Example Application of Set/ Graph methods in HEP

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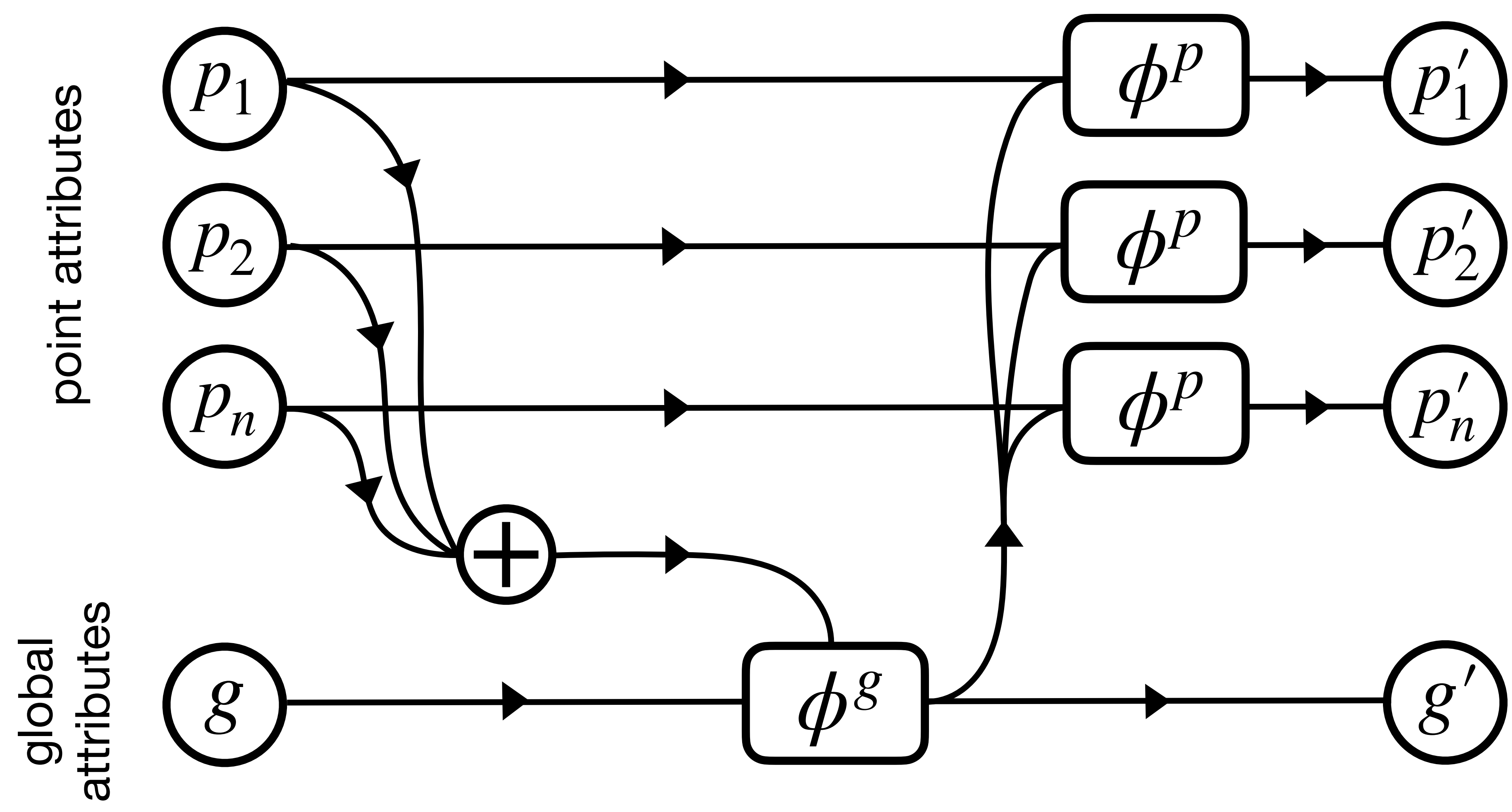
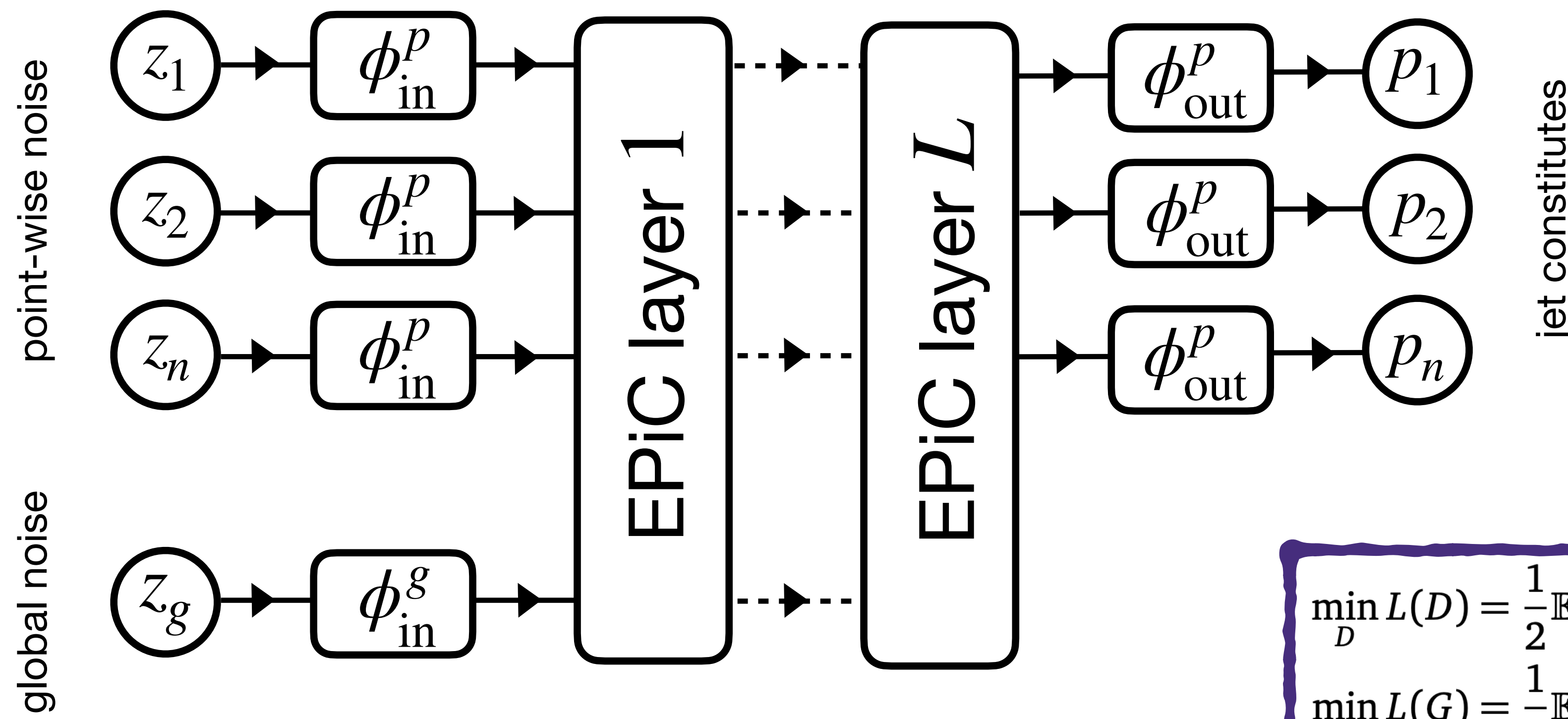
Point cloud generation

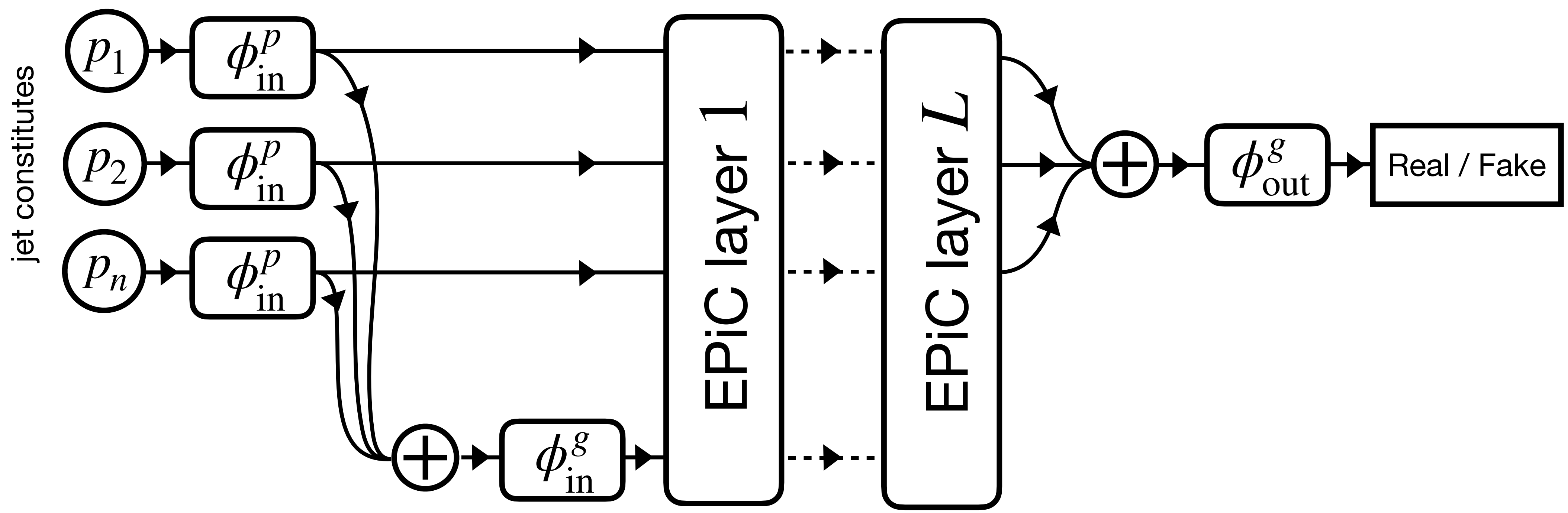
EPIC paper as an example : arXiv 2301.08128 / https://github.com/uhh-pd-ml/EPiC-GAN/tree/main



