DeGeSim – Pileup Modelling using AI

10-11-23

Stephen Jiggins - DESY

Brief

Problem:

Pileup from multiple proton interactions currently miss-model data. This trend worsens with the number of interactions per bunch crossing leading to an explosive issue moving towards the HL-LHC:

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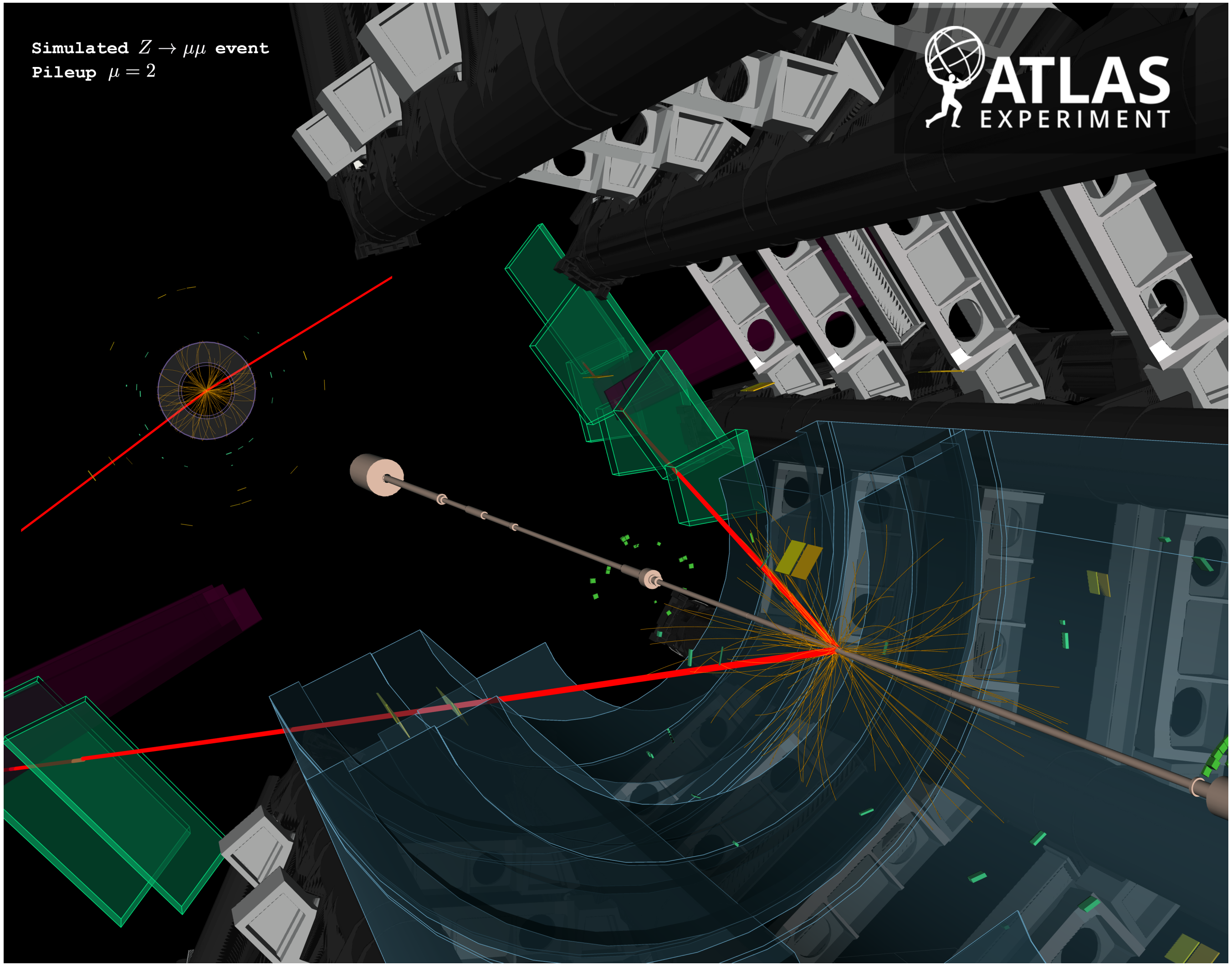

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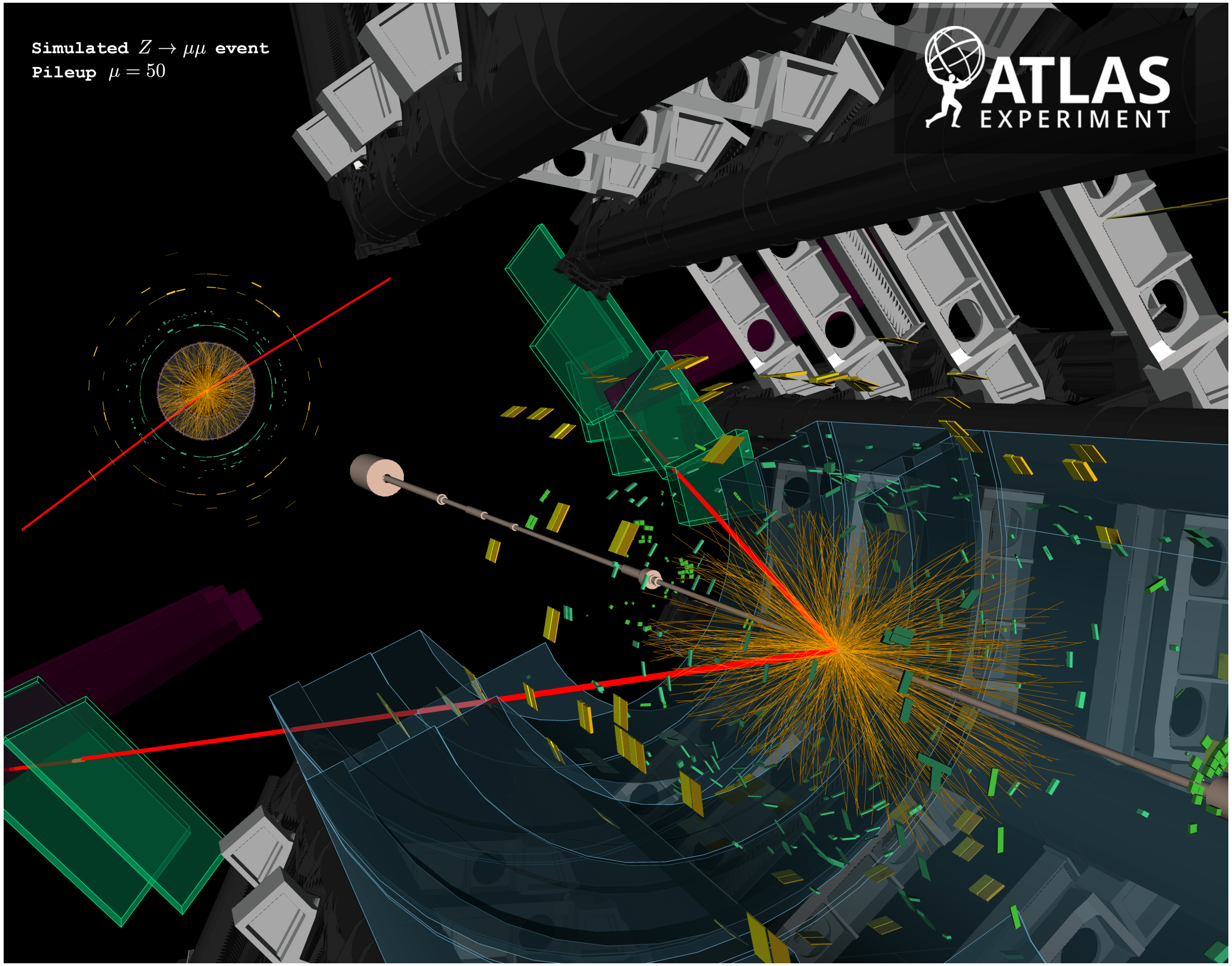

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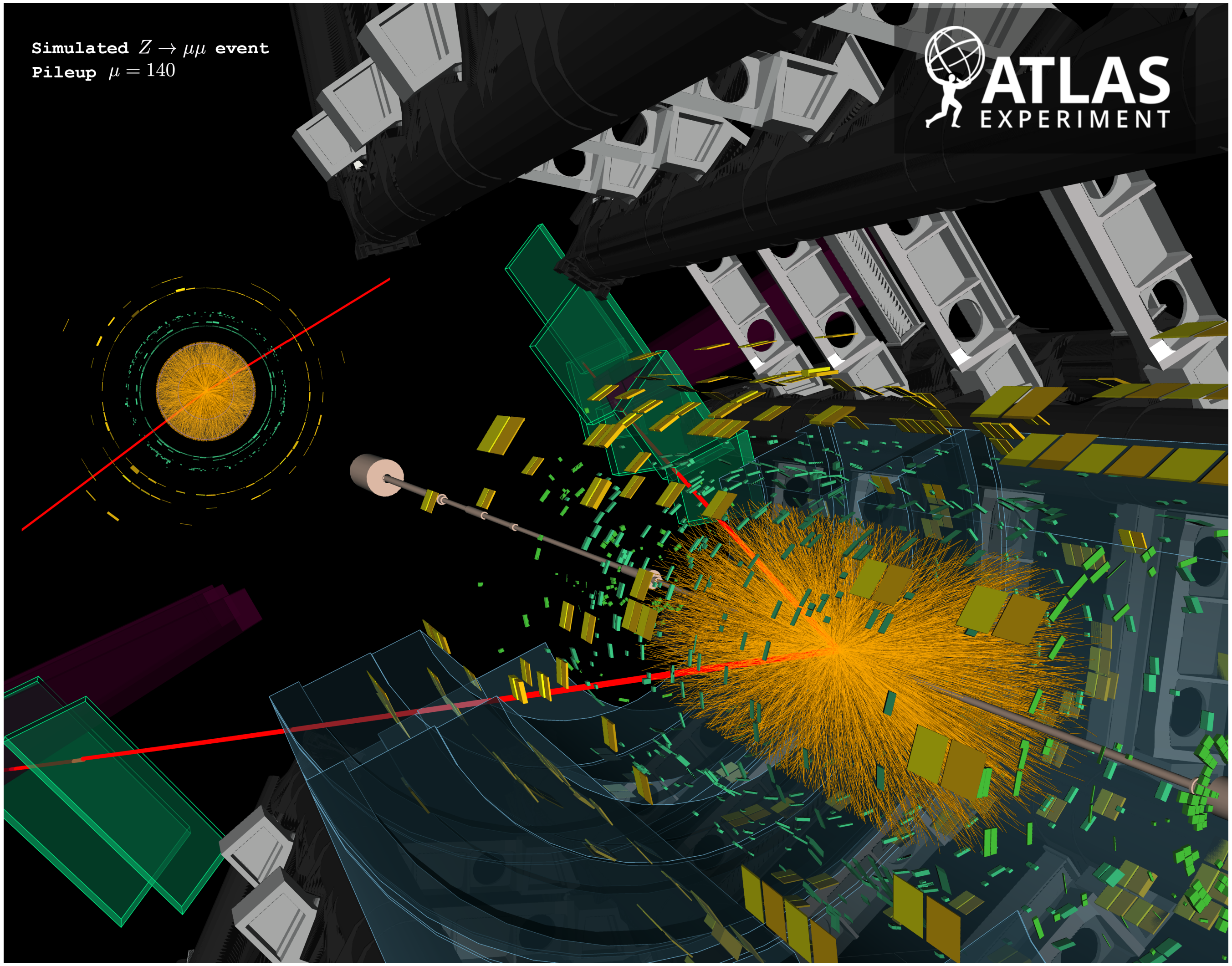

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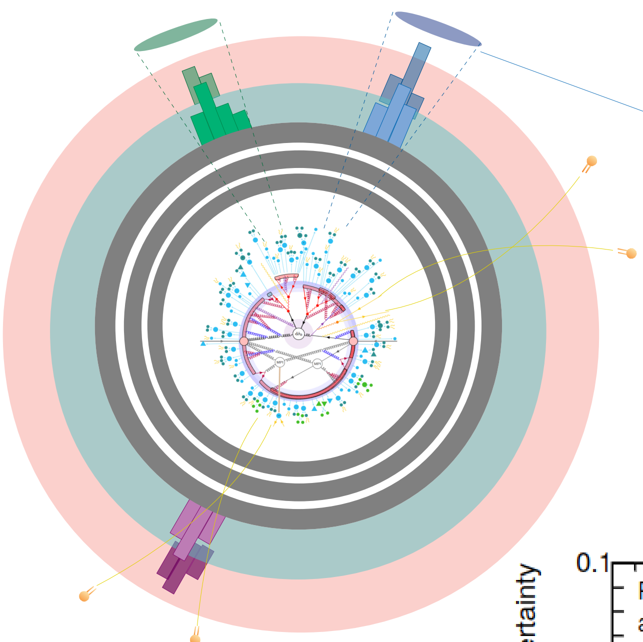
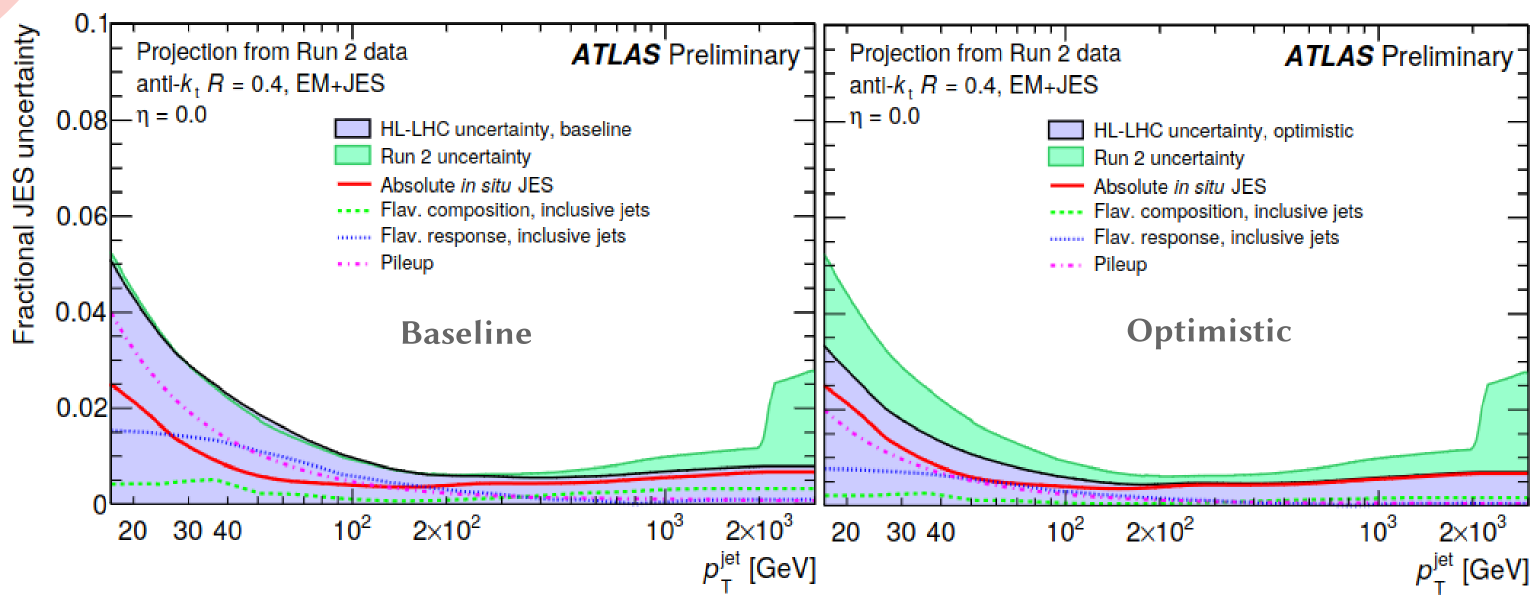


⟶ HL-LHC jet performance projections for ATLAS 1902.10229:

Baseline ~ Run-2

Optimistic: Requires improved understanding of jet fragmentation & pile-up



Source: 1902.10229

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Project Aim:
Generative modelling of pileup interactions using zero-bias data instead of MC simulations using ML image synthesis techniques

DeGeSim:
Helmholtz AI funded project for simulating detector simulations in proton-proton colliders using deep generative ML models as joint project with CMS + Juelich + TRIUMF:

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ATLAS (DESY)


CMS (DESY)



Juelich

TRIUMF

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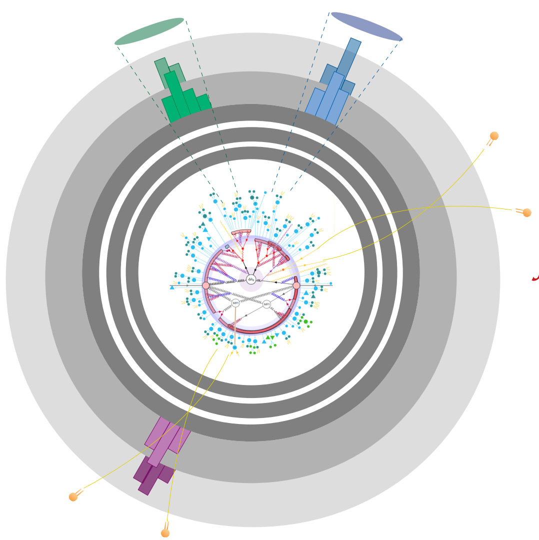
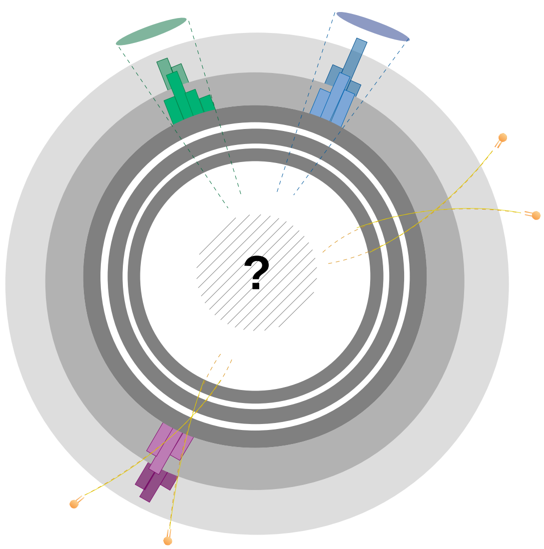
Monte Carlo (MC)

EPOS+Pythia8 simulated
soft-QCD



$f\colon \boldsymbol{X}_{MC} \longrightarrow \boldsymbol{X}_{D}$

Zero-Bias Data



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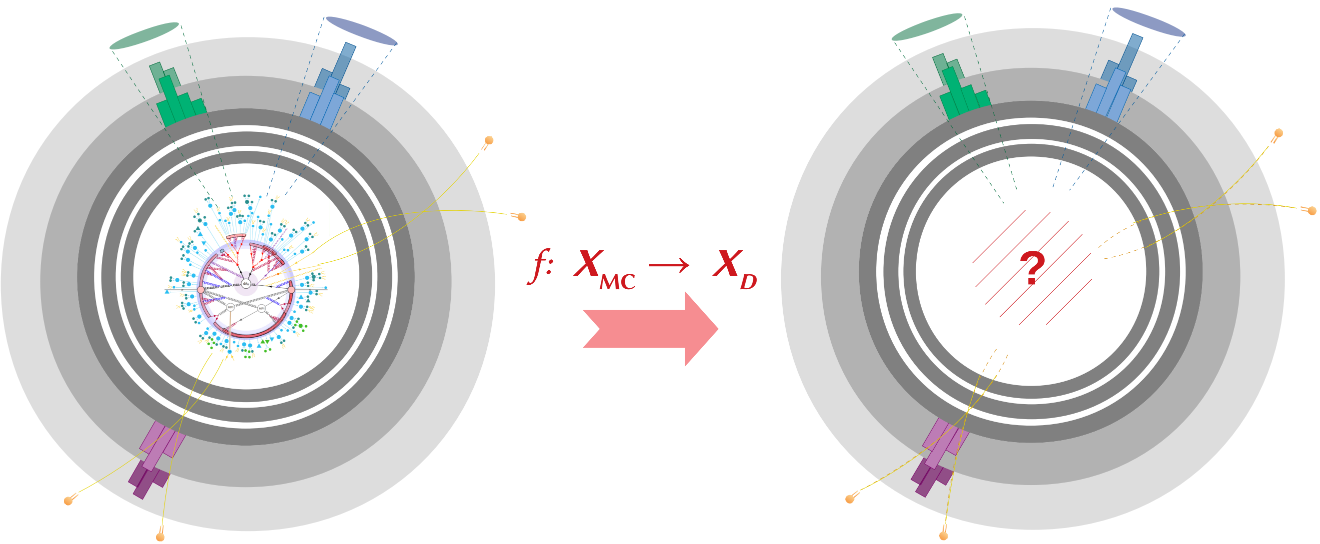

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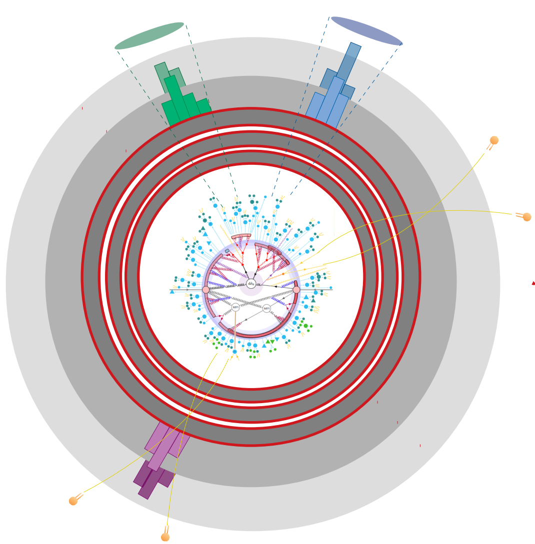

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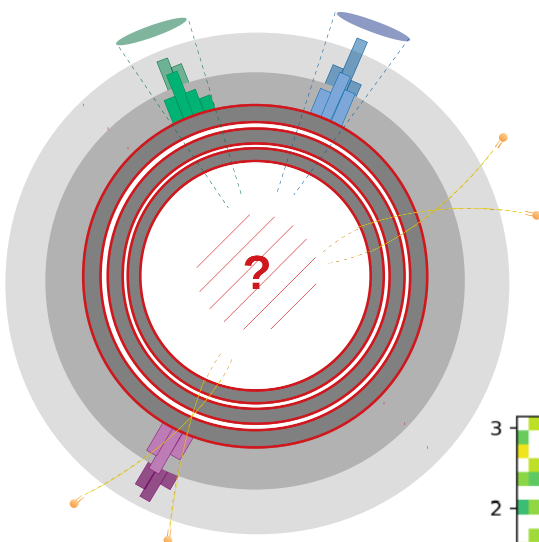

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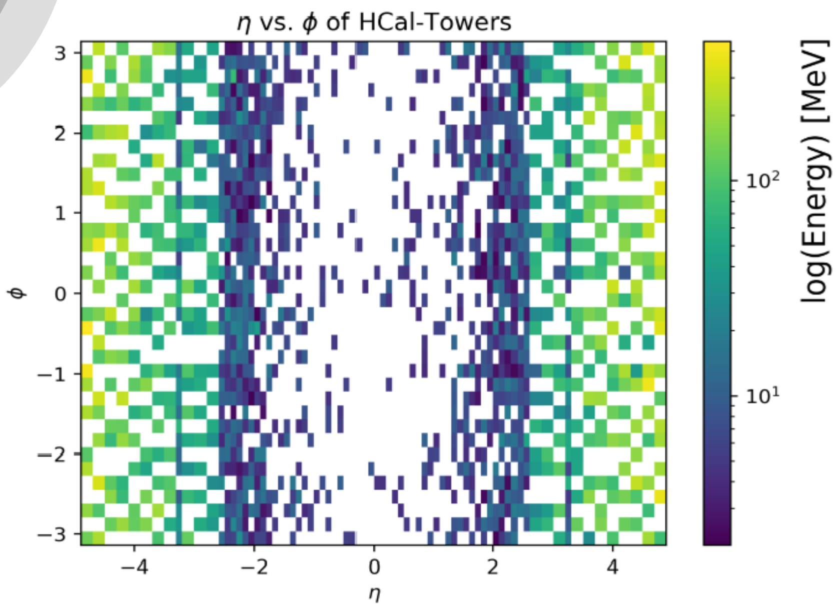

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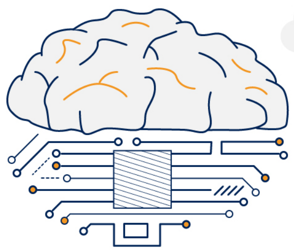

Which model?

