Generative Models and Calorimeter Fast Simulation for the LHCb

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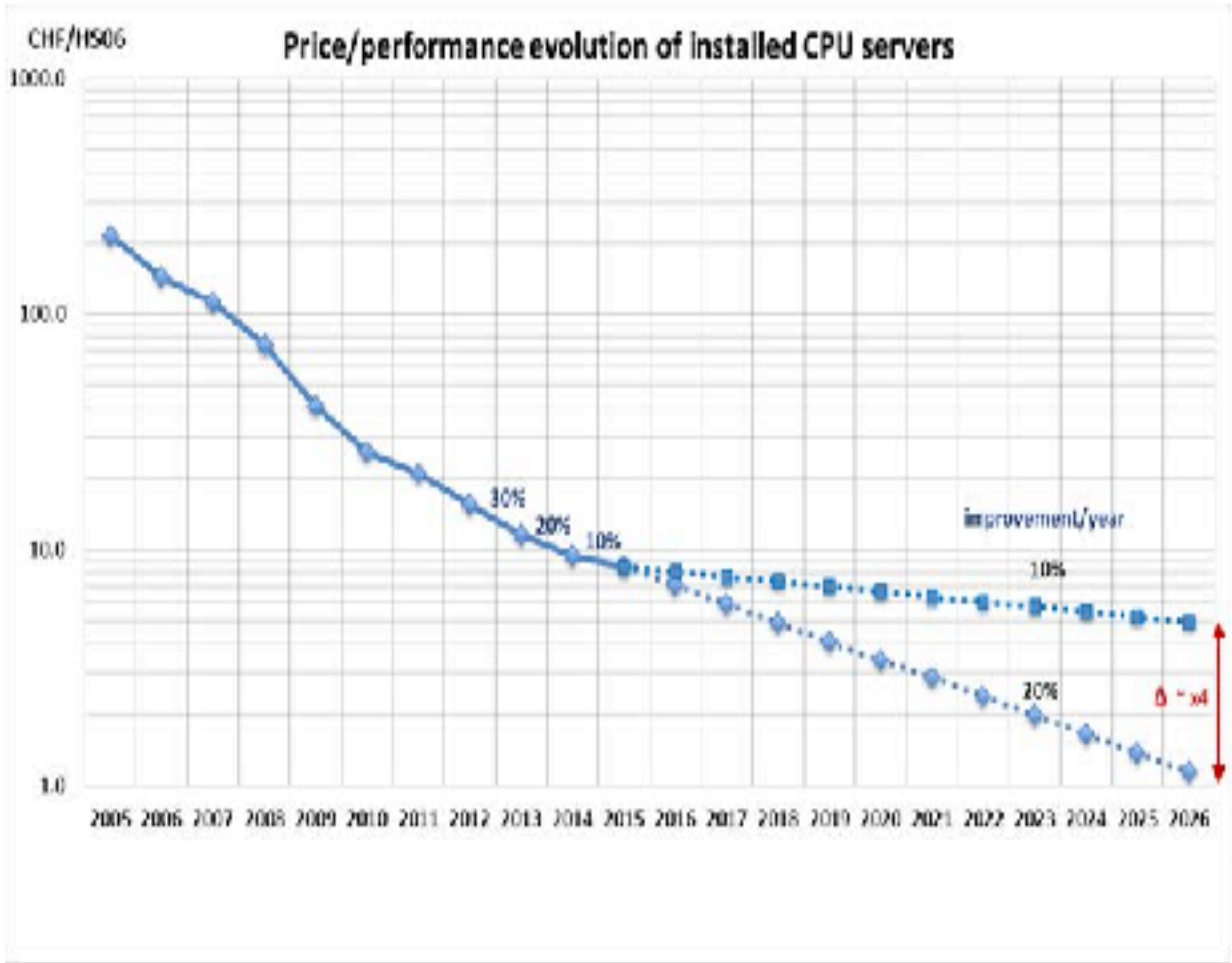
Library Approach

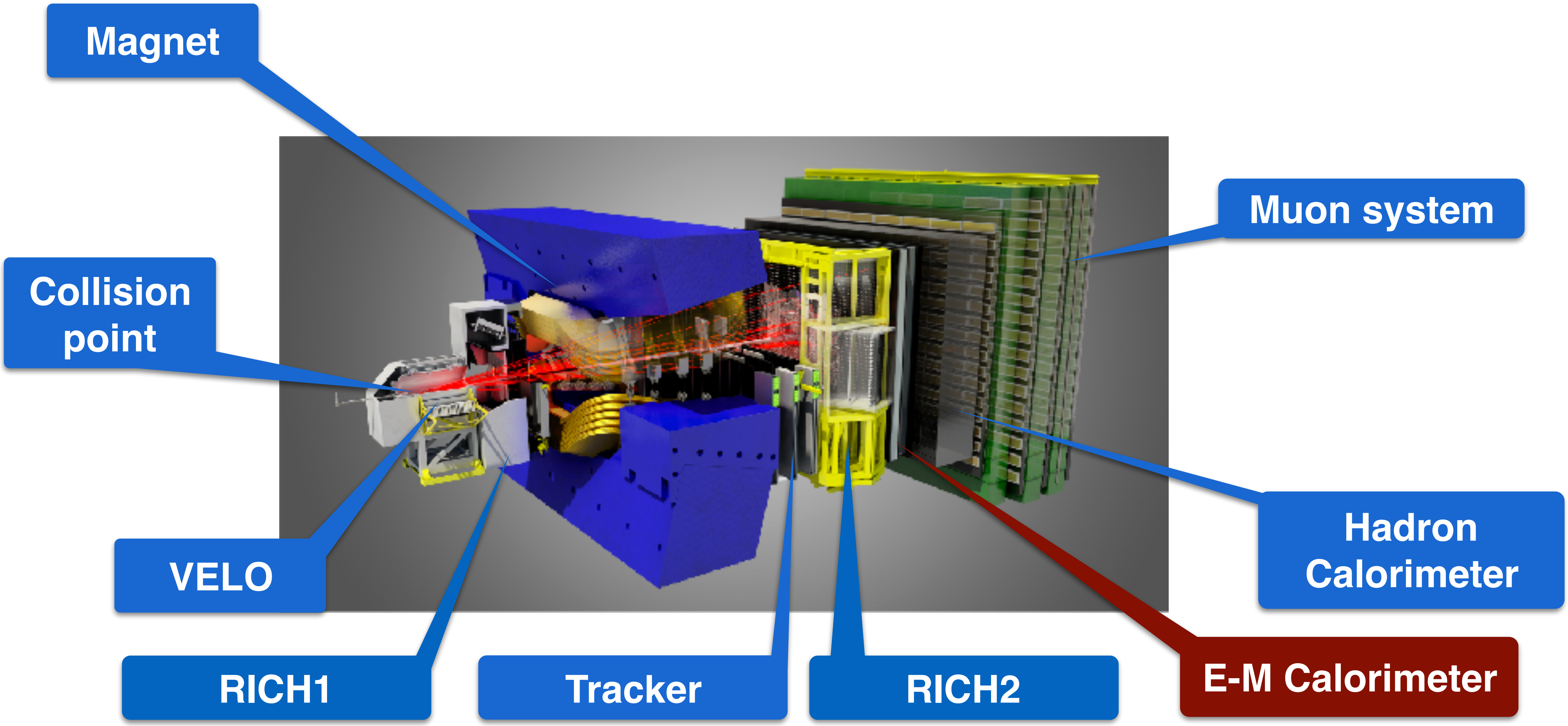
- We have train sample for the generative model
  - consistency with this train sample is a figure of merit for the generative model
- Objects of the train sample may be used for generation directly
  - remember KNN classification algorithm
  - k=1 - straightforward
    - the only drawback - search for the object with appropriate conditions in the (presumably huge) data library
  - k>1 - problem to interpolate between objects
    - short distance objects interpolation, more robust than global generation
- NB: this approach by construction uses full information which is contained in the training sample

