

# HGPflow: Particle flow as a Hypergraph learning task

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*On behalf of the HGPflow team*

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# Reconstructing particles in jets using set transformer and hypergraph prediction networks

**Francesco Armando Di Bello**<sup>1,a</sup>, **Etienne Dreyer**<sup>2,b</sup>, **Sanmay Ganguly**<sup>3</sup>, **Eilam Gross**<sup>2</sup>,  
**Lukas Heinrich**<sup>4</sup>, **Anna Ivina**<sup>2</sup>, **Marumi Kado**<sup>5,6</sup>, **Nilotpall Kakati**<sup>2,c</sup>, **Lorenzo Santi**<sup>6</sup>,  
**Jonathan Shlomi**<sup>2</sup>, **Matteo Tusoni**<sup>6</sup>

<sup>1</sup> INFN and University of Genova

<sup>2</sup> Weizmann Institute of Science

<sup>3</sup> ICEPP, University of Tokyo

<sup>4</sup> Technical University of Munich

<sup>5</sup> Max Planck Institute for Physics

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Received: date / Accepted: date

<https://arxiv.org/pdf/2212.01328.pdf>

# Reconstructing particles in jets using set transformer and hypergraph prediction networks

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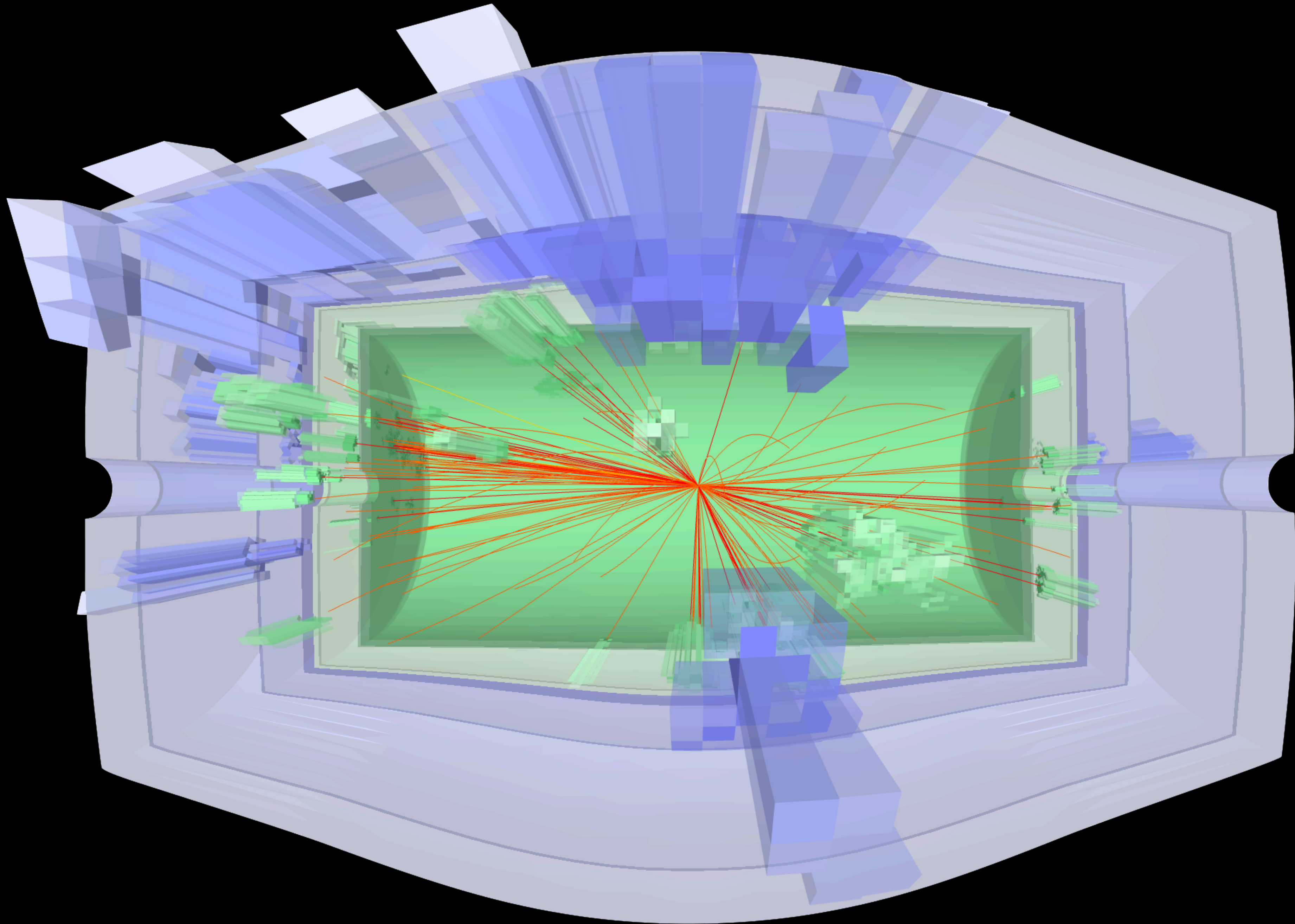
<https://arxiv.org/pdf/2212.01328.pdf>

- Focus on **Hypergraph (HGPflow)**

# The roadmap...

- Dataset
- The Hyper graph approach (HGPflow)
- Performance
- Future work





# COCOA

- **C**onfigurable **Cal**Orimeter simulation for **A**I

- ✓ Open source

- ✓ PYTHIA8-GEANT4

- ✓ Nearly hermetic

- ✓ Easily configurable (json)

- 3 ECAL layers, 3 HCAL layers

- Inner tracker immersed in magnetic field

- **U**ser friendly **o**utput

- ✓ Track, cells, topoclusters, truth particles

- ✓ Full truth record of energy deposit

- ✓ Jet clustering

- ✓ Nearest neighbor graph

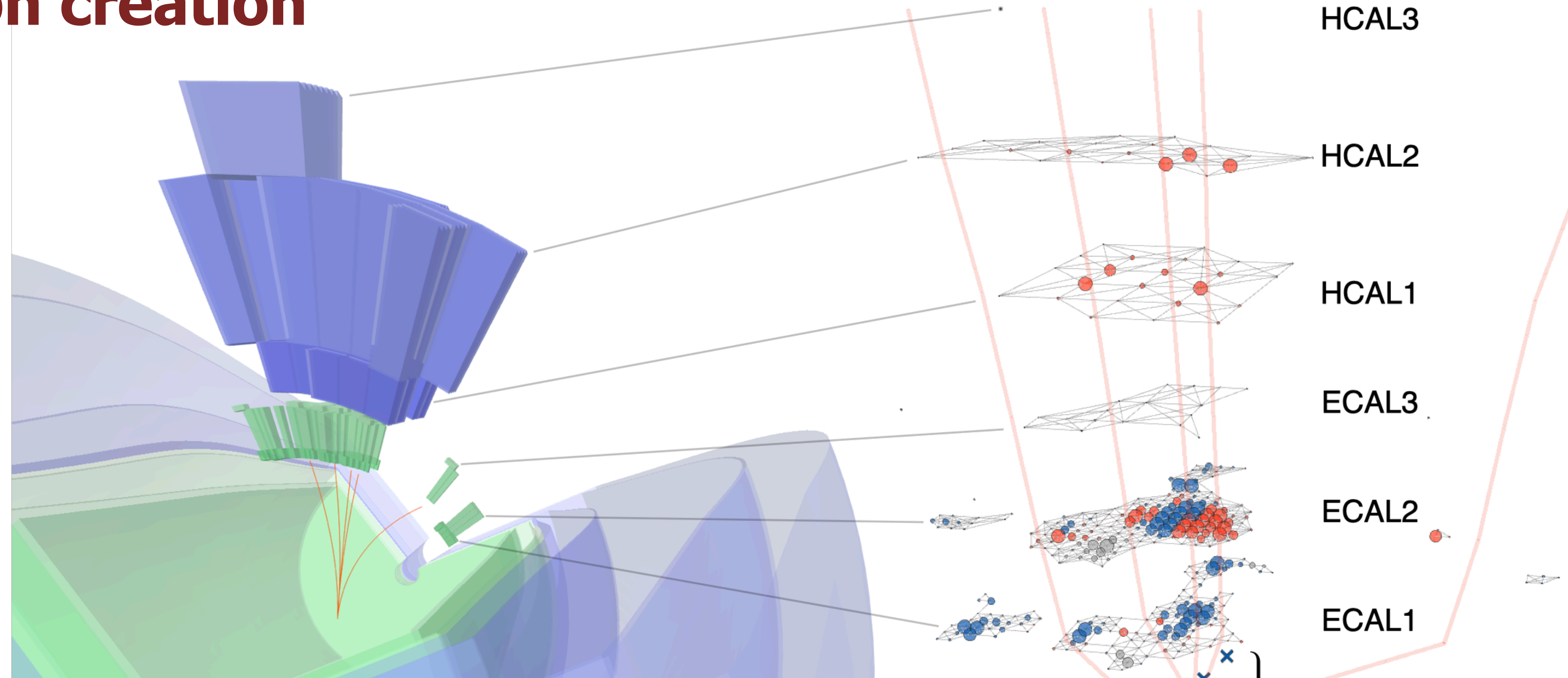


<https://arxiv.org/abs/2303.02101>

[Read the doc link](#)



# Graph creation

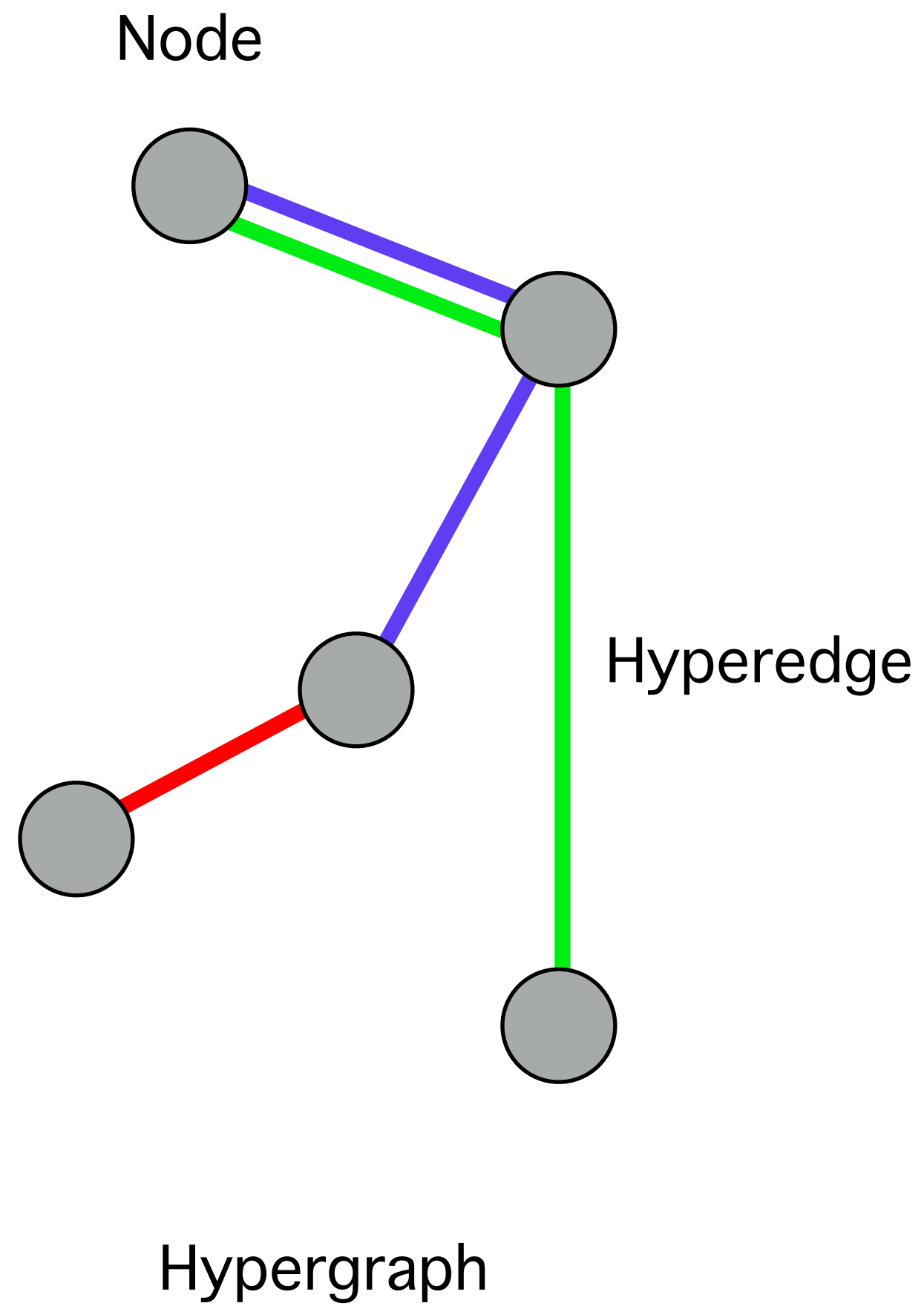


- **Focusing on dense environment**
  - Challenging, but also the building block for full event Pflow
- Single jet (quark/gluon initiated)
- No pileup