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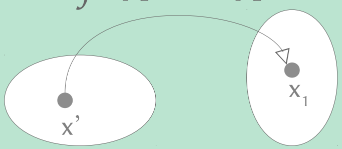
ATLAS (DESY)

Fully Generative

*Sample from a known function $P_s(\overline{x}' \,|\, \overline{\theta})$ to get **X'** and then find a transformation from **X'** to **X**:*

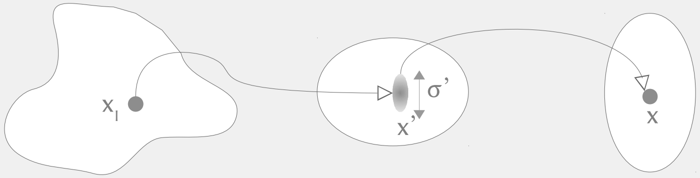
$$f\colon \boldsymbol{X'} \rightarrow \boldsymbol{X}$$



Seeded Generative

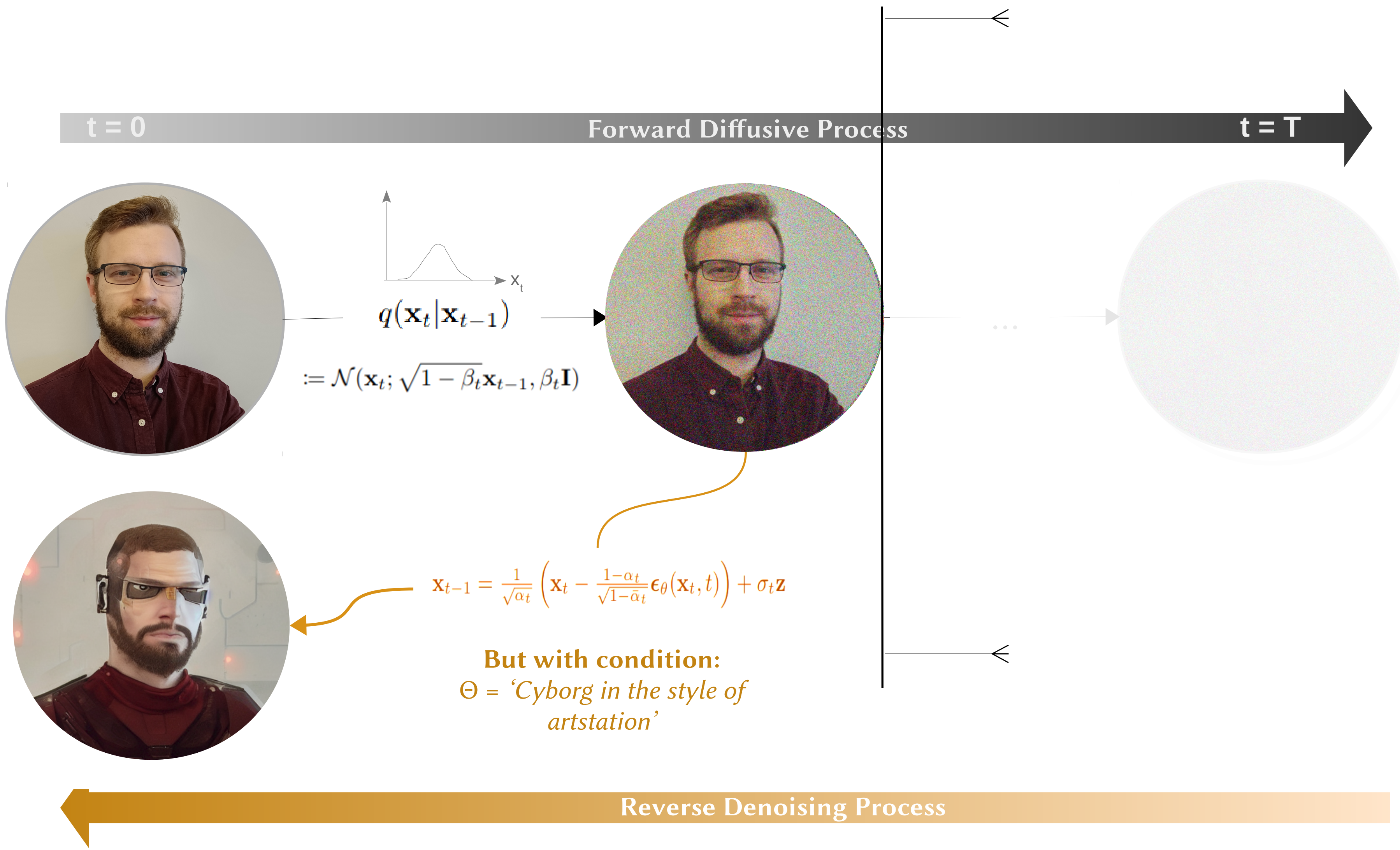
*Transform from a sampled point $\boldsymbol{X_I}$ of a complex function $P_I(\overline{x} \,|\, \overline{\theta})$ and find a transformation from $\boldsymbol{X_I}$ to **X**:*

$$f\colon \boldsymbol{X_I} \rightarrow \boldsymbol{X}$$



Denoising Diffusion Probabilistic Models

Generative DDPM



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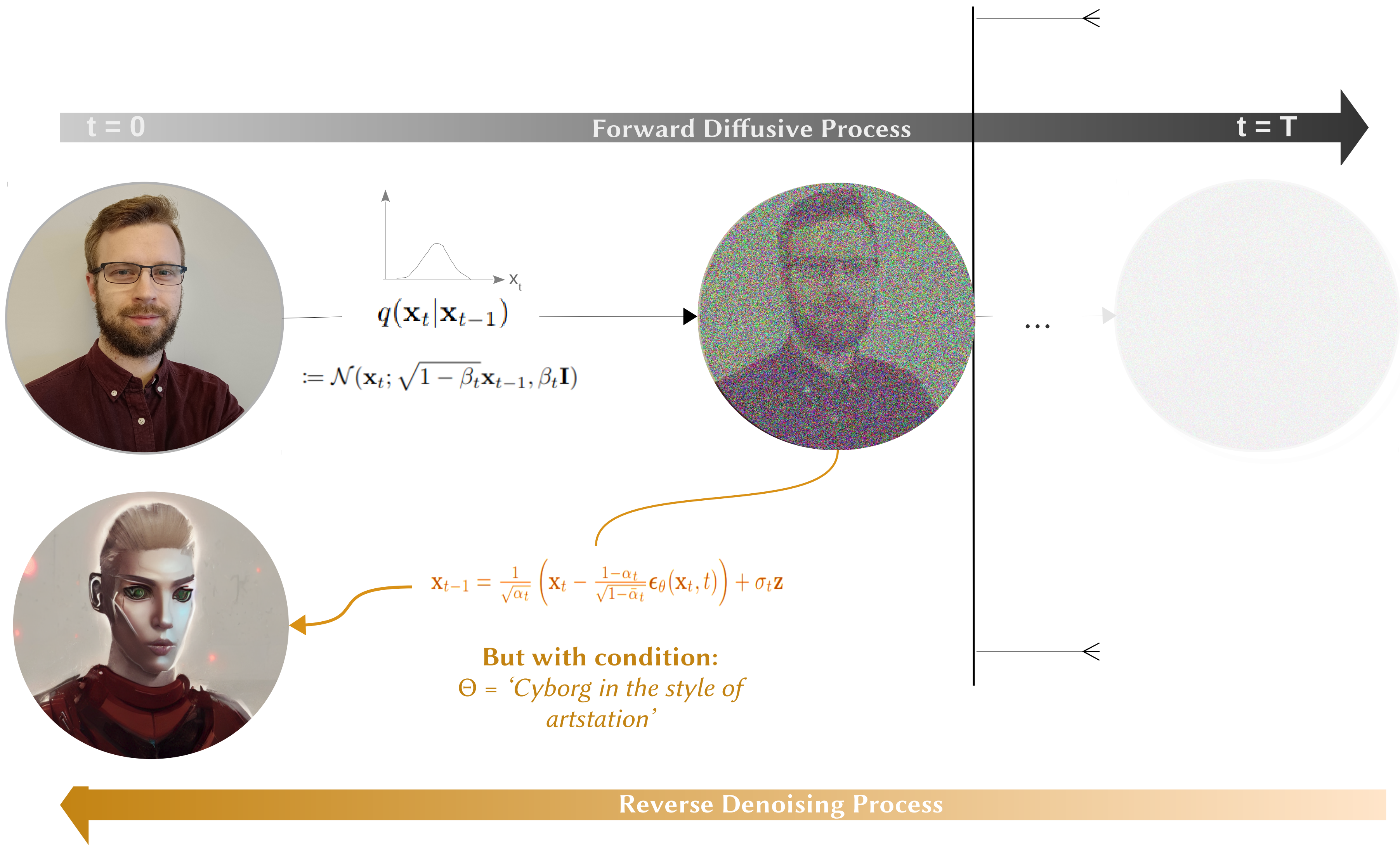

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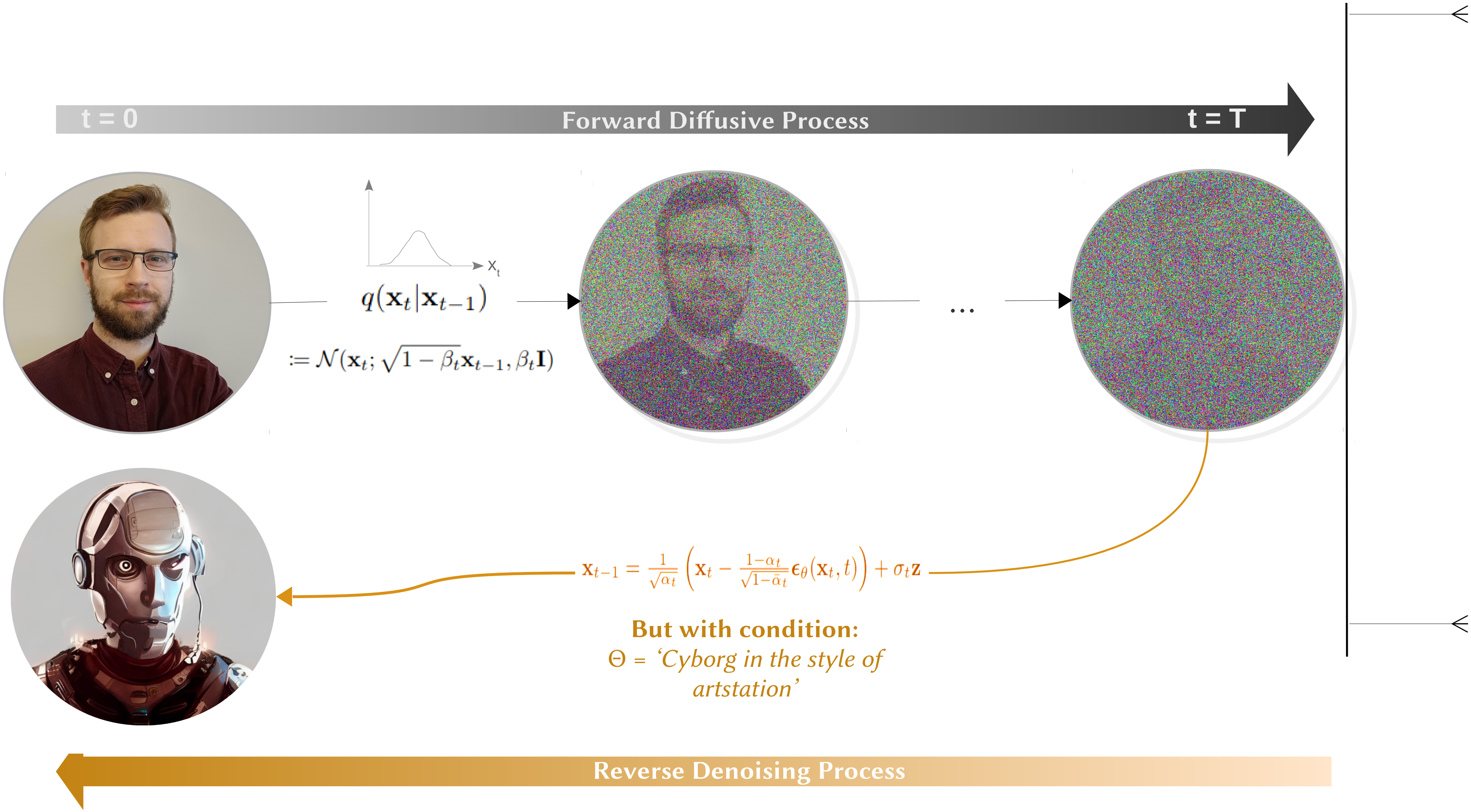

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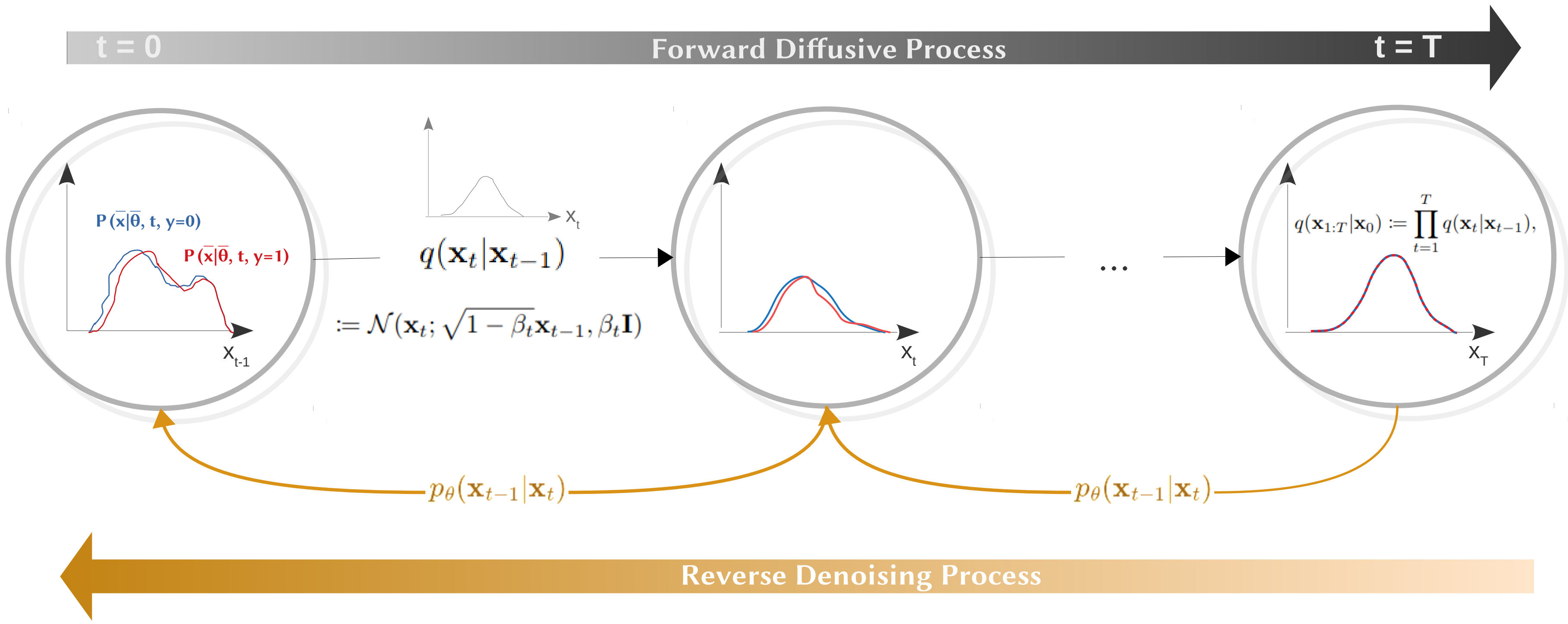

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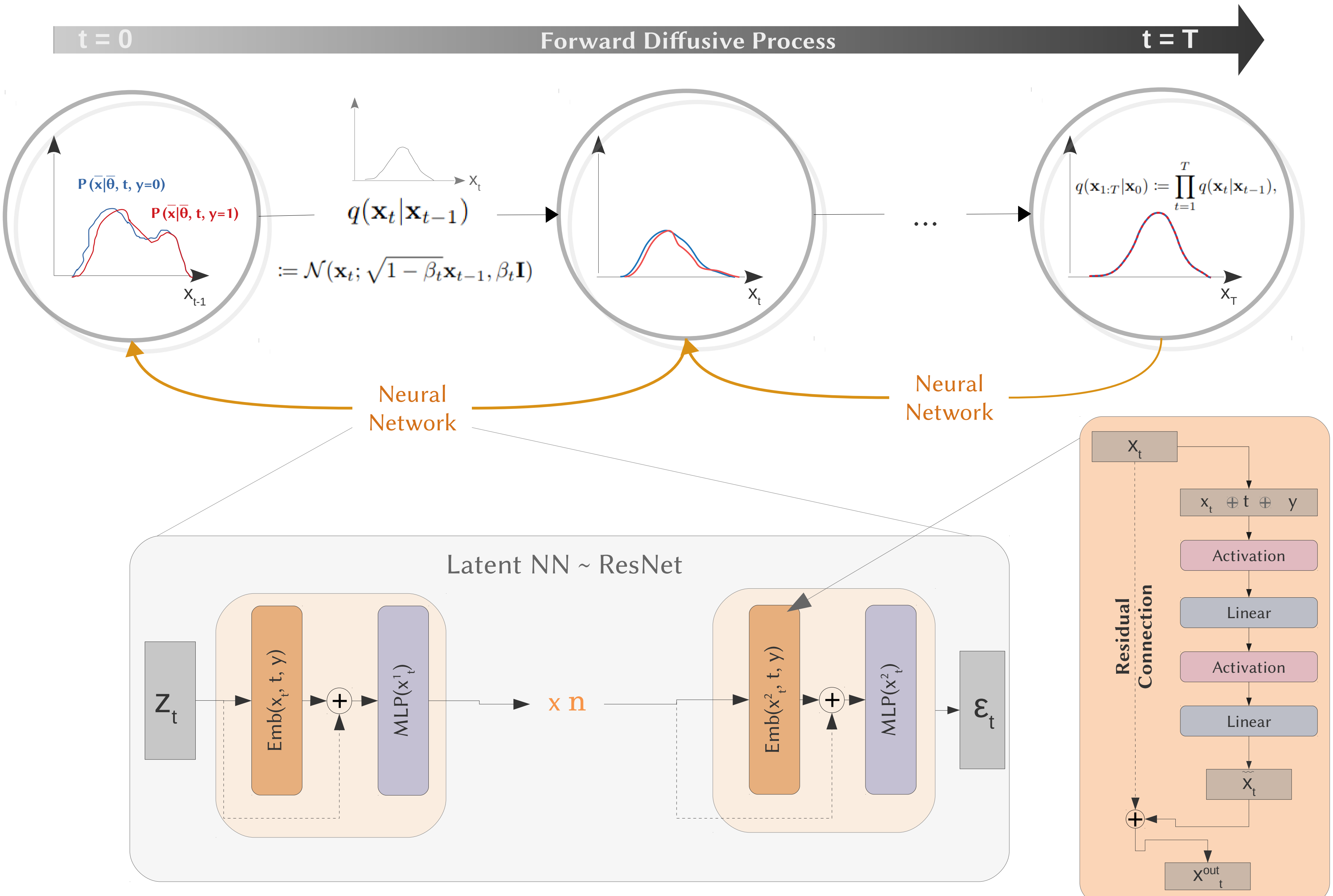
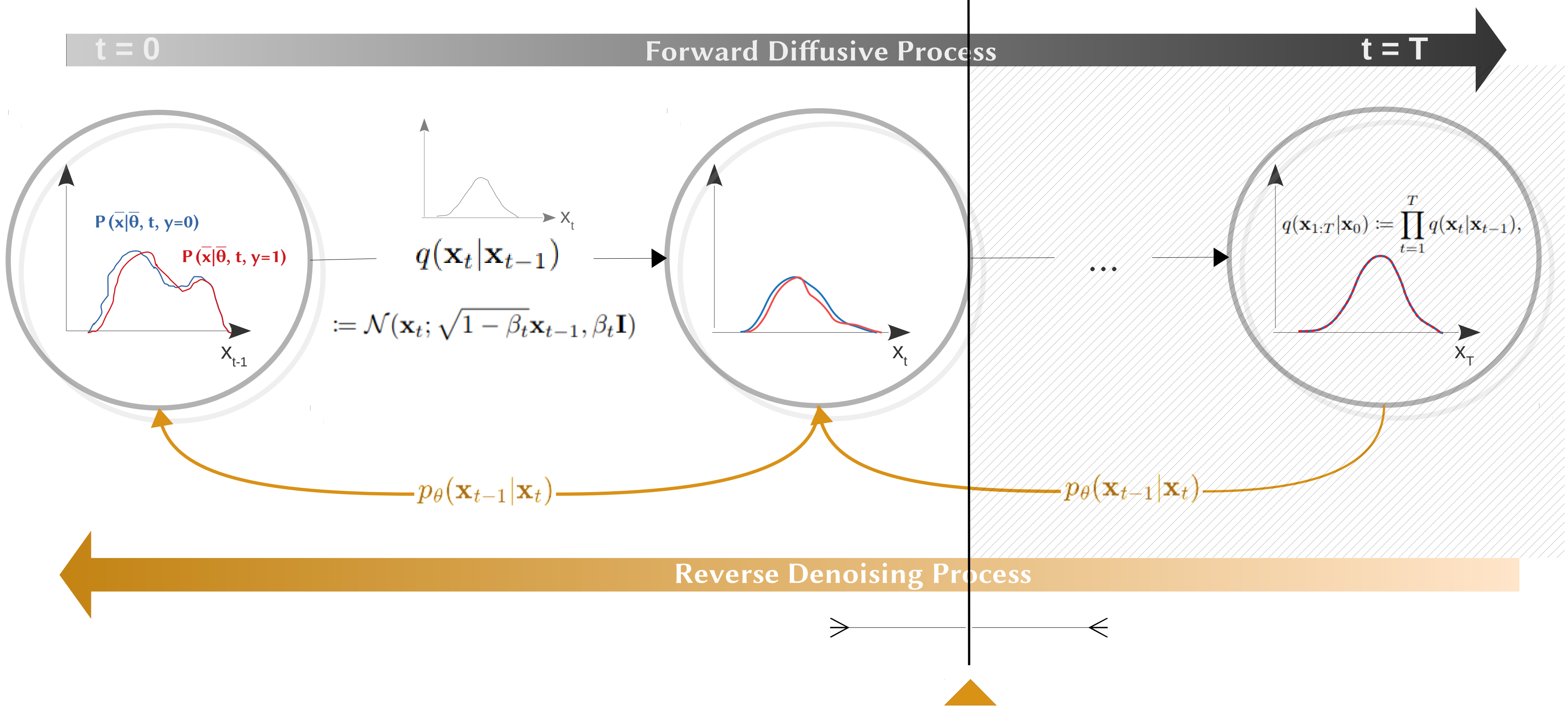


Generative DDPM

Partially diffuse the image to retain features from the original image!

