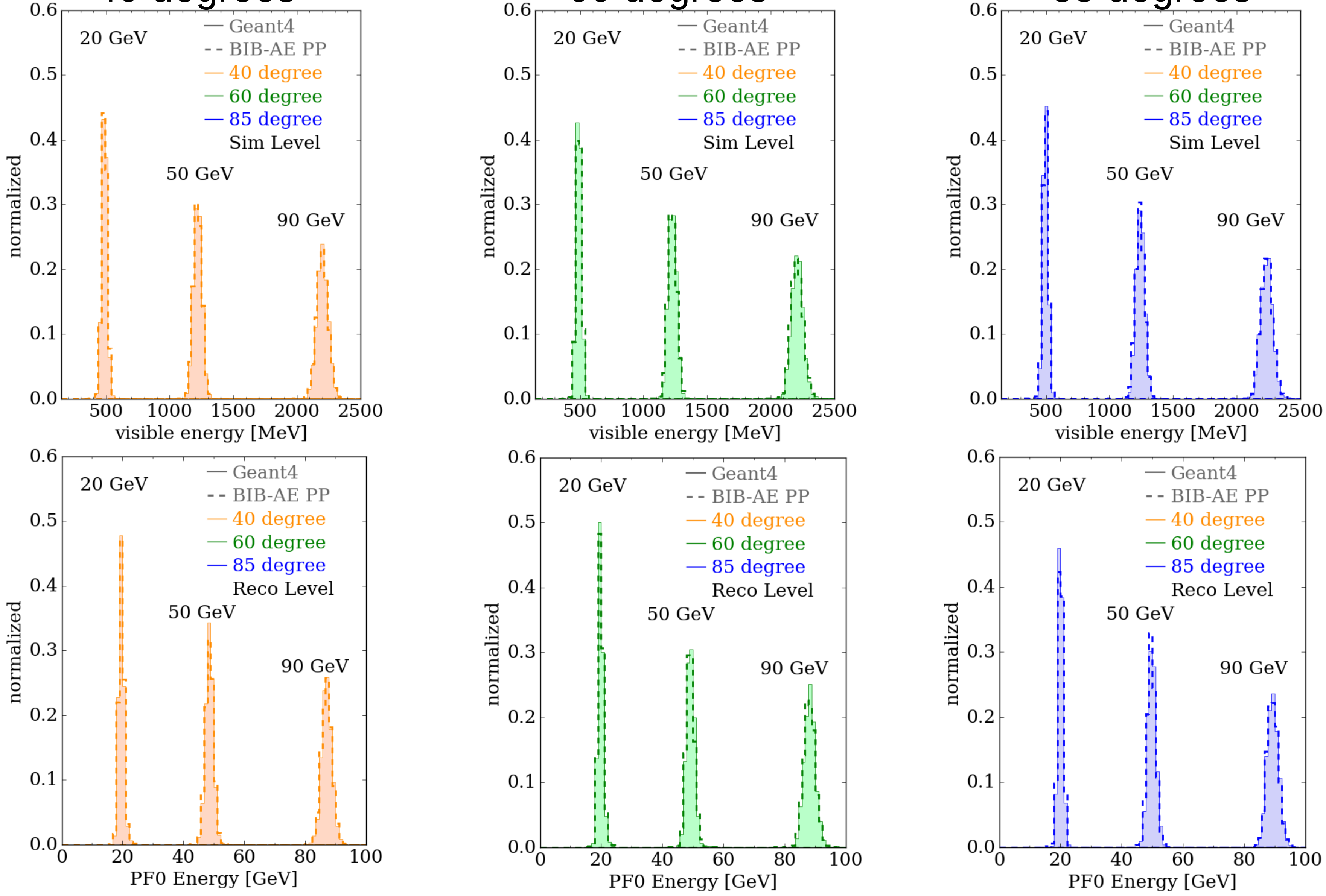


Results: Visible Energy Sum- Sim vs Reco

40 degrees | 60 degrees | 85 degrees

Sim Level

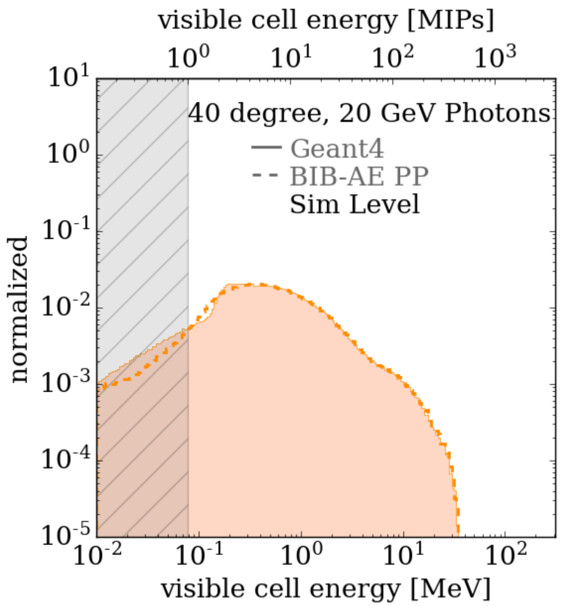
Reco Level

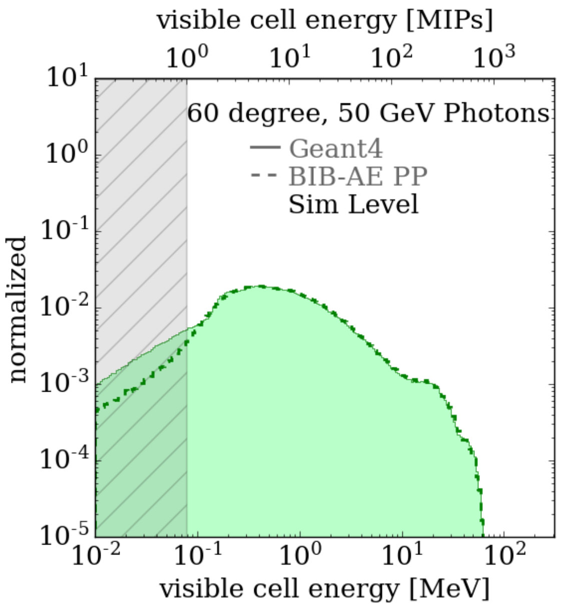


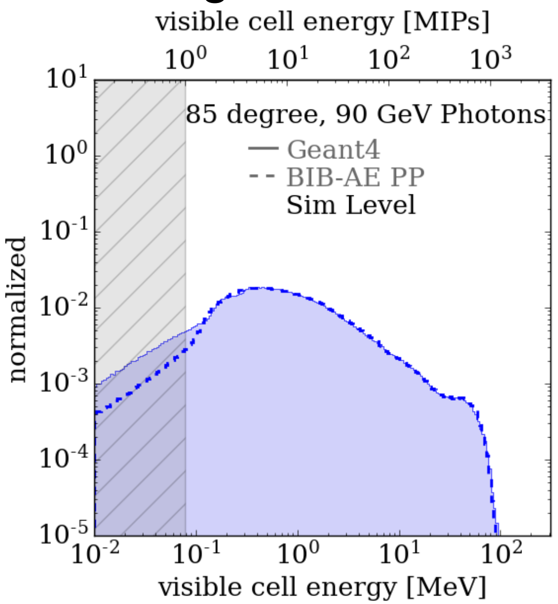
Results: Cell Energy Examples Sim vs Reco