Generative Models at LHC

- About 80% of computing resources are used for MC simulation in HEP experiments
  - Calorimeter simulation is one of bottlenecks
  - RICH is the next in the row for LHCb detector
    - > 85% of simulation is taken by these
- Can not expect exponential rise of CPU performance
- Need work around for Run3 and HL-LHC
- Generative models trained on the detailed GEANT simulation may be a solution



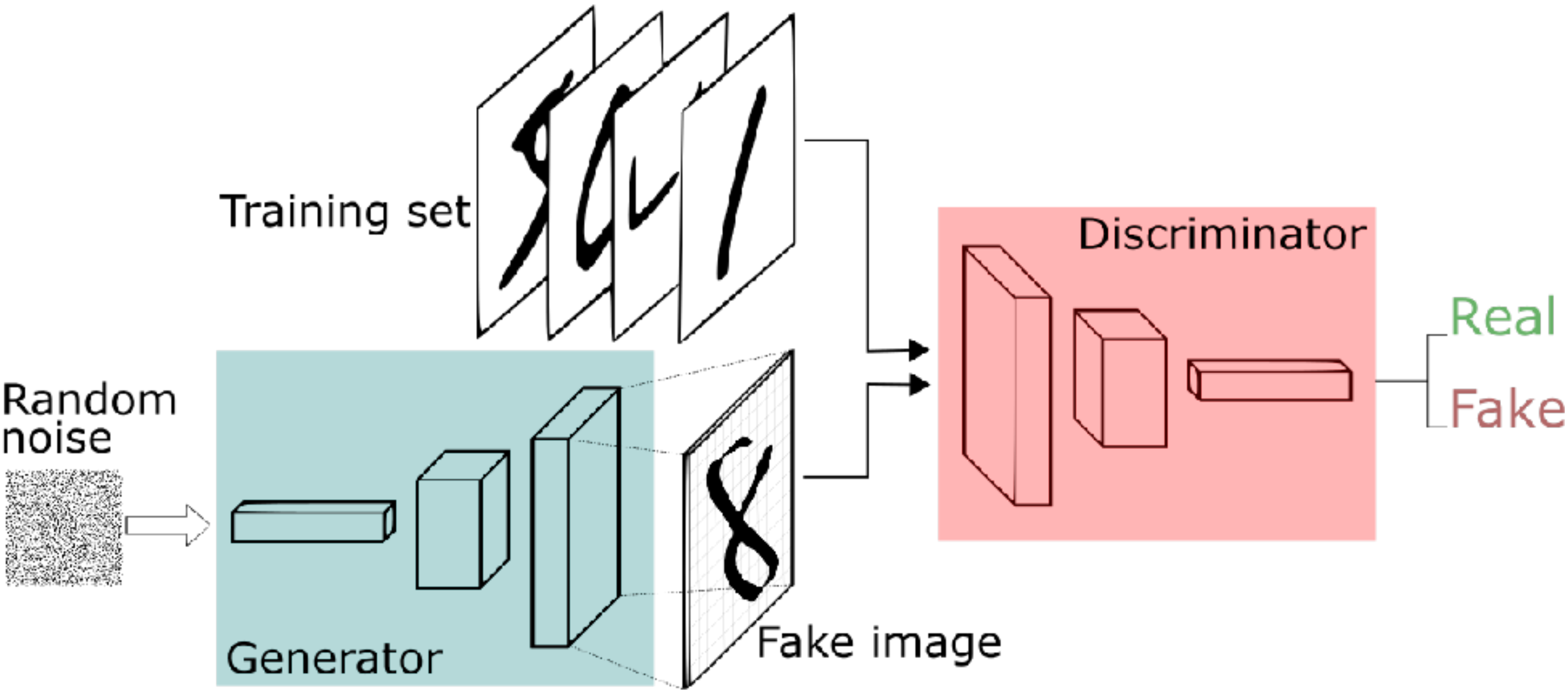
Example: Fast Simulation of the ECAL Response