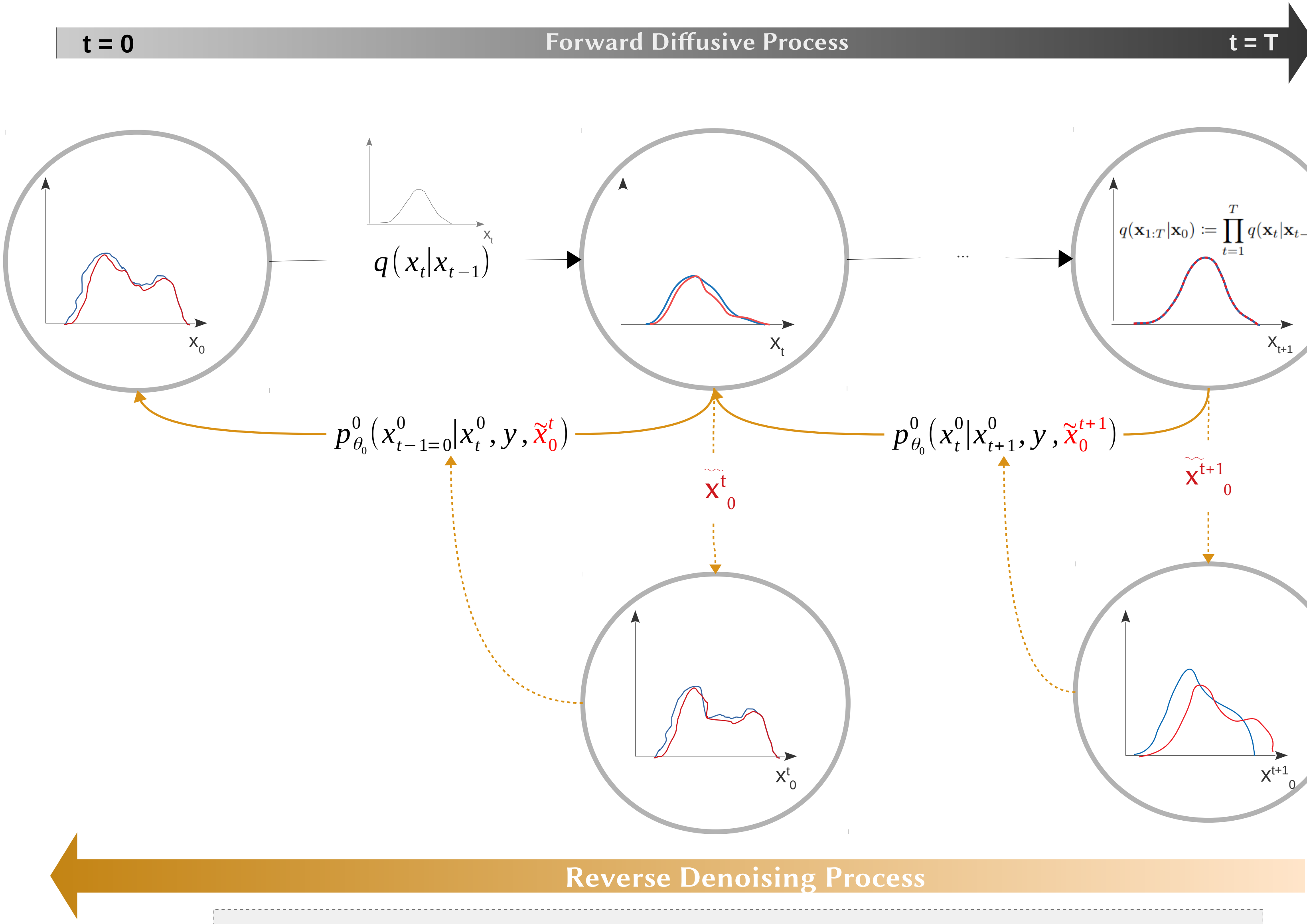
Stop the diffusive process when the two processes are **indistinguishable**



Approach 1

Train a conditional DDPM and partially diffuse a sample to a *release time* **t_r**. Then switch class label ($0 \longrightarrow 1$) and denoise.

Self-Conditioned DDPM



Approach 2

Train a conditional DDPM with concatenated predictions of the origin $\tilde{x}_0$ and partially diffuse a sample to a *release time* **t_r**. Then switch class label ($0 \longrightarrow 1$) and denoise.

JetNet Data Test

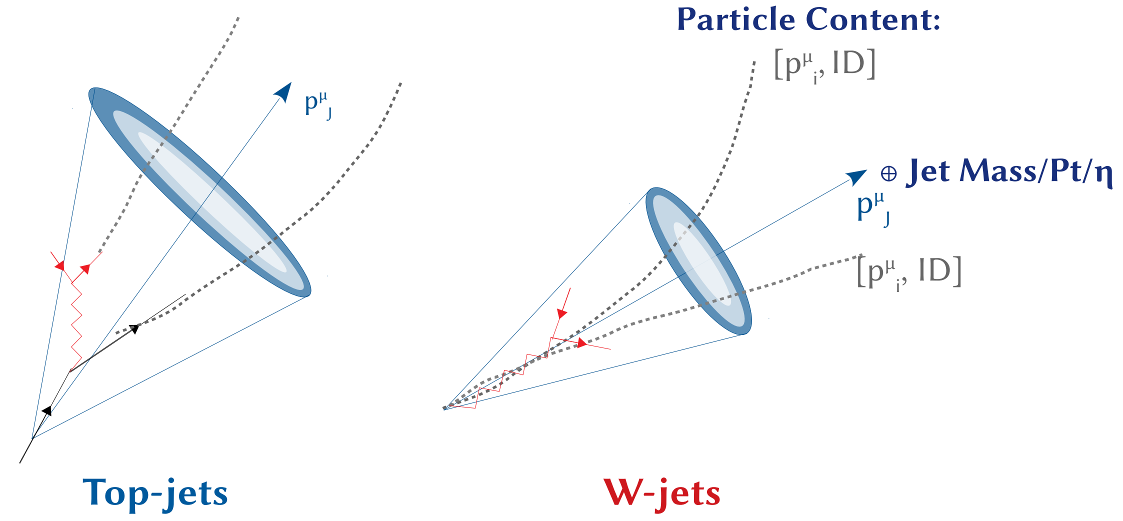
JetNet: Top -vs- W jets

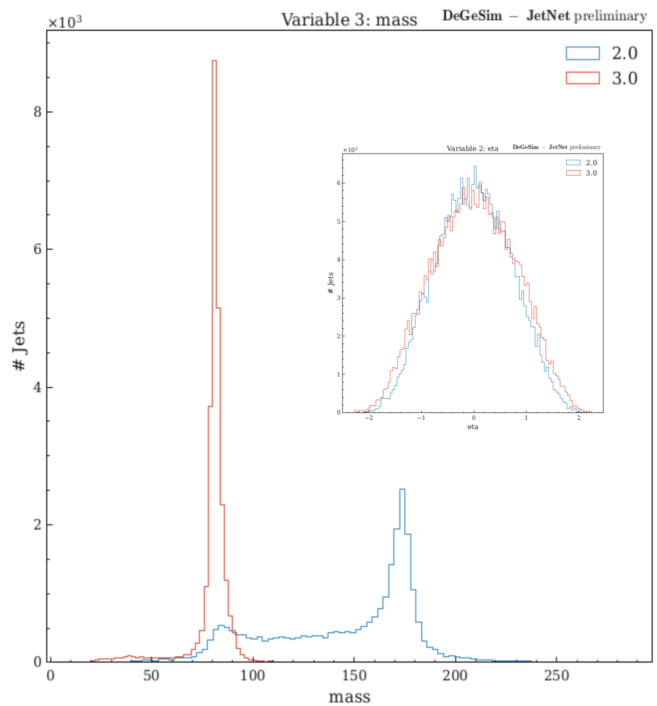
Data - JetNet

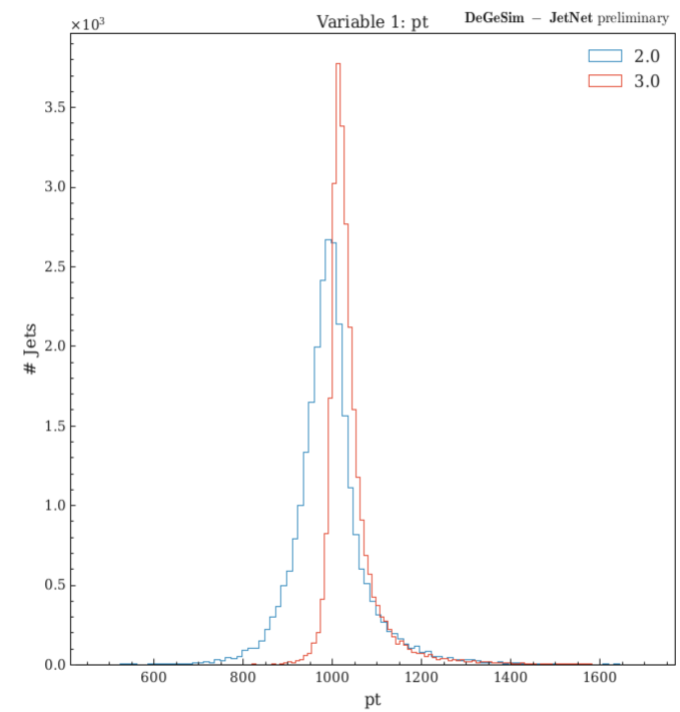
→ **Test using top vs W-jets**
W-jets are a sub-component of top-jets from the top-decay

→ **Implemented using JetNet Python API** - link

→ **Diffusion Model input domain defined by jet features & b-hadrons:**
- $p^\mu_J = [p_T, \eta, m_J]$
- *# of b-hadrons inside jet*







Results

JetNet: Top -vs- W jets

Key

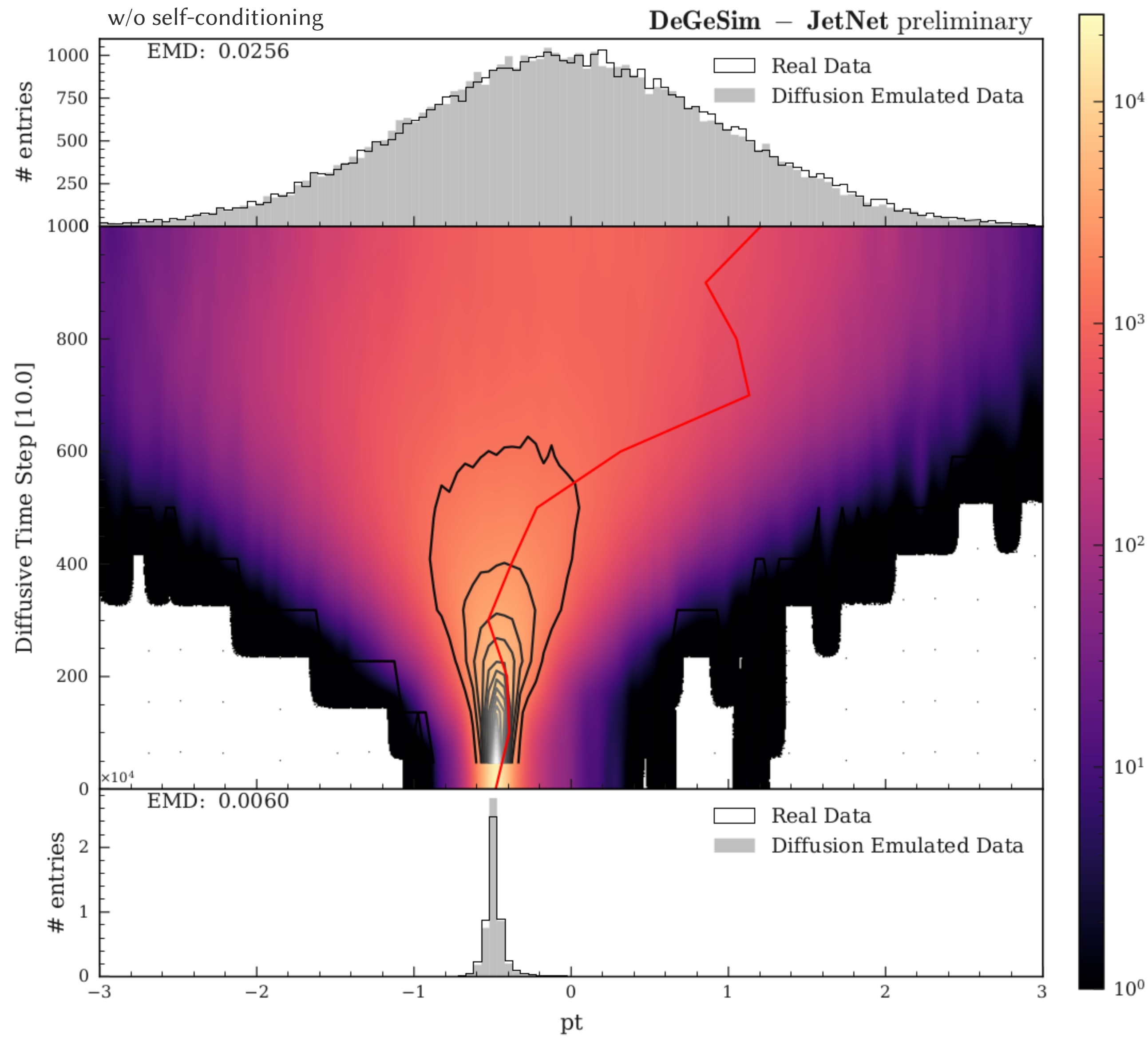
⟶ **Top Pane:** Gaussian emulated (Gen.) sampling with forward diffused *real data*

⟶ **Middle Pane:** Time evolution of emulated (generative) data $p_\theta(x_{t-1}|\ y,\ x_t)$ for time each 10th time step:

Black contours = equal probability
Red line = random event path

⟶ **Bottom Pane:** Real data vs diffusion emulated data from a guassian prior (top pane).

⟶ **Metrics:** Wasserstein distance in 1D projection



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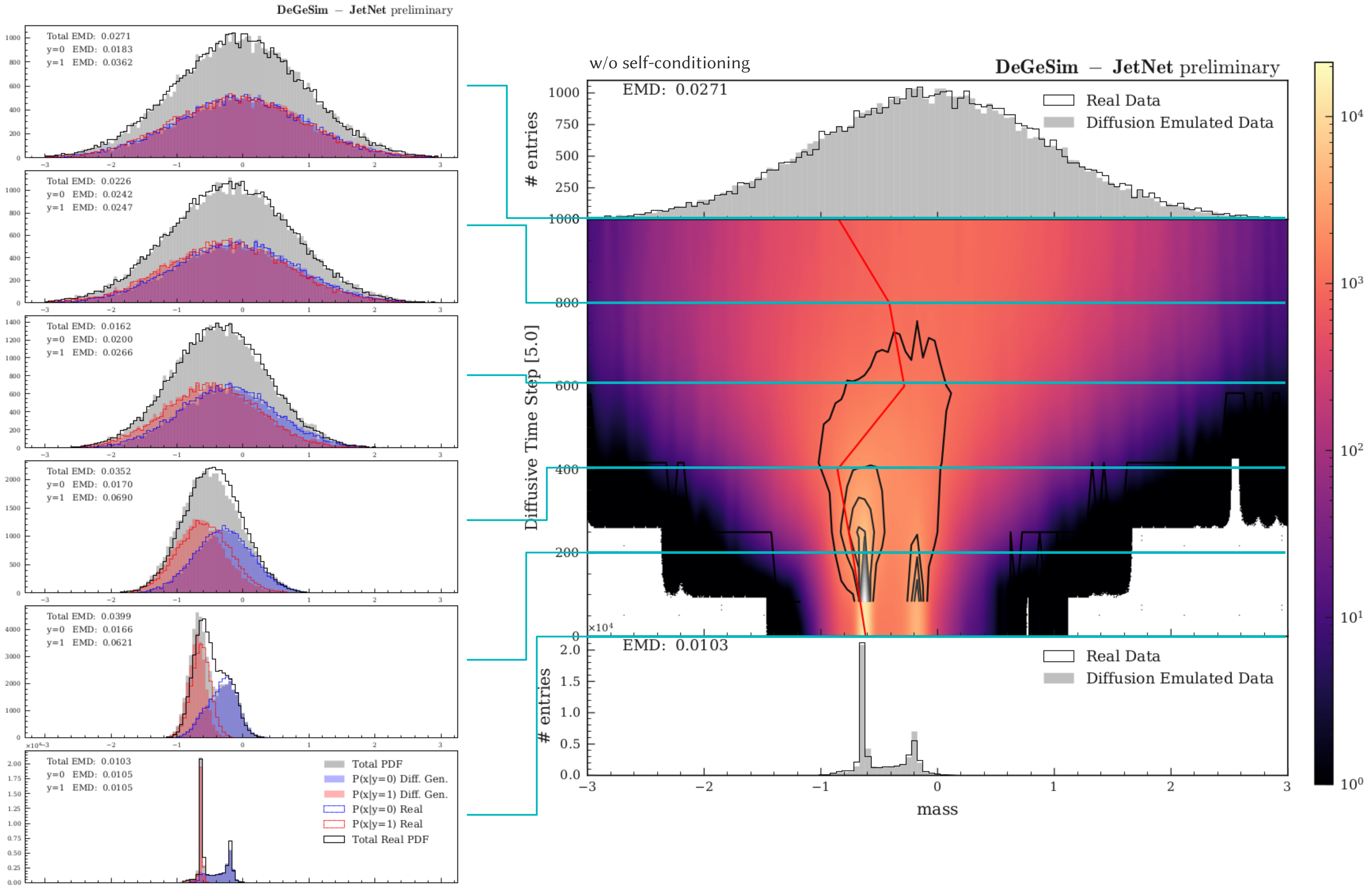

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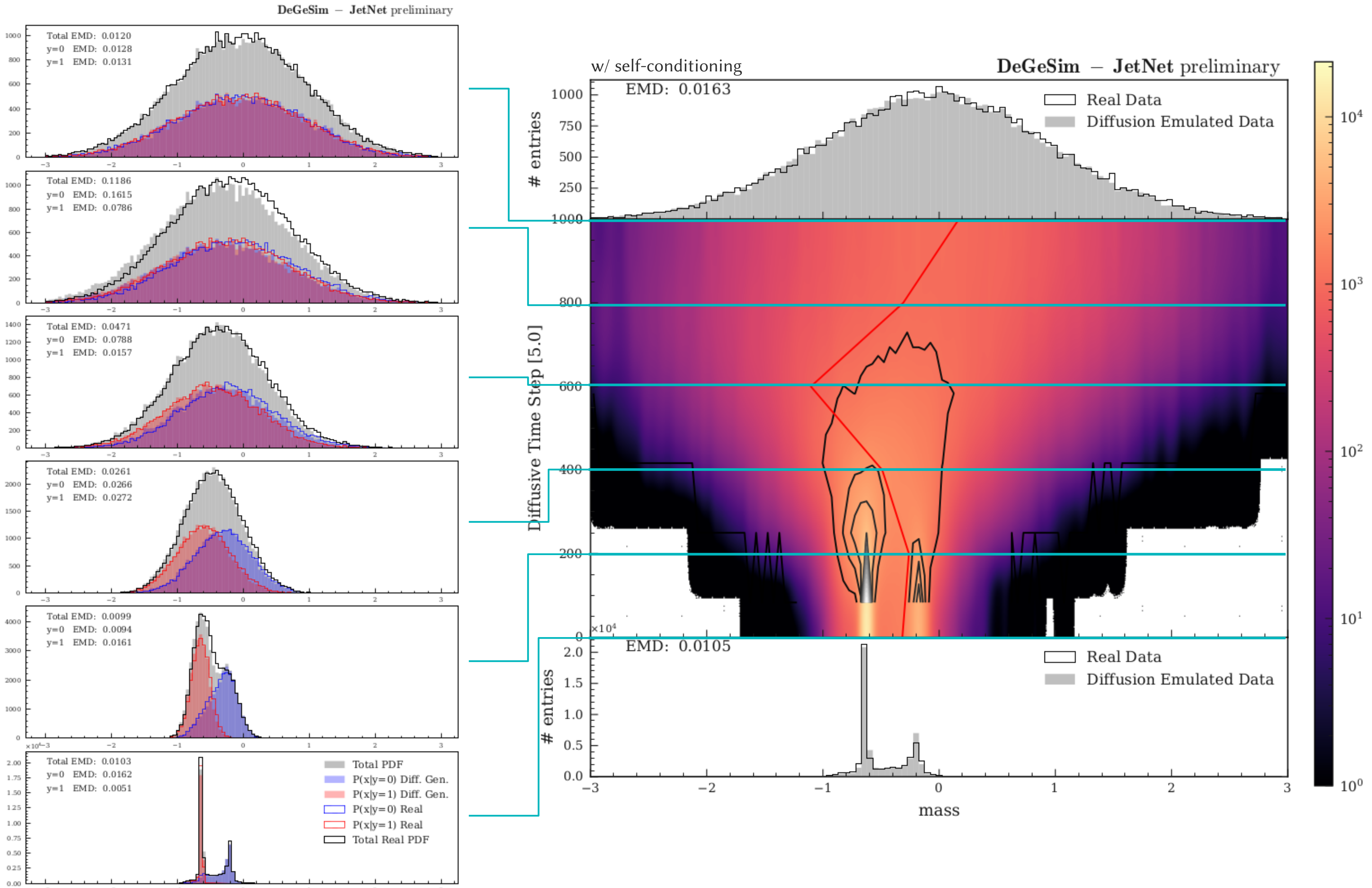

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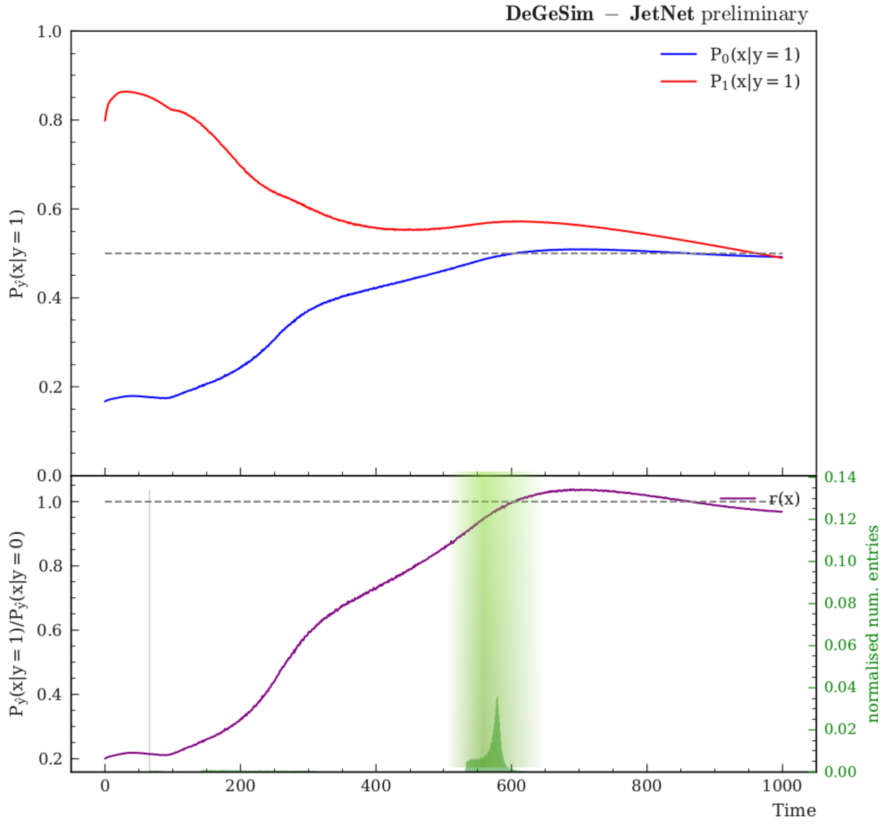
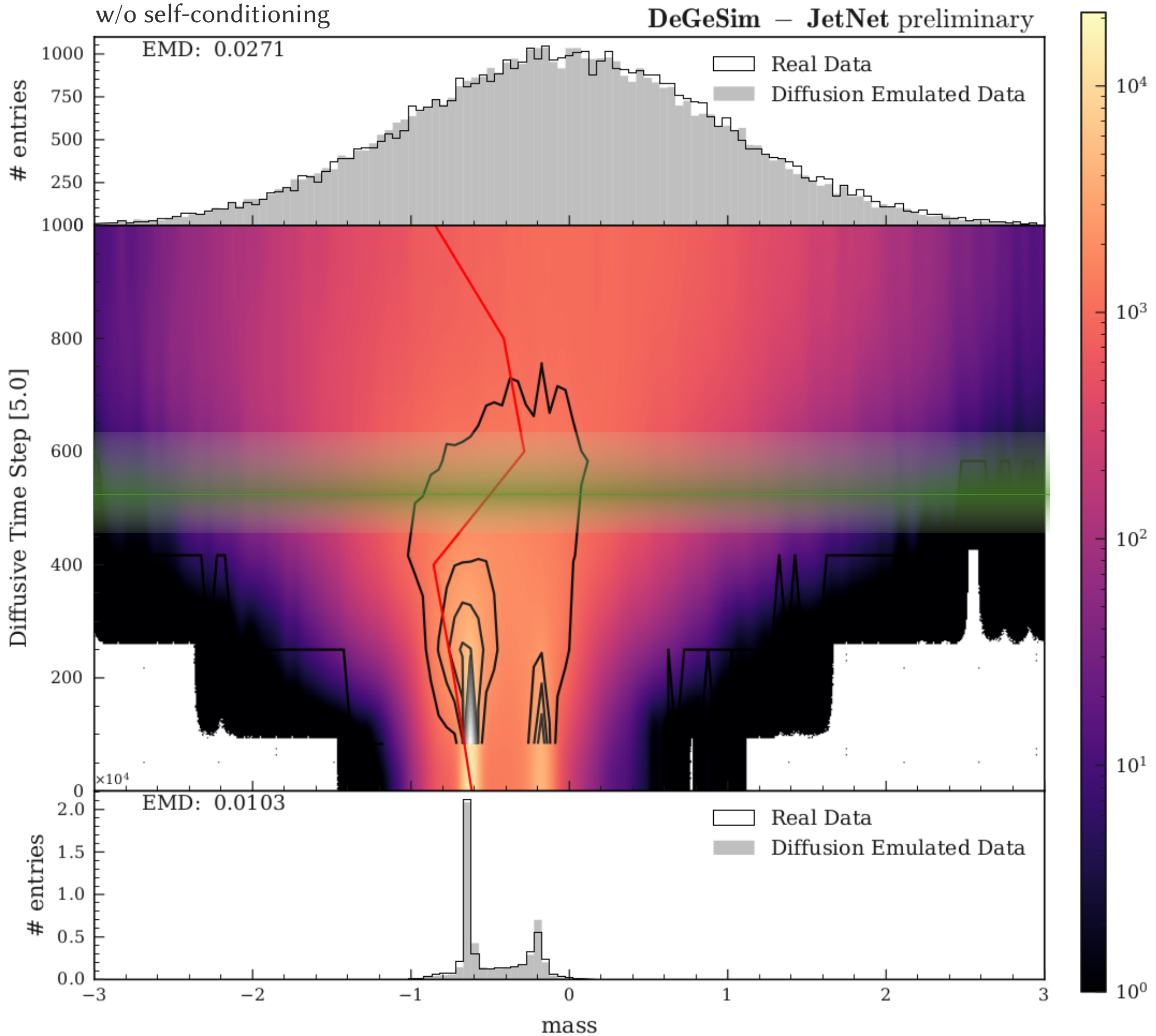