40 degrees, 20 GeV | 60 degrees, 50 GeV | 85 degrees, 90 GeV

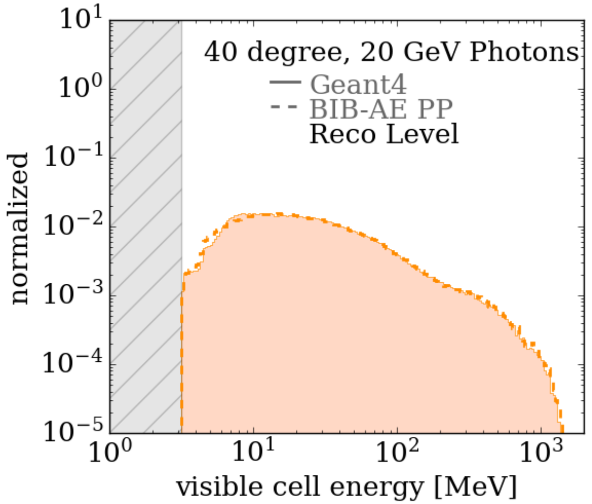
Sim Level

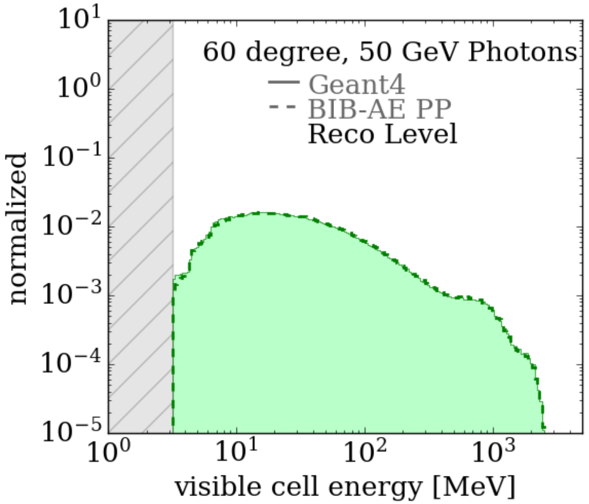


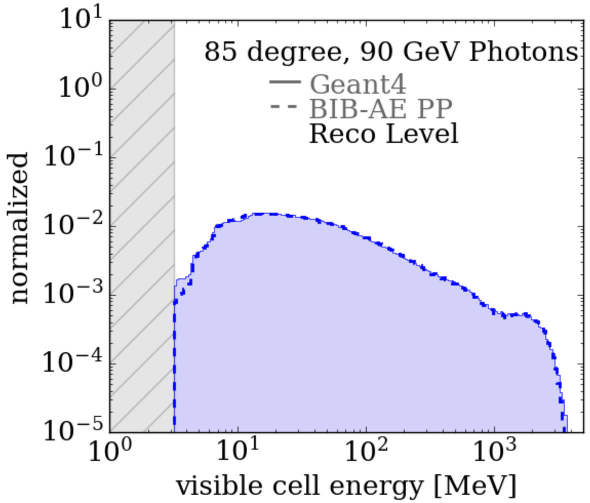




Reco Level





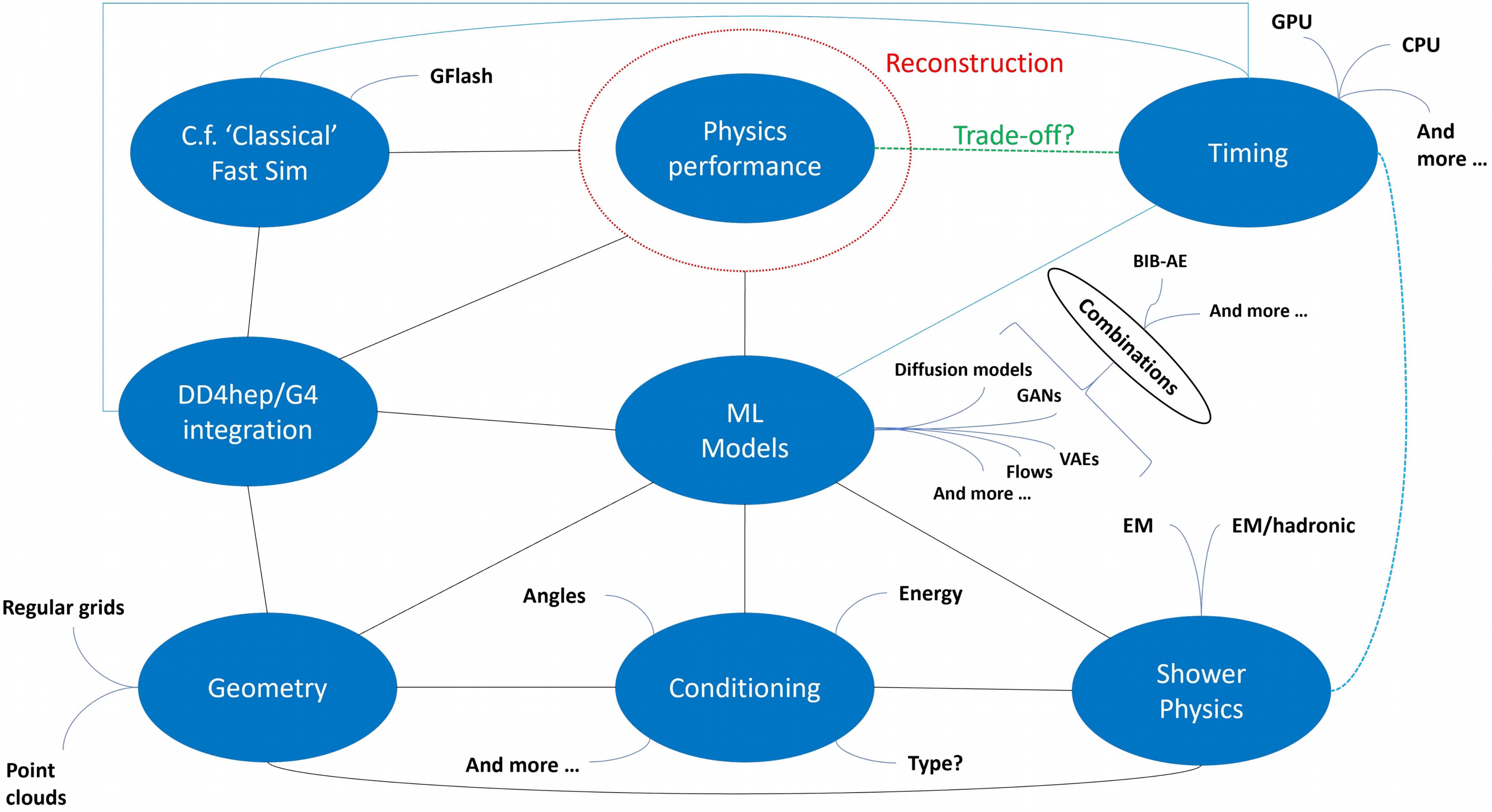


Computing Time for Inference

Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	4417 ± 83	$\times 1$
	BIB-AE	362 ± 2	$\times 12$
GPU	BIB-AE	4.32 ± 0.09	$\times 1022$

Speed-up of as much as three orders of magnitude on single core of Intel® Xeon® CPU E5-2640 v4 and NVIDIA® A100 for the best performing batch size

Map of Generative ML for Fast Calo Sim



Conclusion

Achieved

- Generative models hold promise for **fast** simulation of calorimeter showers with **high fidelity**
- Demonstrated high fidelity simulation of **photon** showers with **angular and energy conditioning**
- Investigated generative model performance after **reconstruction with Pandora**
  - **Performance remains high**

Paper out soon!

Next Steps

- Develop strategy for dealing with **arbitrary incident positions**
- Integration into **DD4hep/Geant4** and study **physics performance**