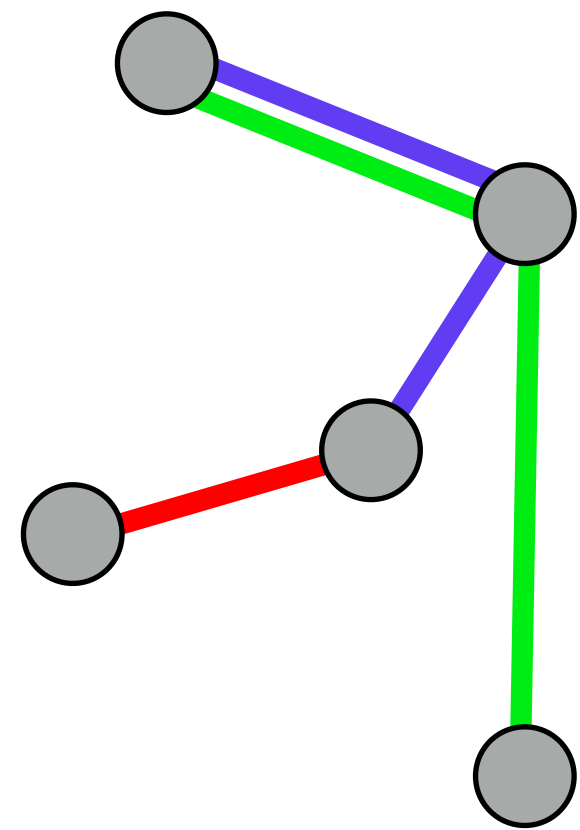
⊗ ●	photon
⊗ ●	neutral hadron
⊗ ●	charged hadron
—	track, extrapolation