→ The classification neural network approximates the classifier s(x):

$$s(x,t)=\frac{P(y=1|x,t)}{P(y=0|x,t)+P(y=1|x,t)}$$

→ When the densities are equivalent we define the *release time* of each event/data point

$$r(x,t_{release})=\frac{s(x,t_{release})}{1-s(x,t_{release})}\approx 1$$



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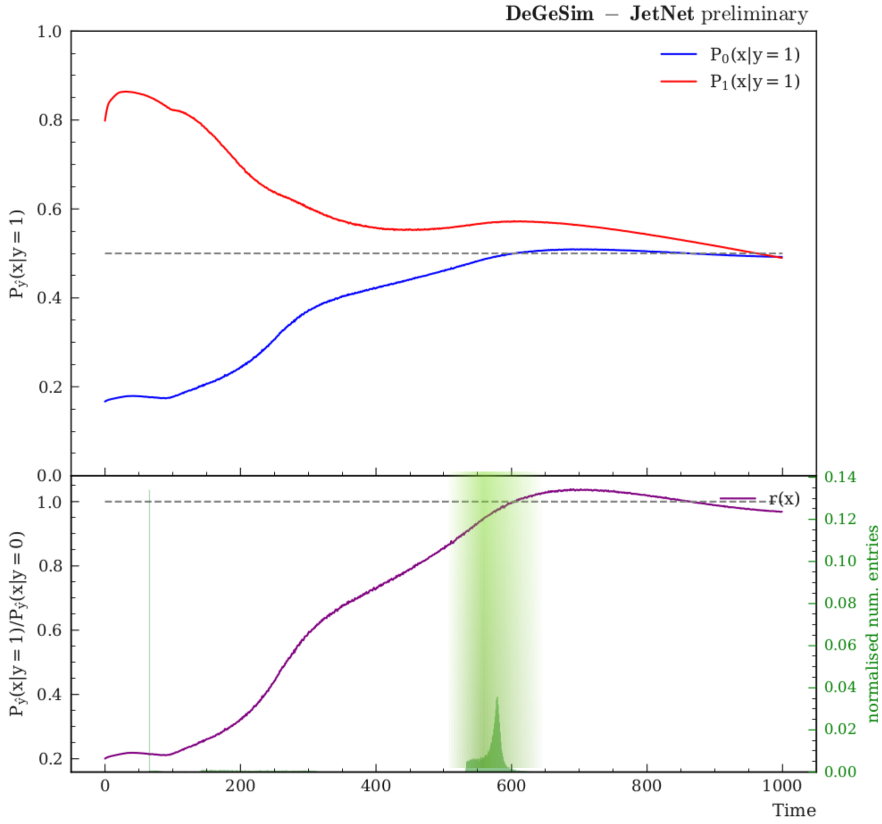

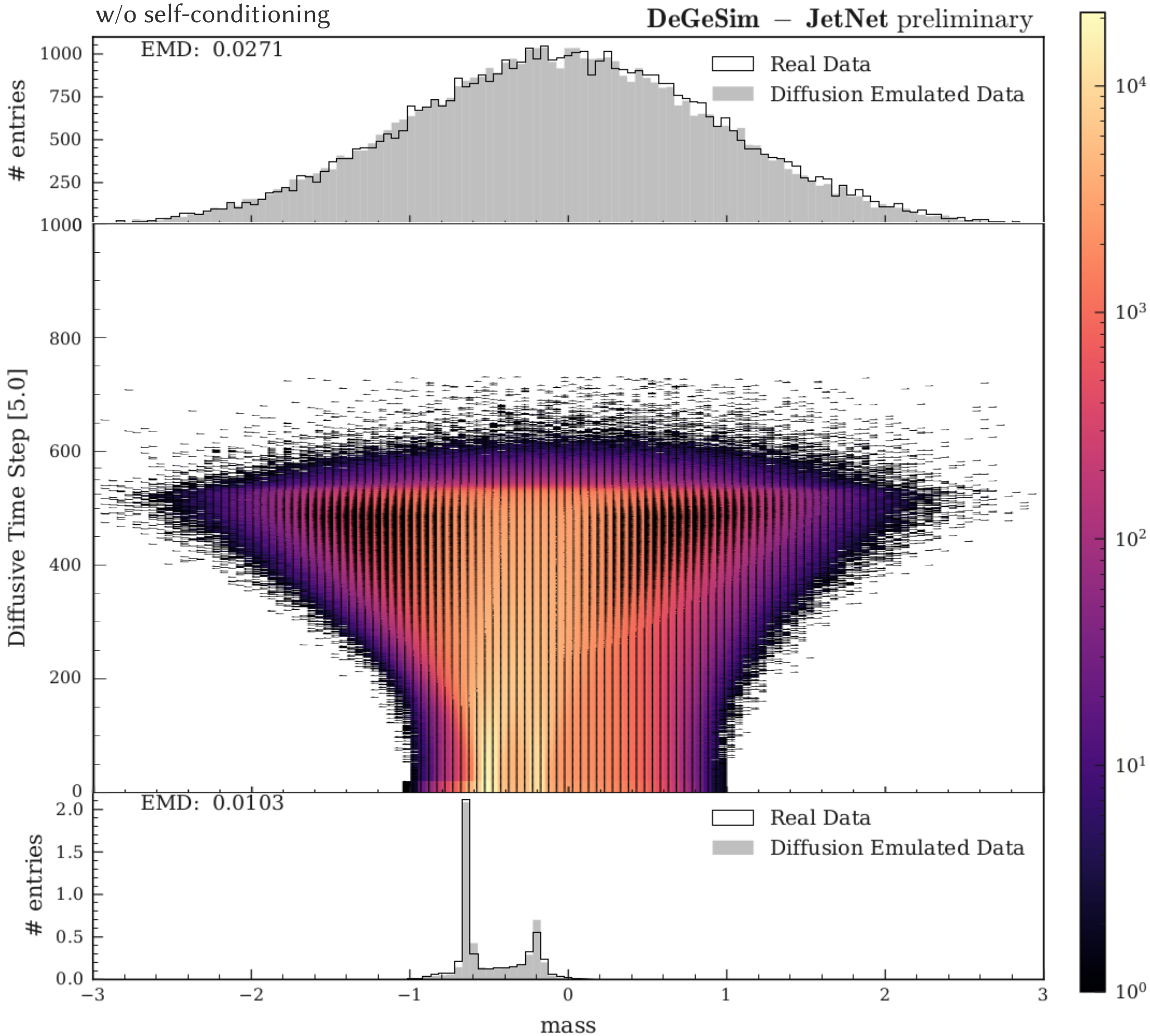

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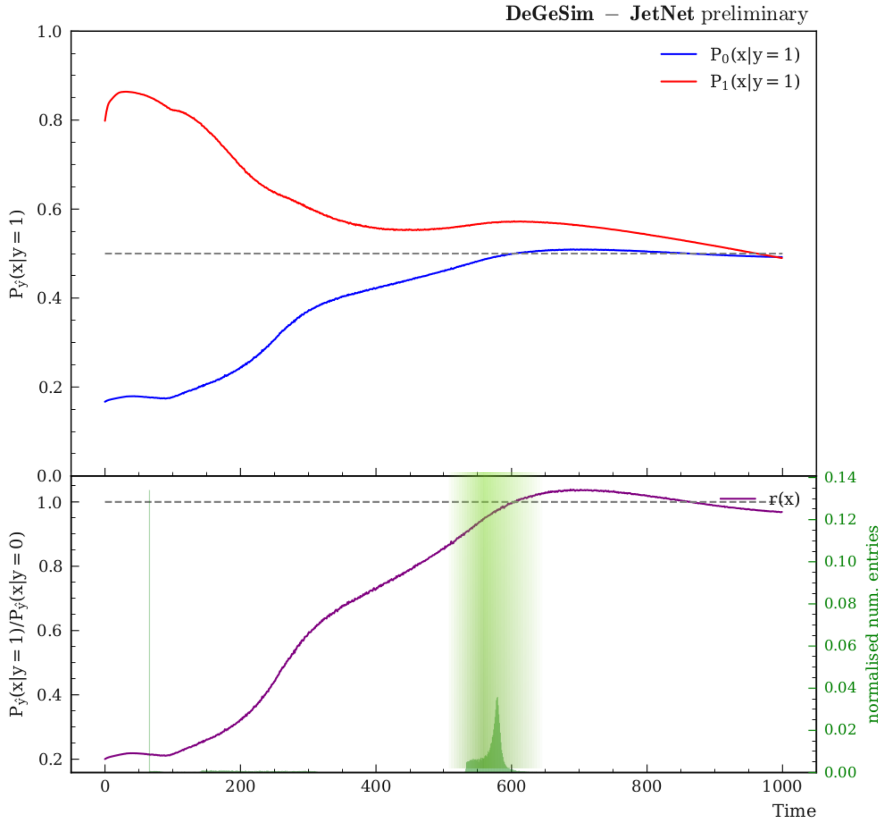

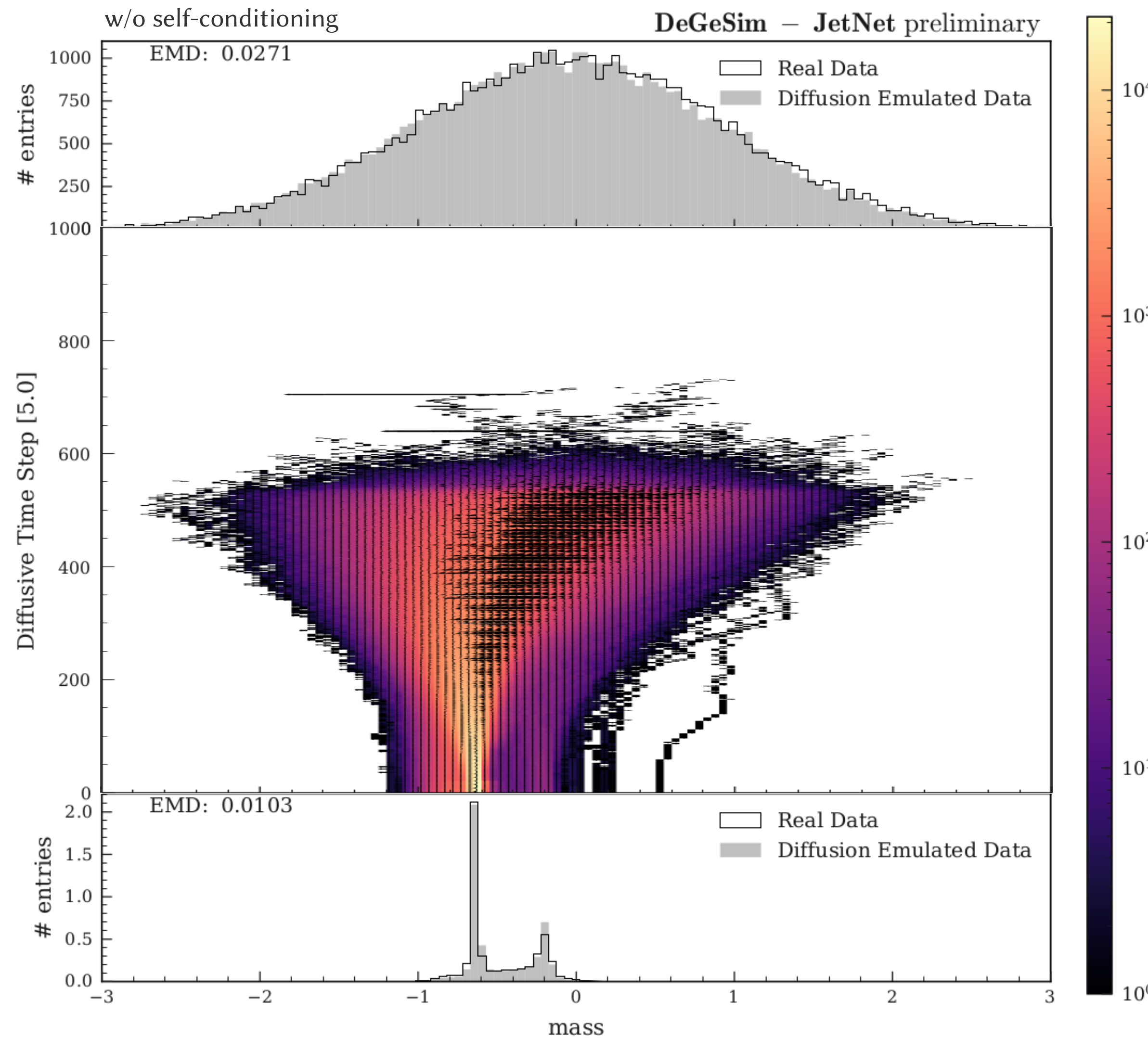

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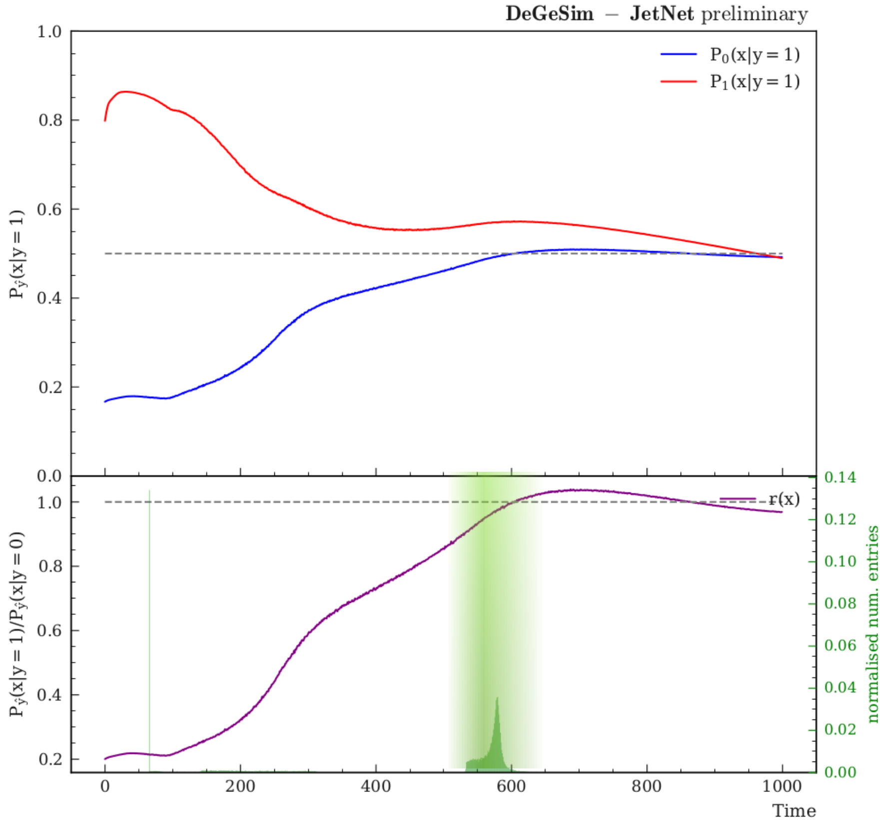

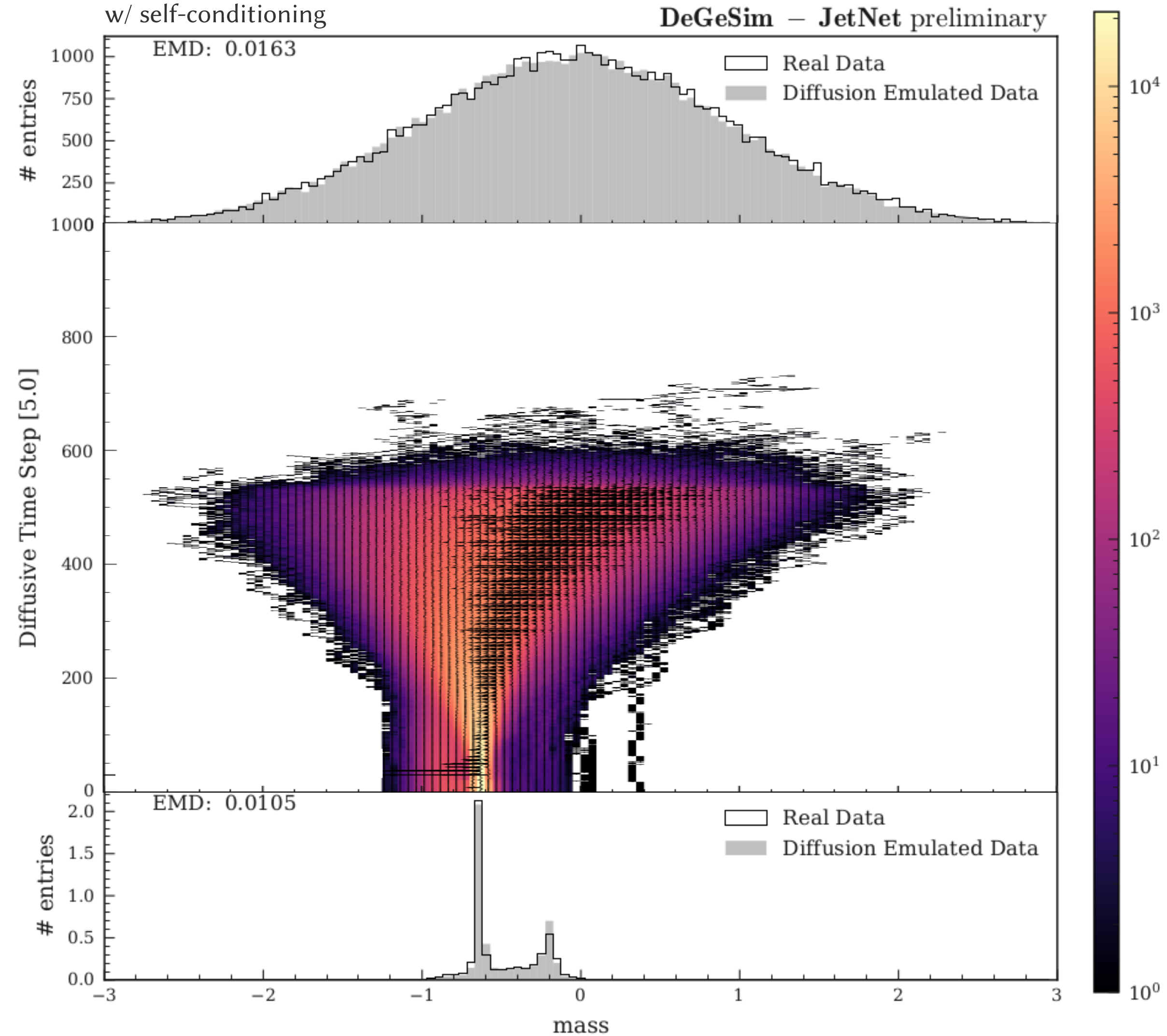

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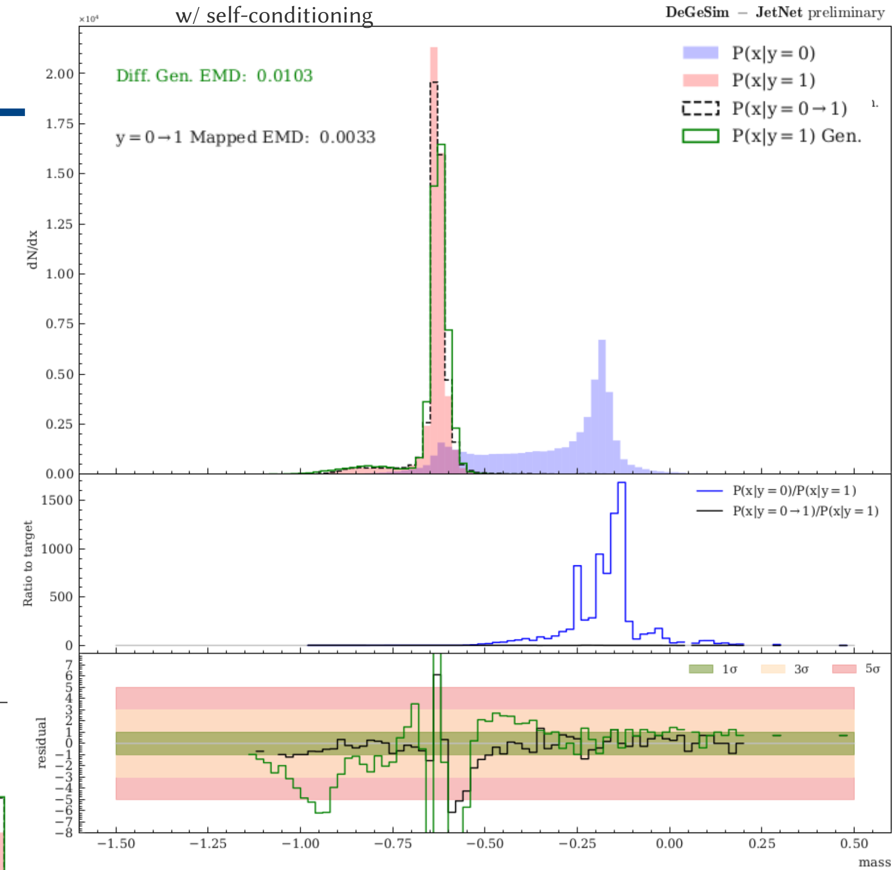

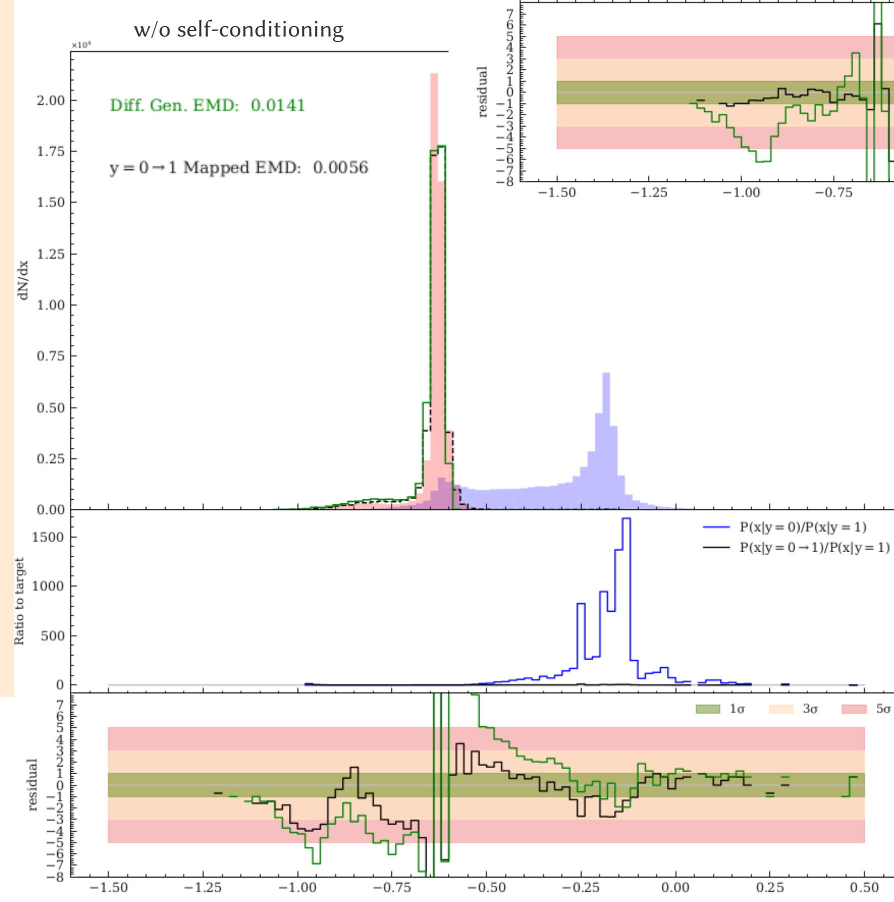

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→ **Top Pane:** Real data (shaded histograms) split based on class label

y = 0 – Top-Jets

y = 1 - W-Jets

→ **Middle Pane:** Ratio to target (y=1)