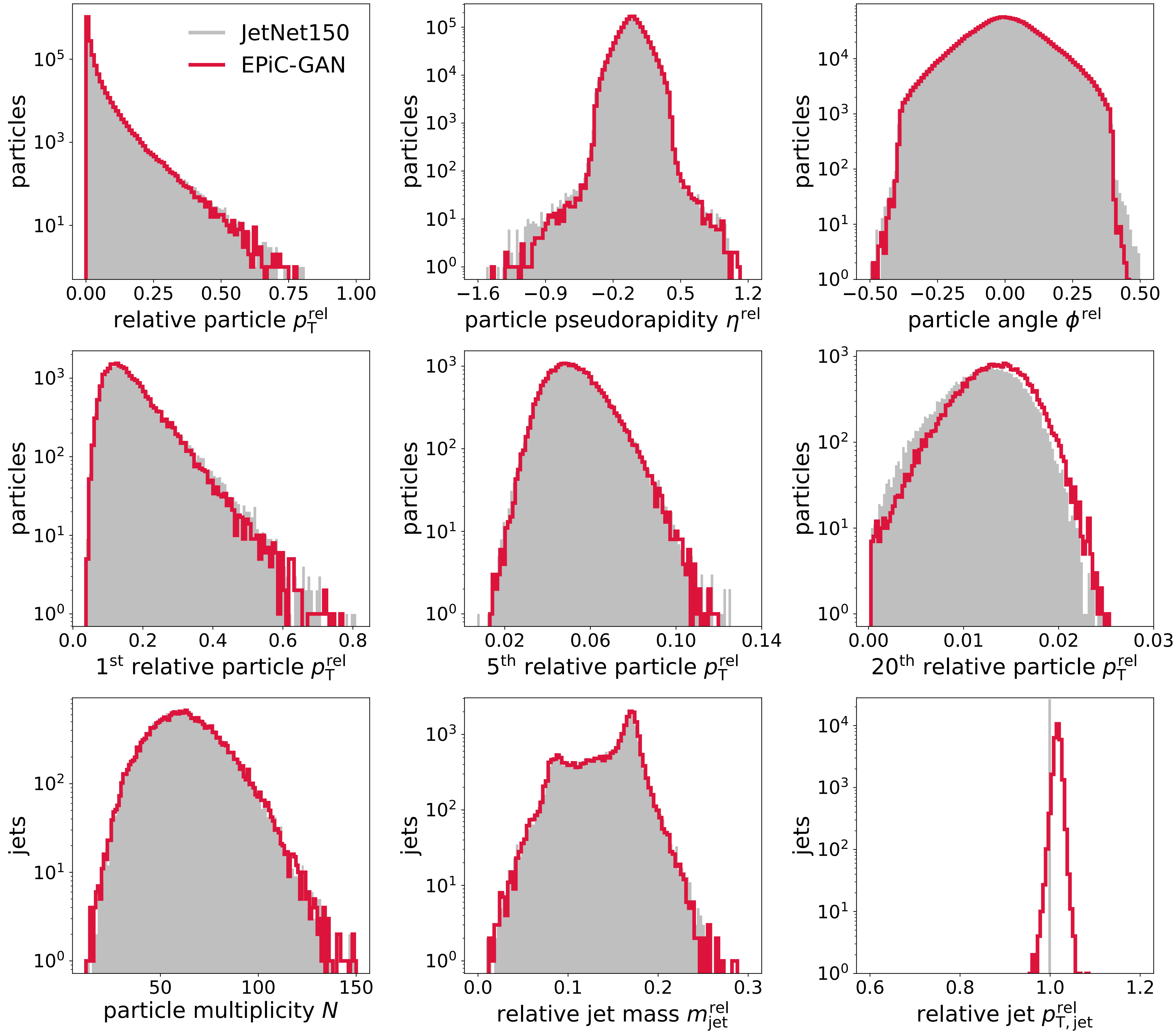
The generator and discriminator



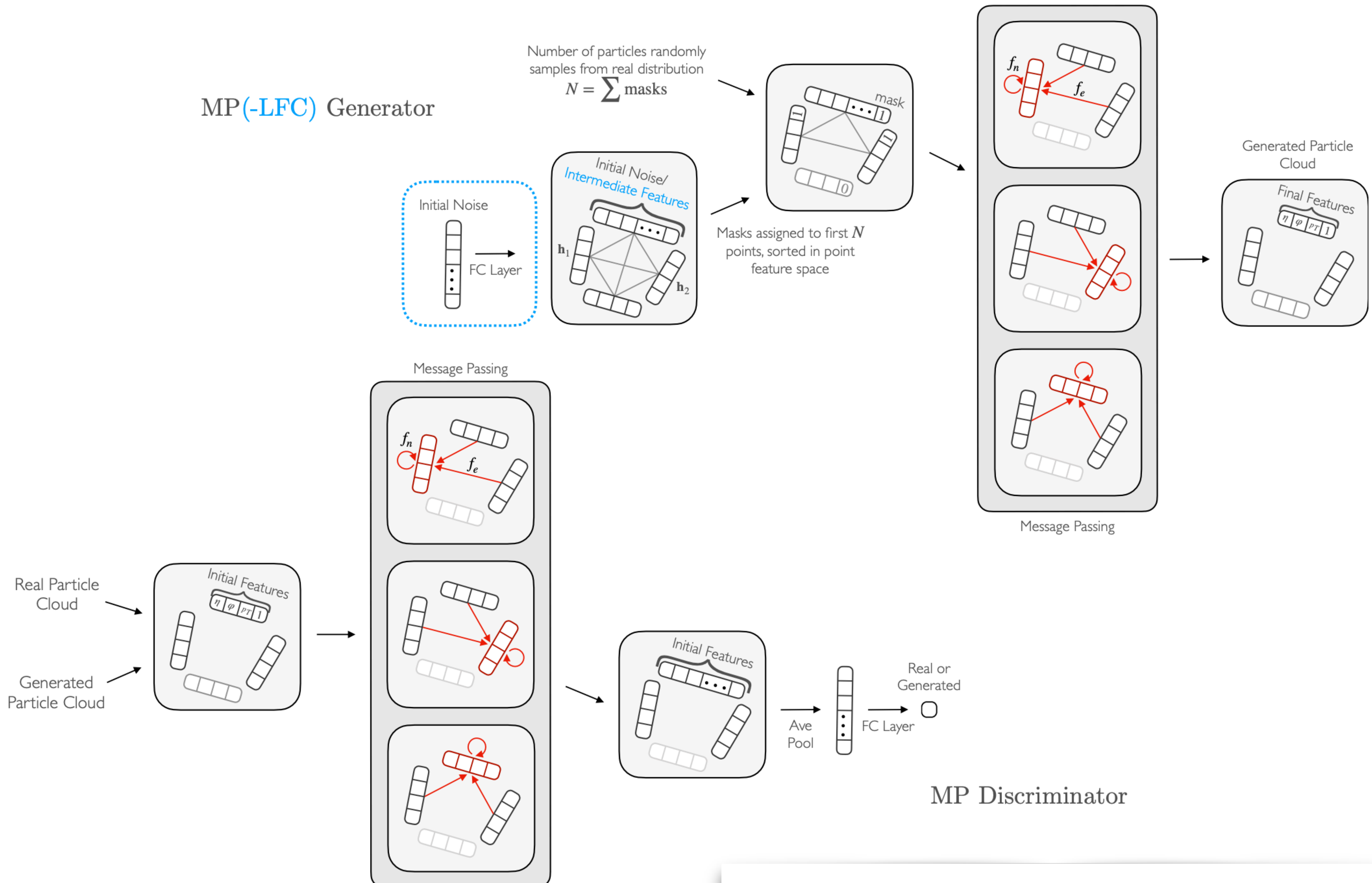
$$\min_D L(D) = \frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[(D(\boldsymbol{x})-1)^2] + \frac{1}{2}\mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[(D(G(\boldsymbol{z})))^2],$$
$$\min_G L(G) = \frac{1}{2}\mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[(D(G(\boldsymbol{z}))-1)^2].$$