- ECAL takes the most time in the LHCb event simulation

GAN

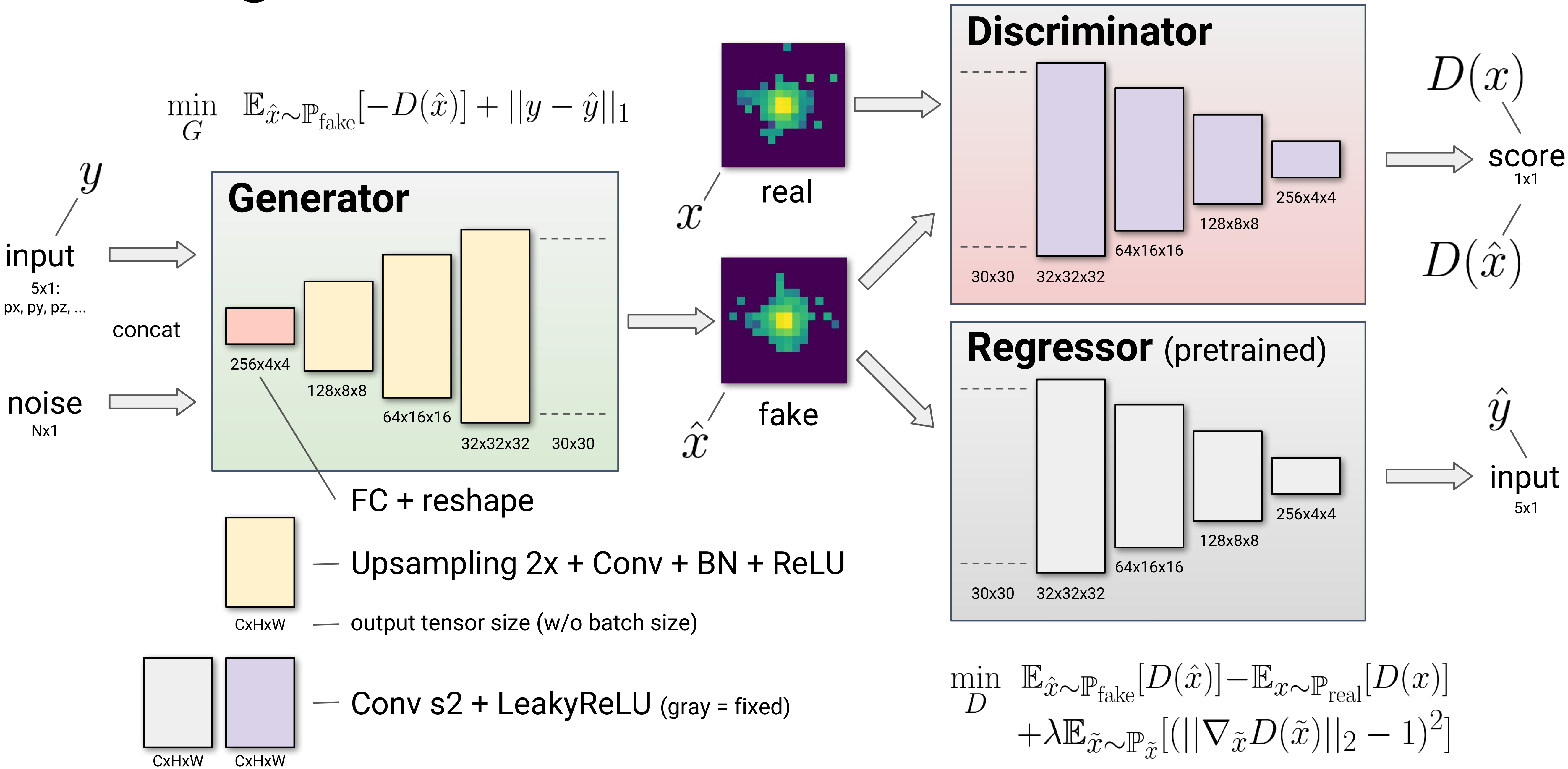
https://medium.freecodecamp.org/an-intuitive-introduction-to-generative-adversarial-networks-gans-7a2264a81394



- Implicit p(xly), sampling only

LHCb ECAL Fast Simulation: GAN

Training scheme



$$\min_{G} \mathbb{E}_{\hat{x}\sim\mathbb{P}_{\text{fake}}}[-D(\hat{x})] + ||y - \hat{y}||_1$$

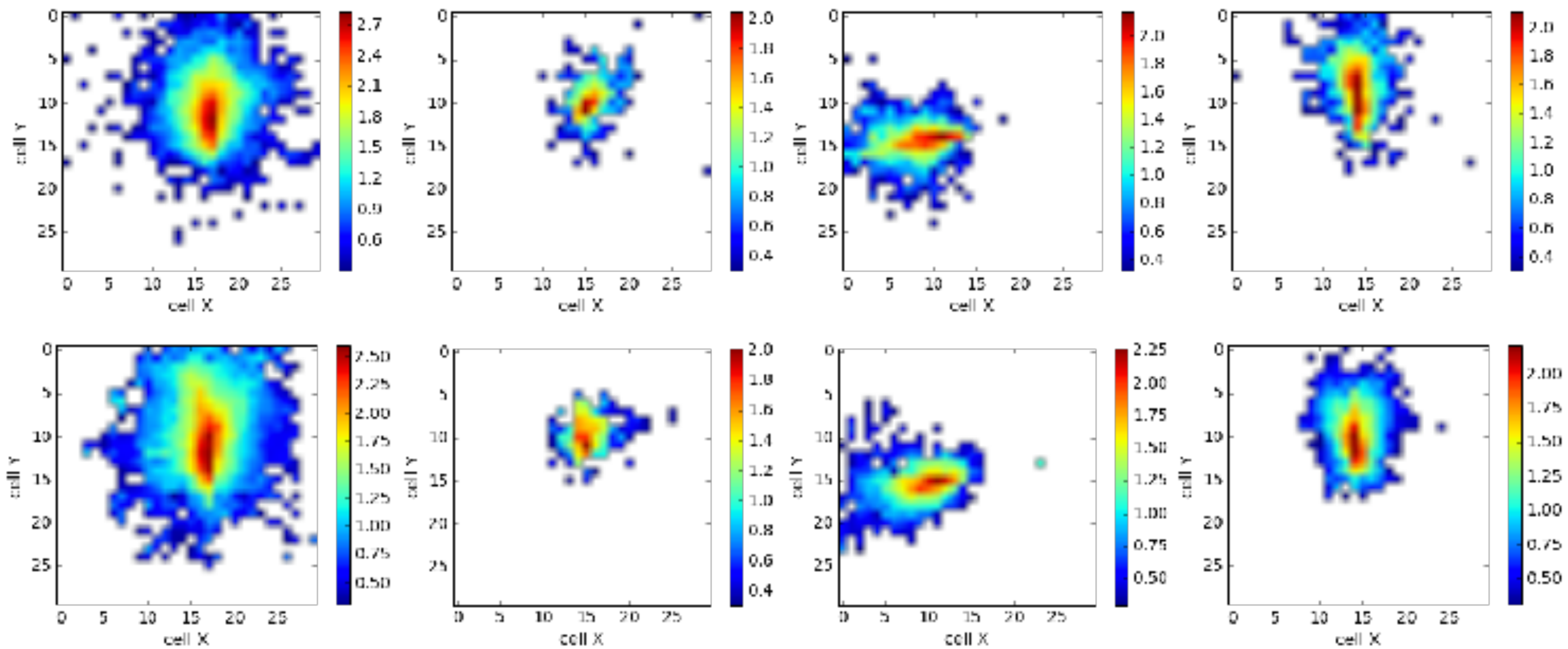
$$\min_{D} \mathbb{E}_{\hat{x}\sim\mathbb{P}_{\text{fake}}}[D(\hat{x})] - \mathbb{E}_{x\sim\mathbb{P}_{\text{real}}}[D(x)] + \lambda\mathbb{E}_{\tilde{x}\sim\mathbb{P}_{\tilde{x}}}[(||\nabla_{\tilde{x}} D(\tilde{x})||_2 - 1)^2]$$

LHCb ECAL Simulation

GEANT Simulated

log10(cell energy)