# Hypergraphs?

# Hypergraph 101

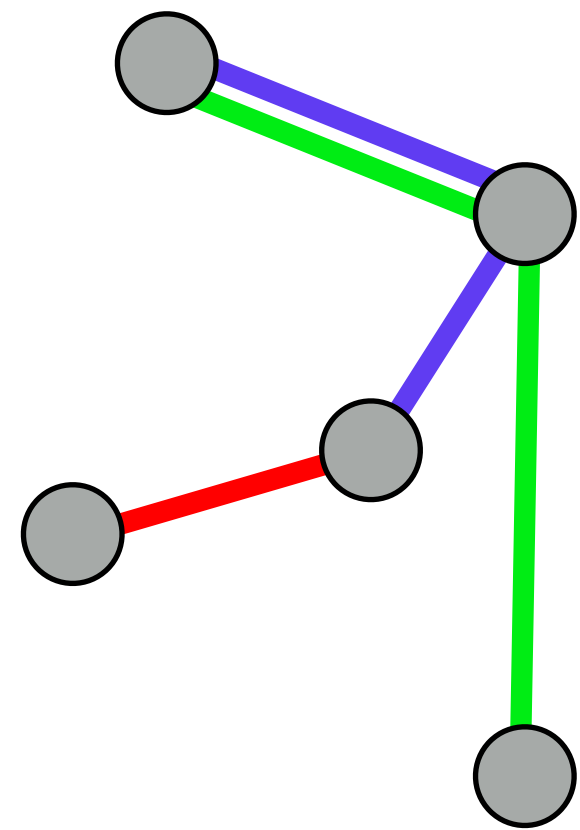


# Hypergraph 101



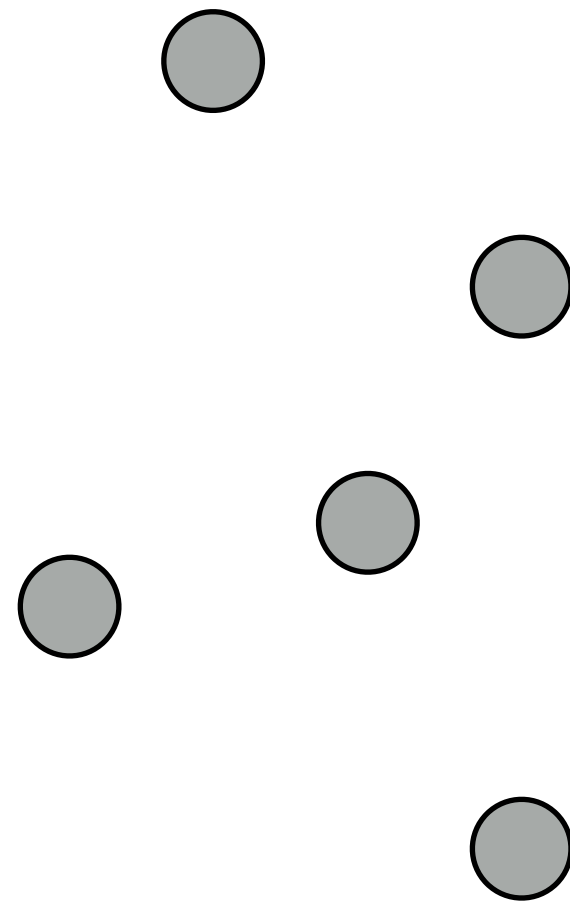
Hypergraph

# Hypergraph 101

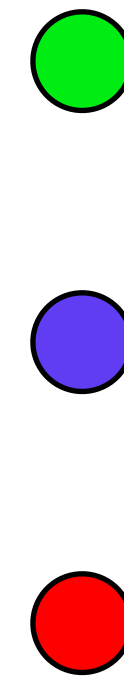


Hypergraph

Nodes

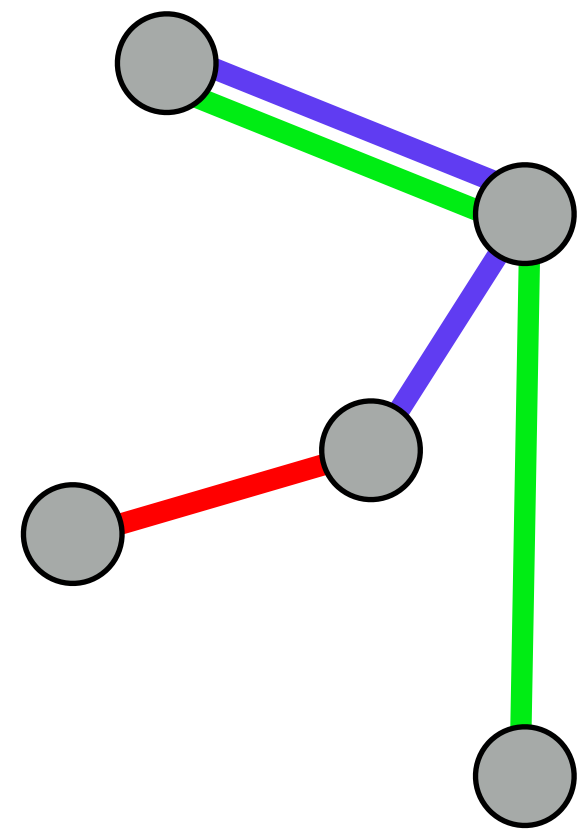


Hyperedges

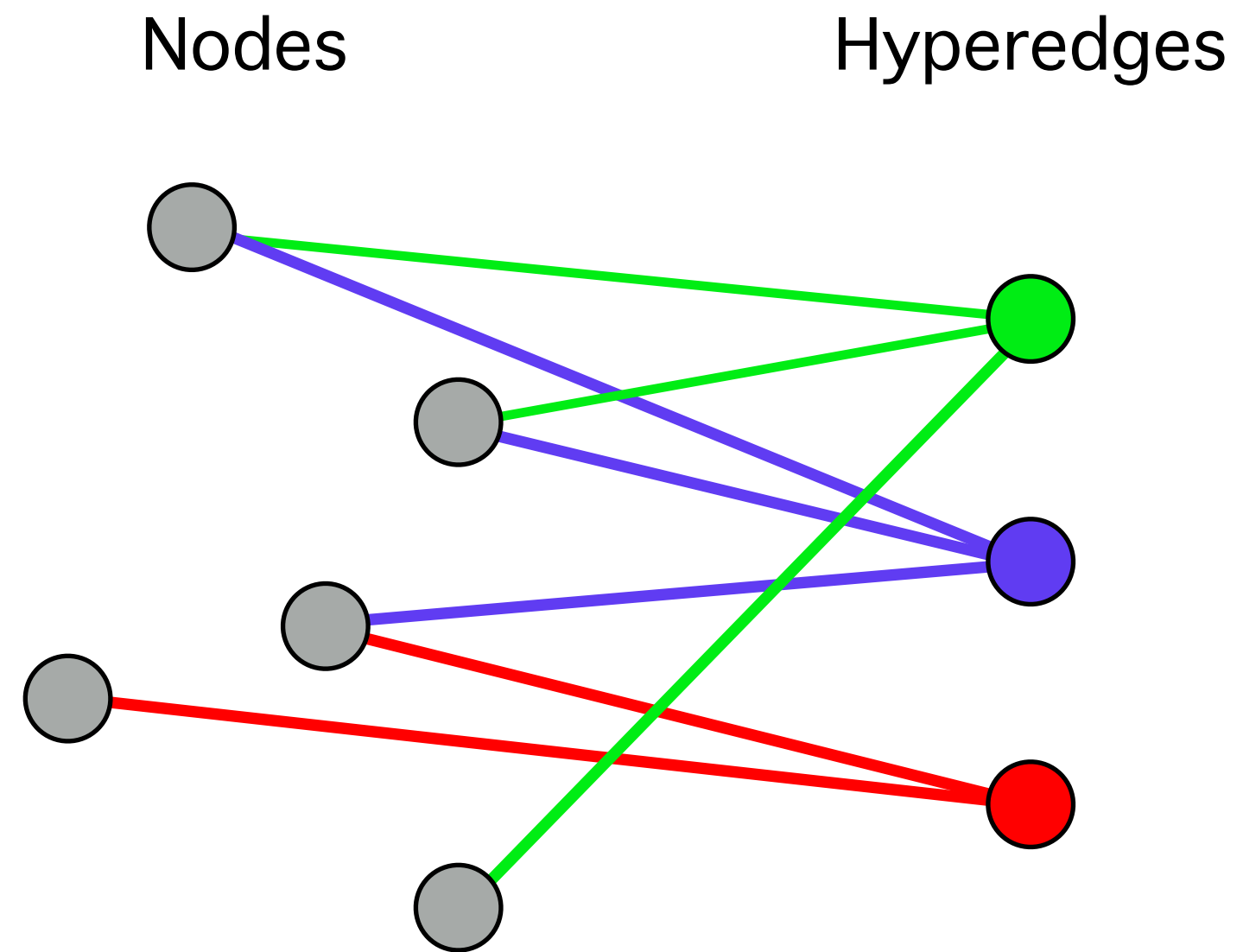




# Hypergraph 101

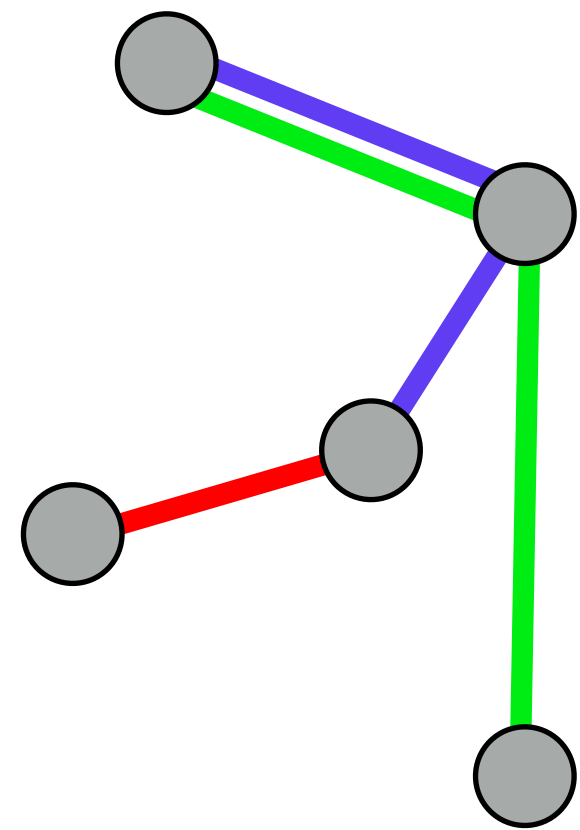


Hypergraph

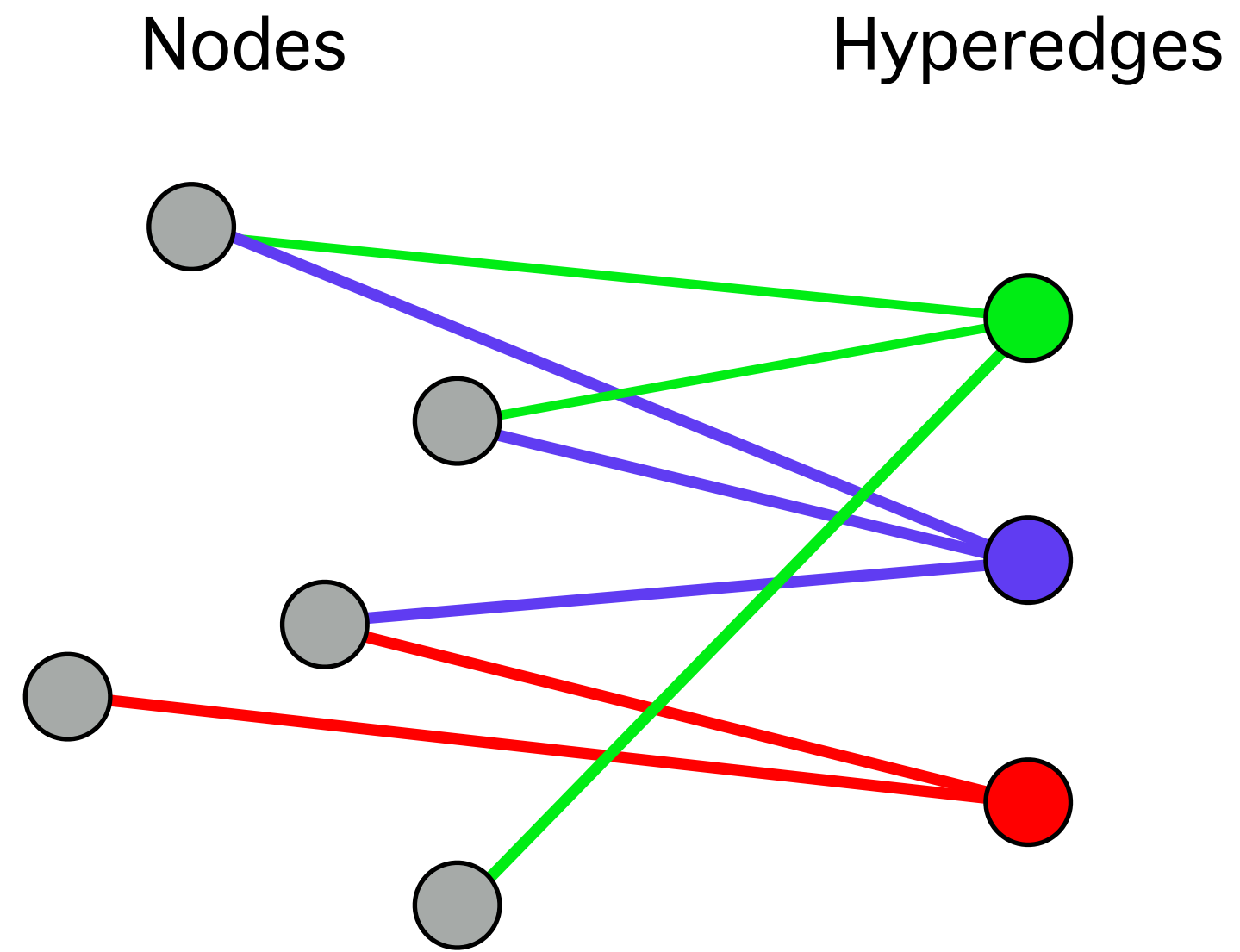