The performance



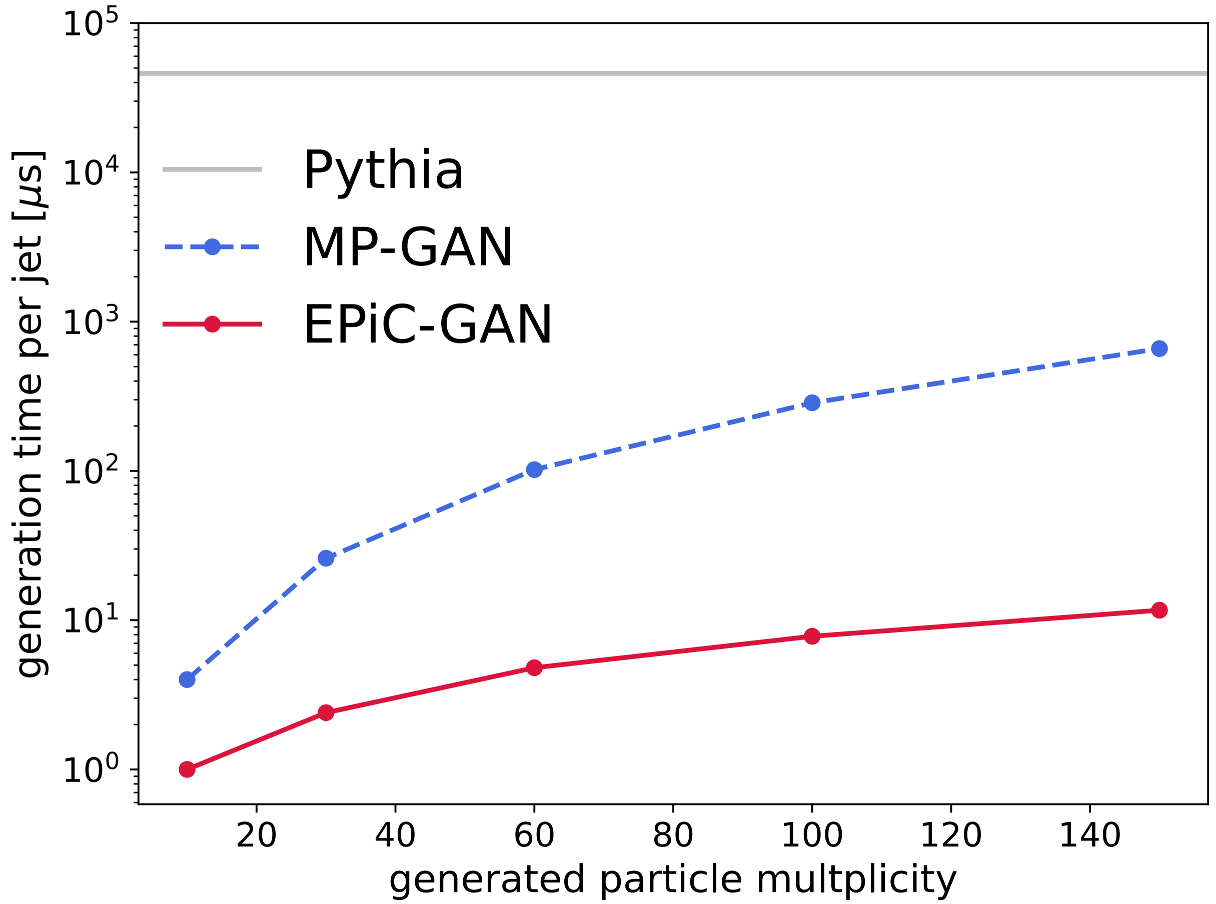
The MPGAN

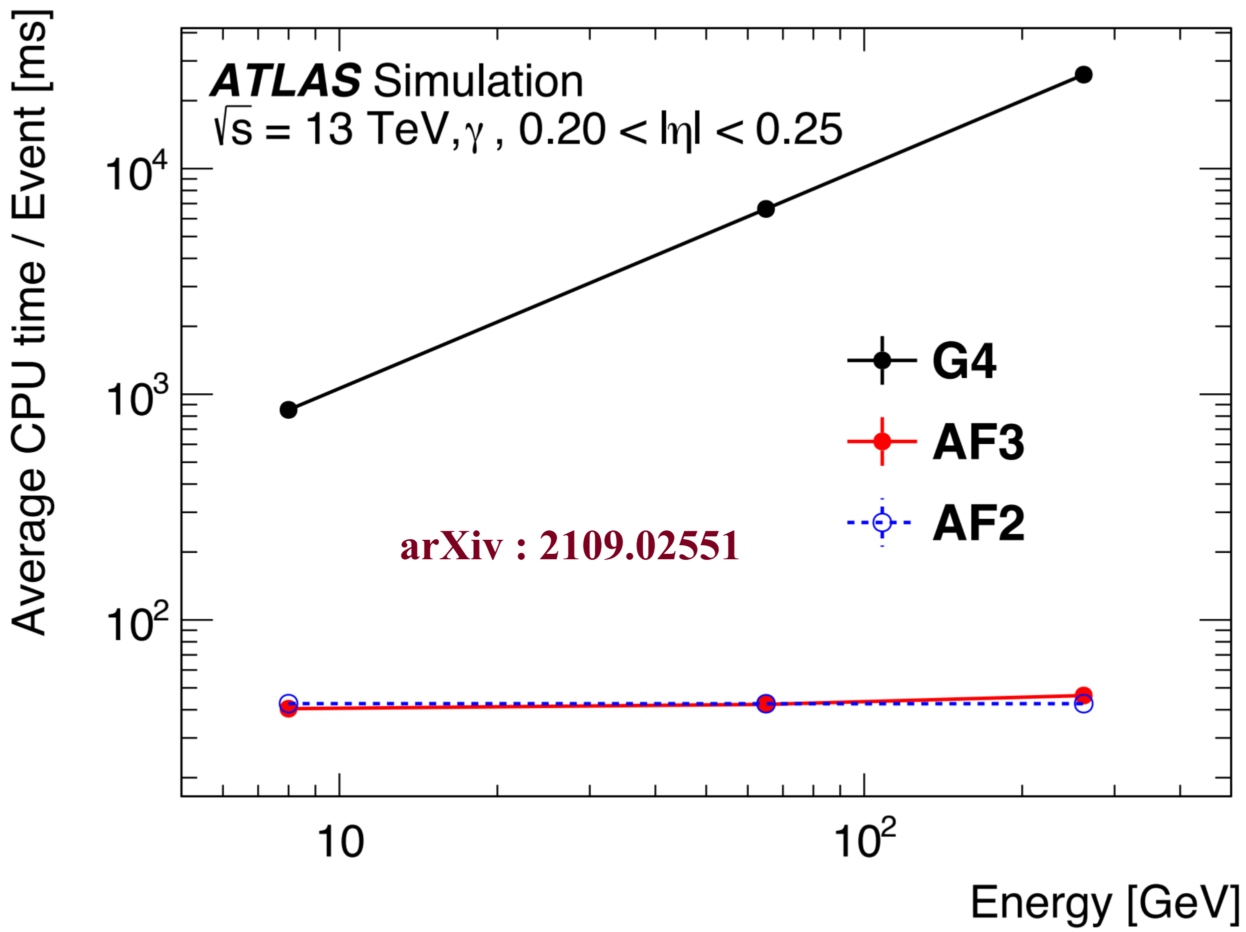


$$\mathbf{m}_{ij}^{t+1} = f_e^{t+1}(\mathbf{h}_i^t \oplus \mathbf{h}_j^t),$$

$$\mathbf{h}_i^{t+1} = f_n^{t+1}(\mathbf{h}_i^t \oplus \sum_{j \in J} \mathbf{m}_{ij}^{t+1}),$$