GAN Generated



GEANT Simulated

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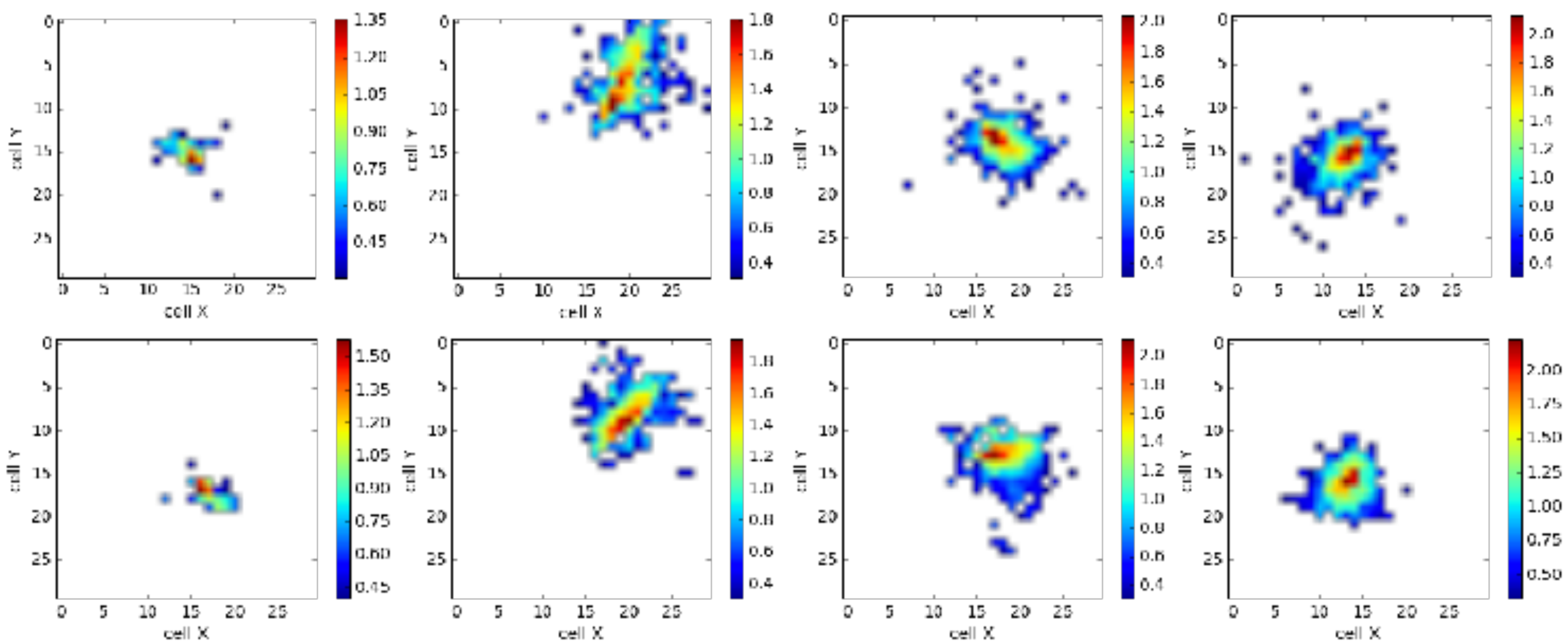
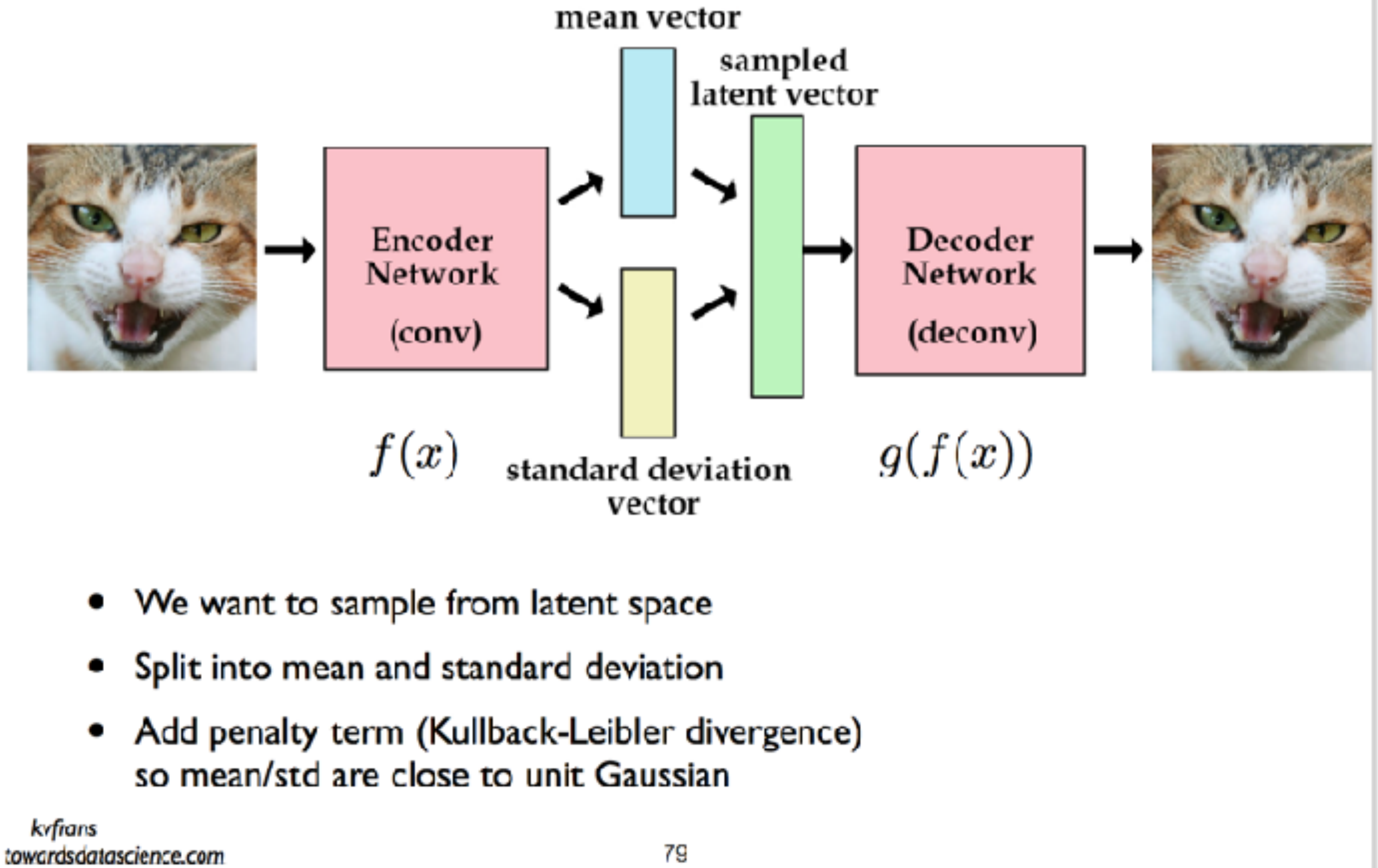
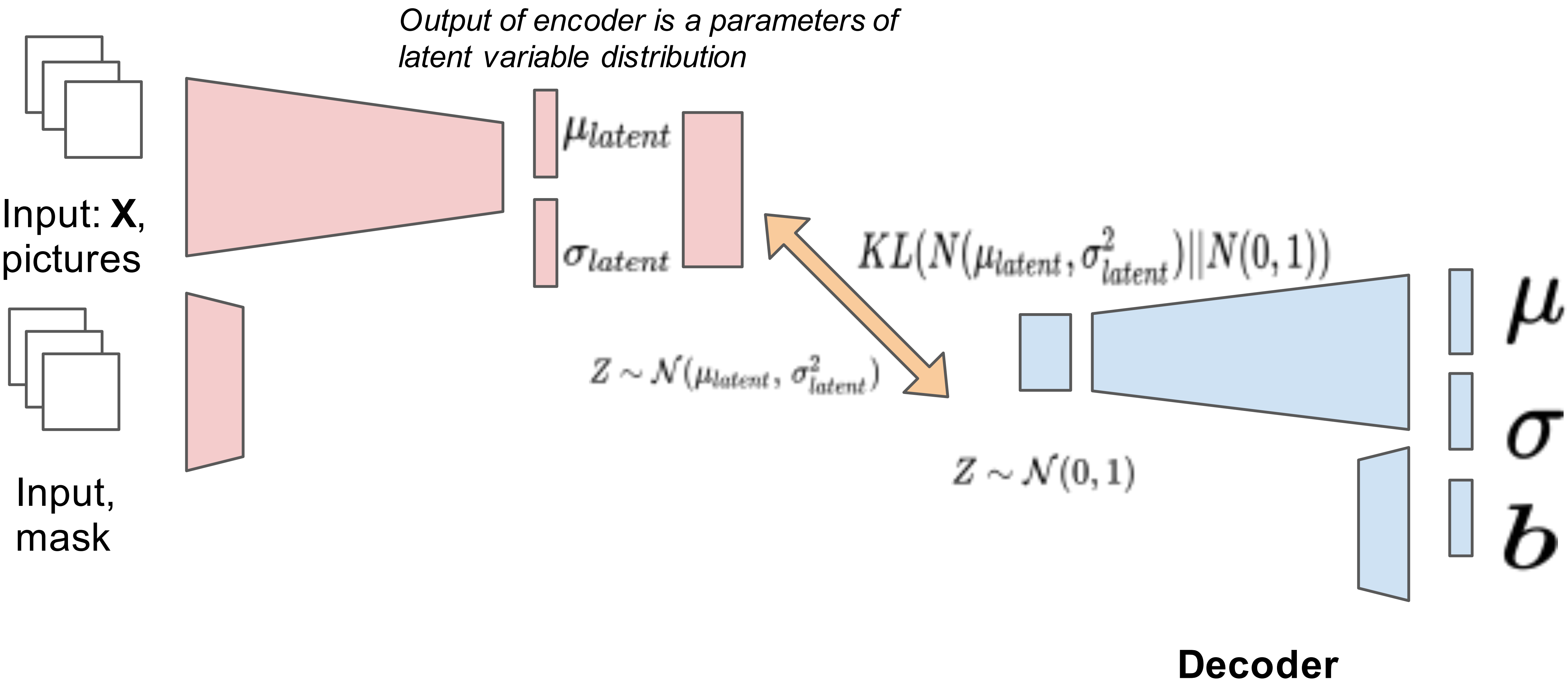