Bipartite graph

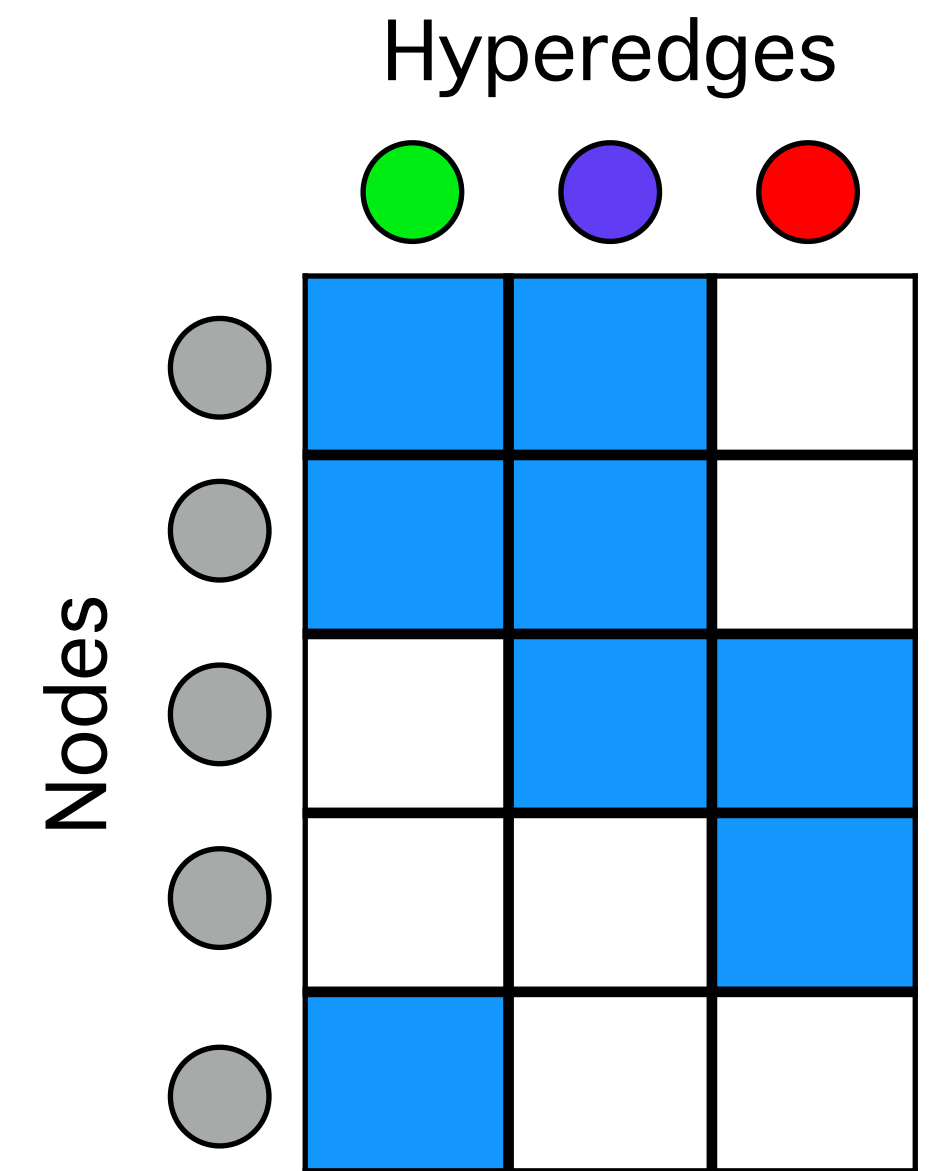
# Hypergraph 101



Hypergraph

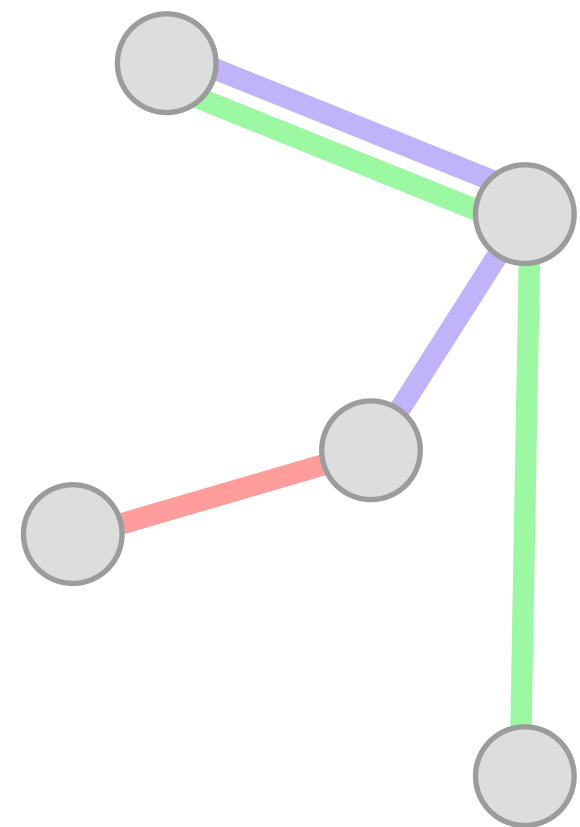


Bipartite graph

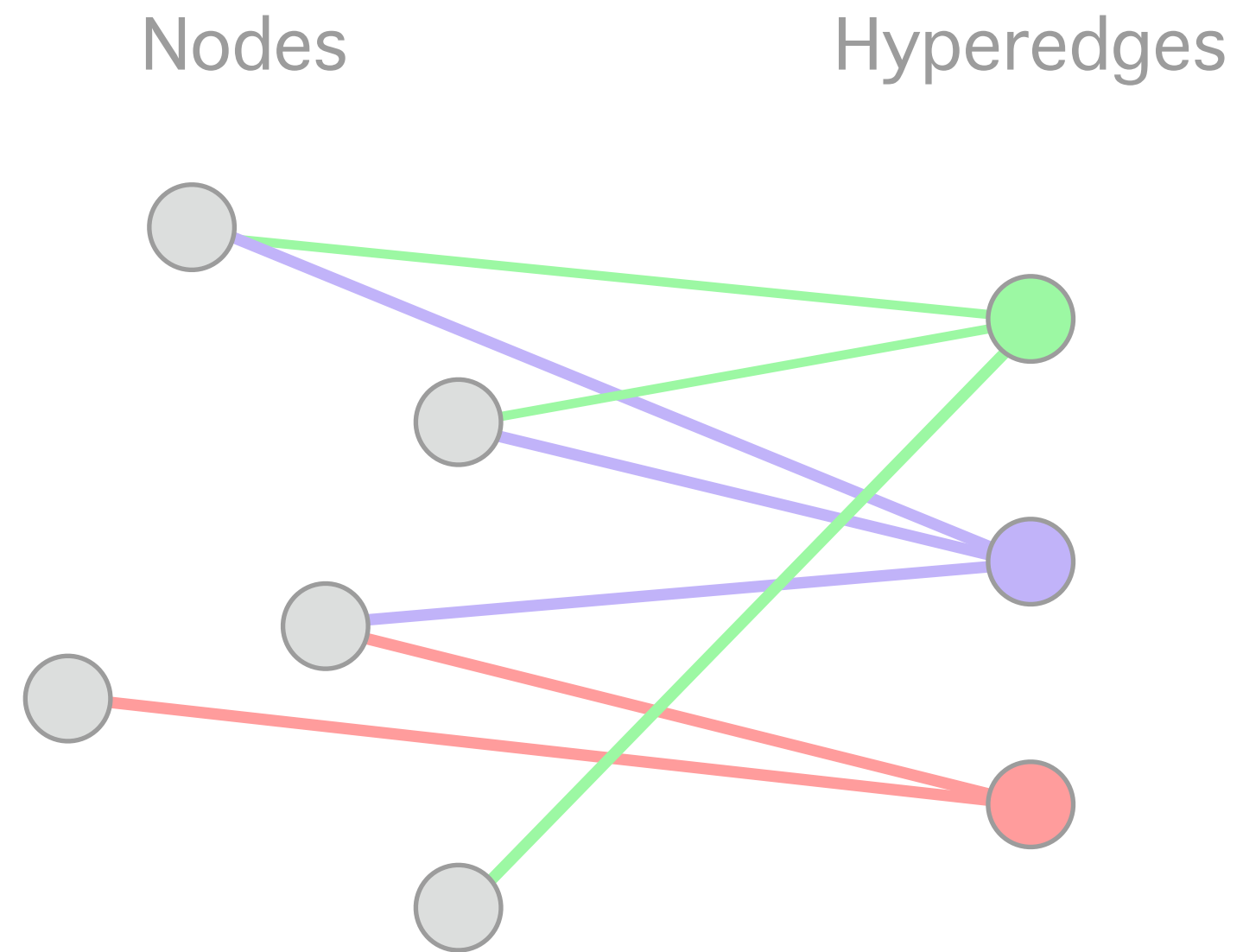


Incidence matrix

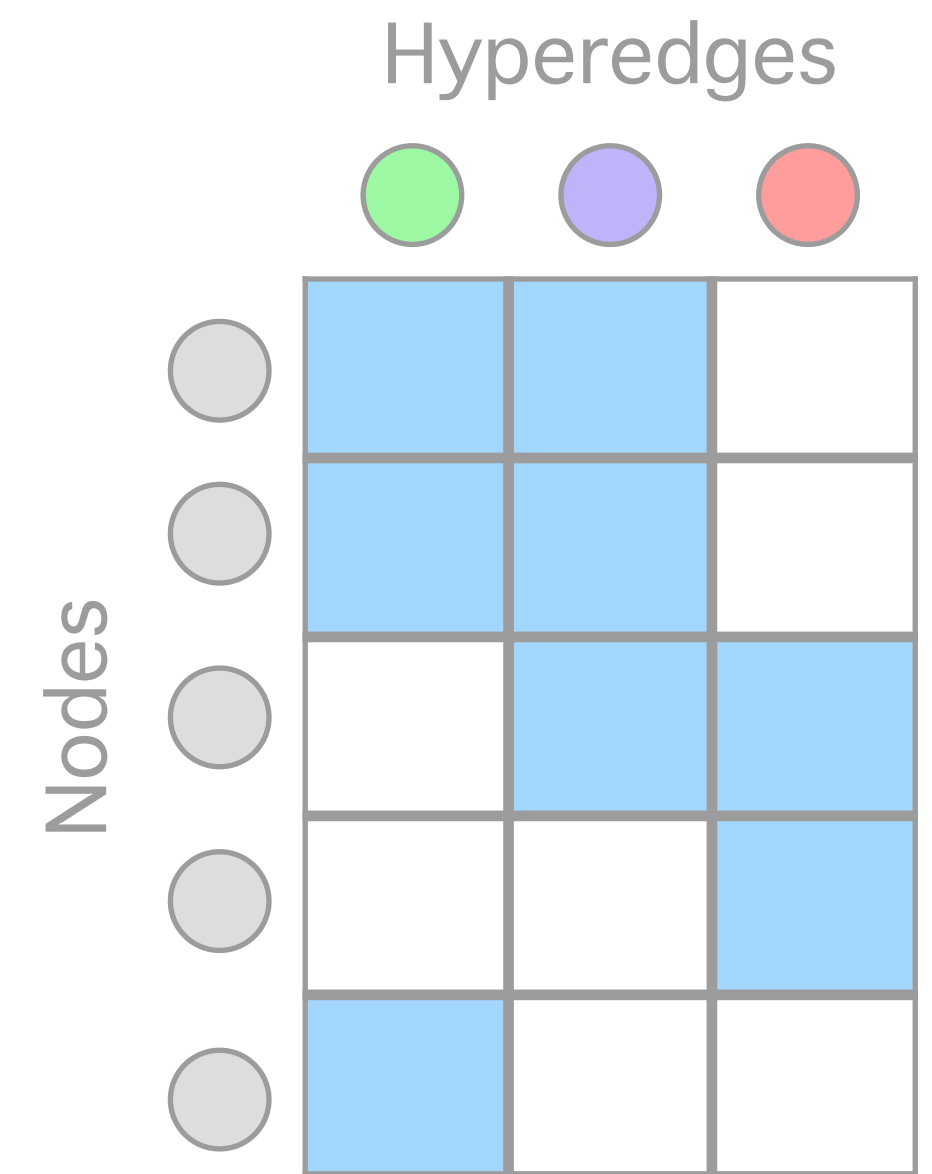
# Hypergraph 101



Hypergraph



Bipartite graph



Incidence matrix

$$\text{Hypergraph} \equiv G(\mathcal{V}, \mathcal{E}, \mathcal{I})$$

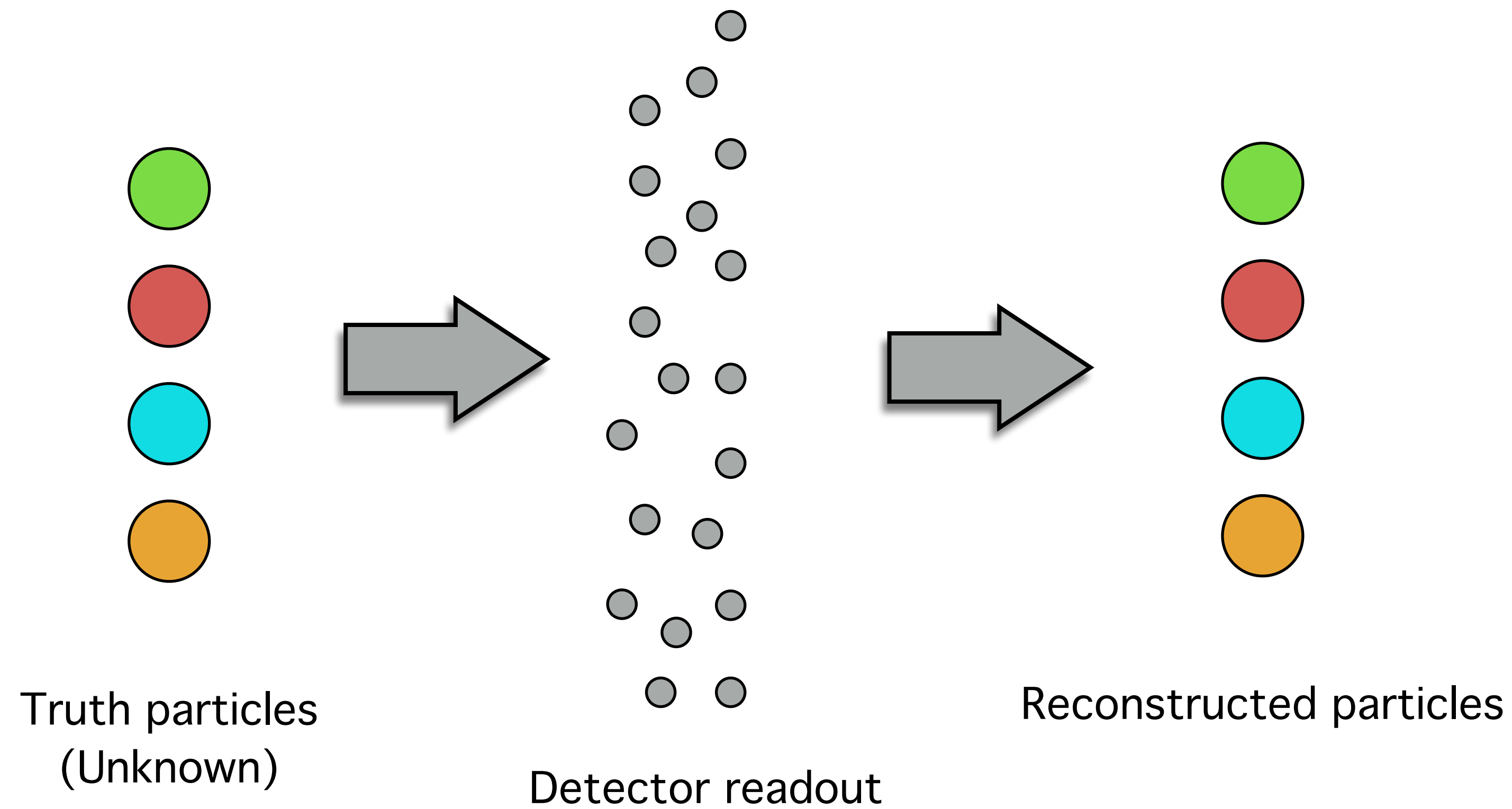
# Why Hypergraphs?