Black = Mapped Distrbution

Blue = y=0 / y=1

→ **Bottom Pane:** Residuals to target for each component:

$$Residual = a\text{-}b \,/\, [\sigma_a^{\,2} + \sigma_b^{\,2}]^{1/2}$$

Target is P(x|y=1), i.e. W-boson jets

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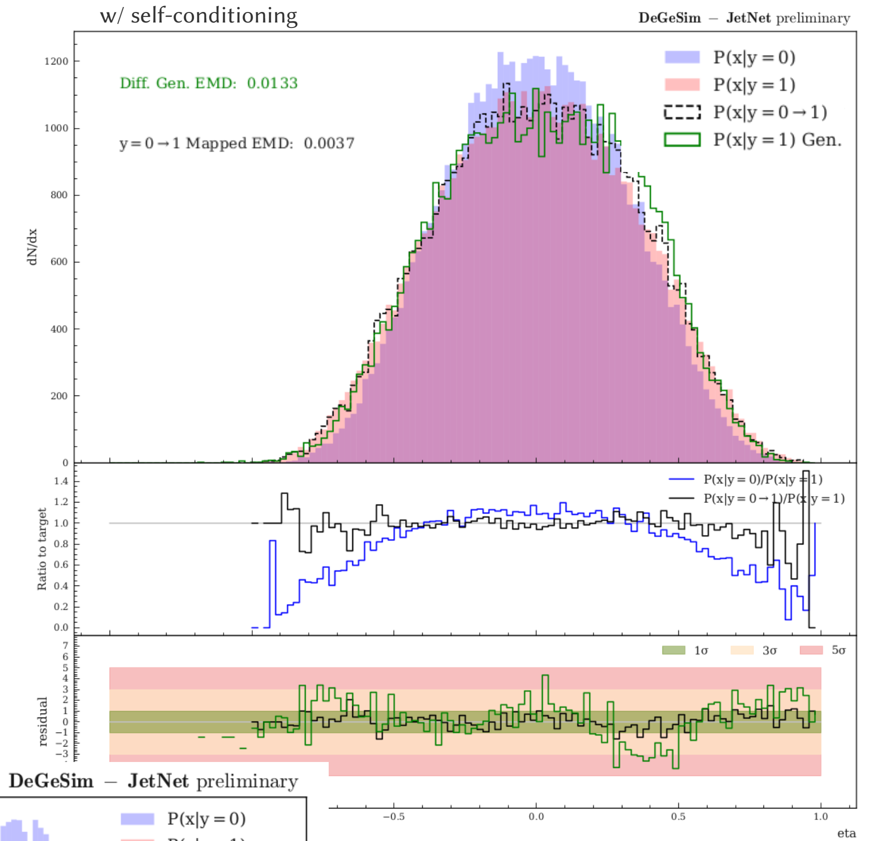

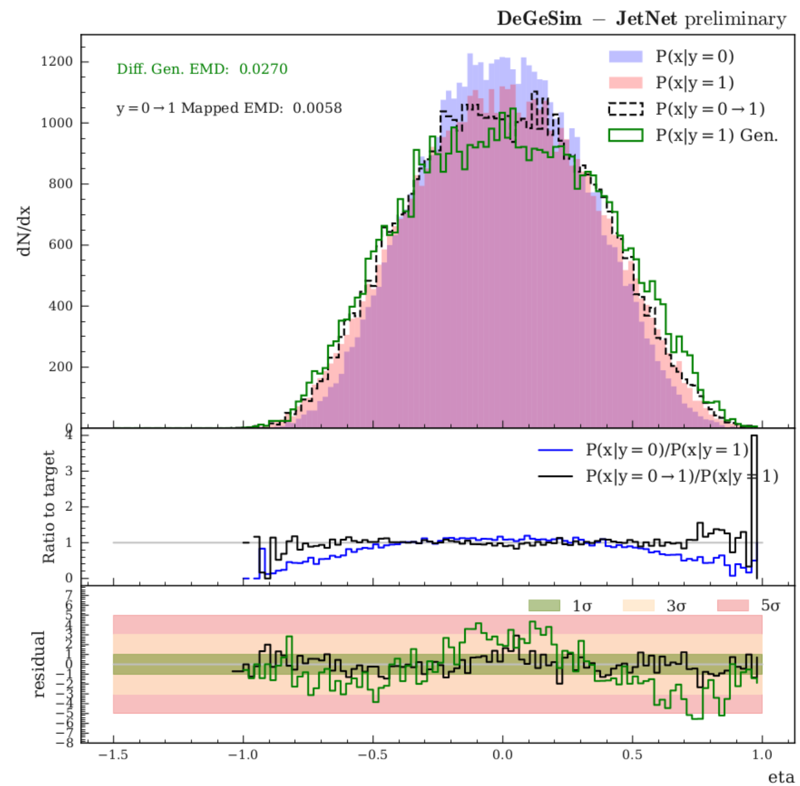

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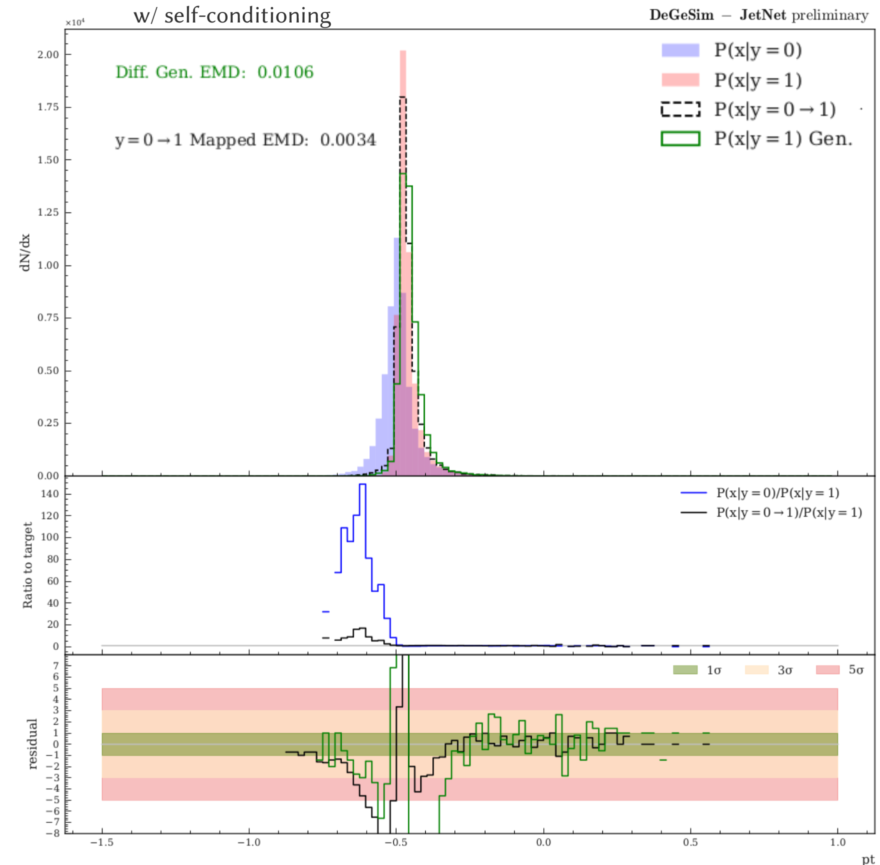

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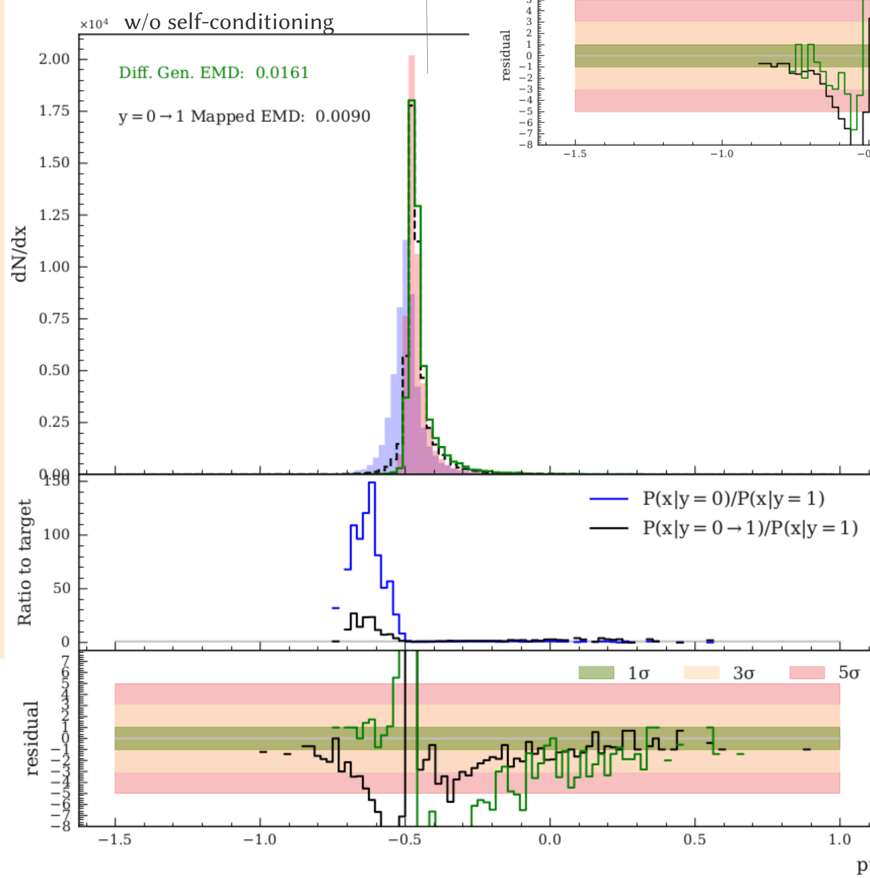


Summary

→ **Goal:** Emulate calorimeter *images* of pileup (minimum/zero bias) seeded from MC based simulations

→ **Status:** Partial diffusion using self-conditioning and classifier free guidance to preserve class-specific features prior to image denoising

→ *Image-to-image (I2I) translation using partial information loss*

→ **Problems:** Null value sparsity injection into calorimeter images:

→ CNNs struggle with noisy images and null-value injection

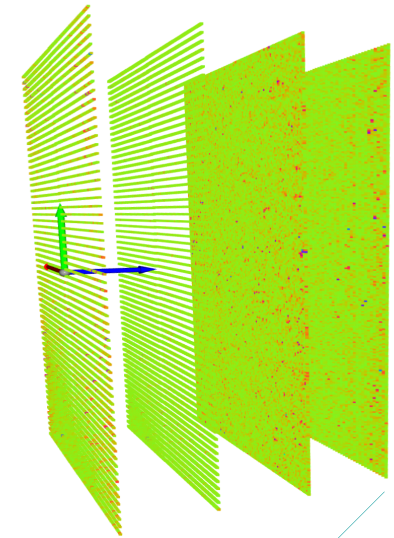
→ Point clouds introduce cell ↔ point assigment ambiguity

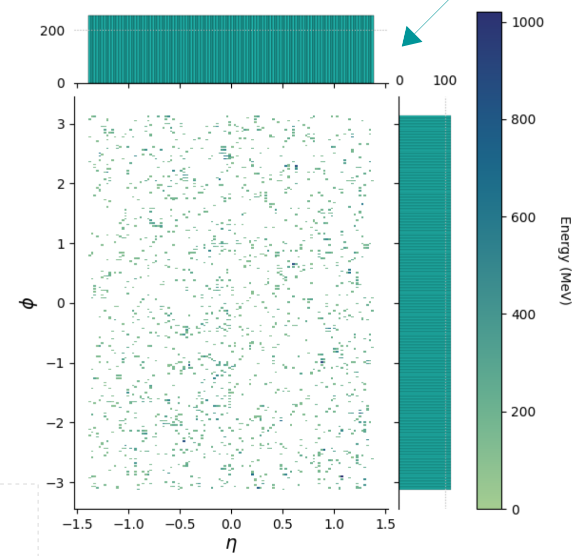
→ Sparse convolutional operations

→ **Further work** will include:

→ Cast discrete state spaces into continuous state space for diffusion (**Analog Bits**)

→ **Cross-domain** conditioning to enhance domain translation duing diffusion





CONTINUOUS & DISCRETE STATE SPACE SAFE CONDITIONAL DENOISING DIFFUSION PROBABILISTIC MODELS USING SELF & CROSS-DOMAIN CONDITIONING FOR MULTI-DIMENSIONAL MAPPING

A PREPRINT

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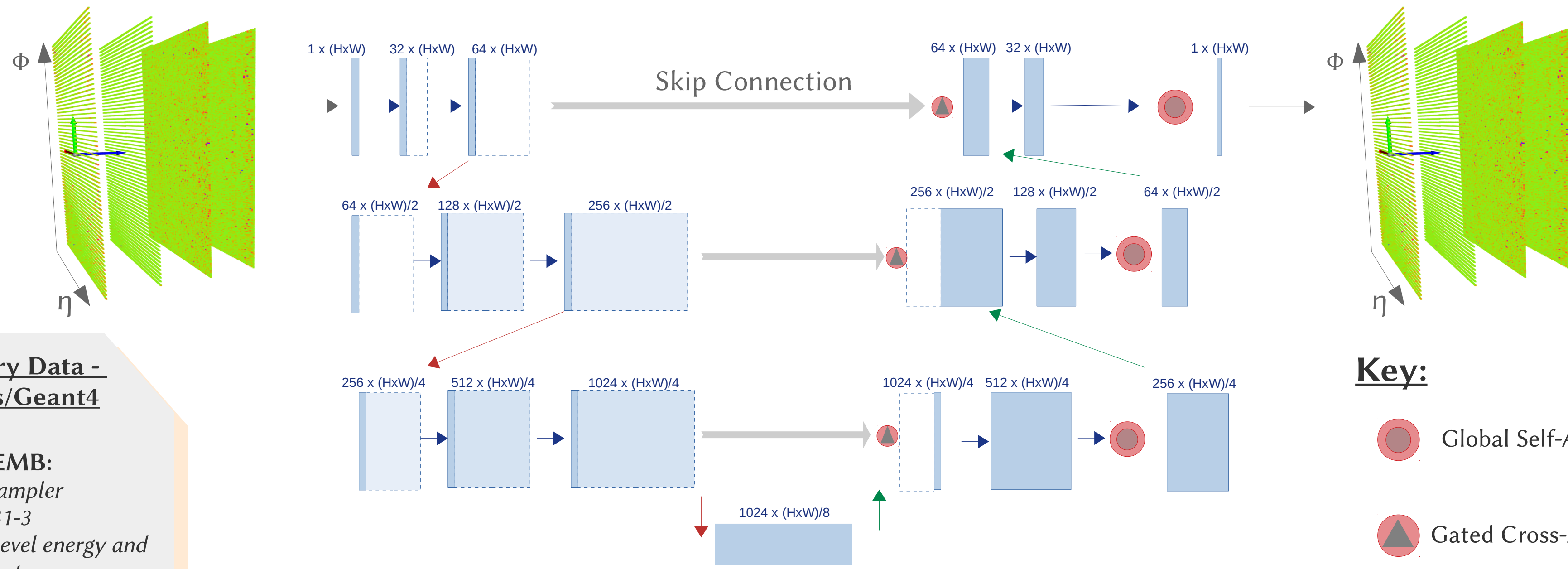
arXiv coming soon...

Backup

Neural Network Architecture

Latent DDPM



Calorimetry Data - Delphes/Geant4

→ **ATLAS EMB:**
- → *Pre-sampler*
- → *EMB1-3*
- → *Cell level energy and geometry*

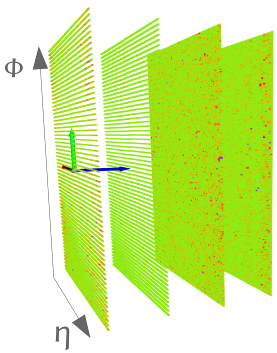
→ **Delphes:**
- → *ECAL*
- → *HCAL*

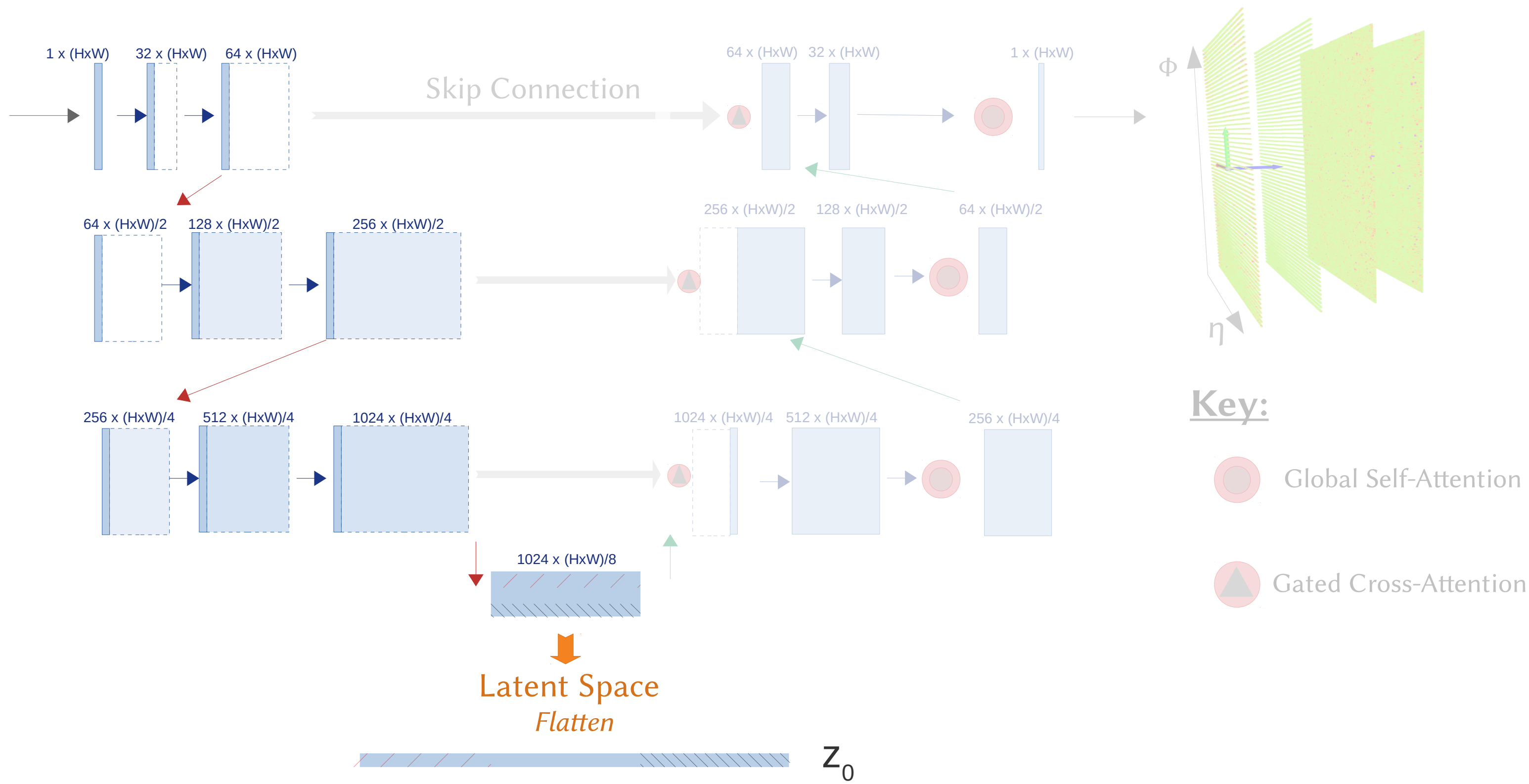
Key:

Global Self-Attention

Gated Cross-Attention

Latent DDPM





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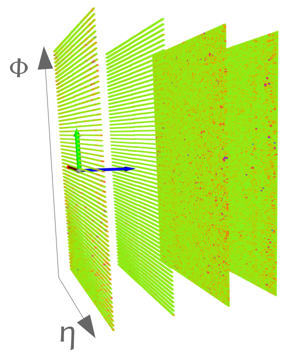

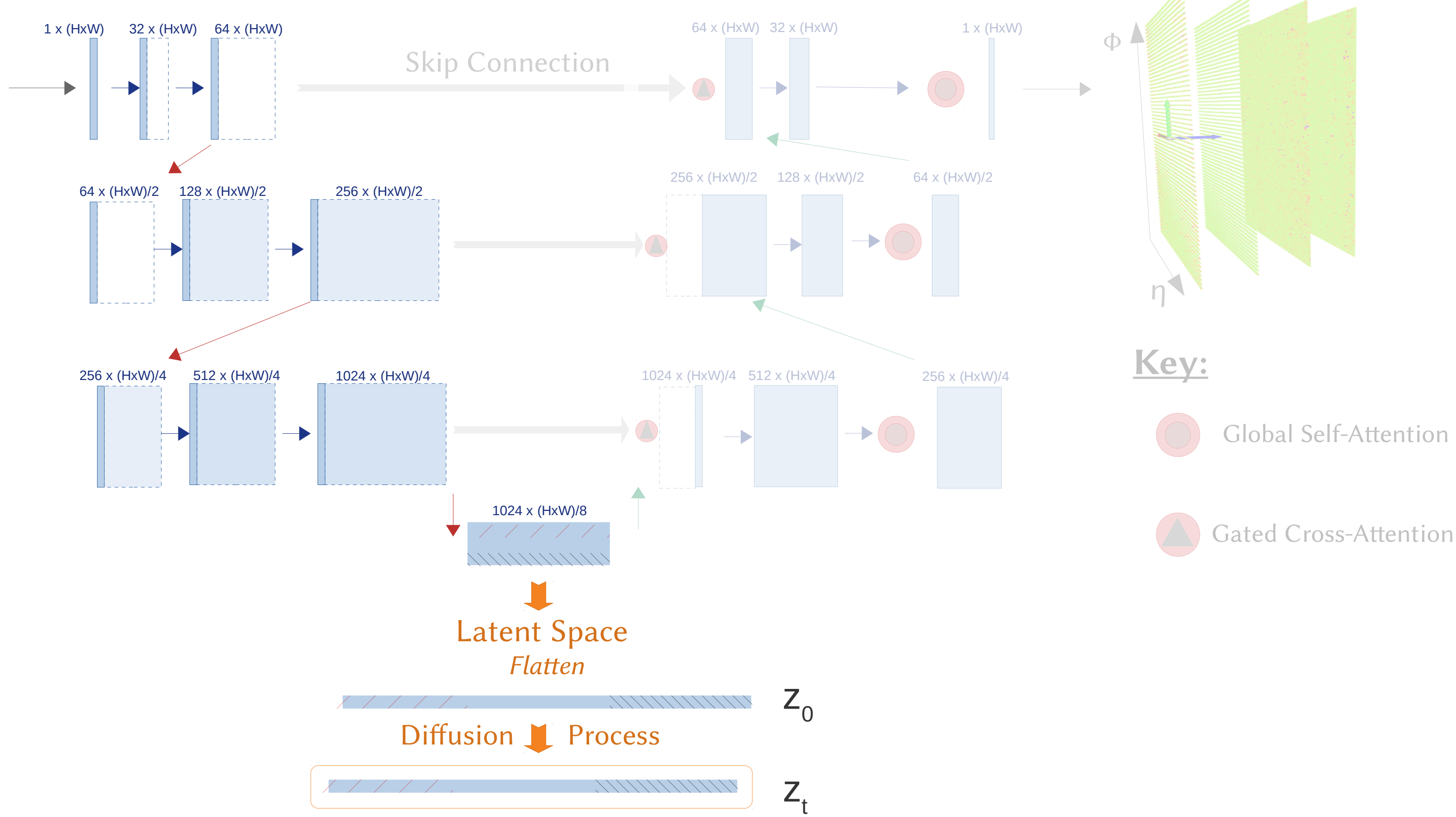

Calorimetry Data - Delphes/Geant4

→ **ATLAS EMB:**
- → *Pre-sampler*
- → *EMB1-3*
- → *Cell level energy and geometry*