Variational Autoencoder



- VAE allows calculate p(x|y) explicitly
  - NB: GAN only allows sampling from p(x|y)
- ... but smaller size of latent dimensions
  - blurry objects

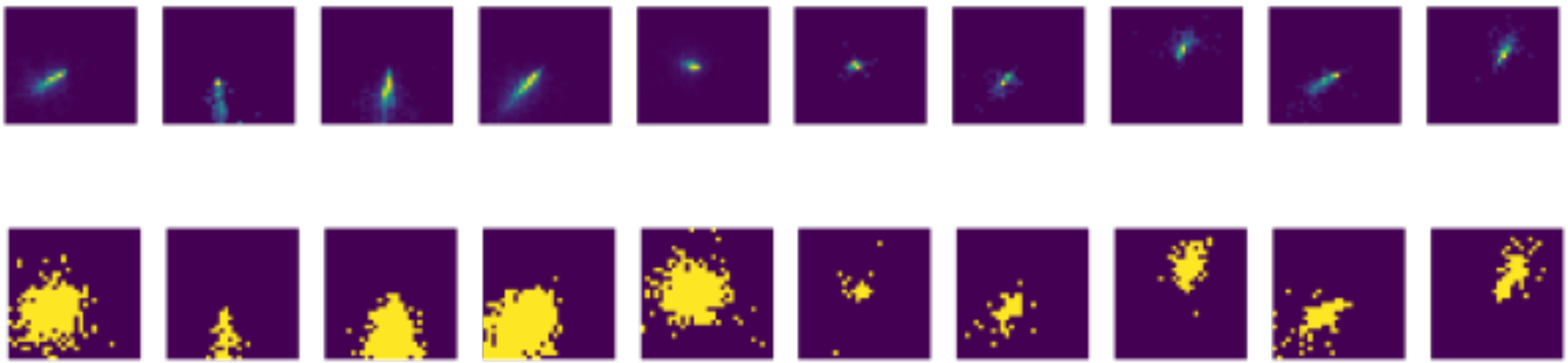
LHCb ECAL Fast Simulation: VAE



$$Loss = KL(N(\mu_{latent}, \sigma^2_{latent})||N(0,1)) + Logprob(X, (\mu, \sigma)) + Logprob(mask, b)$$