# Why Hypergraphs?

- Particle Flow = Learning a Hypergraph

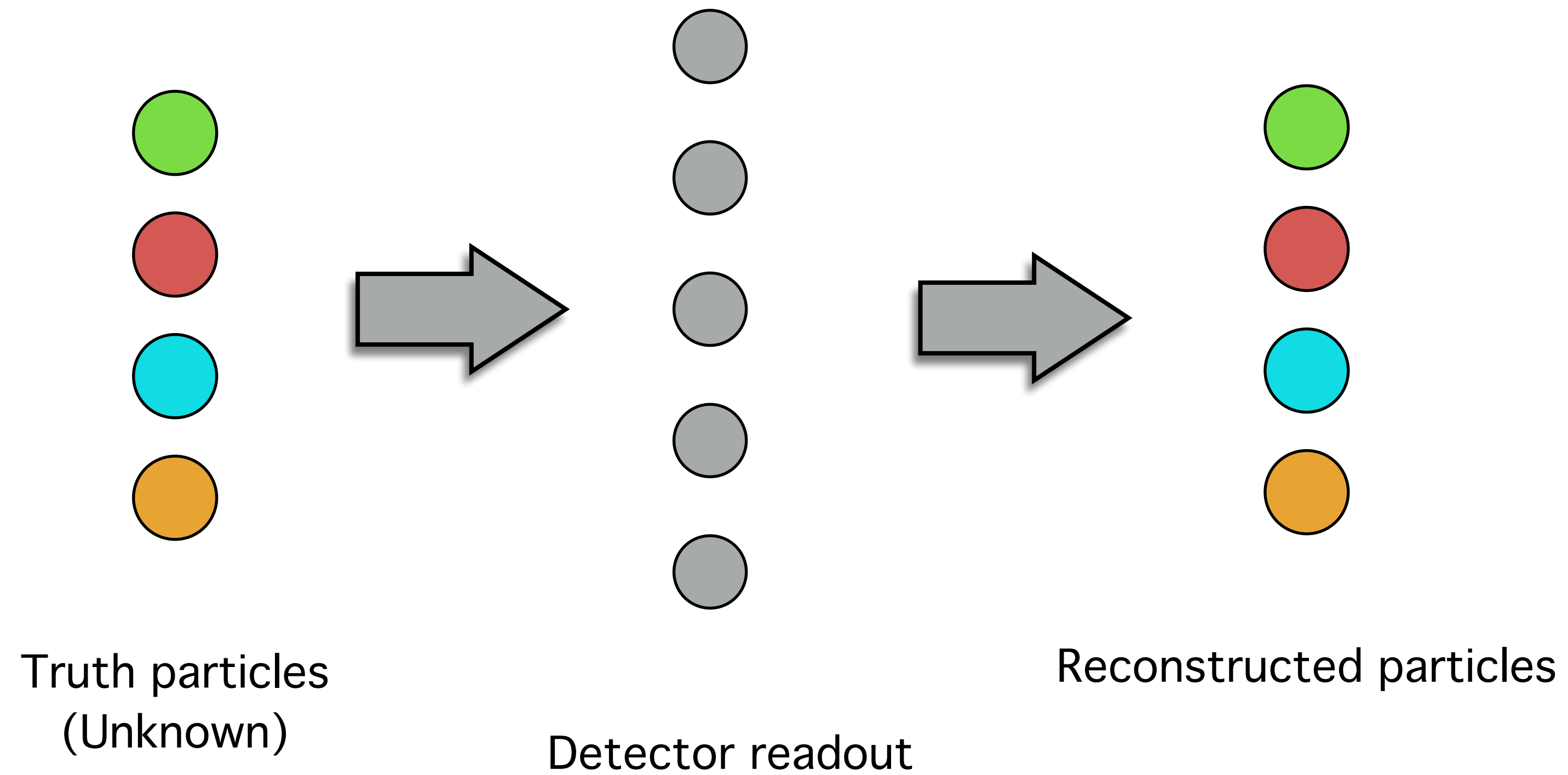
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# Why Hypergraphs?

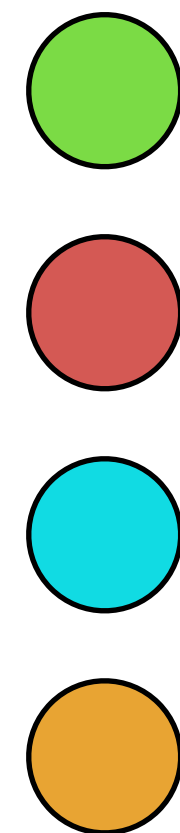
- Particle Flow = Learning a Hypergraph



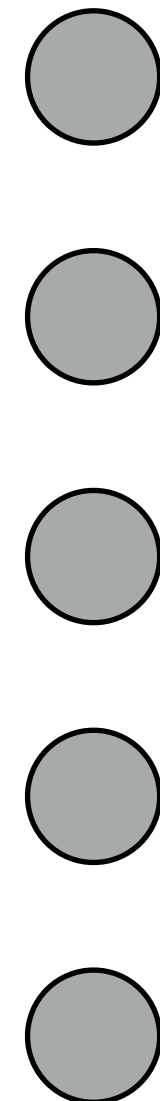


# Why Hypergraphs?

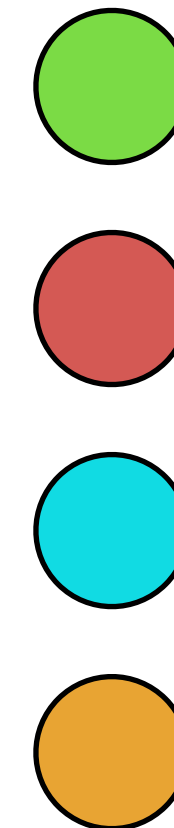
- Particle Flow = Learning a Hypergraph



Truth particles  
(Unknown)



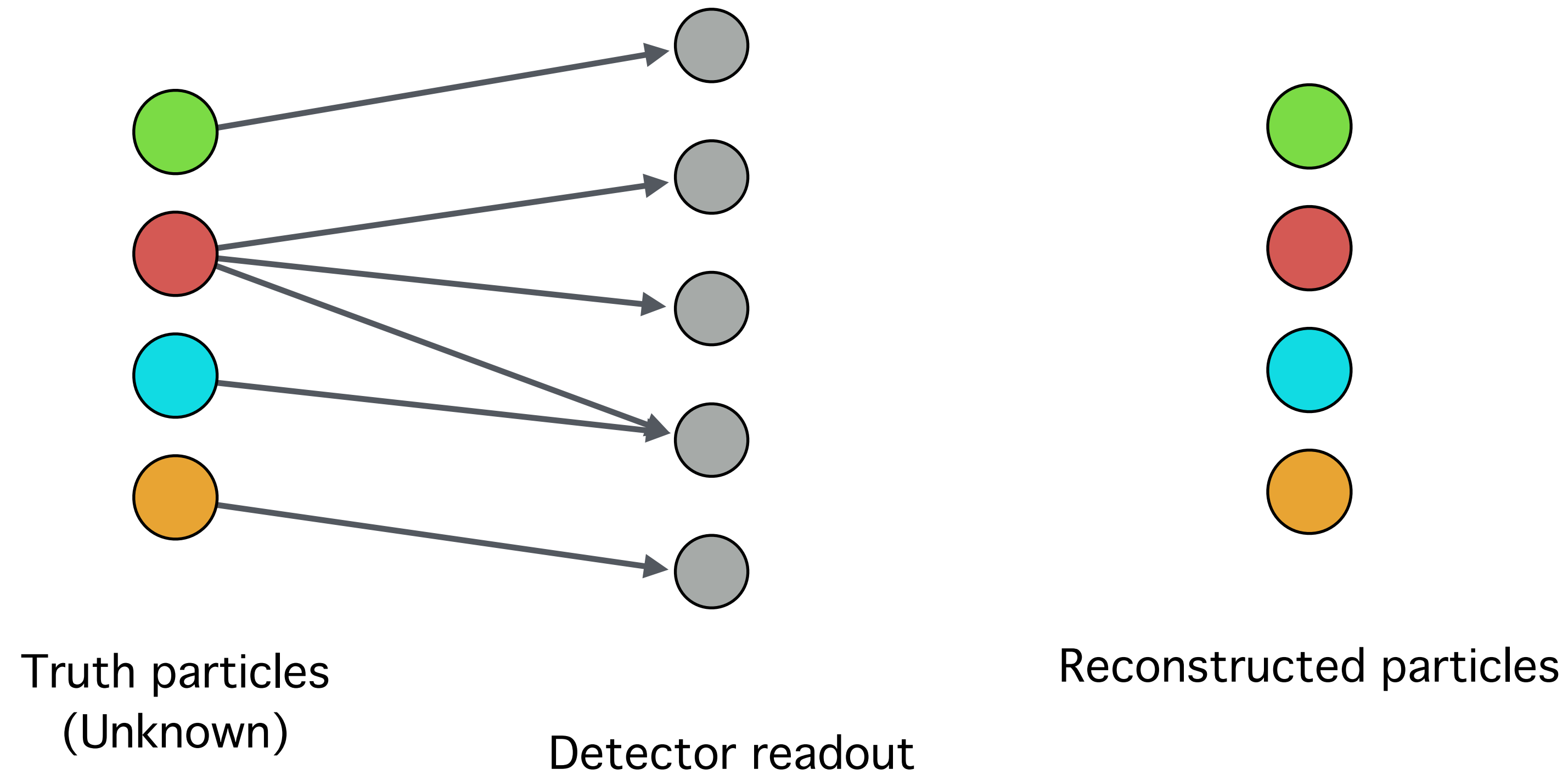
Detector readout



Reconstructed particles

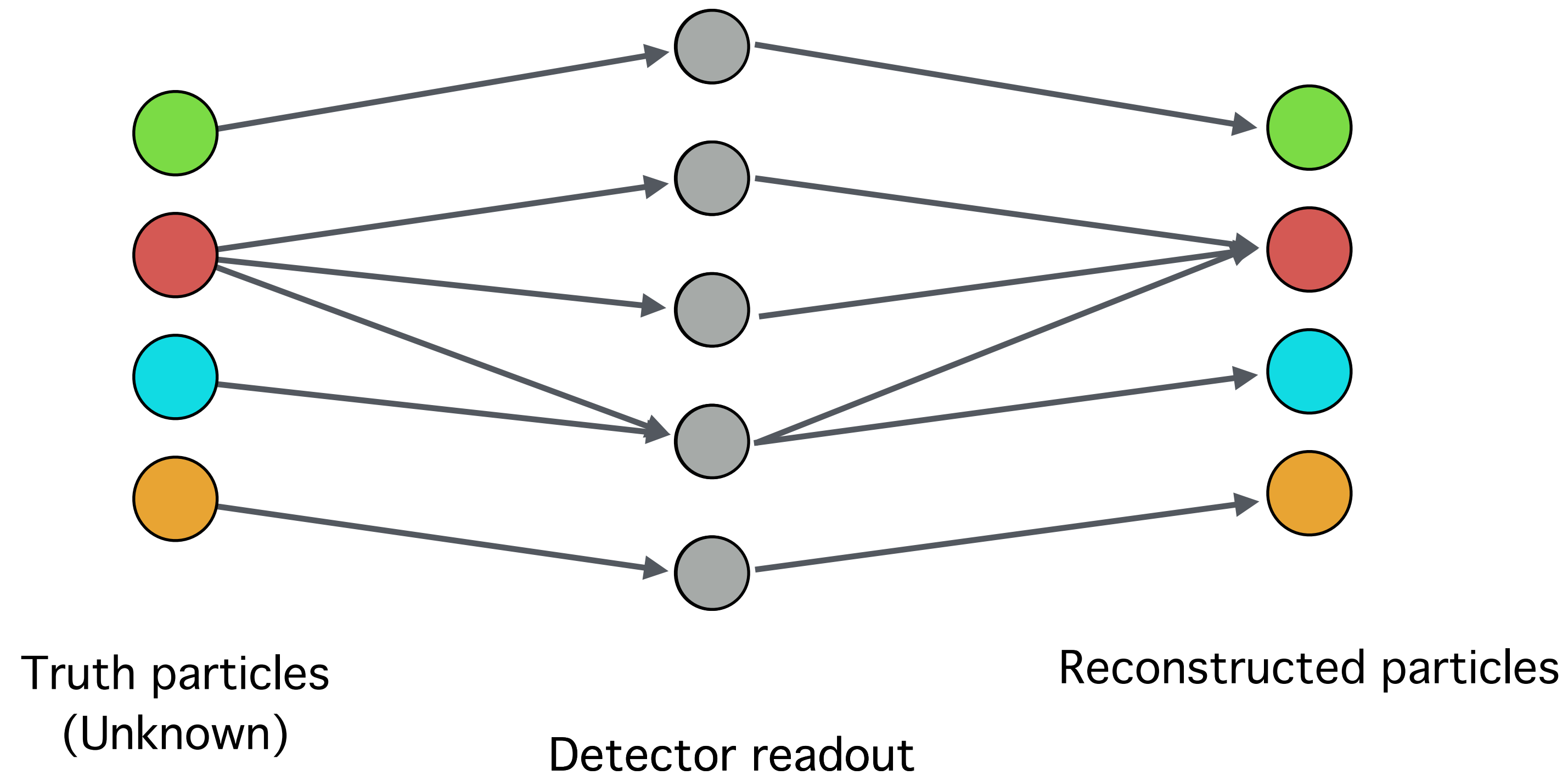
# Why Hypergraphs?