→ **Delphes:**
- → *ECAL*
- → *HCAL*

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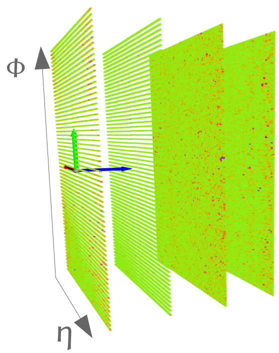

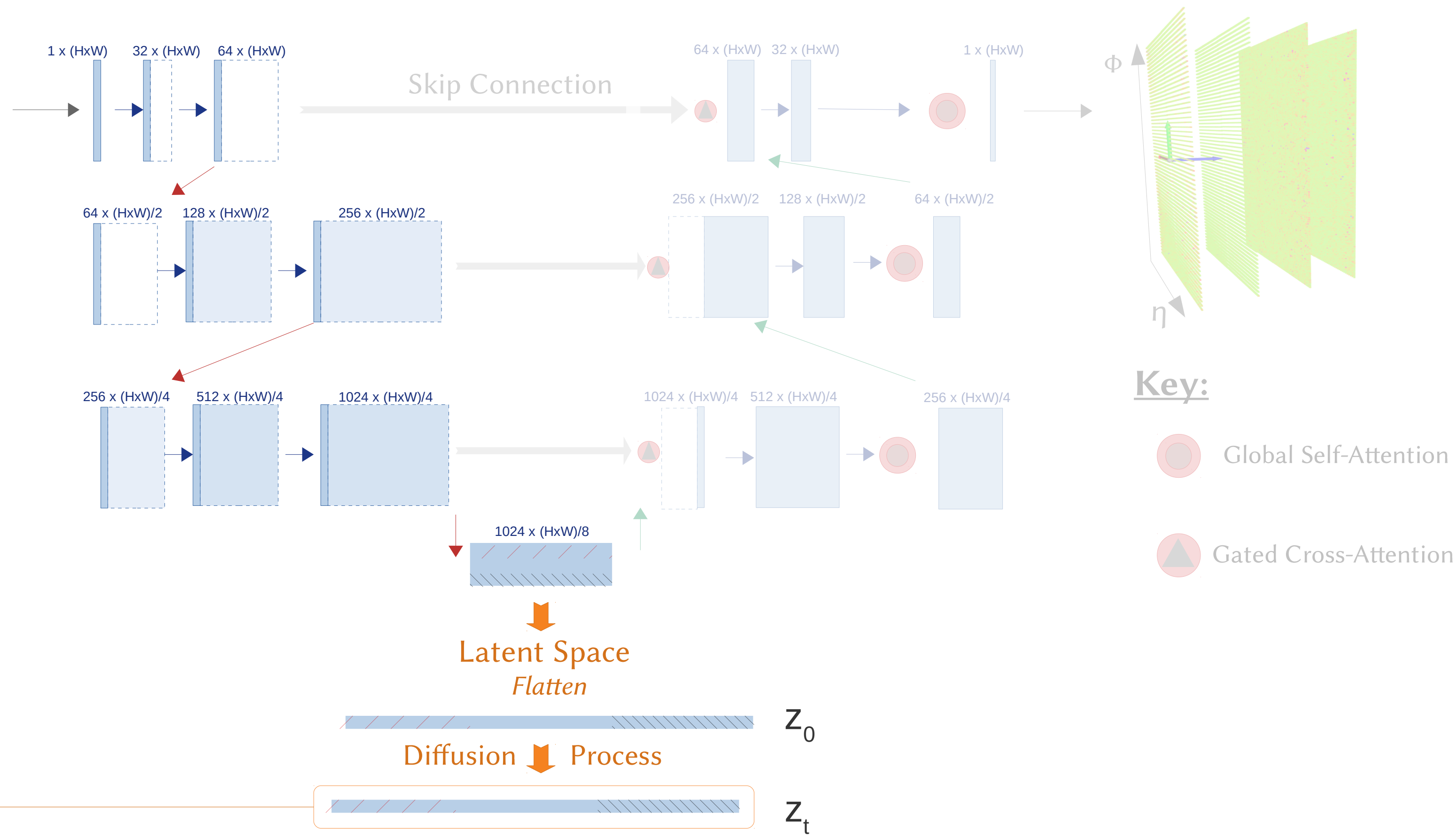

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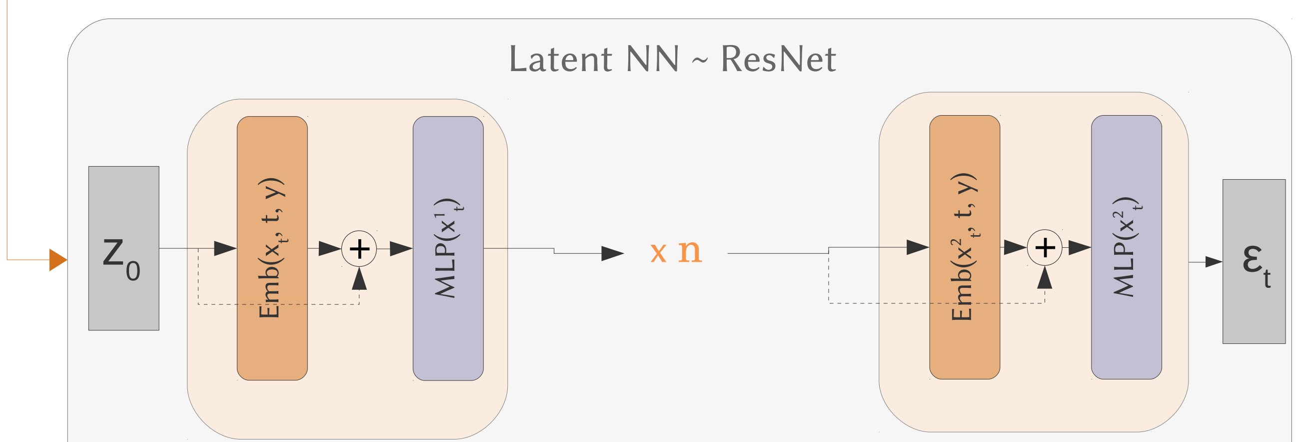

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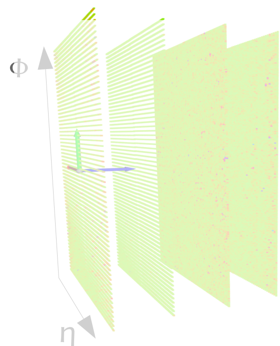

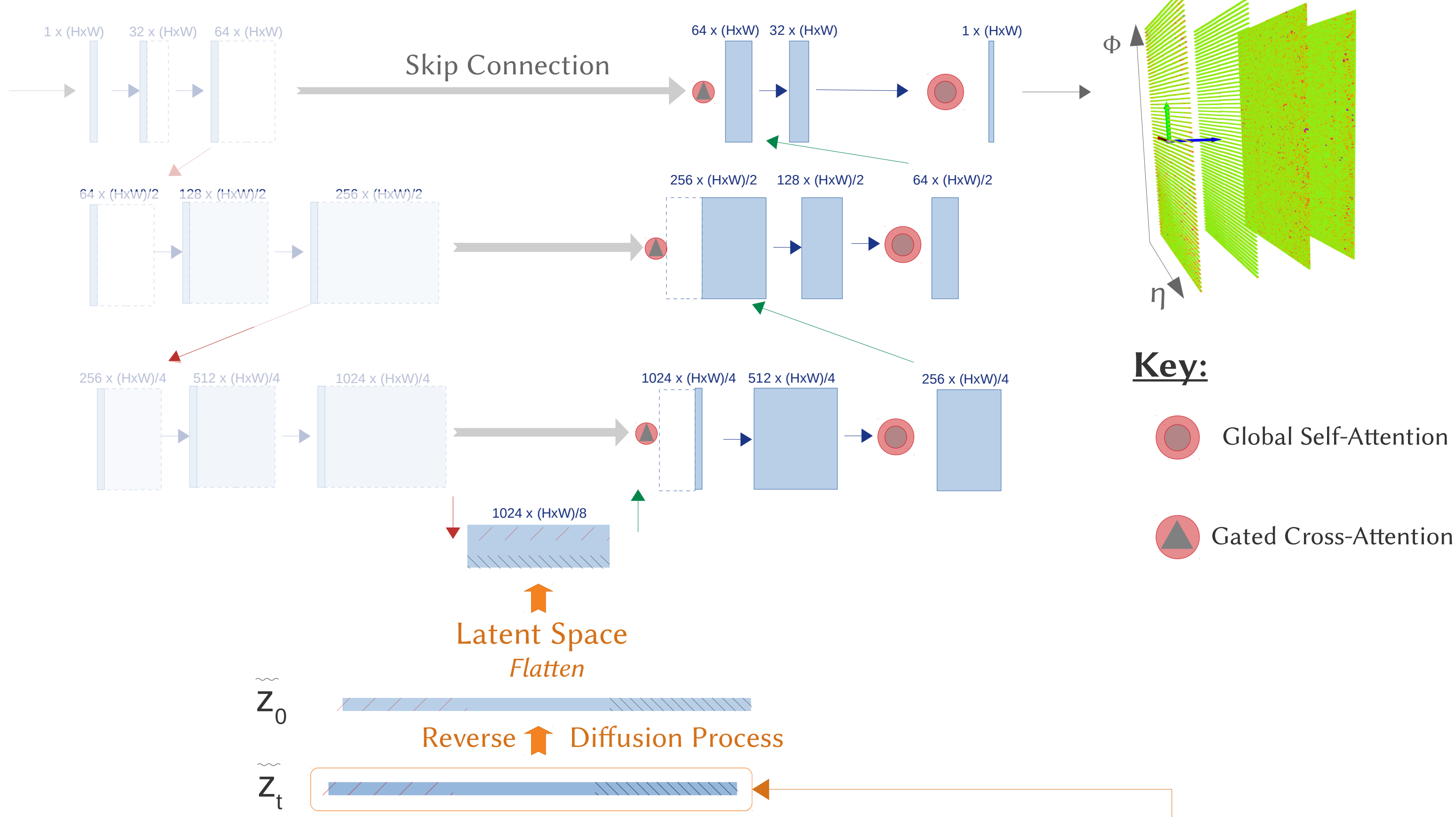

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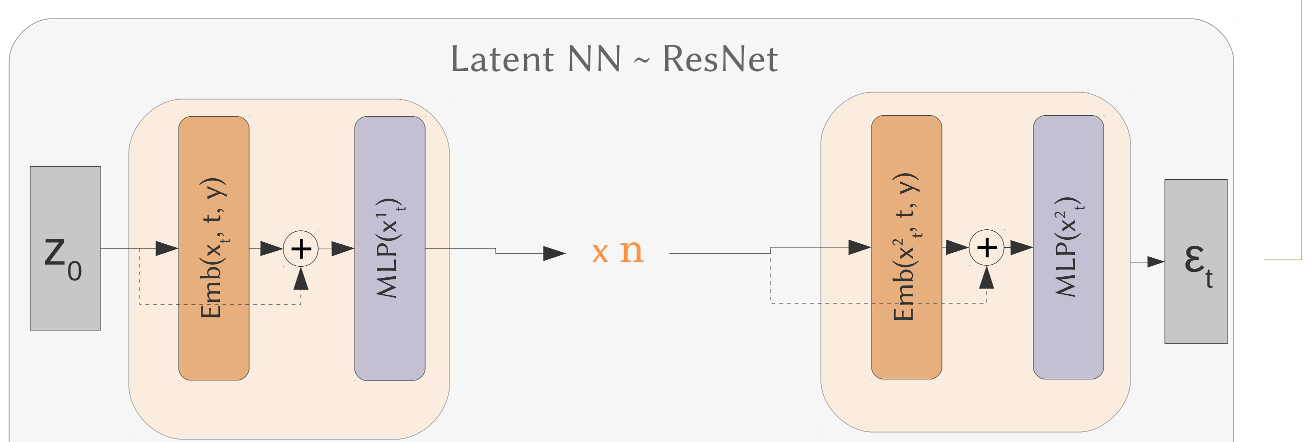

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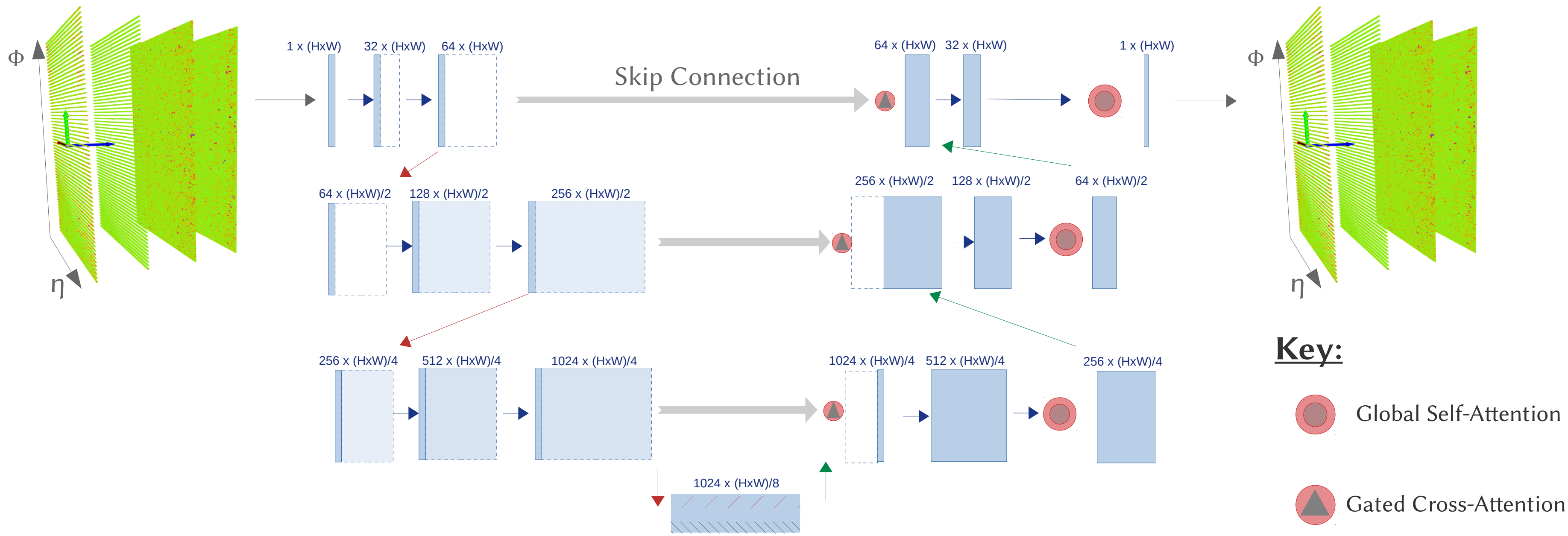
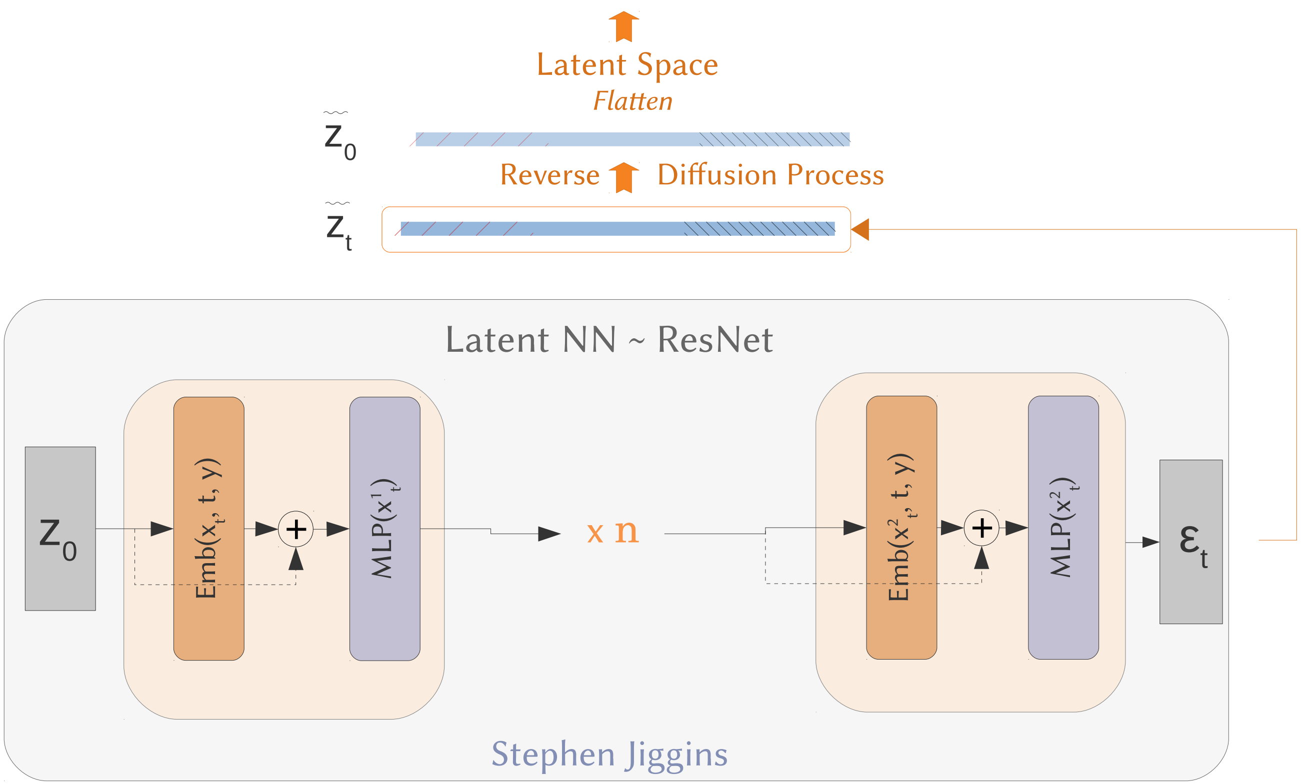


Φ
η
1 x (HxW)
32 x (HxW)
64 x (HxW)
Skip Connection
64 x (HxW)
32 x (HxW)
1 x (HxW)
64 x (HxW)/2
128 x (HxW)/2
256 x (HxW)/2
256 x (HxW)/2
128 x (HxW)/2
64 x (HxW)/2
256 x (HxW)/4
512 x (HxW)/4
1024 x (HxW)/4
1024 x (HxW)/4
512 x (HxW)/4
256 x (HxW)/4
1024 x (HxW)/8
Latent Space
Flatten
Key:
Global Self-Attention
Gated Cross-Attention



z̃0
Reverse Diffusion Process
z̃t
Latent NN ~ ResNet
Z0
Emb(xt, t, y)
MLP(x1t)
x n
Emb(x2t, t, y)
MLP(x2t)
εt

Denoising Diffusion Probabilistic Models

DDPMs – Recipe

→ **Noise Scheduler:**

Cosine β-scheduling noise injection:

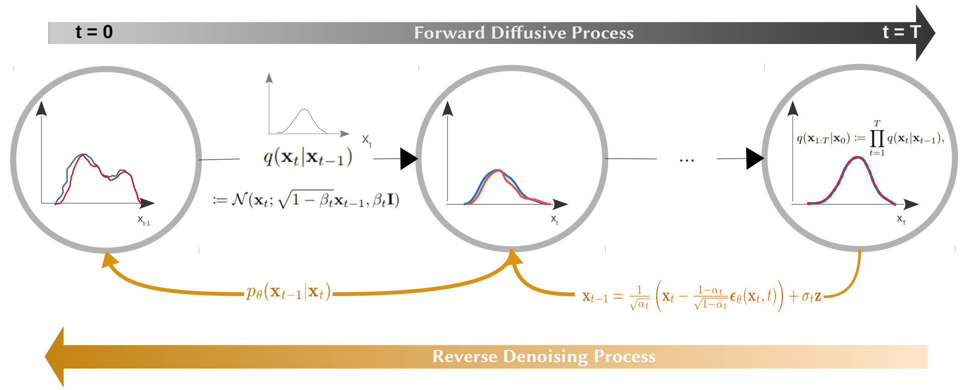
$$\beta_t = 1 - \frac{\overline{\alpha}_t}{\overline{\alpha}_{t-1}} \qquad \overline{\alpha}_t = f(t)/f(0) \qquad f(t) = \cos\left(\frac{(t/T+s)\pi}{2.(1+s)}\right)$$

→ **Denoising Score Matching**

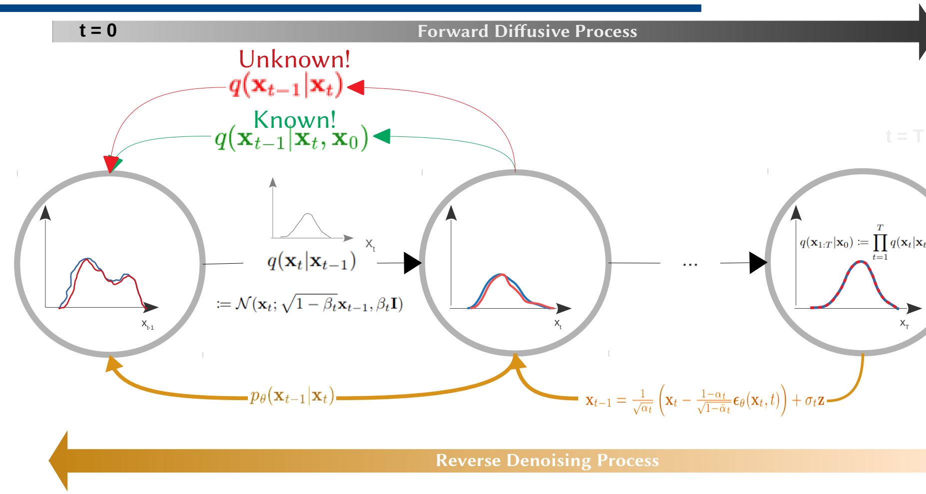
$$L(\theta) = \mathbb{E}_{t,x_0,\epsilon}\left[\left|\epsilon - \epsilon_\theta(x_t(x_0,\epsilon),t)^2\right|\right]$$

→ **Density Ratio Estimating Classifer**

$$L_{DRE} = \sum \left[p_c(t,x_0)\log(\widehat{p}_c(t,x_0))\right]$$



Denoising Diffusion Probabilistic Models



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→ **Density Ratio Estimating Classifer**

$$L_{DRE} = \sum \left[p_c(t,x_0)\log(\hat{p}_c(t,x_0))\right]$$

→ The *origin* conditional probability is tractable:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)}$$

→ Network needs to learn the reverse process:

$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

→ Lower variational bound objective:

$$L_{\text{VLB}} = \mathbb{E}_{q(\mathbf{x}_{0:T})}\left[\log\frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\right]$$

→ DSM needs to learn the term:

$$L_{\text{VLB}} = L_T + \underbrace{L_{T-1} + \cdots}_{} + L_0$$

$$\sum_{t=2}^{T} \underbrace{D_{\text{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}}$$

Denoising Diffusion Probabilistic Models

DDPMs – Recipe

→ **Noise Scheduler:**

Cosine β-scheduling noise injection:

$$\beta_t = 1 - \frac{\overline{\alpha}_t}{\overline{\alpha}_{t-1}} \qquad \overline{\alpha}_t = f(t)/f(0) \qquad f(t) = \cos\left(\frac{(t/T+s)\pi}{2.(1+s)}\right)$$

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$$L(\theta) = \mathbb{E}_{t,x_0,\epsilon}\left[\left|\epsilon - \epsilon_\theta(x_t(x_0,\epsilon),t)\right|^2\right]$$

→ **Density Ratio Estimating Classifer**

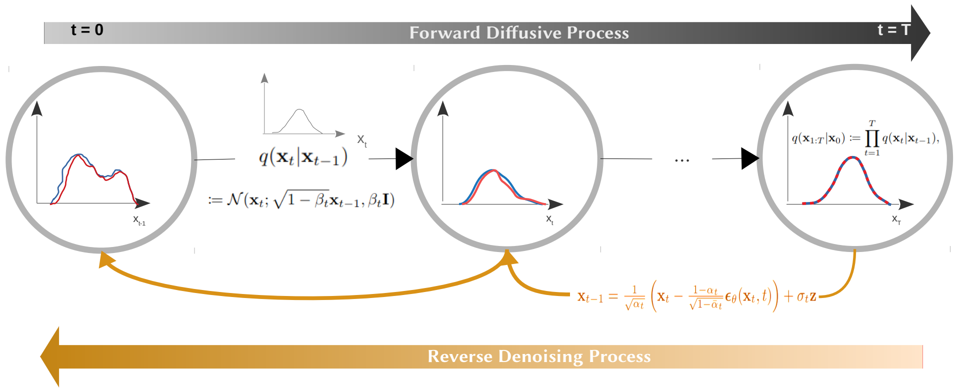
$$L_{DRE} = \sum \left[p_c(t,x_0)\log(\widehat{p}_c(t,x_0))\right]$$