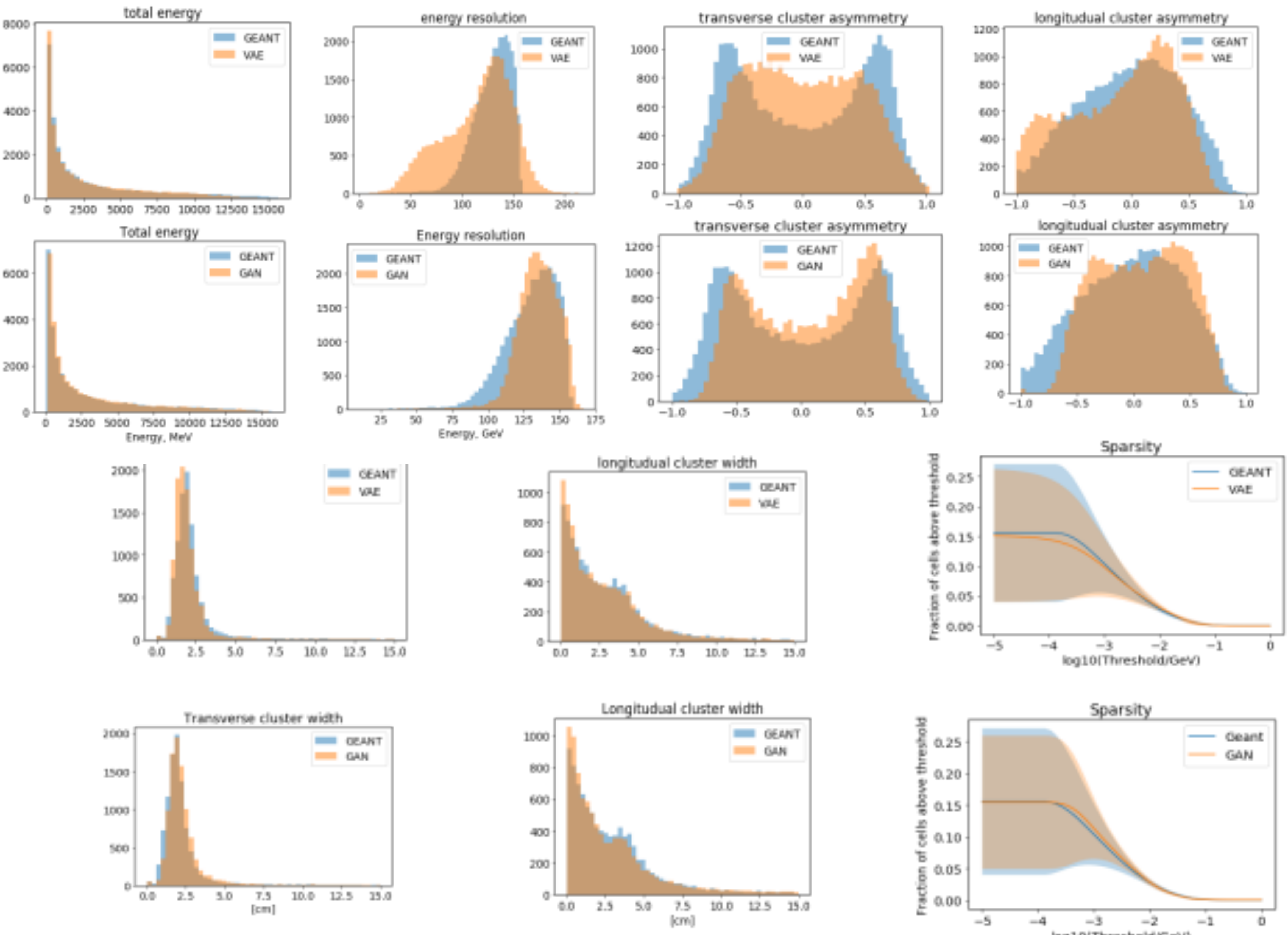
VAE in 5D

GEANT Simulated



VAE Simulated

ECAL Single Cluster Properties



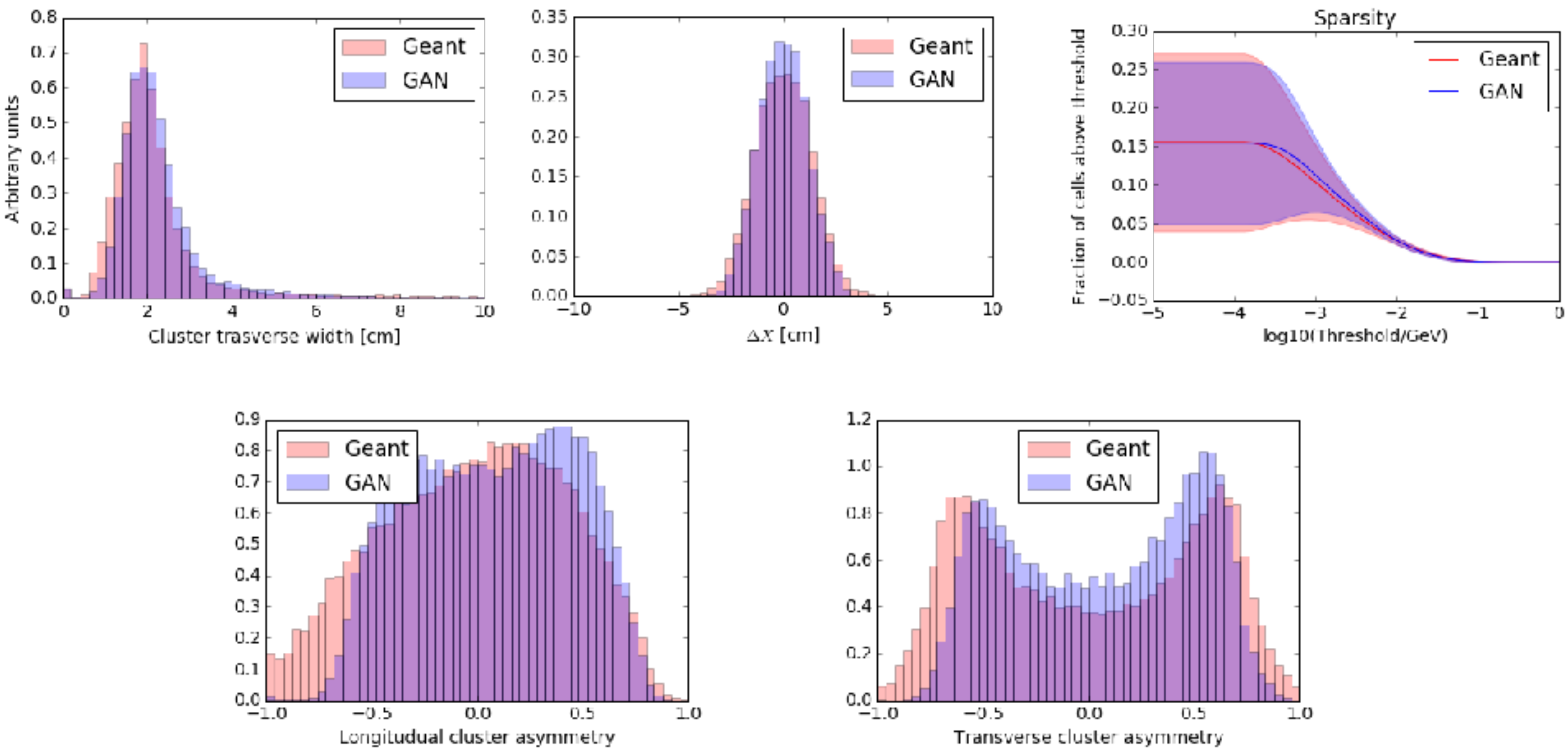
VAE

GAN

VAE

GAN

Primary and Marginal Distributions



- ◇ Is hard to fit marginal distributions
  - ◇ unless the model is aware that those are important for us

Natural Requirements

- For image generation we are usually happy if the result looks like it is desired
- In science we need the result to reasonably well match the given set of requirements. This target set is driven by scientific considerations to reach the ultimate scientific goal
  - e.g. we could want $E^2-p^2=m^2$ for generated particles
- Explicit control to satisfy requirements is preferable
  - e.g. exclude E from generated features, set it explicitly from generated p