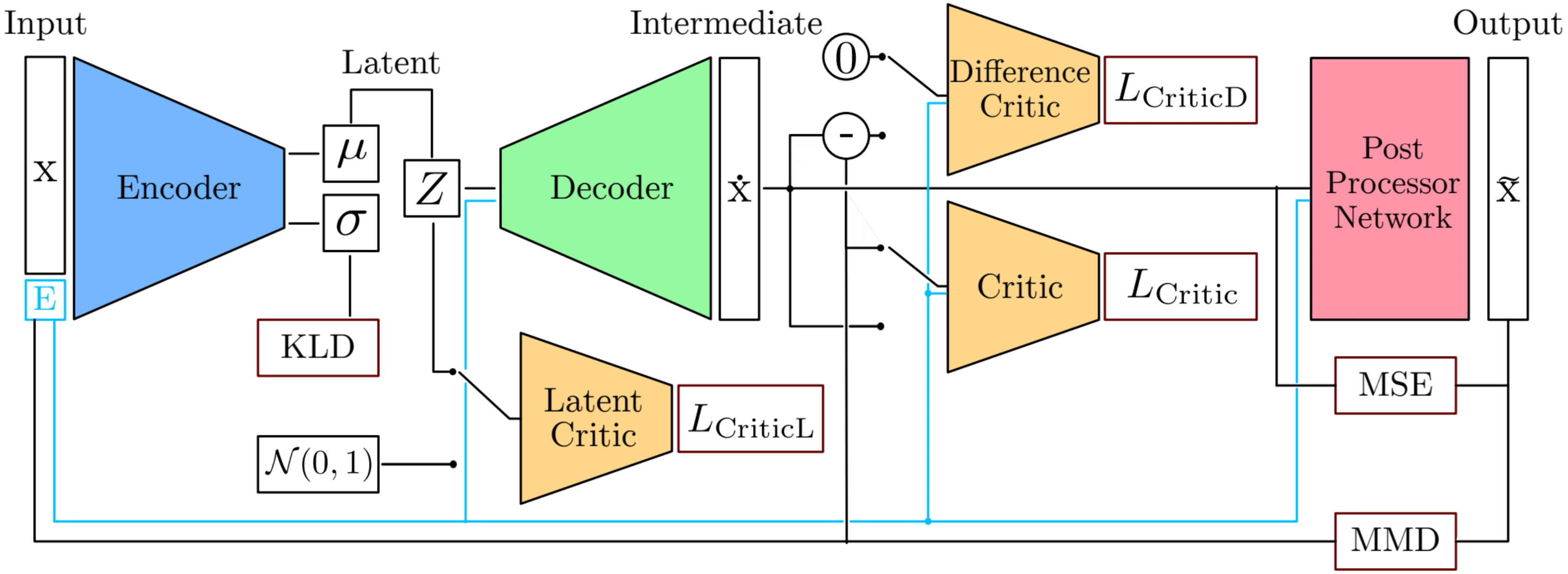
Backup

Architectures: BIB-AE

More Details

- Unifies features of both GANs and VAEs
- Adversarial critic networks rather than pixel-wise difference a la VAEs
- Improved latent regularisation: additional critic and MMD term
- Post-Processor network: Improve per-pixel energies; second training

- Updates and improvements:
  - Dual and resetting critics: prevent artifacts caused by sparsity
  - Batch Statistics: prevent outliers/ mode collapse
  - Multi-dimensional KDE sampling: better modeling of latent space



$$L_{\text{BIB-AE}} = \text{KLD} + L_{\text{CriticL}} + L_{\text{Critic}} + L_{\text{CriticD}}$$

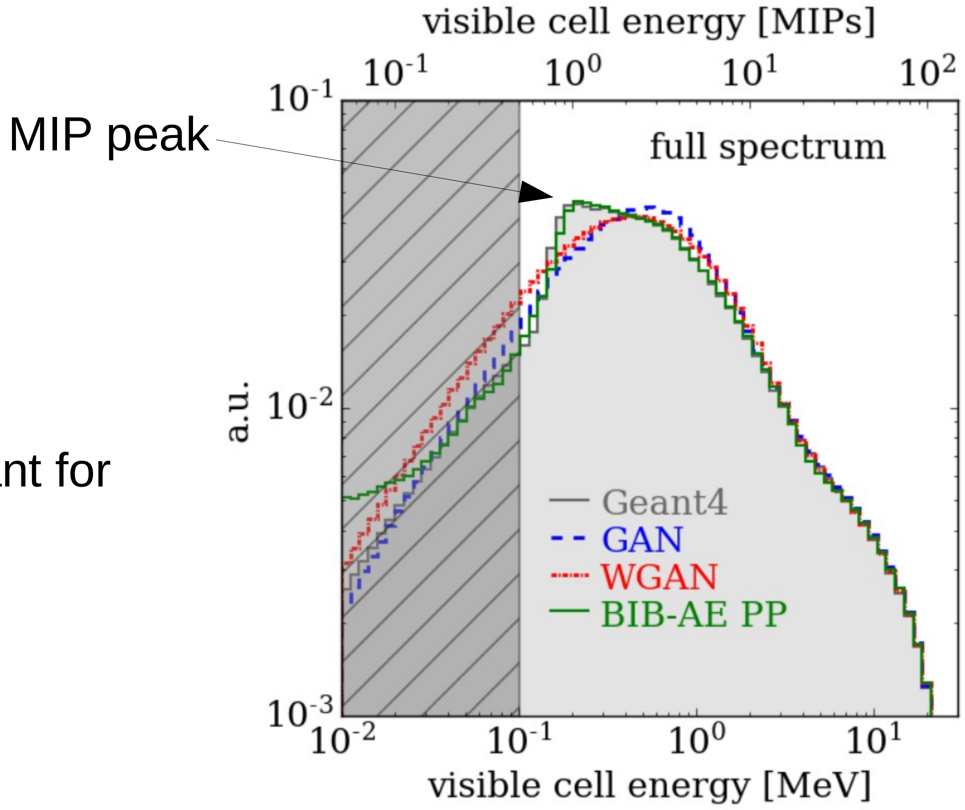
$$L_{\text{Post}} = \text{MMD} + \text{MSE}$$

Adaption to Highly Granular Calorimeter Shower Data

- **Highly granular** calorimeter data is very **sparse**
  - Causes problems for an MSE based loss
  - Switch to a discriminator based approach

- **Cell energy spectrum** has a very steep rise (MIP peak- important for calibration)
  - Difficult to model with an adversarial approach...