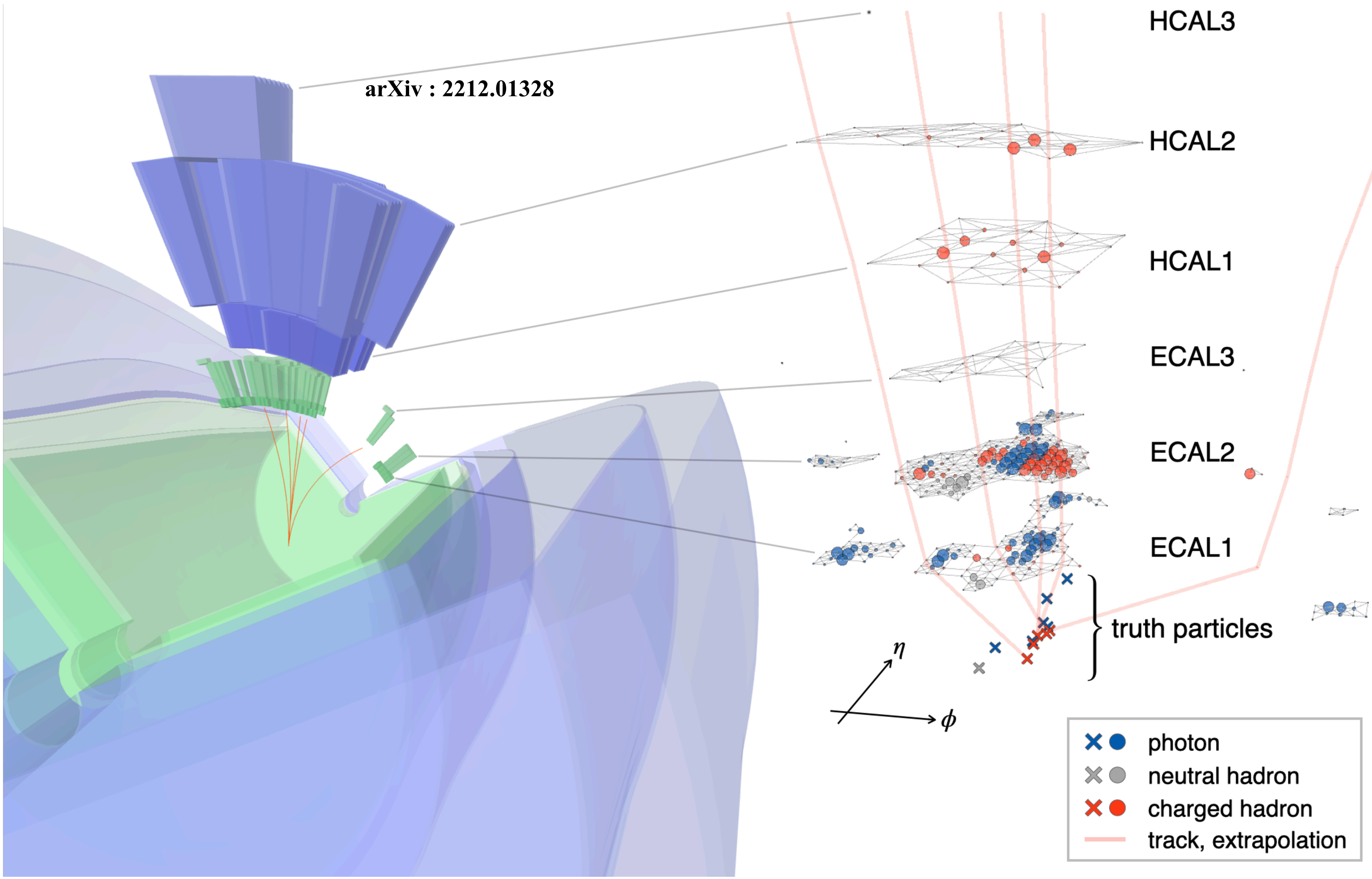
The major gain



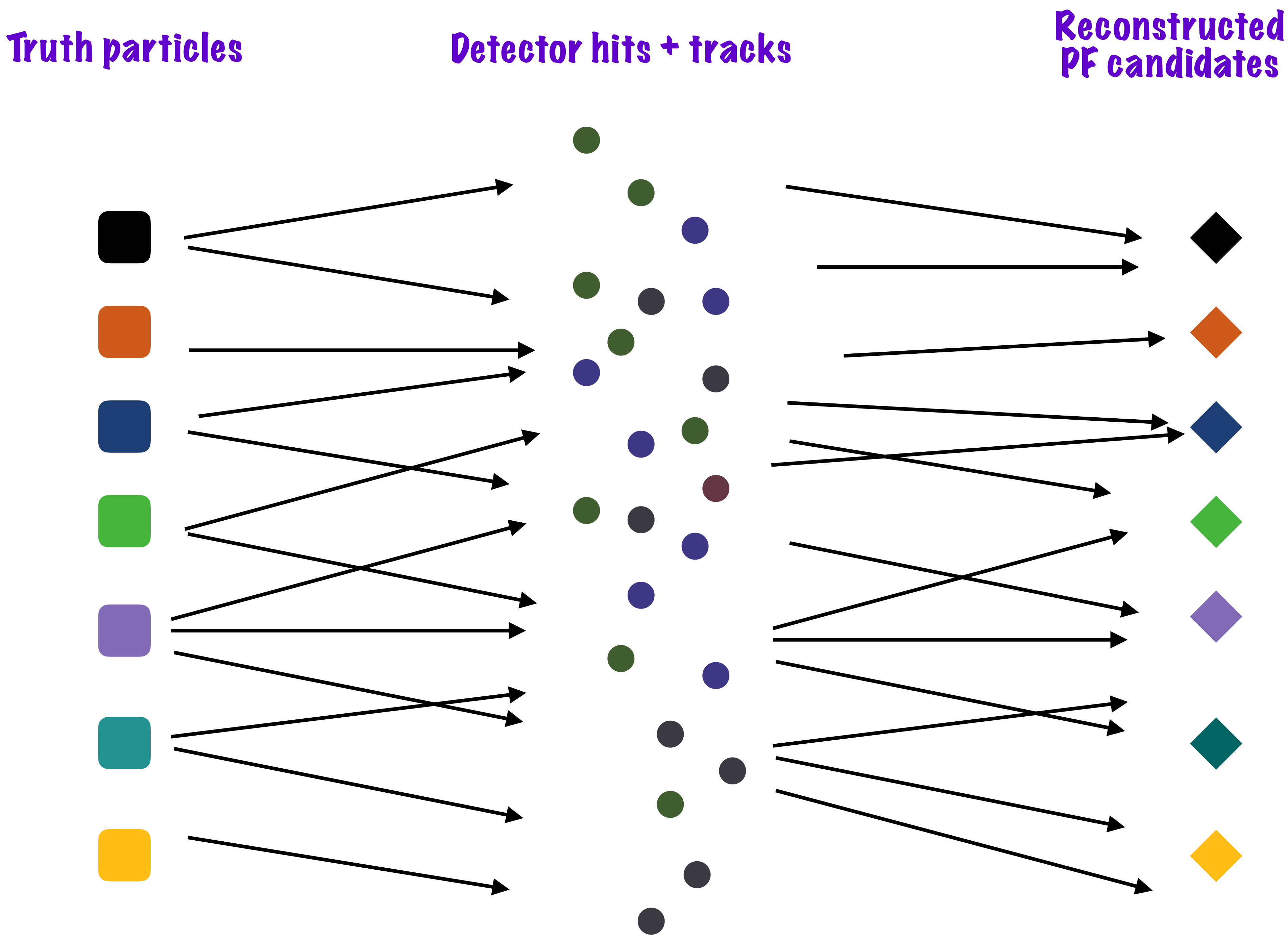


A sure shot motivations to use PC generative models for HEP used cases

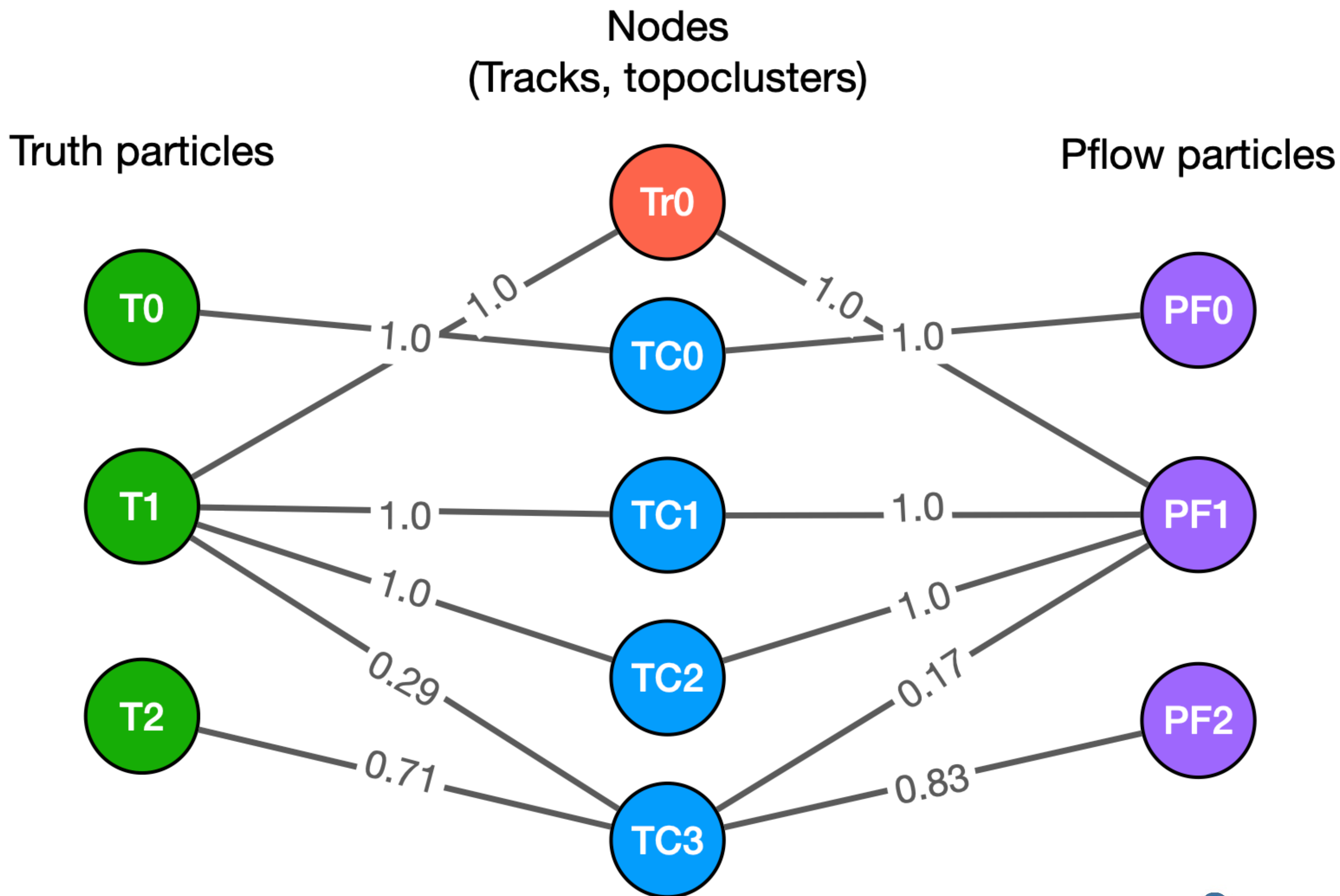
The PF reconstruction algorithm



What's the core data structure?