Enforcing Important Statistics

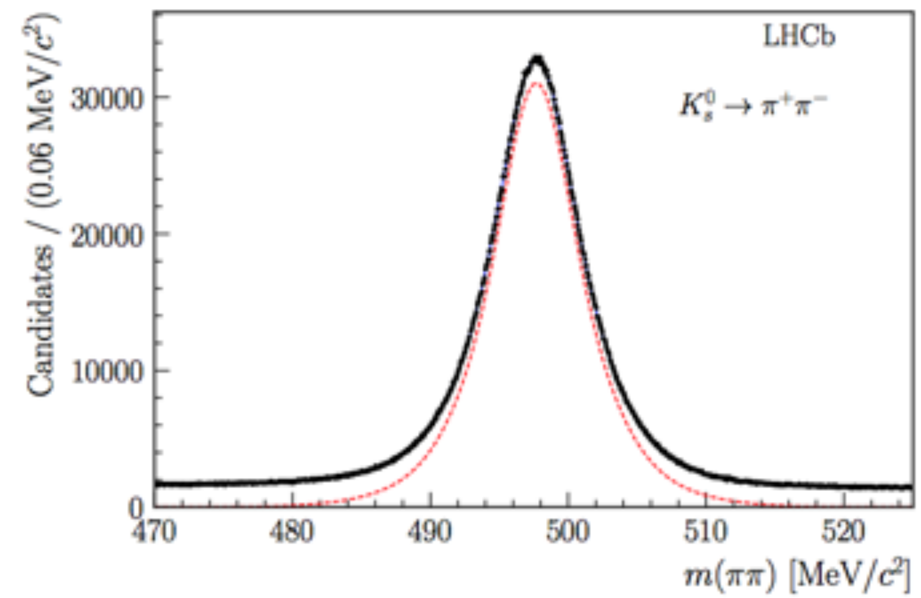
- No generative model is ideal
  - some deviations from the original distribution remain
- Model tends to learn primary statistics of generated objects
- In physics applications we mostly need our model to learn some particular statistics which may be marginal to the generated object
  - e.g. cluster shape fluctuations for fast calorimeter simulation
- Can enforce these statistics by explicit adding them to the los
  - can’t we?

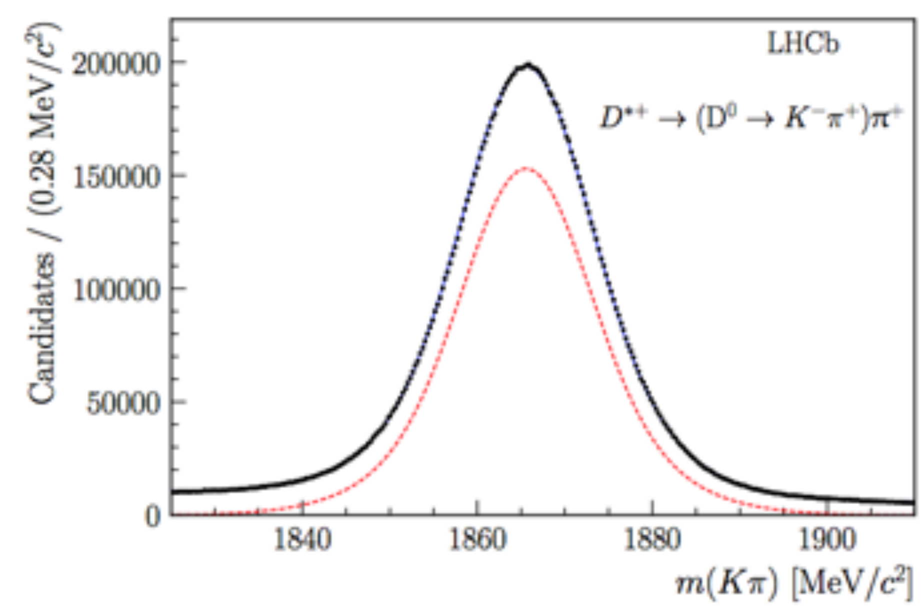
Enforcing Important statistics

- Can enforce statistics by explicit adding them to the los
  - can't we?
- By adding statistics into the loss we do enforce match for these statistics
  - most likely by the price of overtraining these particular statistics
    - … and we lose handle to validate quality of generator on this statistics
- Still can remove those statistics from loss, and see how far they would deviate
  - figure of merit for generating this statistics