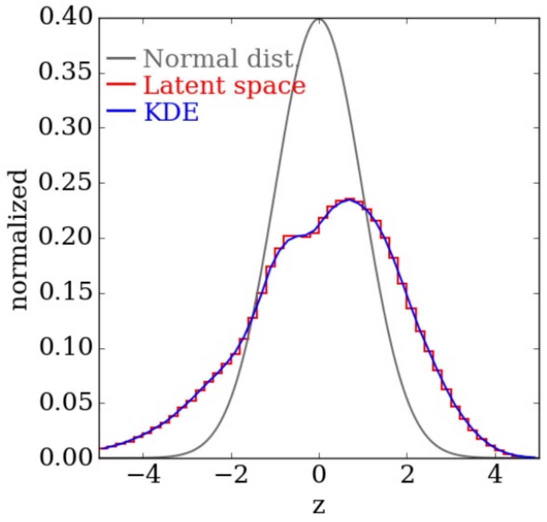
- Offload to separate **Post Processor** network:
  - 3D convolutions, kernel size 1
  - MSE loss and Sorted Kernel MMD loss
  - Encourage network to modify individual pixels

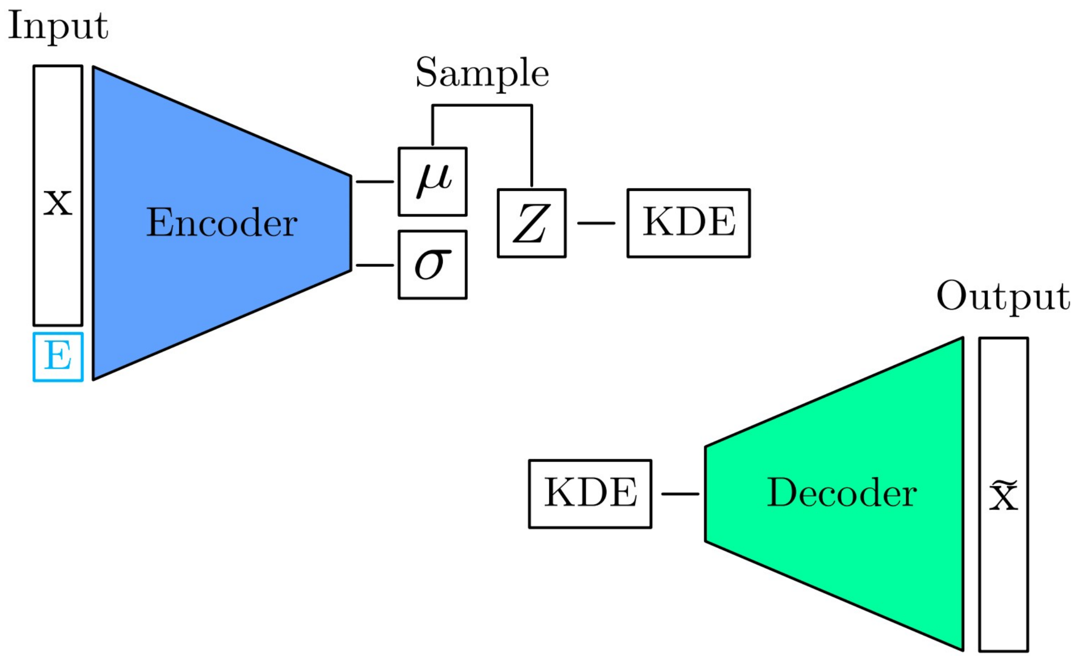


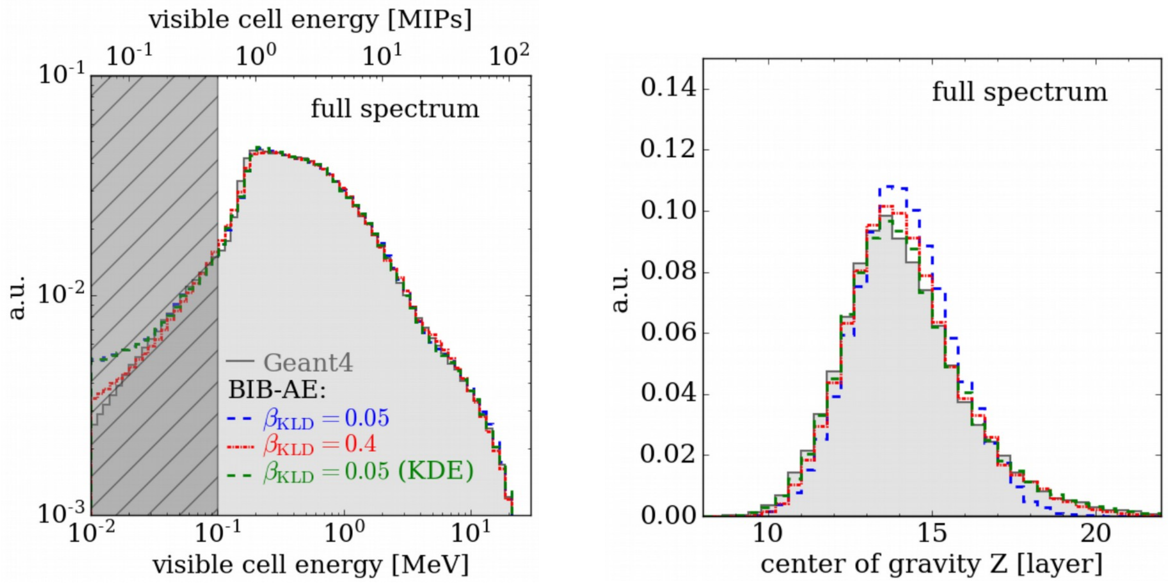
Buhmann et. al: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed**, CSBS 5, 13 (2021)