- Particle Flow = Learning a Hypergraph



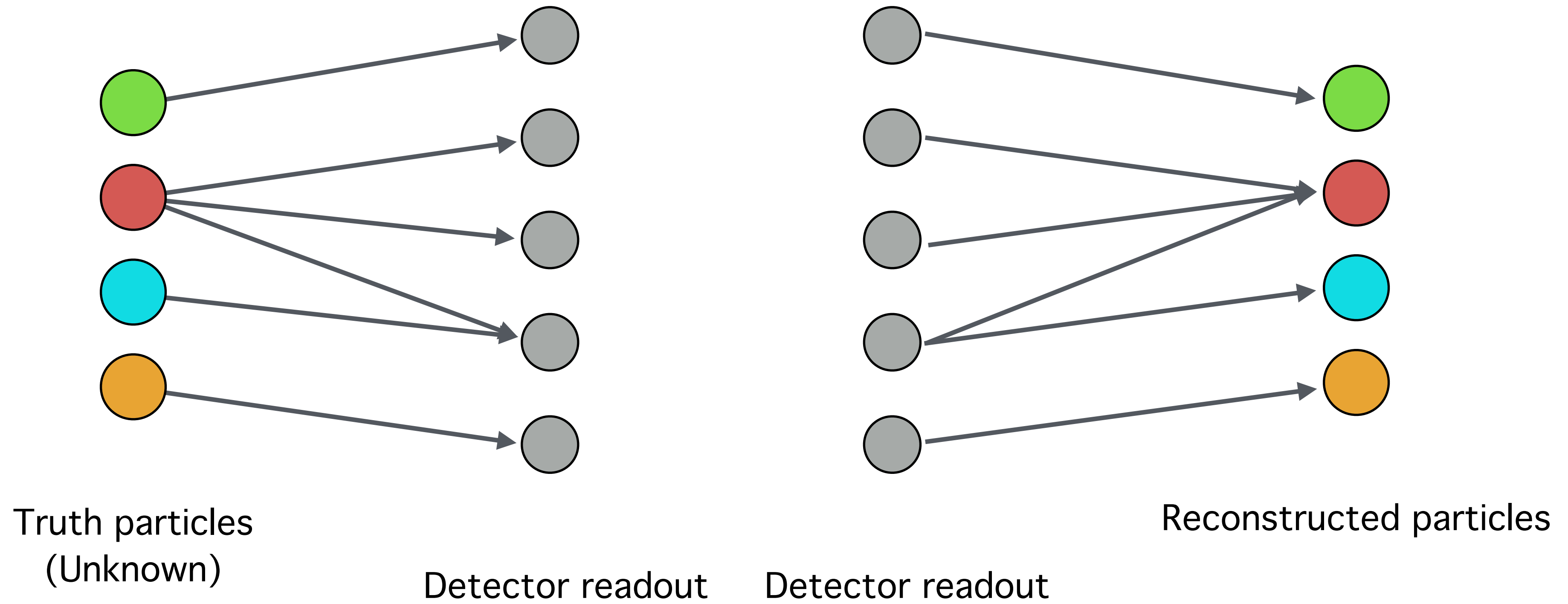
# Why Hypergraphs?

- Particle Flow = Learning a Hypergraph



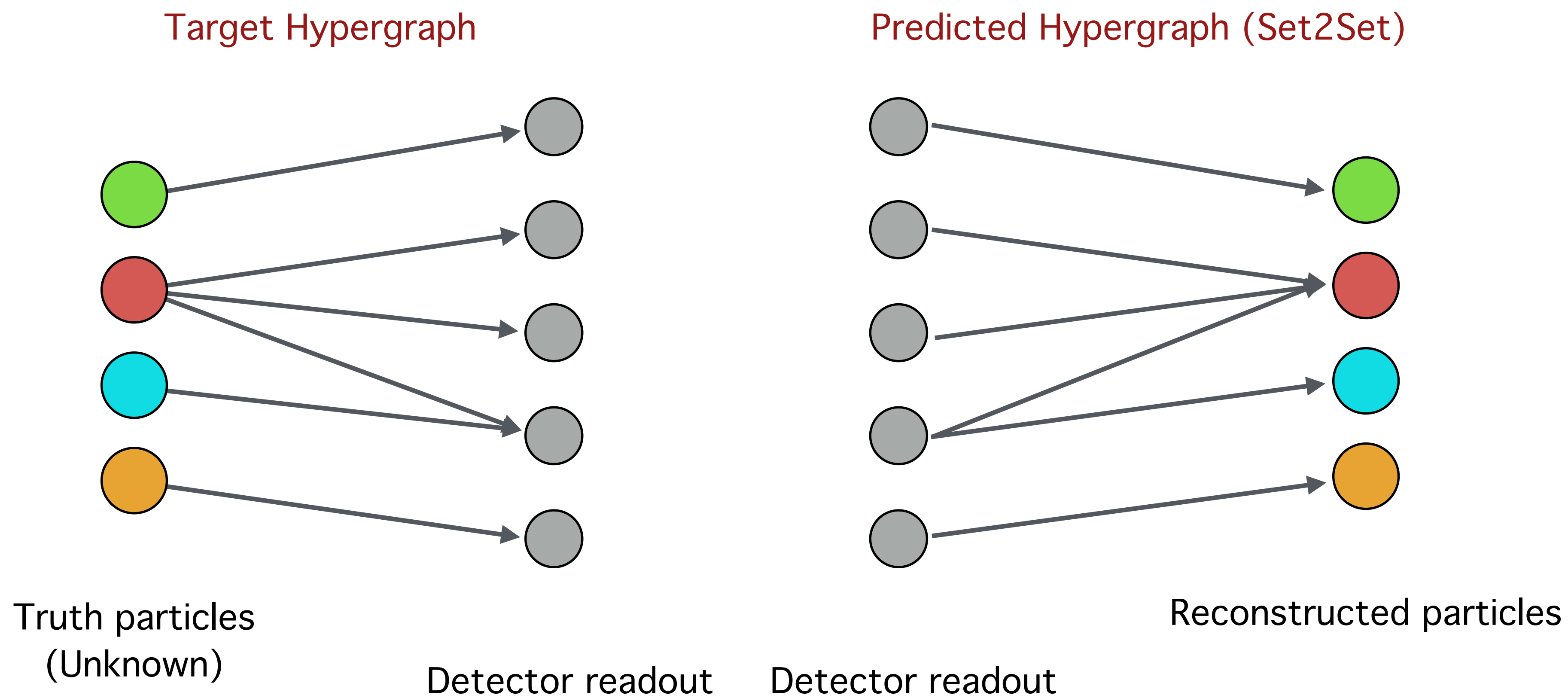
# Why Hypergraphs?

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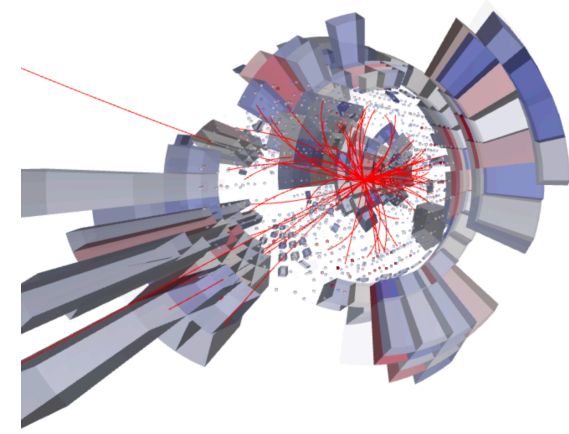
# Why Hypergraphs?

- Particle Flow = Learning a Hypergraph



# The overall plan

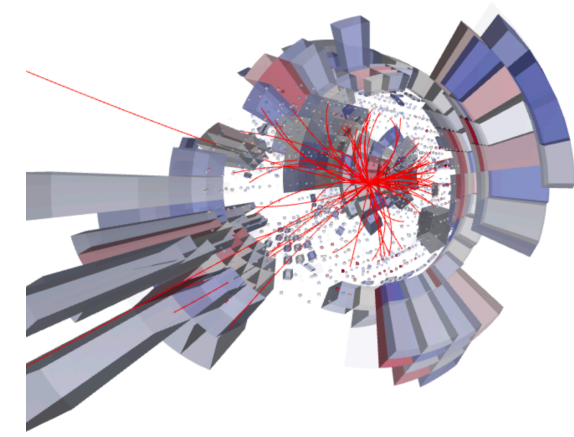
# The overall plan



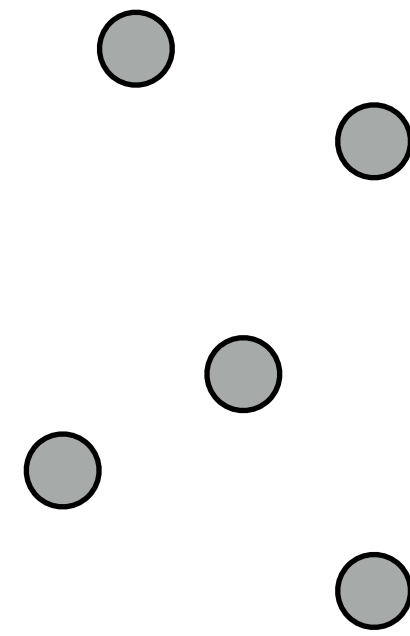
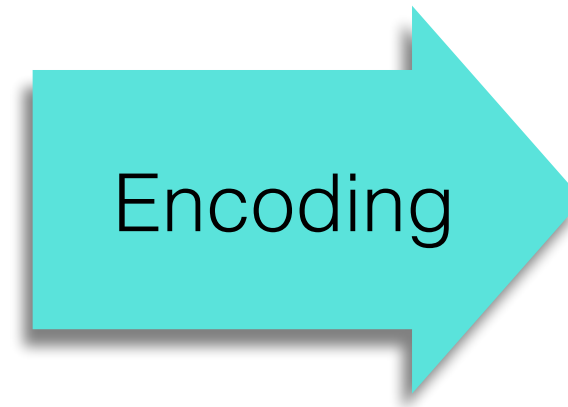
Detector data  
(Tracks, cells)



# The overall plan

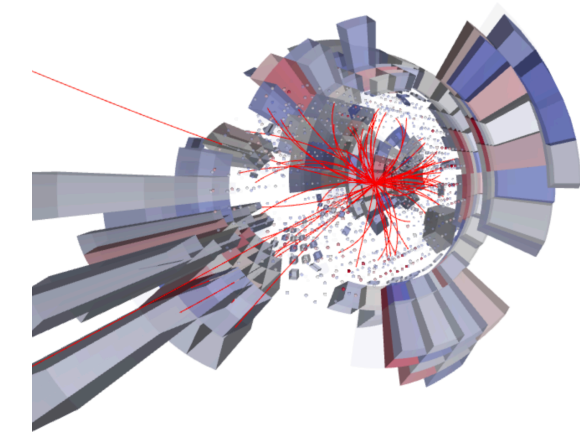


Detector data  
(Tracks, cells)