→ **Conditional Embedding**

$$L(\theta) = \mathbb{E}_{t,x_0,\epsilon,y}\left[\left|\epsilon - \epsilon_\theta(x_t(x_0,\epsilon),y,t)\right|^2\right]$$

→ **Classifier Free Guidance**

$$\overline{\epsilon}_\theta(x_t, y, t) = (w+1)\,\epsilon_\theta(x_t, y, t) - w.\,\epsilon_\theta(x_t, t)$$



→ Conditional dependency can be integrated:

$$q(\mathbf{x}_{t-1}|x_t, x_{0,y}) = q(\mathbf{x}_t|x_{t-1}, x_{0,y}) \cdot \frac{q(x_{t-1}|x_{0,y})}{q(x_t|x_{0,y})}$$

$$p_\theta(\mathbf{x}_{0:T}|y) = p_\theta(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|x_t, y)$$

→ Score estimation naturally extends with this conditionality:

$$\nabla^w_{x_t} \log(p_\theta(\mathbf{x}_t|y)) = (1-w)\nabla_{x_t}\log(p_\theta(\mathbf{x}_t)) + w\nabla_{x_t}\log(p_\theta(\mathbf{x}_t|y))$$

→ Guidance scalar (w) used to control conditional ↔ unconditionally interpolation of score/noise estimators:

$$\overline{\epsilon}(x_t, t, y) = w\,\epsilon_\theta(x_t, t, y) - (1-w)\,\epsilon_\theta(x_t, t)$$

Denoising Diffusion Probabilistic Models

DDPMs – Recipe

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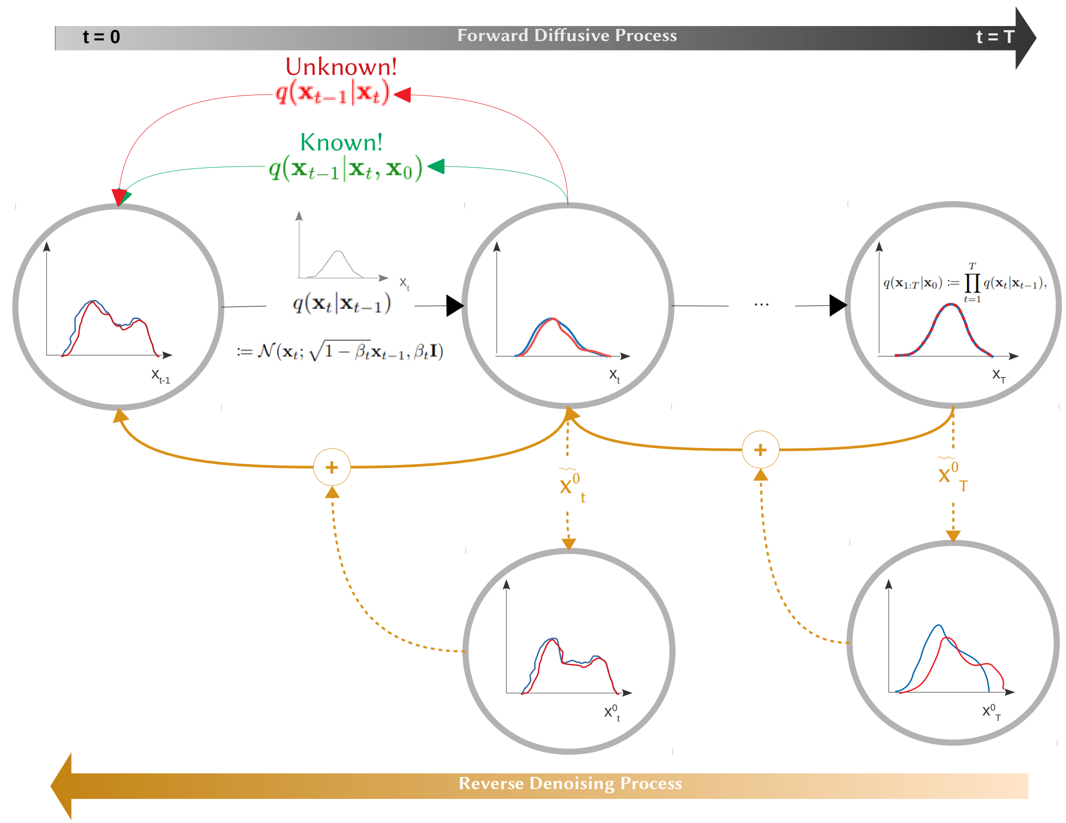
→ **Self-Conditioning**

$$L(\theta) = \mathbb{E}_{t,x_0,\widehat{x}_0,\epsilon,y}\left[\left|\epsilon - \epsilon_\theta(x_t(x_0,\epsilon),y,t,\widehat{x}_0)\right|^2\right]$$



→ Self-conditioned dependency can be integrated:

$$p_\theta(\mathbf{x_{0:T}}|y,\tilde{x}_0) = p_\theta(\mathbf{x_T})\prod_{t=1}^{T} p_\theta(\mathbf{x_{t-1}}|x_t,y,\tilde{x}_0)$$

→ Provided that there is a stop gradient on the estimate of the original image $\tilde{x}_0$:

$$\nabla^w_{x_t}\log(p_\theta(\mathbf{x_t}|y,\tilde{x}_0)) = (1-w)\nabla_{x_t}\log(p_\theta(\mathbf{x_t})) + w\nabla_{x_t}\log(p_\theta(\mathbf{x_t}|y,\tilde{x}_0))$$

→ Scalar based guidance becomes:

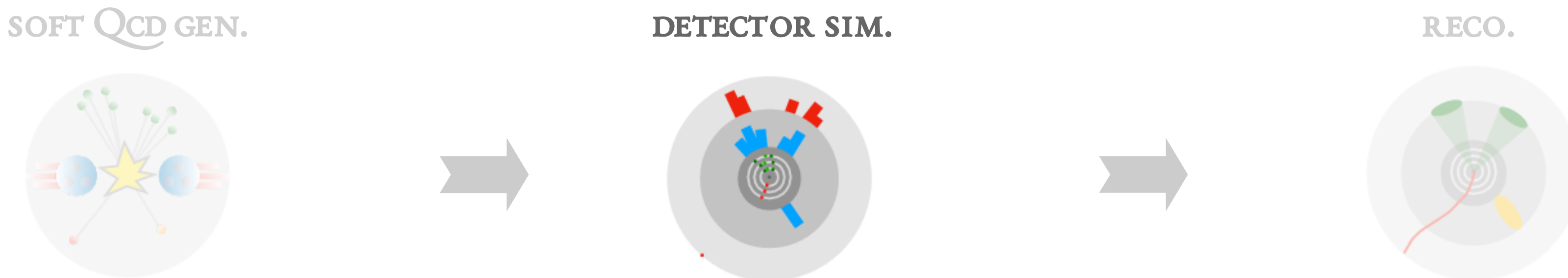
$$\overline{\epsilon}(x_t,t,y) = w\,\epsilon_\theta(x_t,t,y,\tilde{x}_0) - (1-w)\,\epsilon_\theta(x_t,t)$$

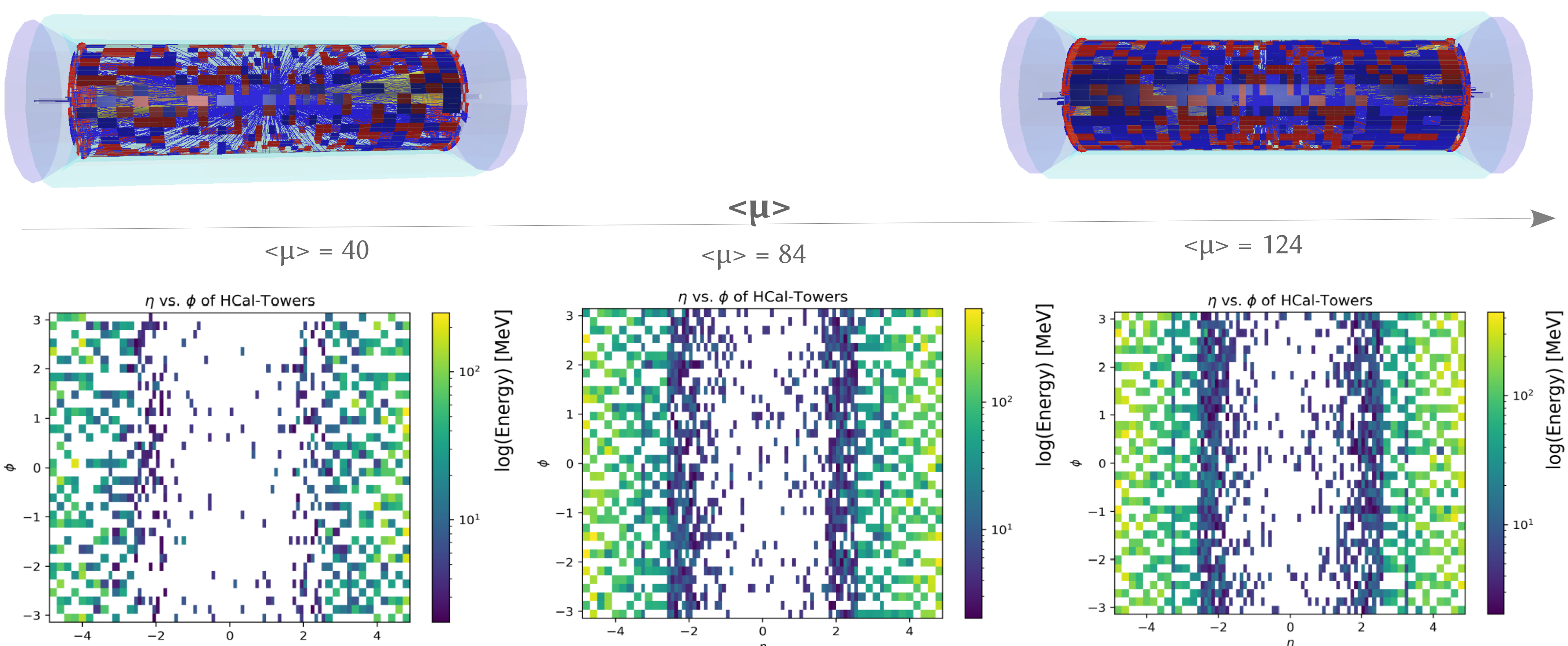
Delphes Pile-up Simulation

Brief

Problem:

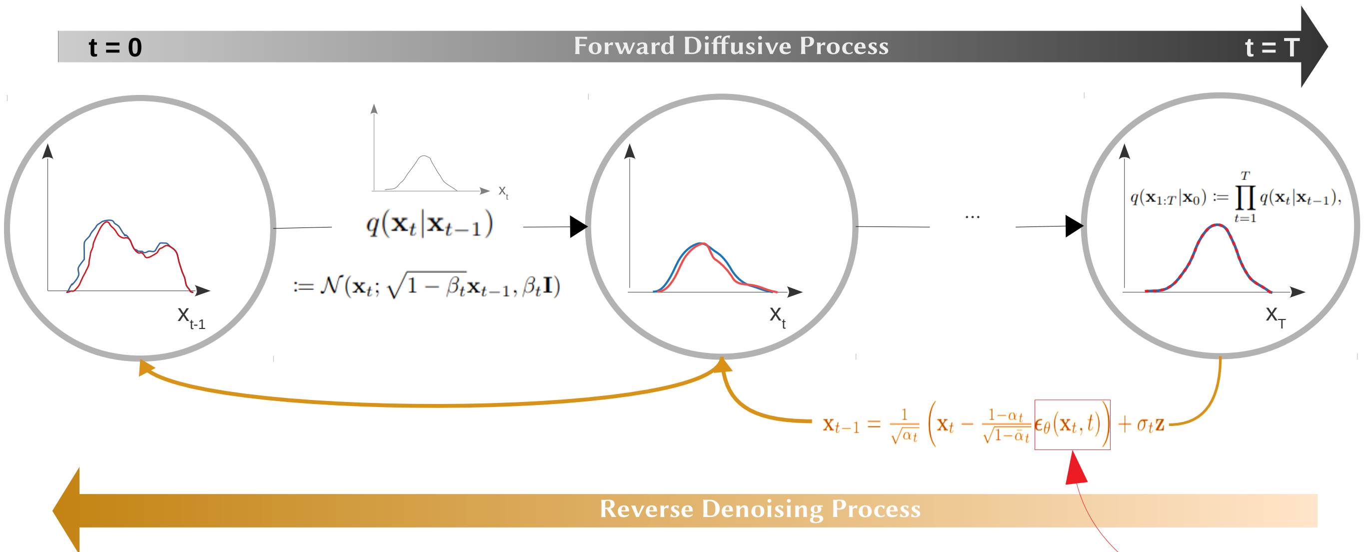
Pileup from multiple proton interactions currently miss-model data. This trend worsens with the number of interactions per bunch crossing leading to an explosive issue moving towards the HL-LHC:

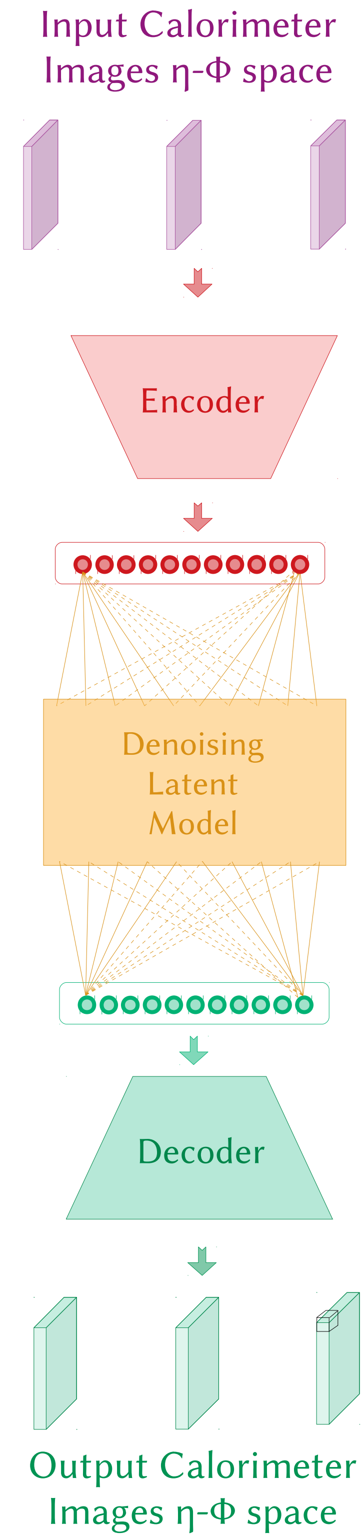




Denoise Score Matching Neural Network

DDPM Model Architecture





Denoising Neural Model

→ Image Reco. Encoder + Decoder:

Using a UNet based architecture with:

- *Cross-Attention*
- *Global Self-Attention*
- *Deep Residual Connections*

Using patch + pixel based reconstruction loss:

→ Denoising Latent Model:

Using a residual block based neural network:

- *Sinusoidal embedding of class+time*
- *Short + Long residual connections*
- *Dense (non-)-linear MLP blocks*

Using noise score matching criteria:

$$L(\theta) = \mathbb{E}_{t,x_0,\hat{x}_0,\epsilon,y}\left[\left|\epsilon - \epsilon_\theta(x_t(x_0,\epsilon), y, t, \hat{x}_0)\right|^2\right]$$

Latent Diffusion Residual Network

Latent Diffusion Resi. Net

→ Residual Neural Network

Deep embedding blocks to prevent mode collapse. Therefore need residual connections to overcome lost gradients

→ Simple Sinusoidal Embedding

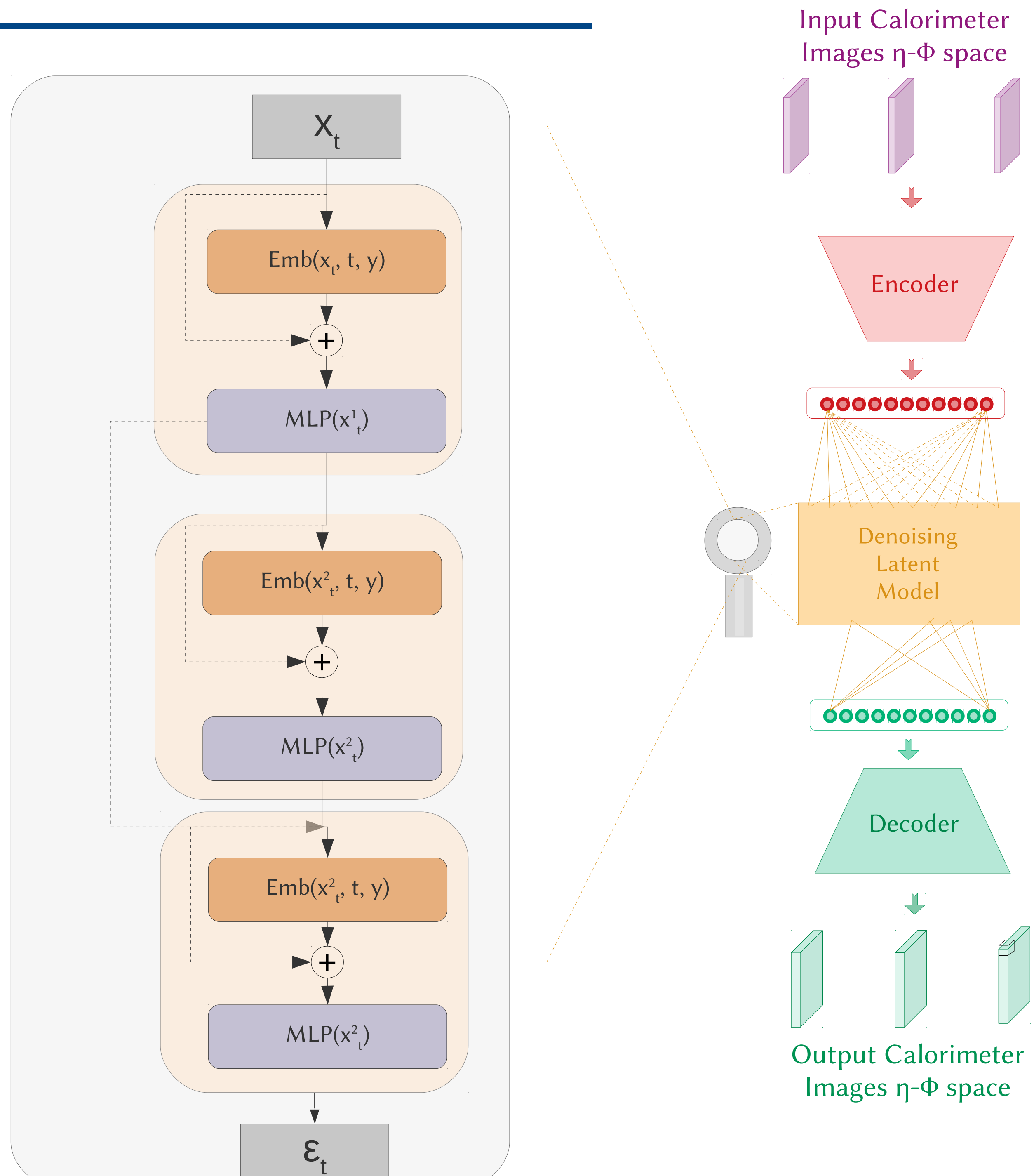
$$PE_{t,2i} = \sin\left(t/\alpha^{2i/d_{emb}}\right)$$

$$PE_{t,2i+1} = \cos\left(t/\alpha^{(2i+1)/d_{emb}}\right)$$

Natural normalisation of conditional variables that scales dimensionally with embedding space

→ FFN Blocks

Simple dense feed-forward neural network blocks for dimensionality scaling and expressibility



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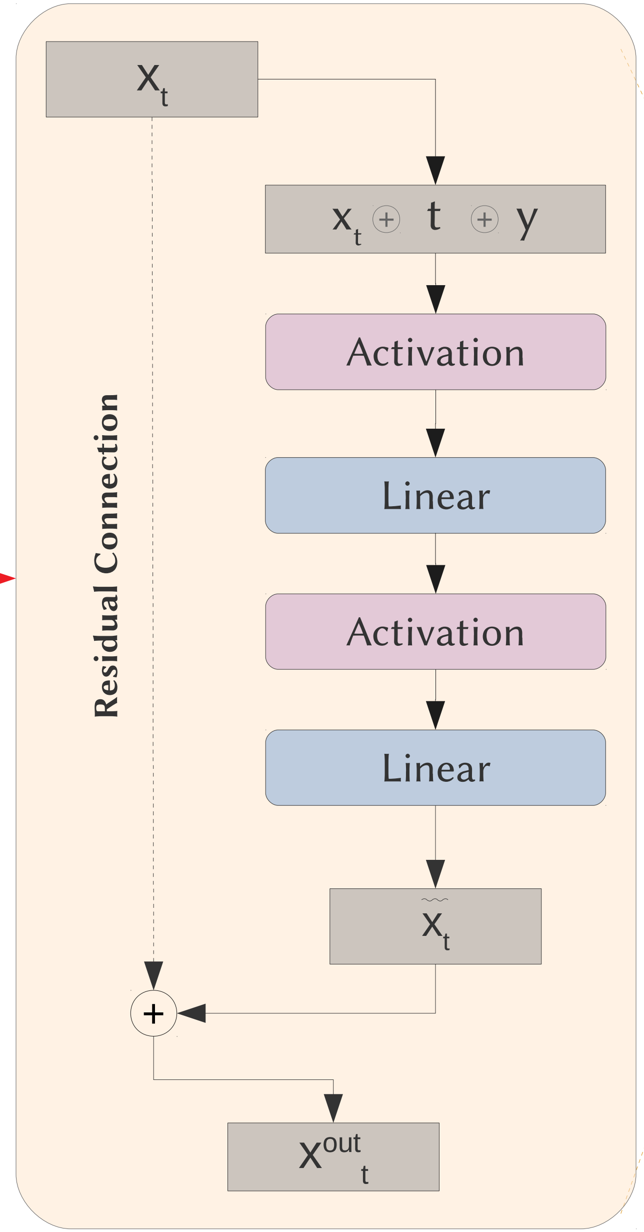