Latent Space sampling

- **Relaxing regularisation** of latent space allows more information to be stored
  - Latent space deviates from a Normal distribution
- Employ **density estimation** to produce latent sample (**normalising flow**)
- **Improve** modeling of **shower shape** (center of gravity)

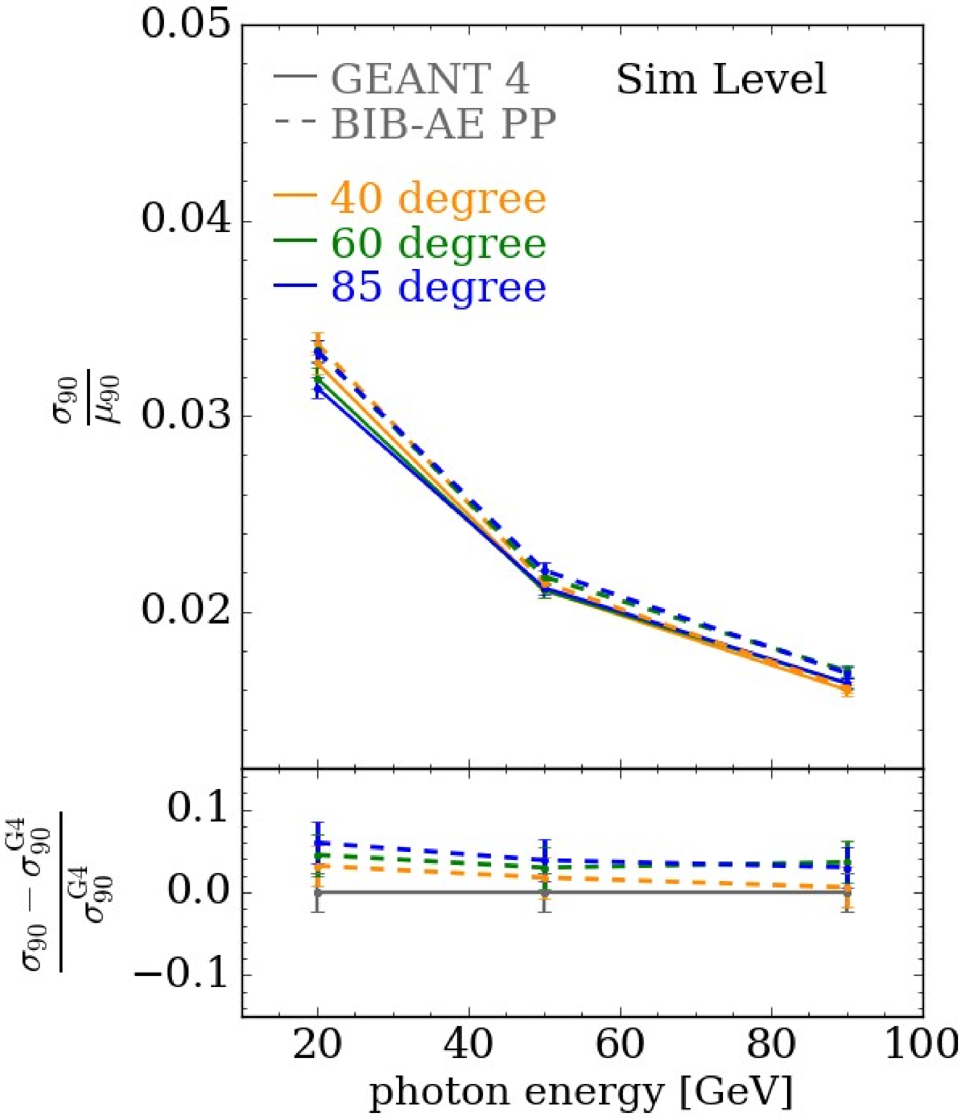


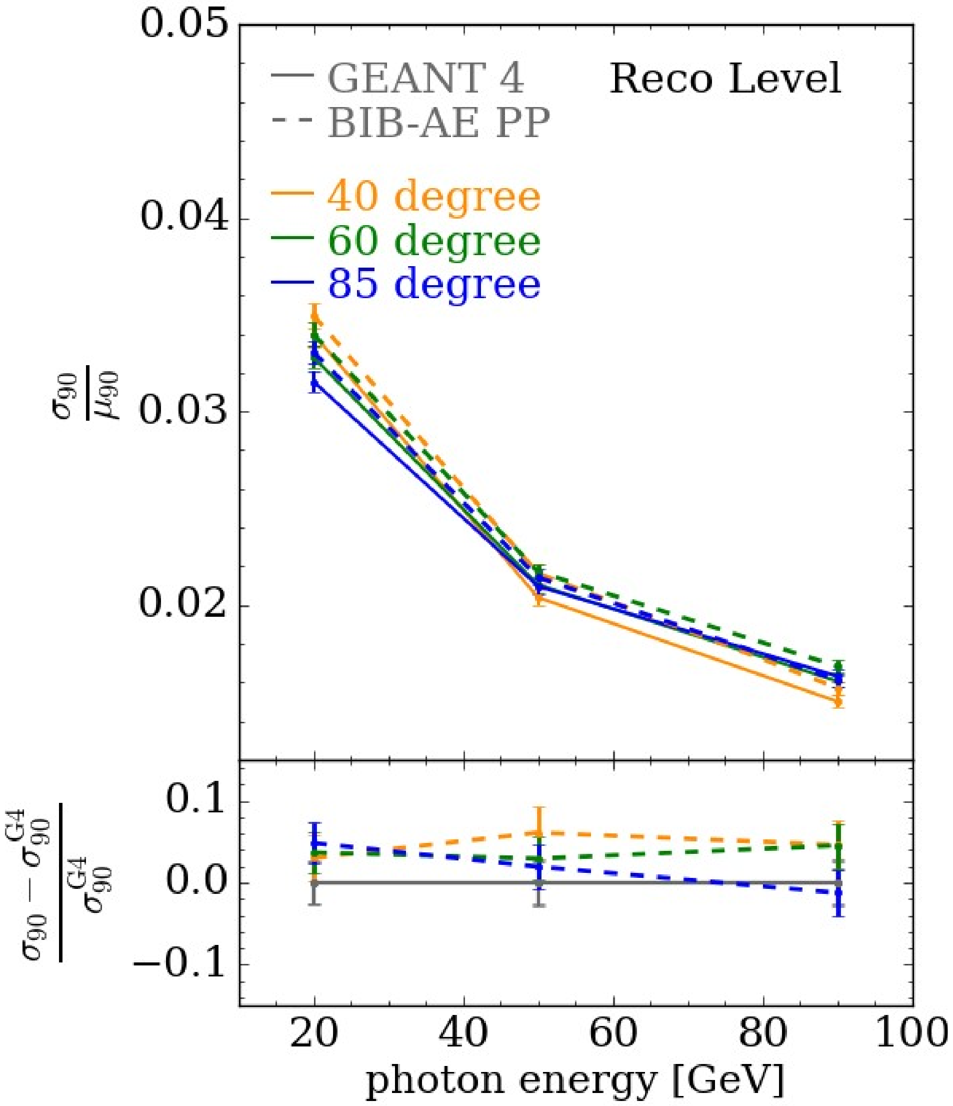




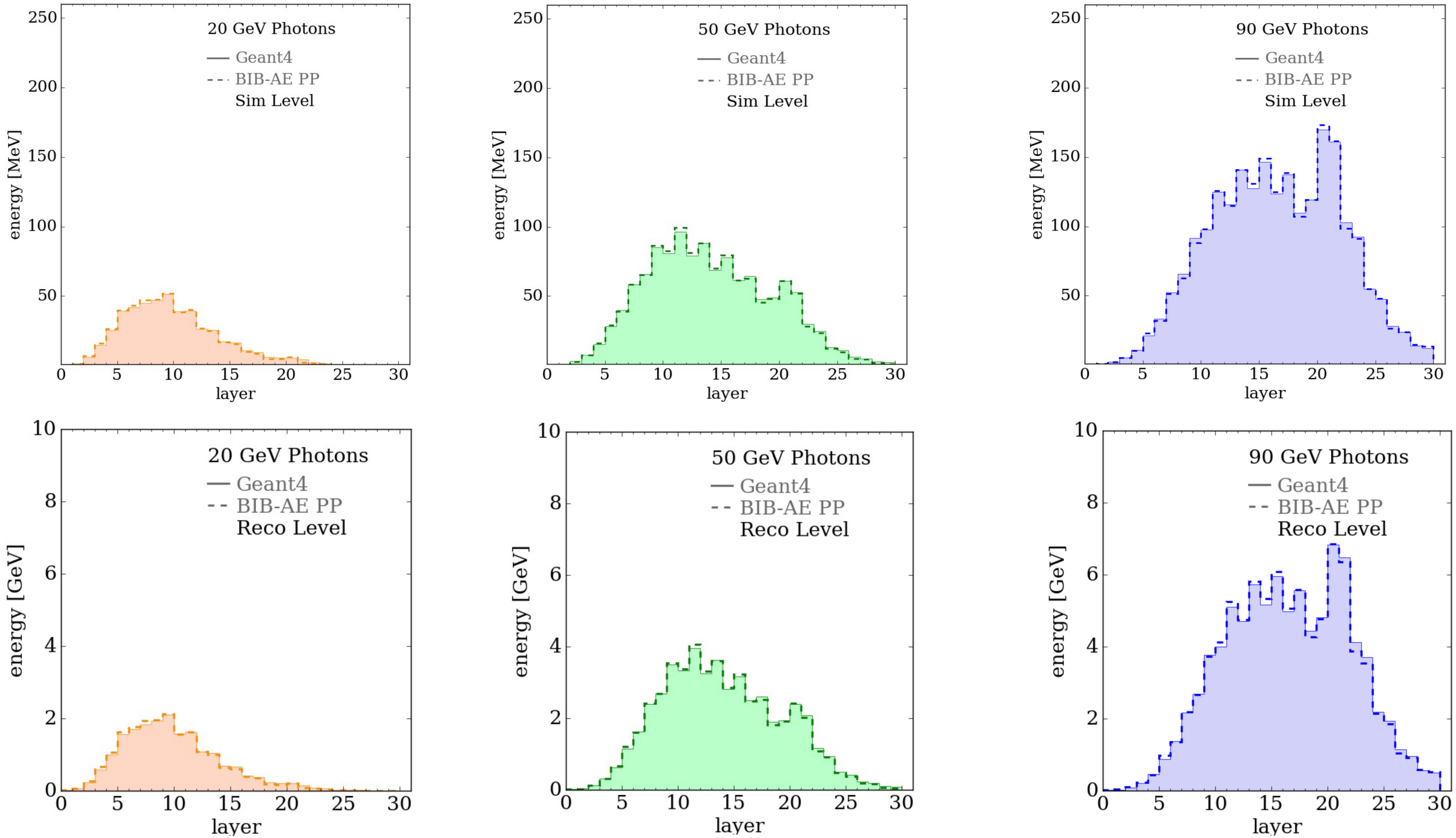
Buhmann et. al: **Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network**, [EPJ Web of Conferences 251, 03003](https://doi.org/10.1051/epjconf/202125103003) (2021)