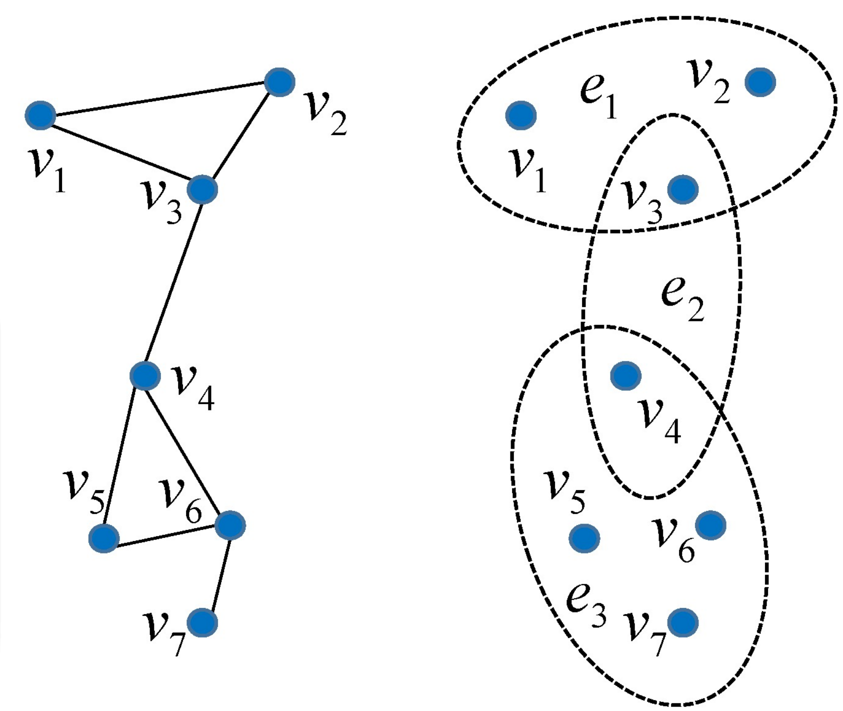


What’s the core data structure?



https://www.mdpi.com/2072-4292/9/5/506

Learning Flow is essentially learning the incidence matrix of a Hypergraph.

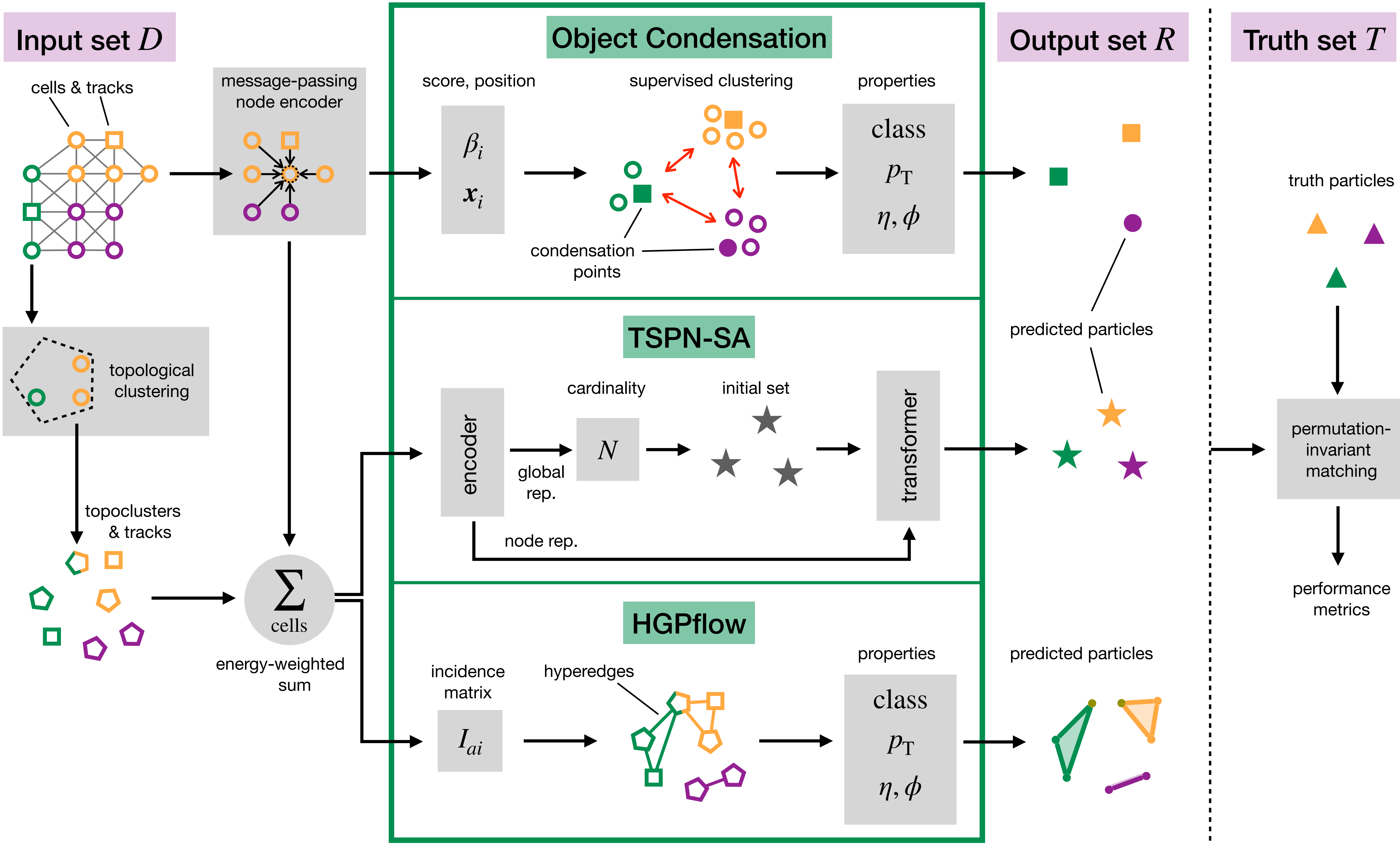


(a) Simple graph (b) Hypergraph **G**

	e_1	e_2	e_3
v_1	1	0	0
v_2	1	0	0
v_3	1	1	0
v_4	0	1	1
v_5	0	0	1
v_6	0	0	1
v_7	0	0	1