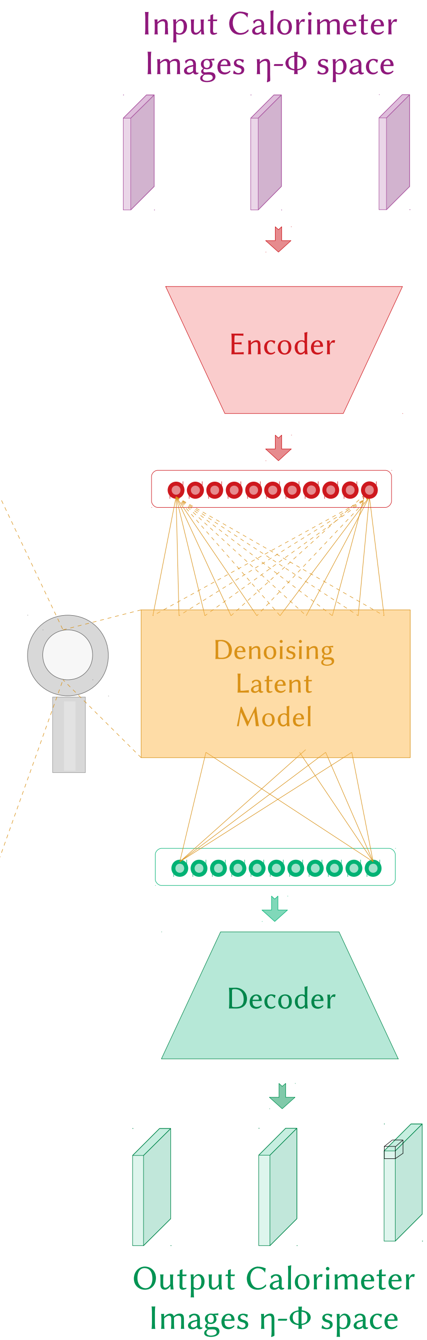

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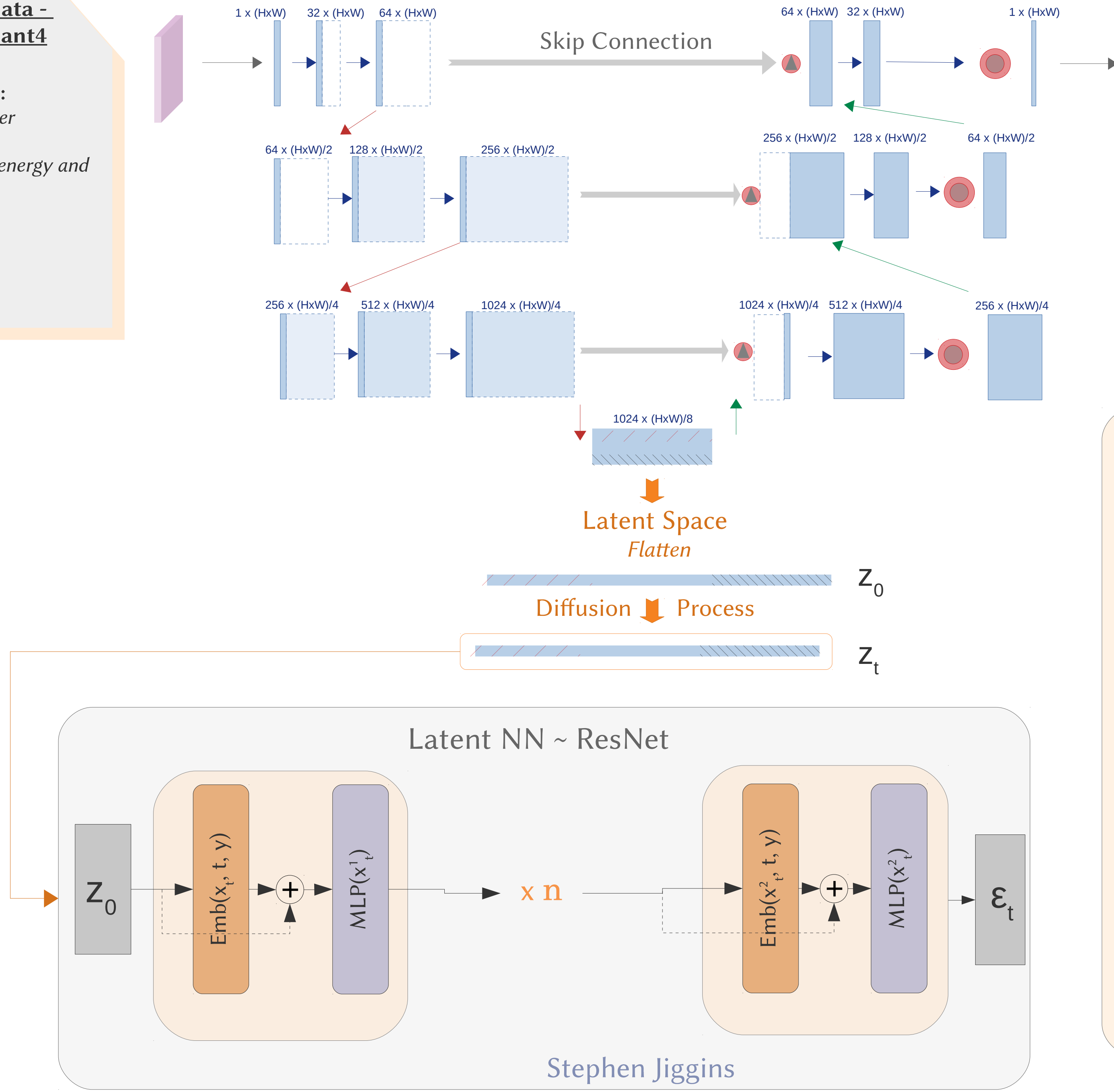
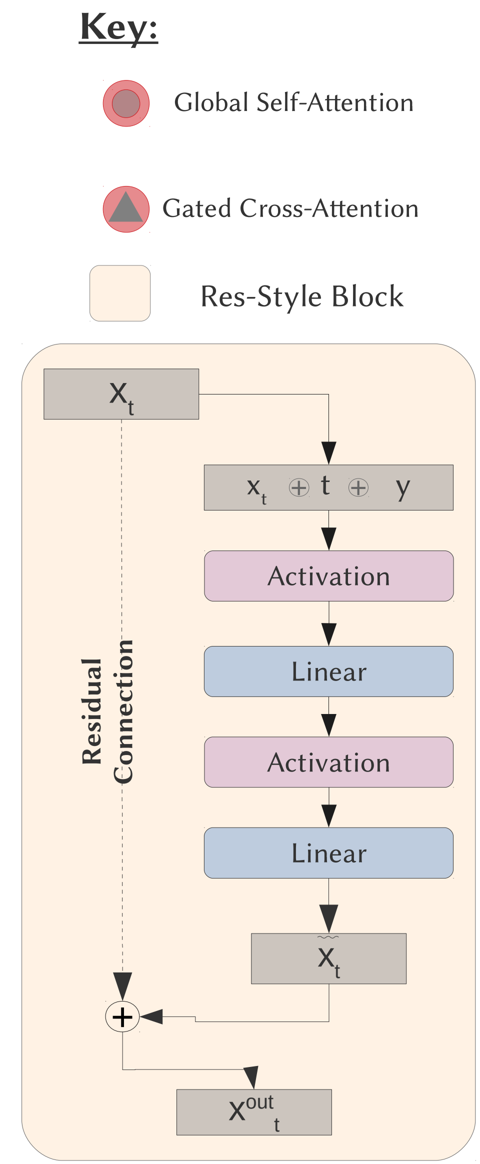
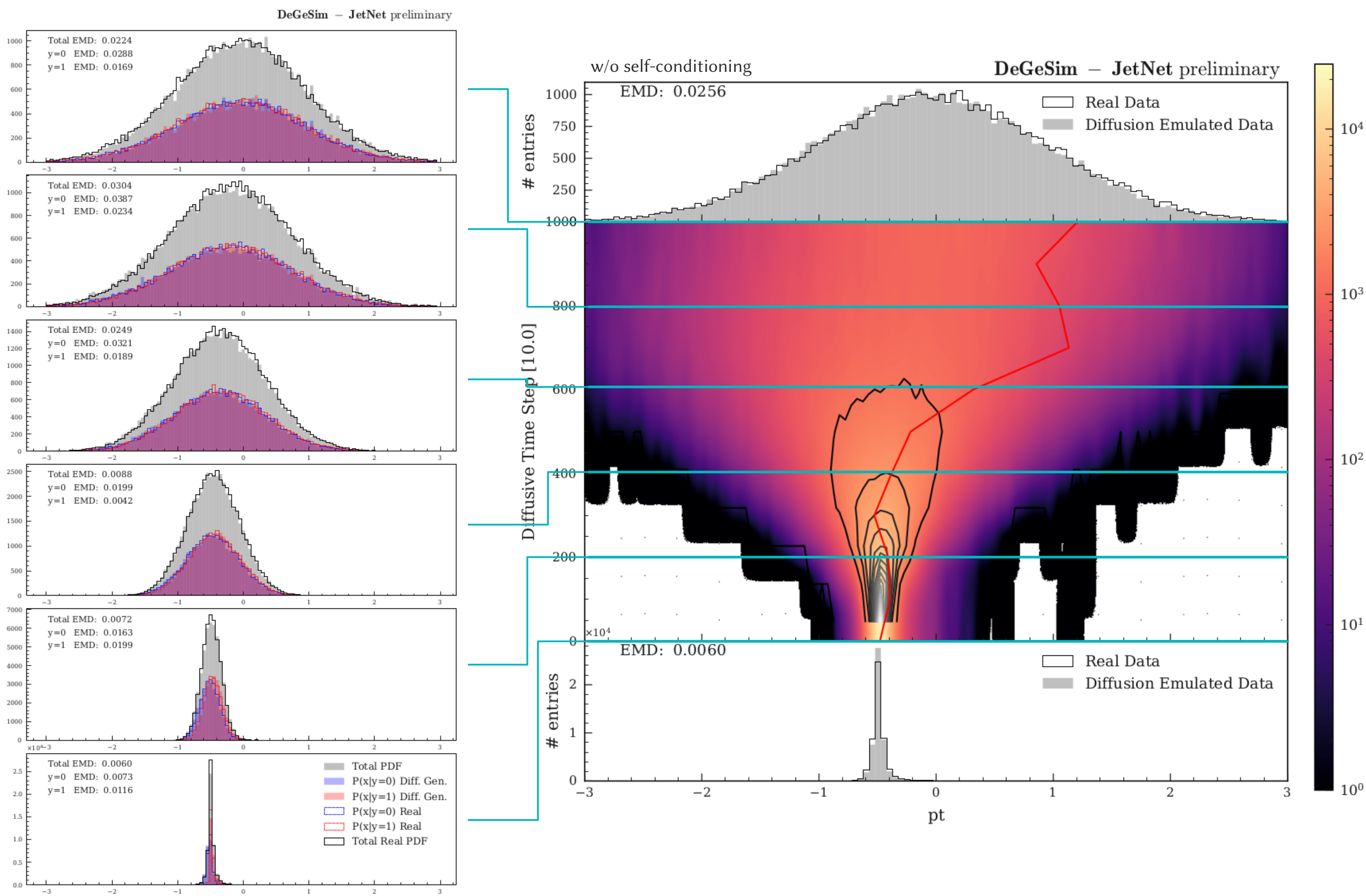




PDF Heat Map – Time Profile

w/ self-conditioning

JetNet: Top -vs- W jets



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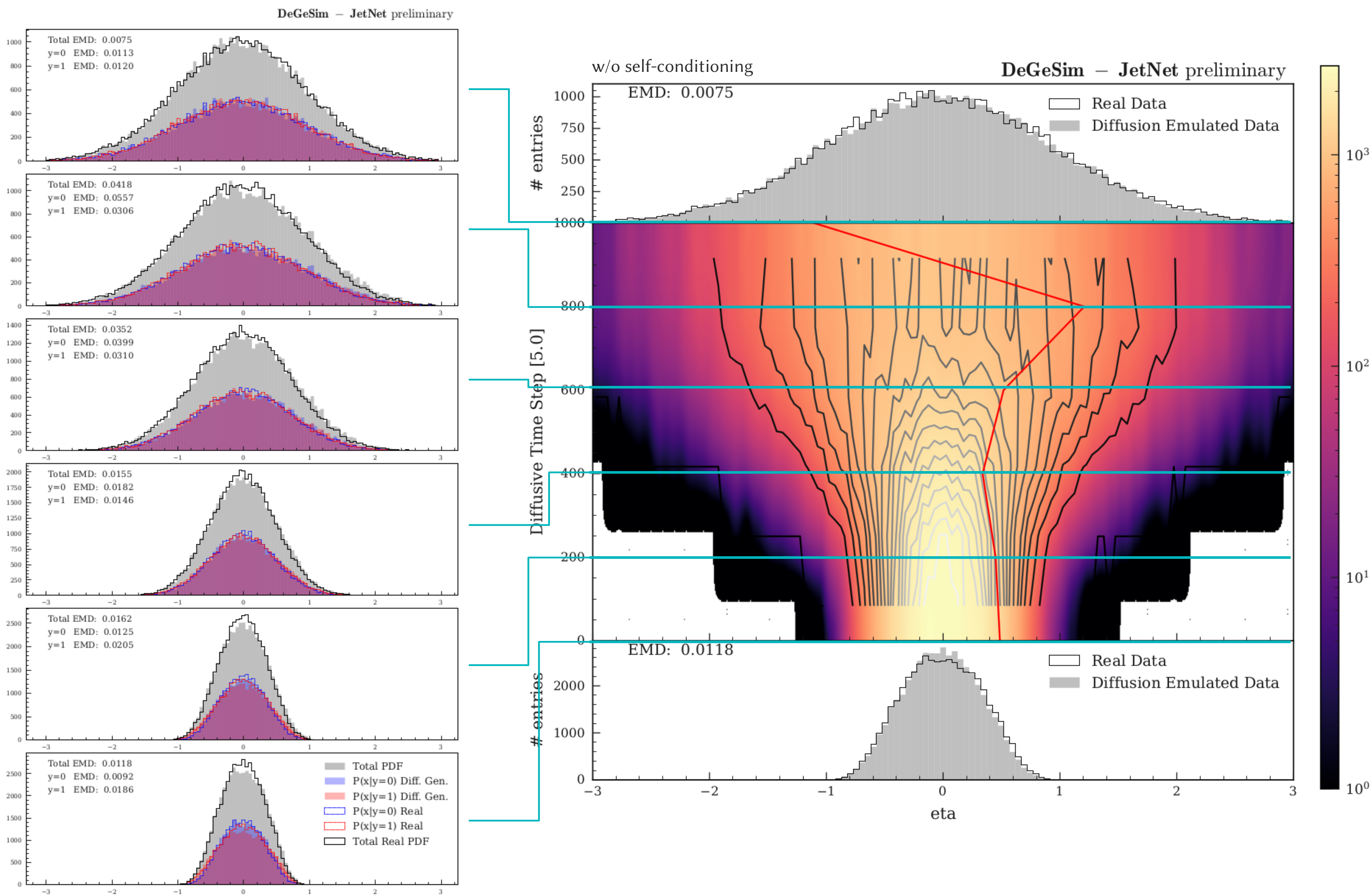

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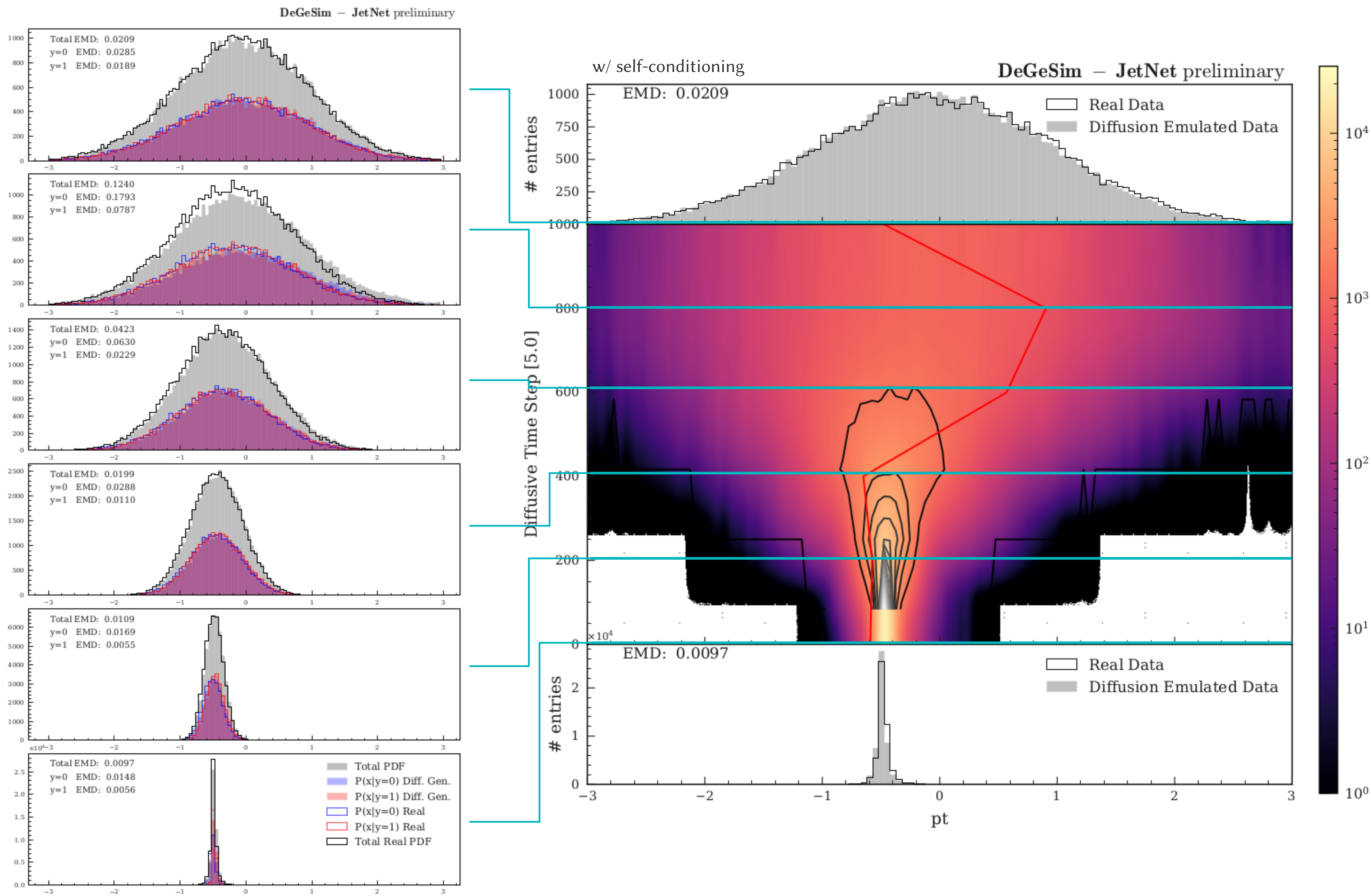

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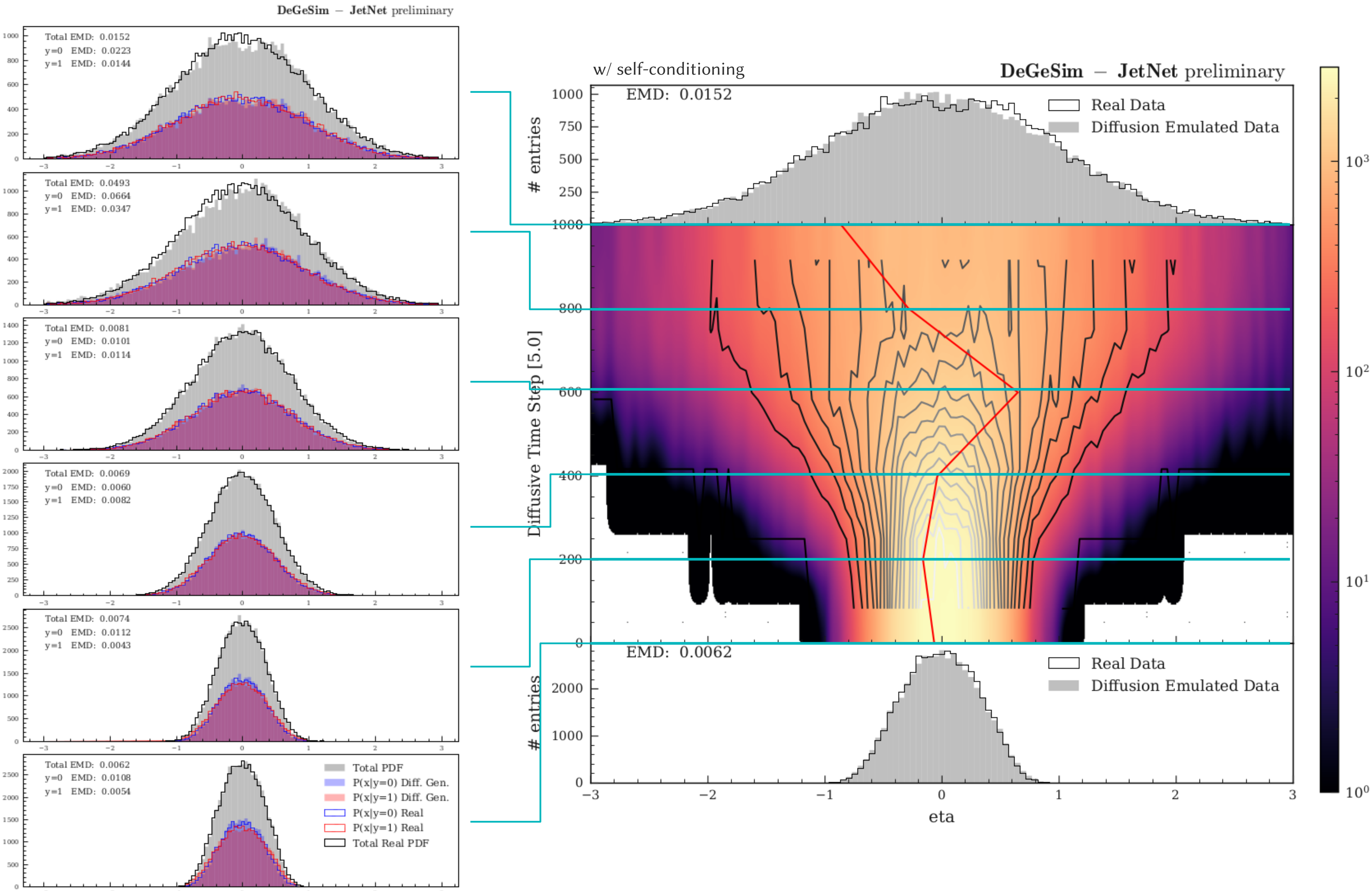
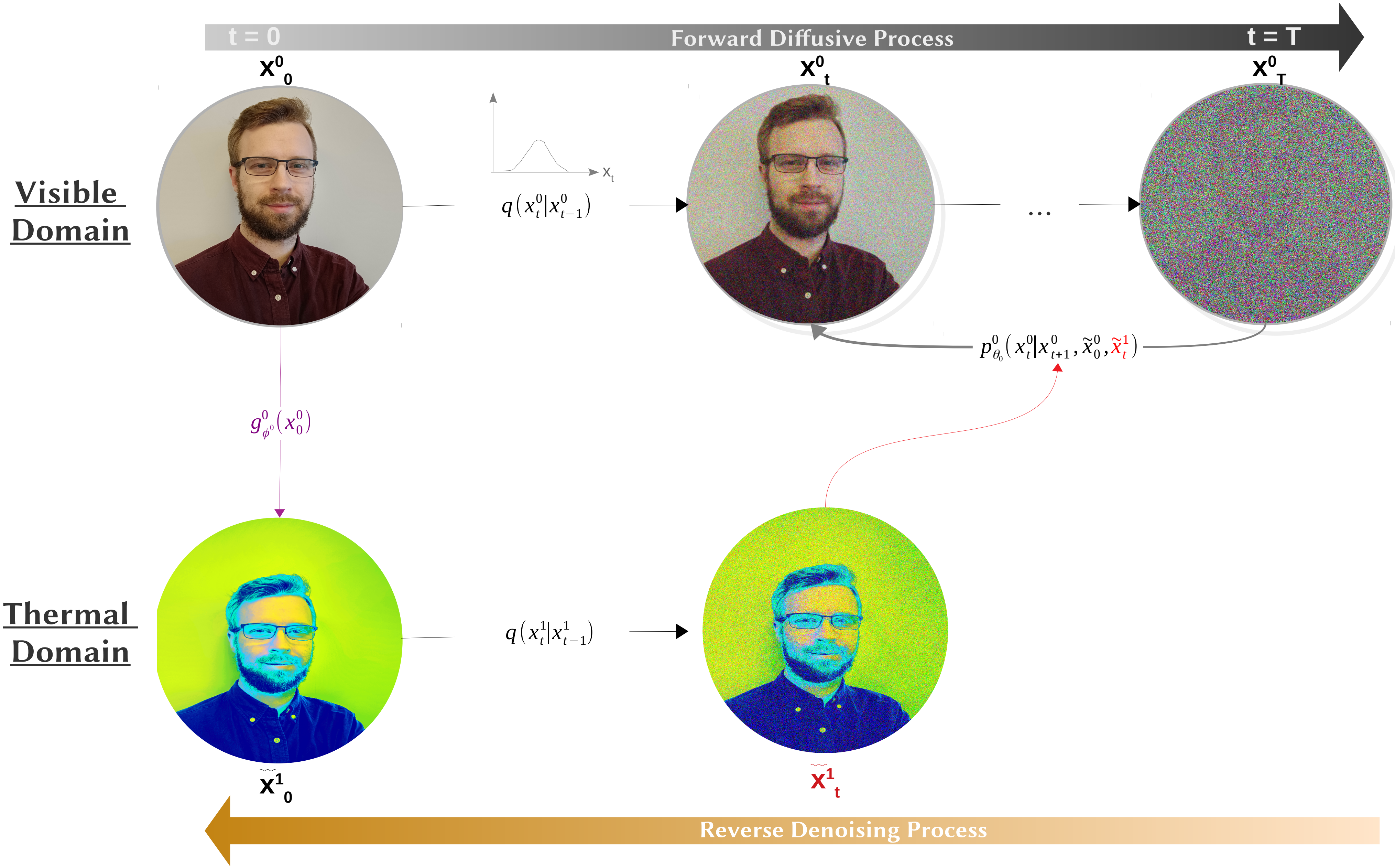


Cross Domain Attention

Unpaired Domain Adaptation DDPM - I2I



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