Results: Energy resolution Sim vs Rec

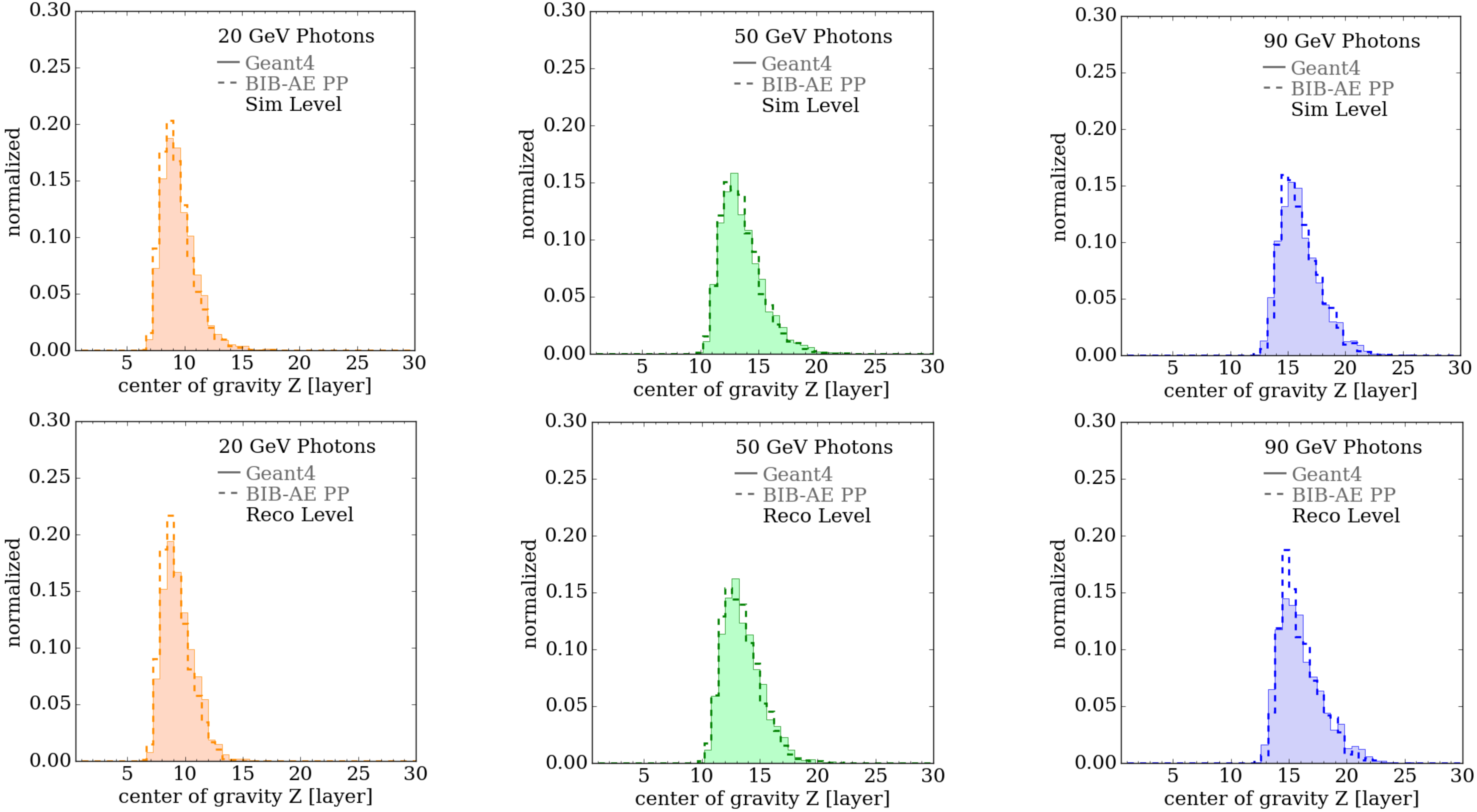




Results: Longitudinal Profile



Results: Center of Gravity



Results: Radial Profile