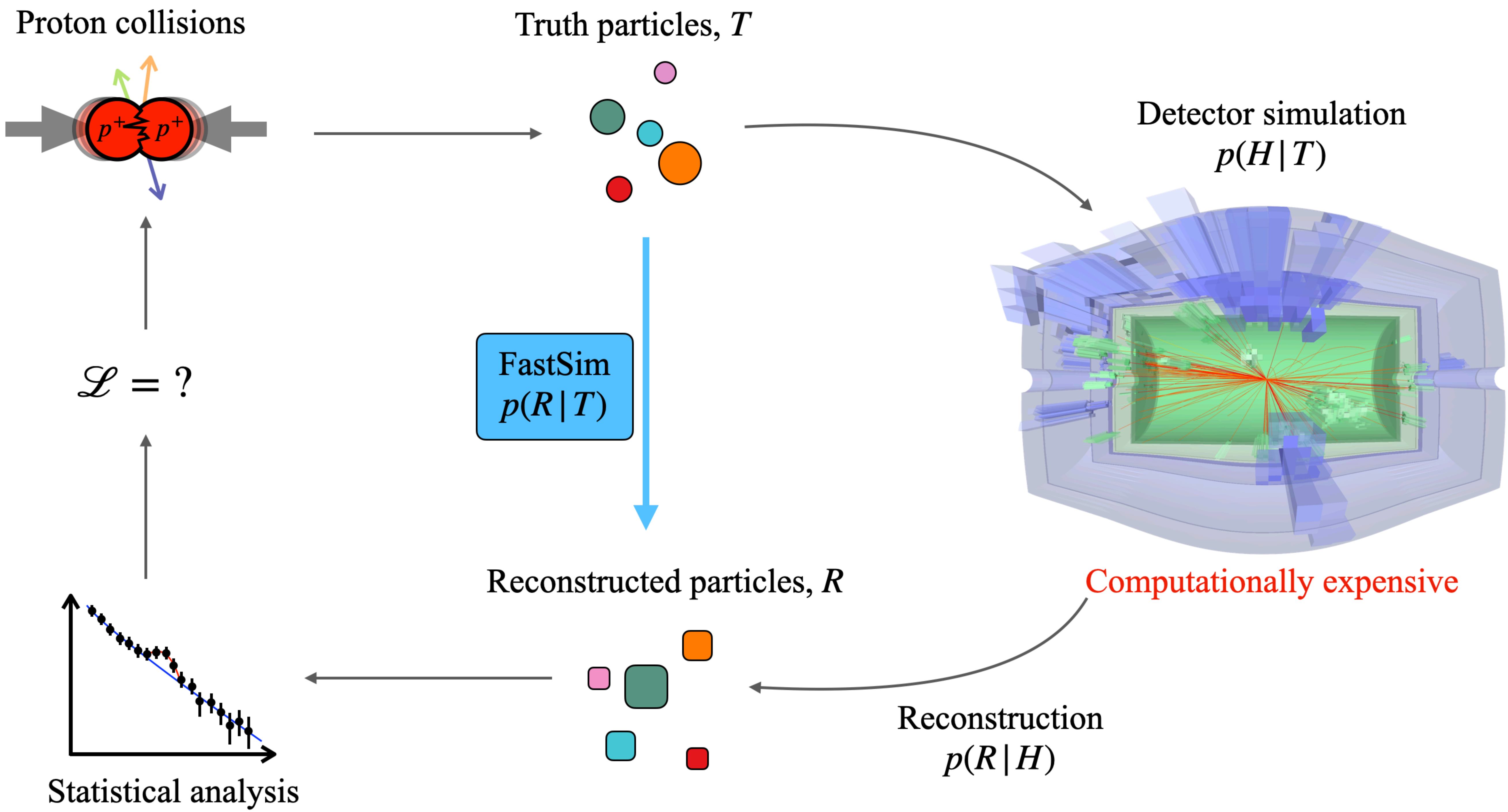
(c) Incidence matrix **H**

The network flow comparisons



A generative model for Flow

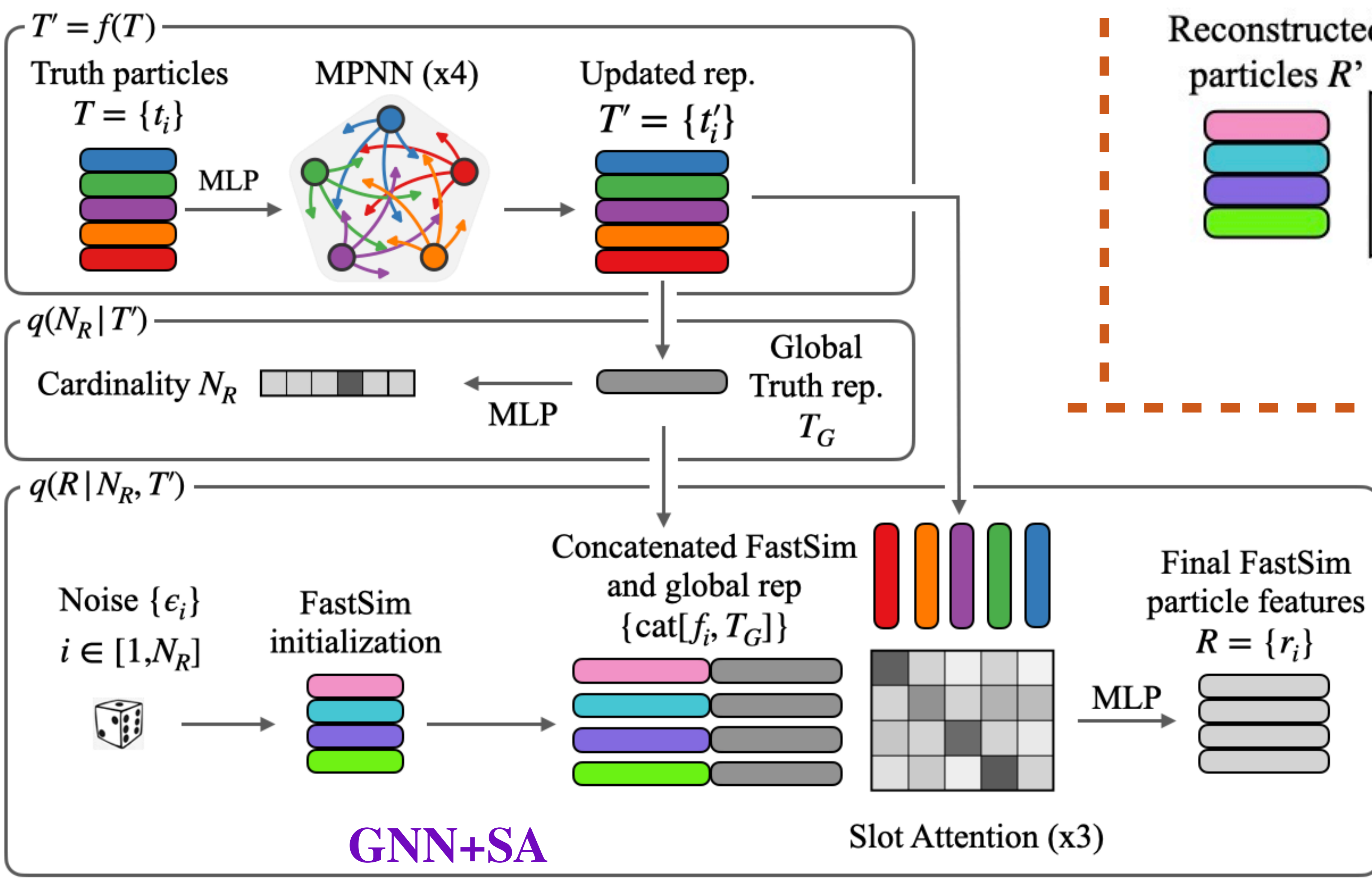
arXiv : 2211.06406

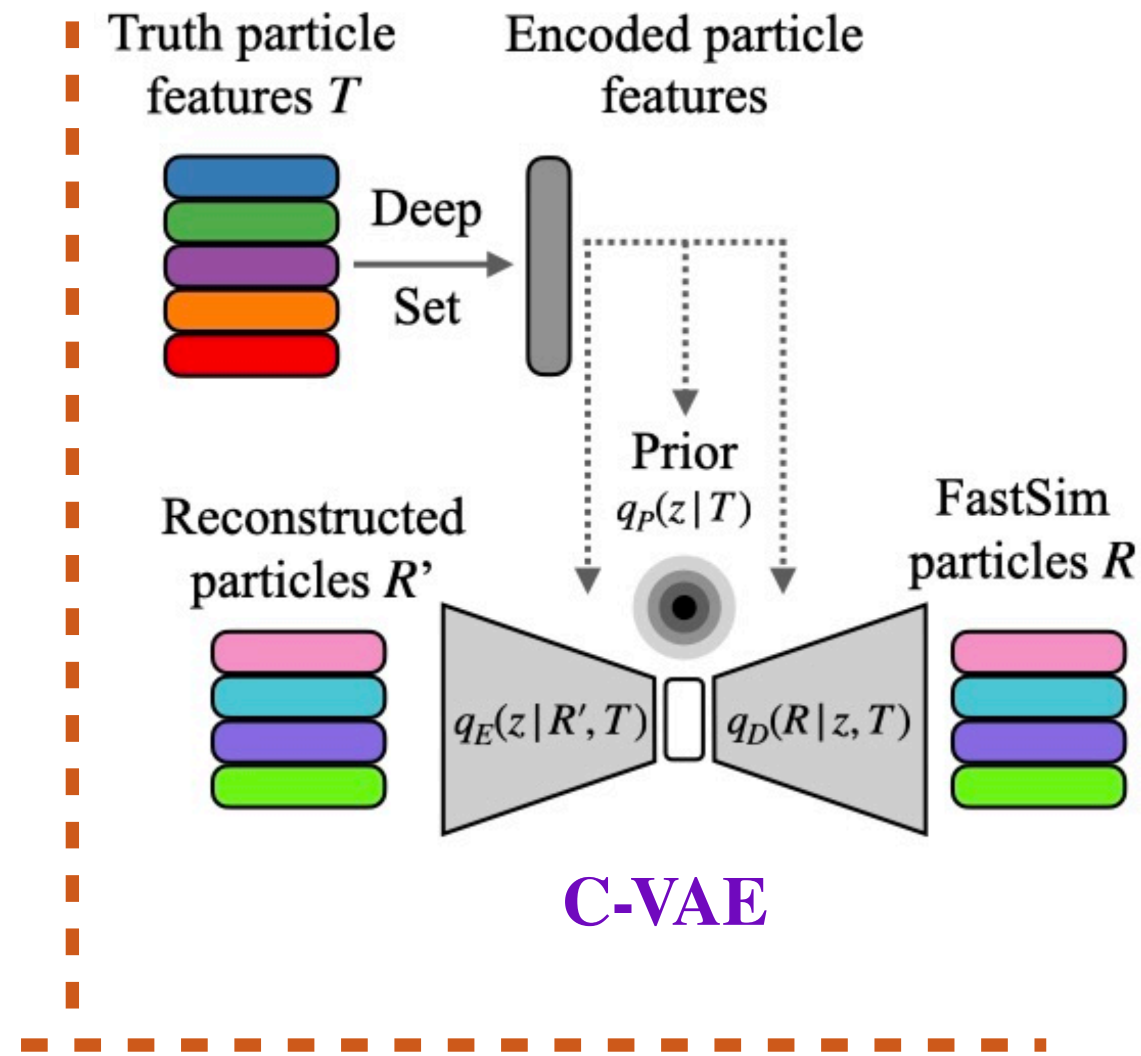


$$R \sim p(R|T) = \int \mathrm{d}H\, \delta(R(H) - R)\, p_{\mathrm{sim}}(H|T).$$

The task of constrained set generation

$$\mathbf{q}_{\theta}(\mathbf{R}\,|\,\mathbf{T}) \sim \mathbf{q}_{\theta_1}(\mathbf{N_R}\,|\,\mathbf{T})\mathbf{q}_{\theta_2}(\mathbf{R}\,|\,\mathbf{N_R},\mathbf{T})$$