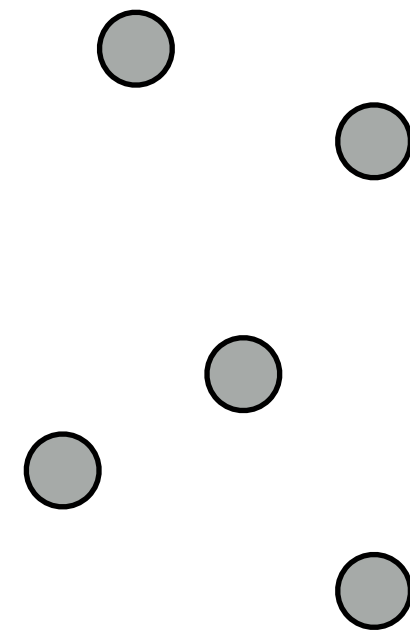
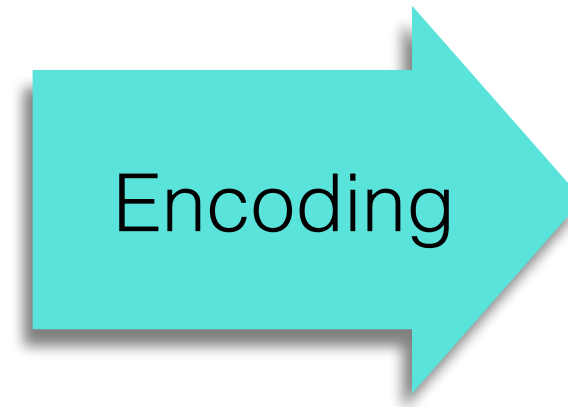


Encoded data

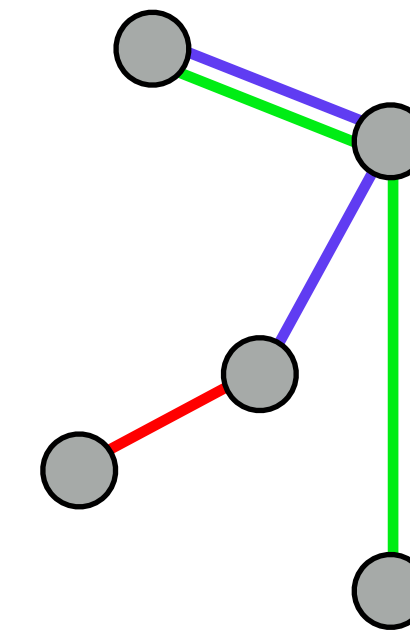
# The overall plan



Detector data  
(Tracks, cells)

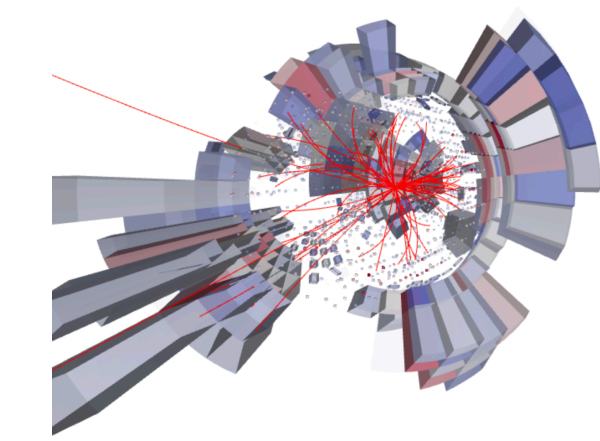


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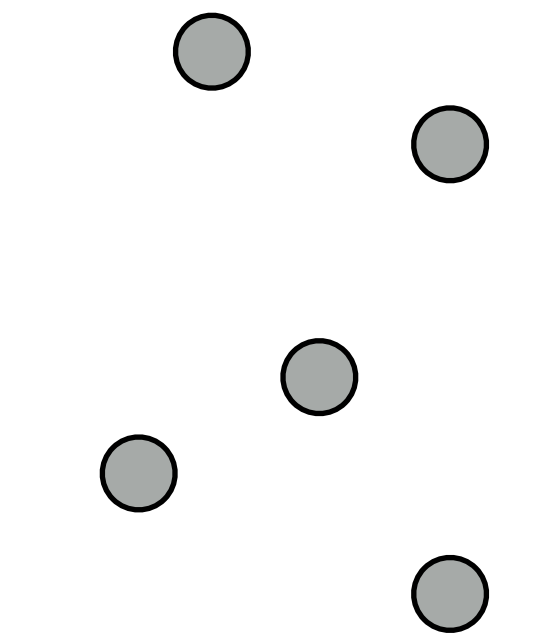
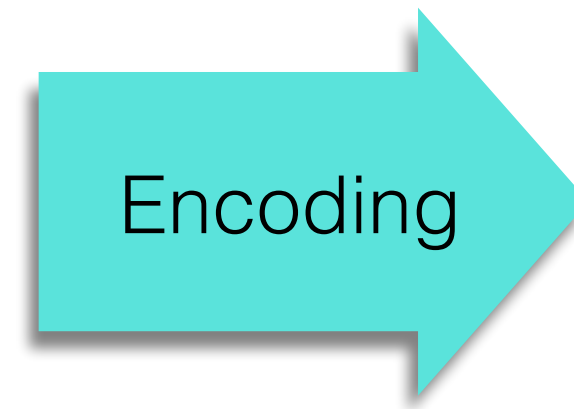


Hypergraph

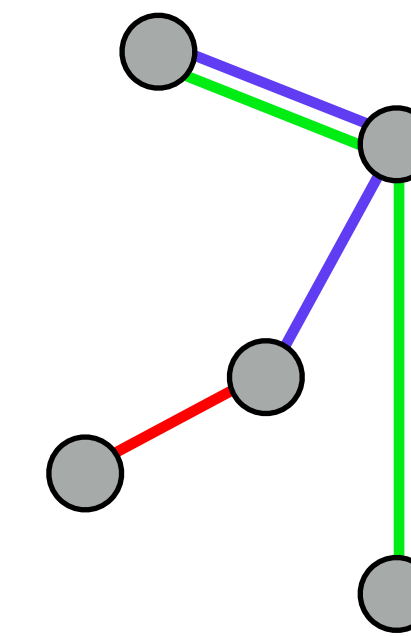
# The overall plan



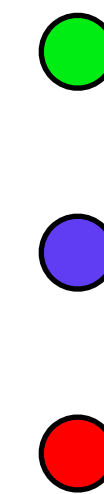
Detector data  
(Tracks, cells)



Encoded data

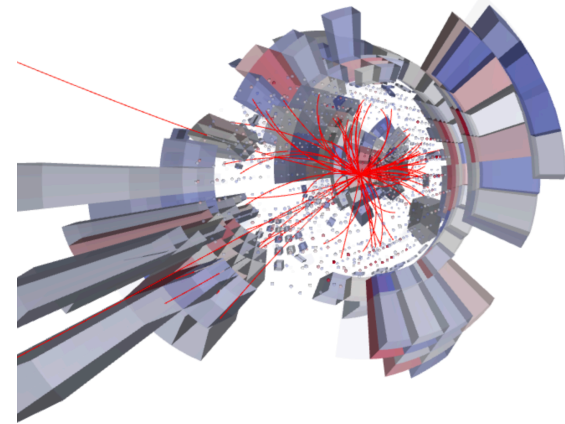


Hypergraph

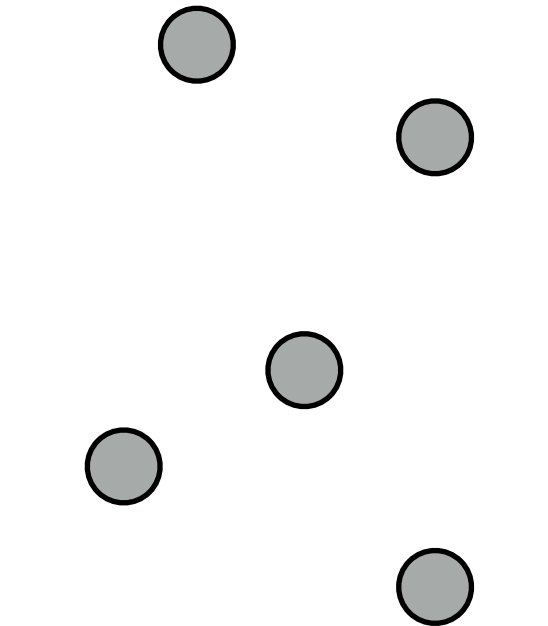
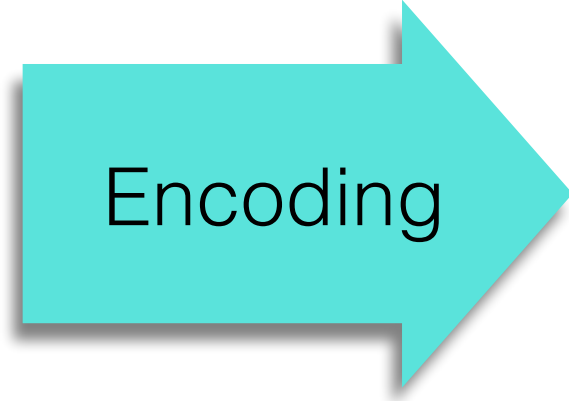


Particles

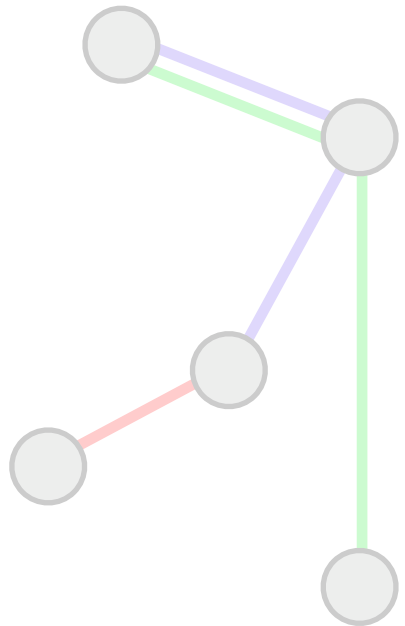
# Step 1



Detector data  
(Tracks, cells)