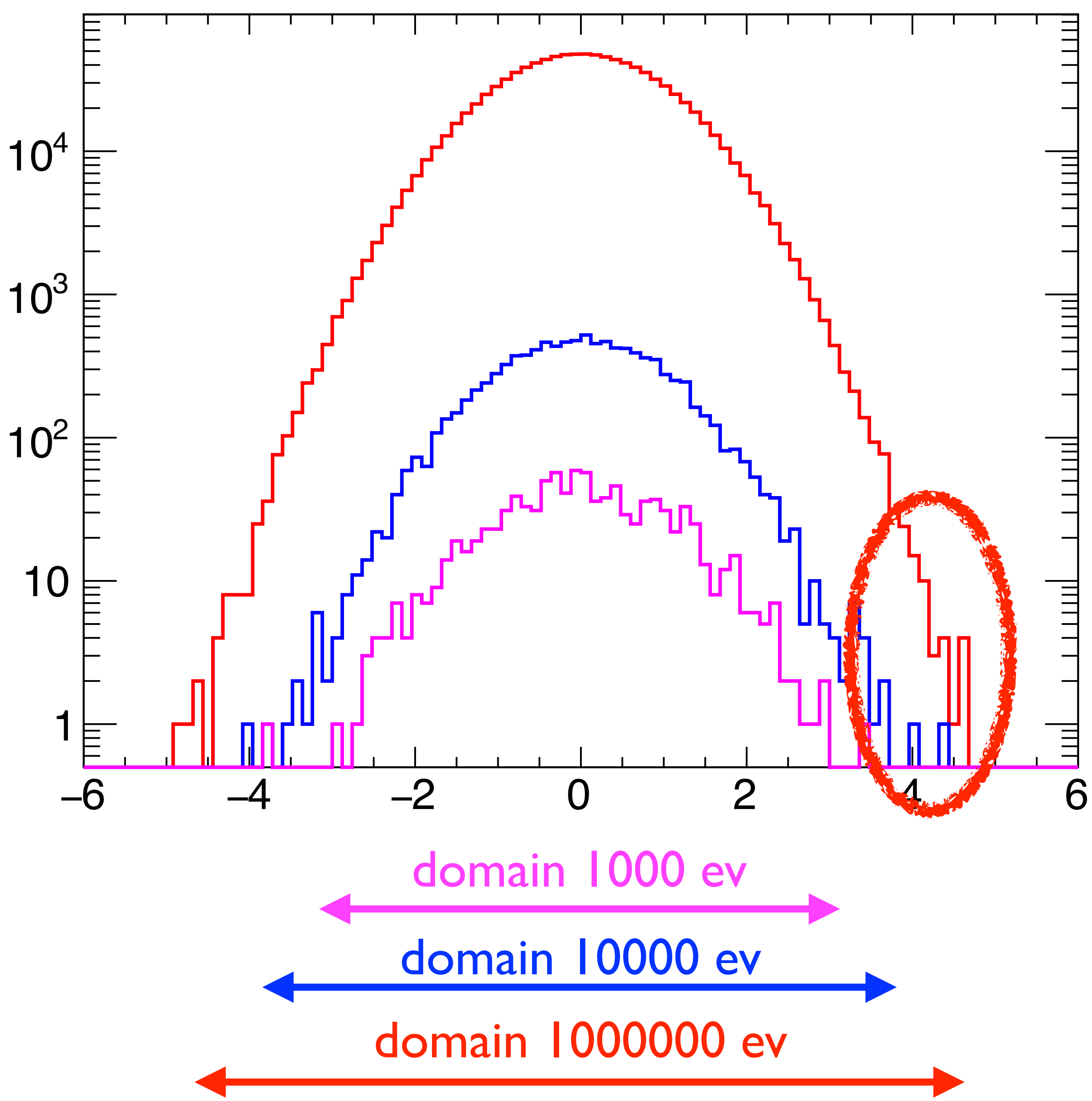
Generative Models Trained on Real Data

- Real data samples, even calibration, are never 100% clean
  - contamination from events with different labels/conditions
- Can not determine label of particular object uniquely
  - however can statistically determine fractions of different labels
- Can use weighted samples to train WGAN and CramerGAN





Completeness



- Domain for the generative model is driven by the training sample
  - model can not extend beyond the train domain even if produces high statistics
    - until explicitly set to behave beyond train domain

Decomposition

- Quality of the generative models is limited by the size of the train data sample
  - generative models may not give profit for producing statistically correct big data sets
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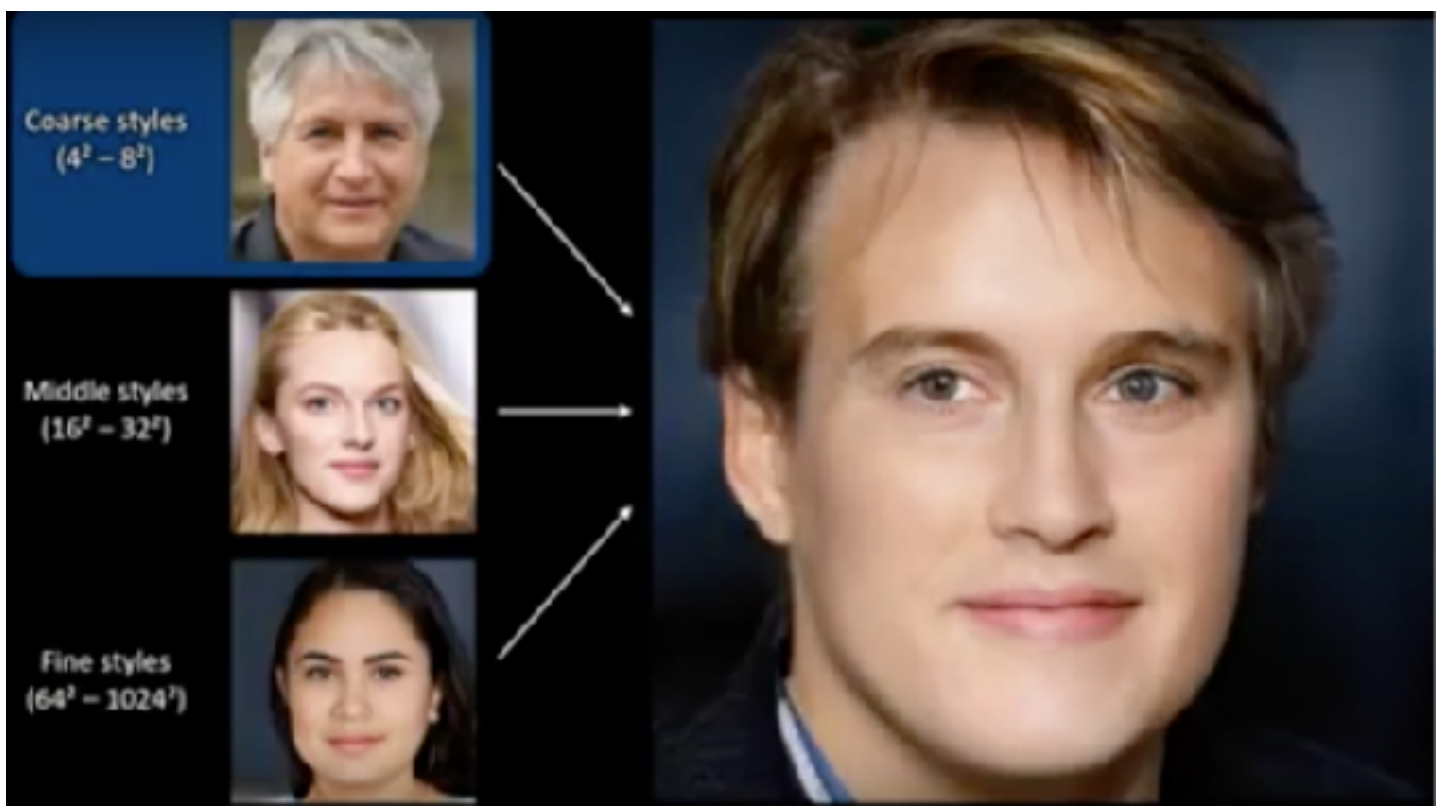

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  - random combinations of different components may drastically increase variativity

Decomposition

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- Not quite if we can decompose generative model into separate components
  - random combinations of different components may drastically increase variativity
- E.g. fast simulation of the calorimeter response
  - generator is trained on 10^6 incident particles
  - $\sim$50 particles in the calorimeter per event
  - total variativity $\sim(10^6)^{50} = 10^{300}$!

Quality Metric

- No generative model is ideal
  - some deviations from the original distribution remain
- Minor deviations are not that important e.g. for image generation
- Minor deviations may be a big deal for physics generative models
  - e.g. we could want $E^2 - p^2 = m^2$ for generated particles to be precise
- Ultimate generative model quality metric is comparing final physics result obtained using generative model, and the one obtained using train data
  - accuracy is limited by the size of the train data

Conclusions

- Surrogate generative models demonstrate extraordinary progress in current years
- Fast simulation for LHC detectors in Run 3 is a natural target
  - fast simulation of calorimeters is a primary target
- Generative models need attention ensure scientifically solid results
  - completeness of generated sample
  - satisfying boundary conditions, control of scientifically important but marginal statistics
  - evaluating quality of the model, propagate model imperfections to systematic uncertainties of the final scientific result
- We developing different approaches for fast generation of calorimeters in LHCb
  - results look promising, but not production quality yet