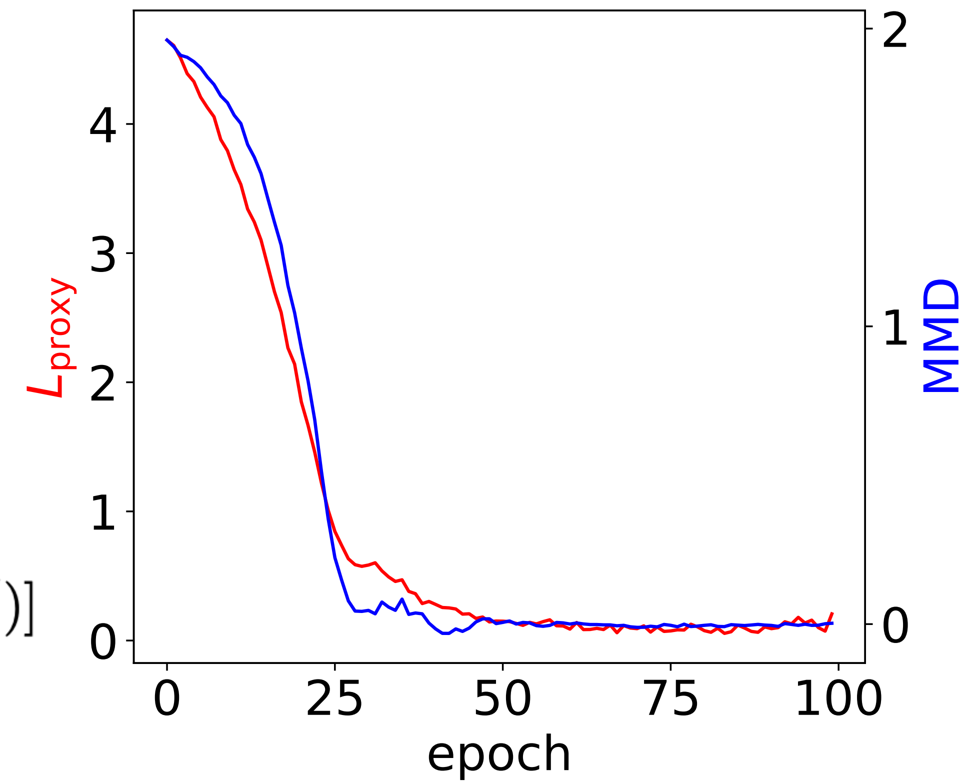




The task of constrained set generation

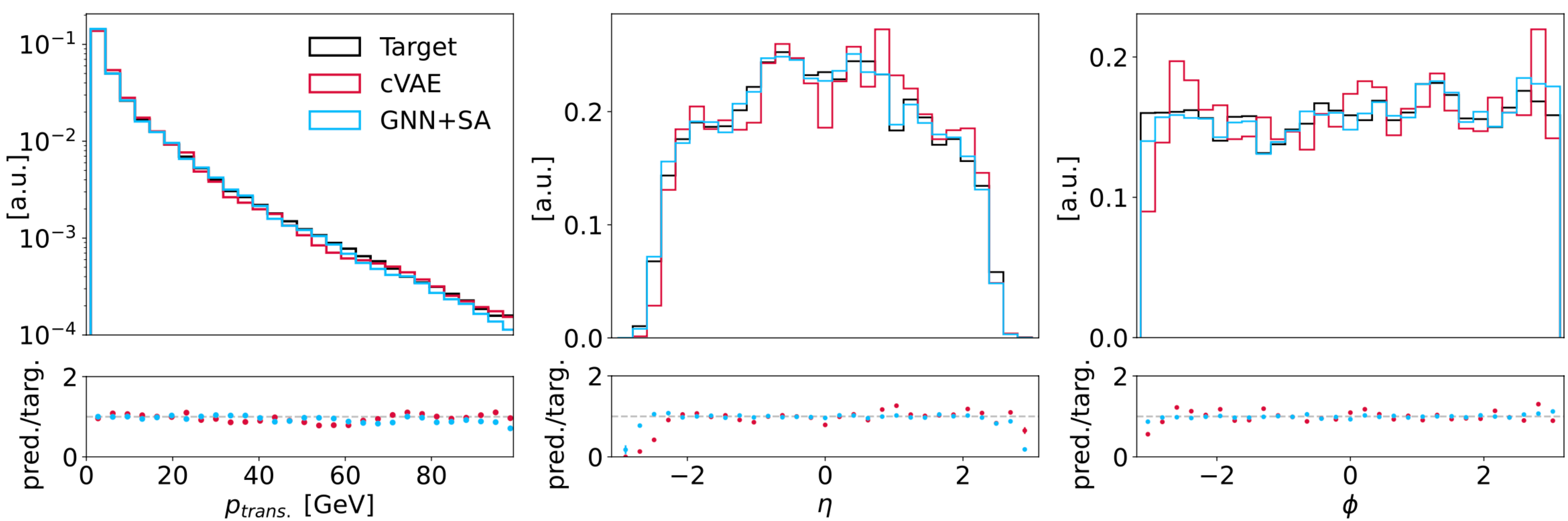
The cVAE training is done by optimizing negative evidence lower bound (ELBO) loss :

$$L = -\mathbb{E}_{T,R}\mathbb{E}_{z\sim q_E(z|R,T)} \log \frac{q_D(R|z,T)q_P(z|T)}{q_E(z|R,T)}$$
$$= -\mathbb{E}_{T,R}\mathbb{E}_z \log q_D(R|z,T) + D_{\mathrm{KL}}(q_E(z|R,T)||q_P(z|T))$$

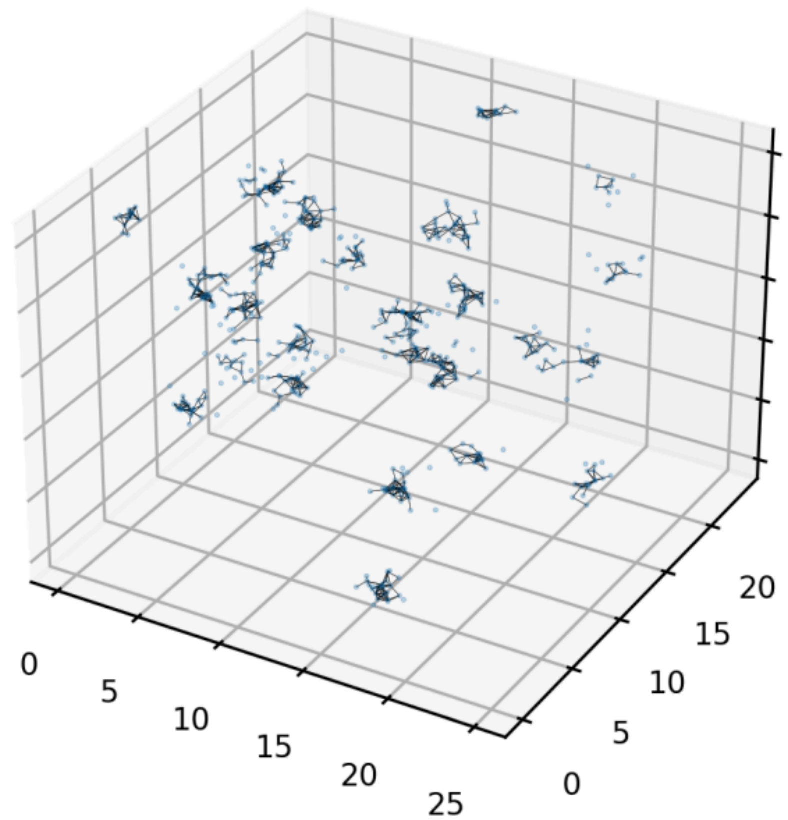


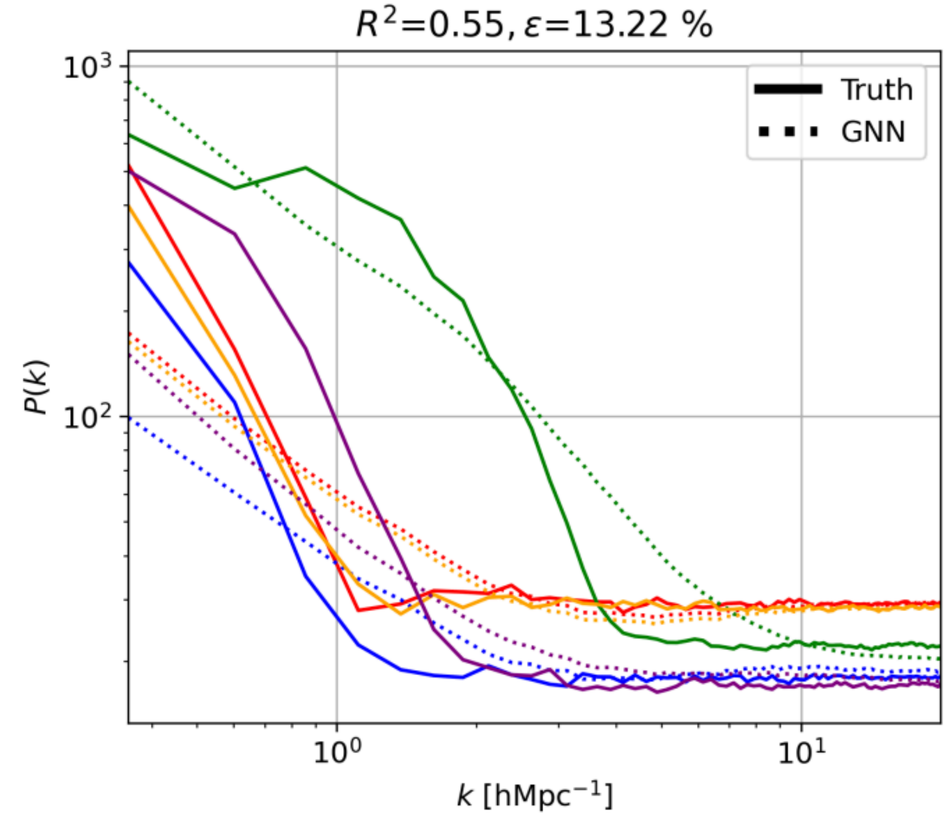
For GNN+SA, we try a regular Hungarian loss and also MMD (maximum mean discrepancy) :

$$\mathrm{MMD}^2 = \mathbb{E}_{(x\sim p,x'\sim p)}[k(x,x')] + \mathbb{E}_{(x\sim q,x'\sim q)}[k(x,x')] - 2\mathbb{E}_{(x\sim q,x'\sim p)}[k(x,x')]$$



GNN in other fields of physics





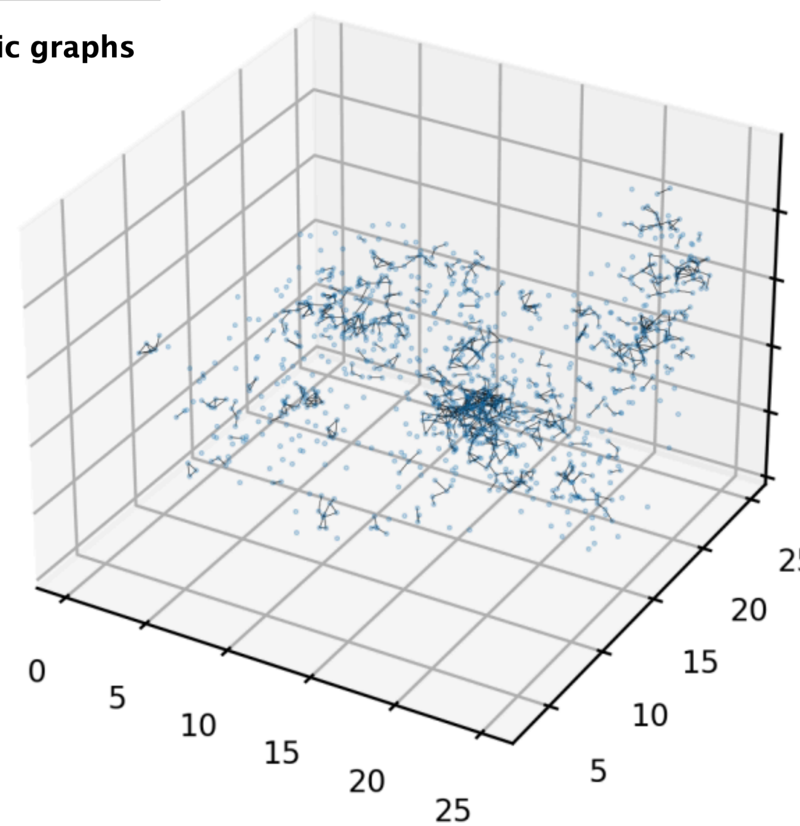
arXiv > astro-ph > arXiv:2204.13713

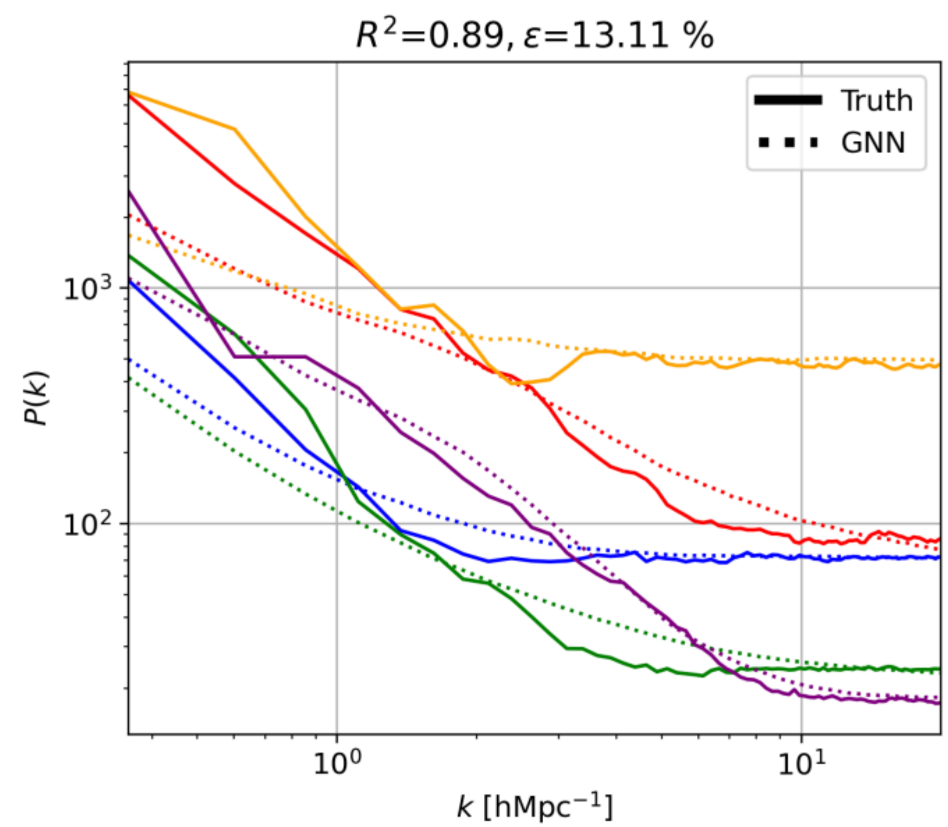
Astrophysics > Cosmology and Nongalactic Astrophysics

[Submitted on 28 Apr 2022 (v1), last revised 8 Feb 2023 (this version, v2)]

Learning cosmology and clustering with cosmic graphs

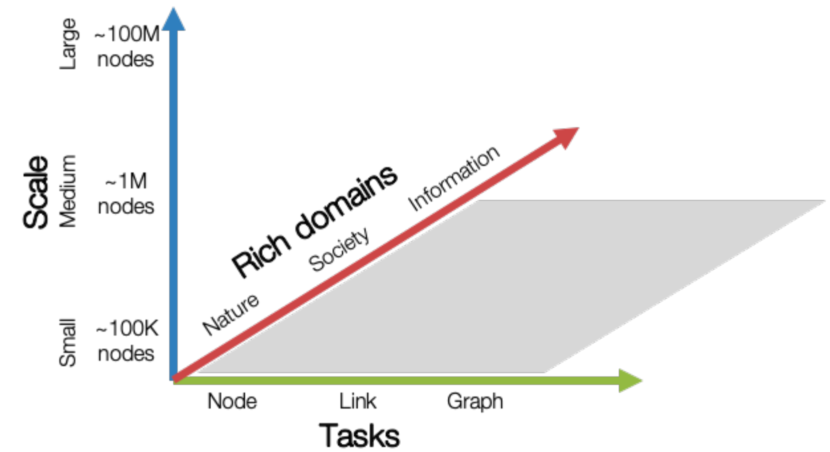
Pablo Villanueva-Domingo, Francisco Villaescusa-Navarro





Open software support

OPEN GRAPH BENCHMARK



PyG
torchgeometricco.slack.com

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PyTorch Geometric Tutorial Project

The PyTorch Geometric Tutorial project provides **video tutorials and Colab notebooks** for a variety of different methods in PyG:

1. Introduction [YouTube, Colab]
2. PyTorch basics [YouTube, Colab]
3. Graph Attention Networks (GATs) [YouTube, Colab]
4. Spectral Graph Convolutional Layers [YouTube, Colab]
5. Aggregation Functions in GNNs [YouTube, Colab]
6. (Variational) Graph Autoencoders (GAE and VGAE) [YouTube, Colab]
7. Adversarially Regularized Graph Autoencoders (ARGA and ARGVA) [YouTube, Colab]
8. Graph Generation [YouTube]
9. Recurrent Graph Neural Networks [YouTube, Colab (Part 1), Colab (Part 2)]
10. DeepWalk and Node2Vec [YouTube (Theory), YouTube (Practice), Colab]
11. Edge analysis [YouTube, Colab (Link Prediction), Colab (Label Prediction)]
12. Data handling in PyG (Part 1) [YouTube, Colab]
13. Data handling in PyG (Part 2) [YouTube, Colab]
14. MetaPath2vec [YouTube, Colab]
15. Graph pooling (DiffPool) [YouTube, Colab]

DEEP GRAPH LIBRARY

DGL
deep-graph-library.slack.com

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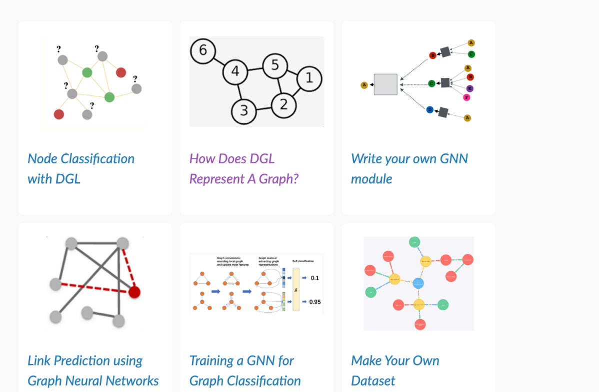
A Blitz Introduction to DGL



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