Encoded data

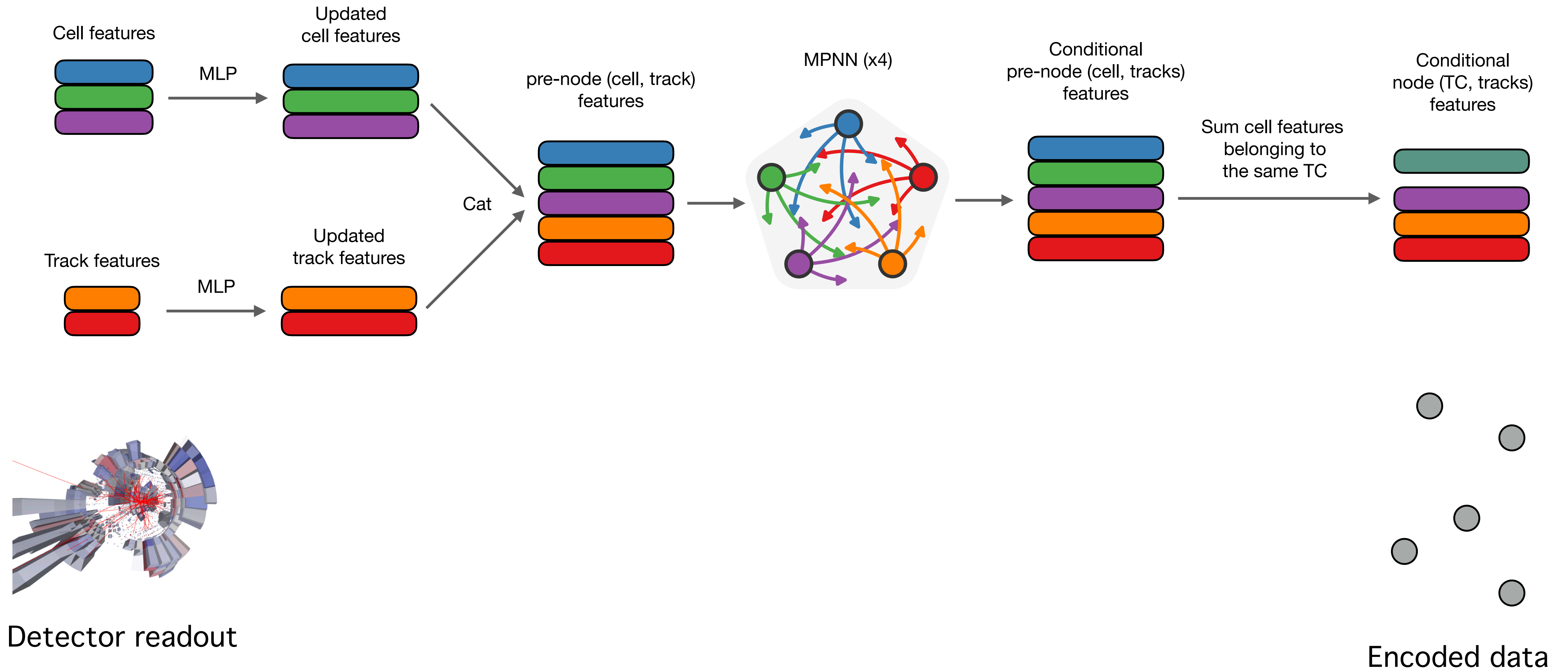


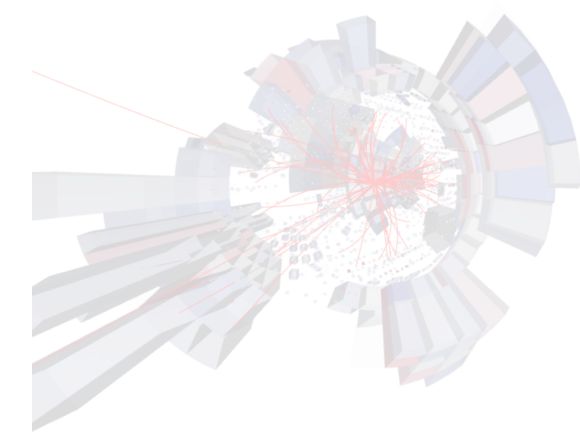
Hypergraph



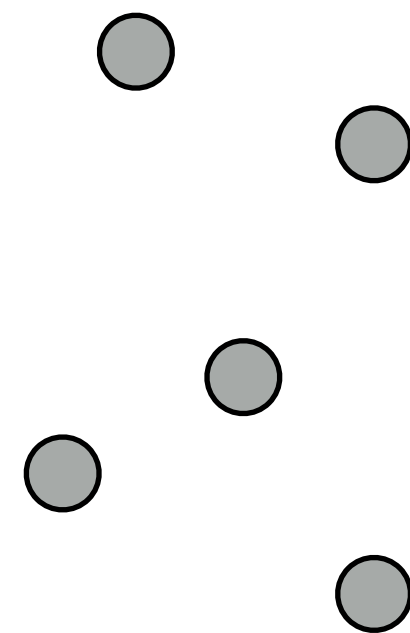
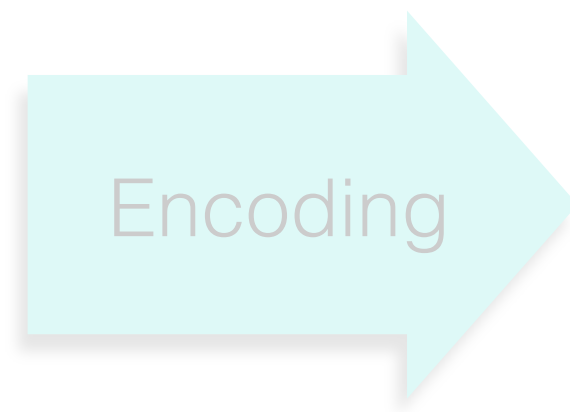
Particles

# Encoding



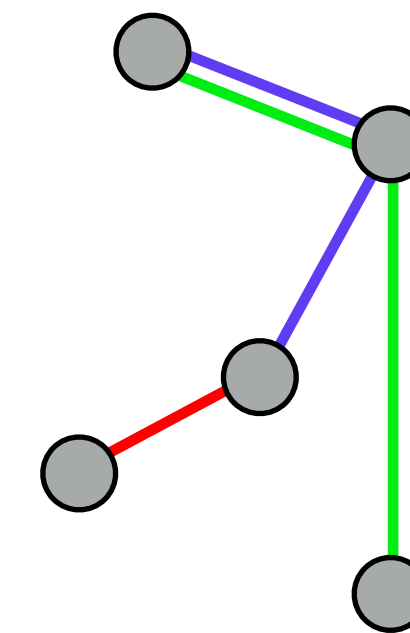


Detector data  
(Tracks, cells)



Encoded data

## Step 2

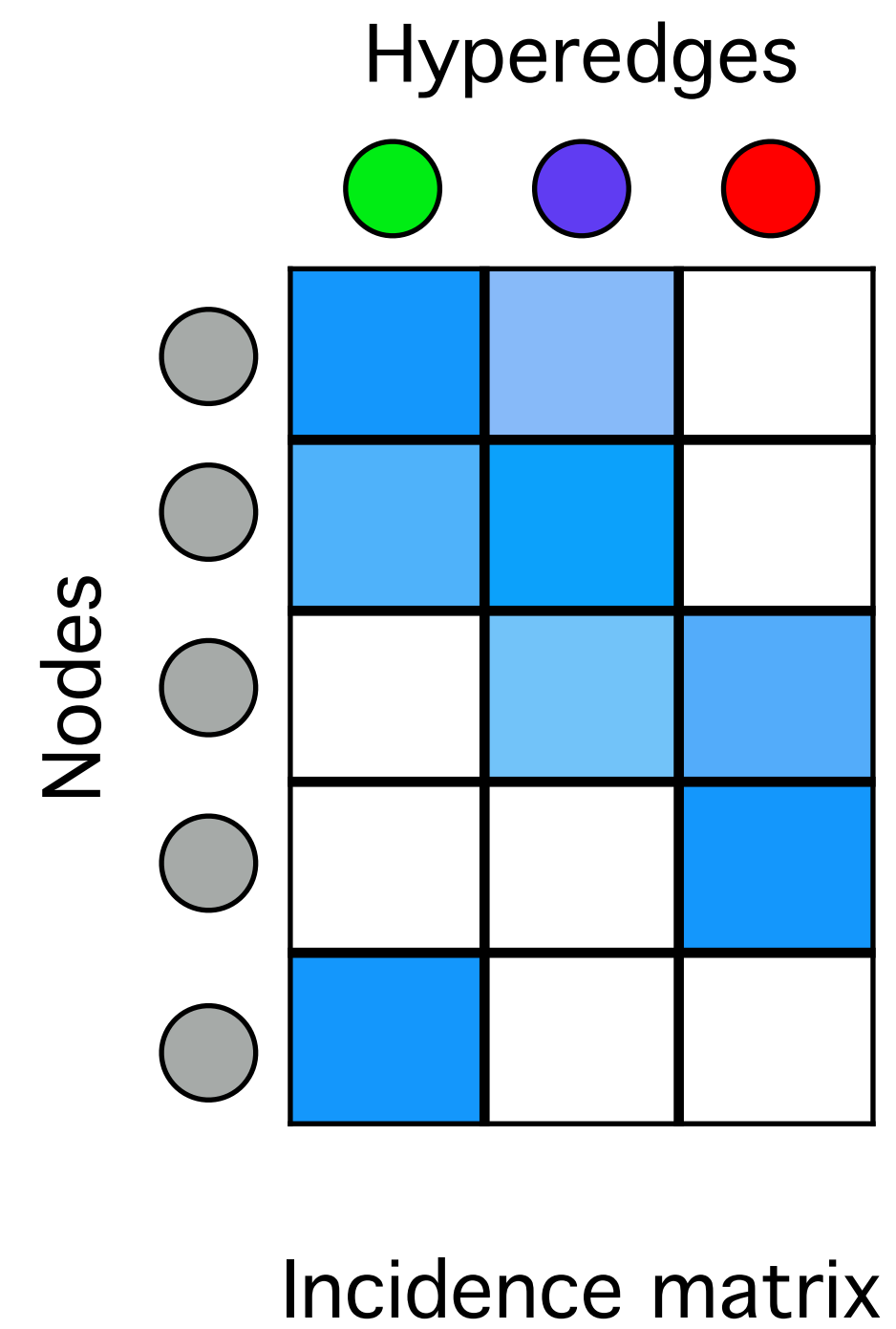


Hypergraph



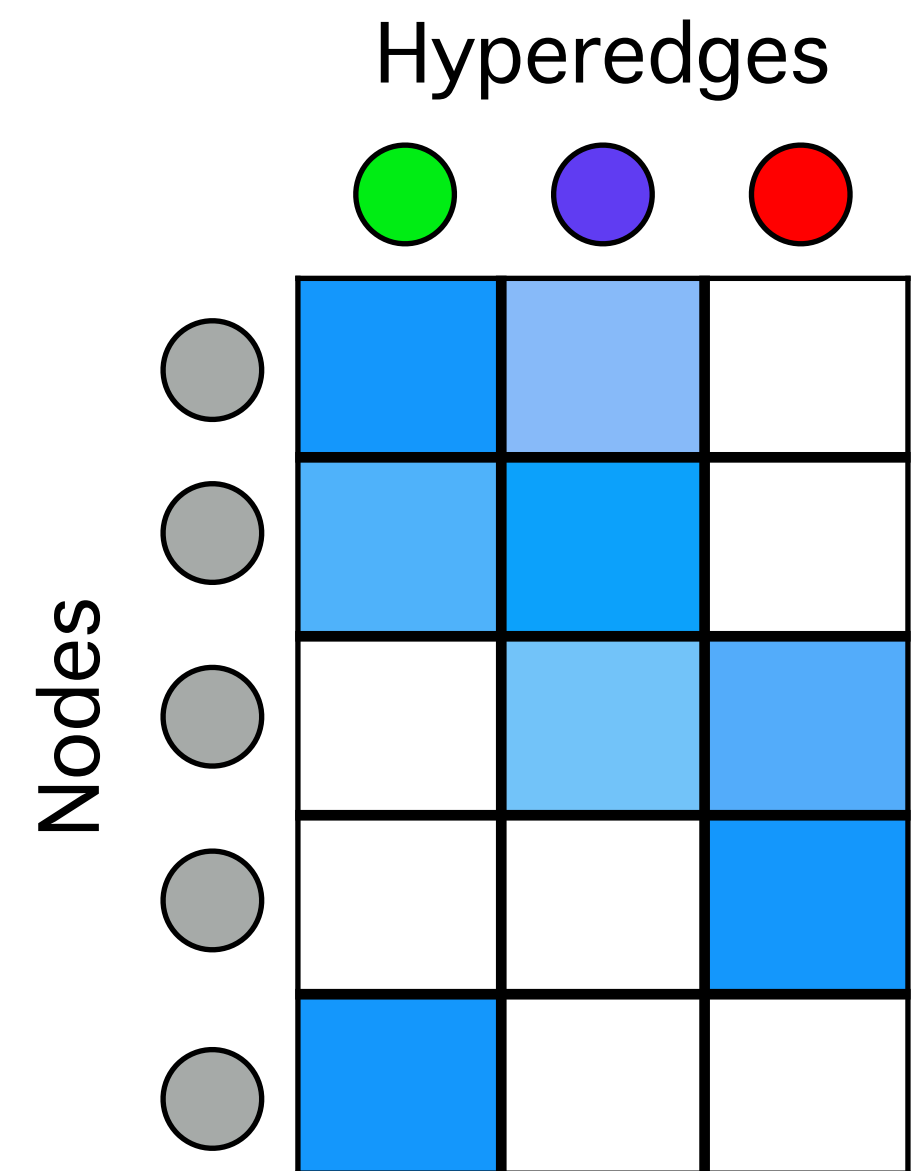
Particles

# Incidence matrix



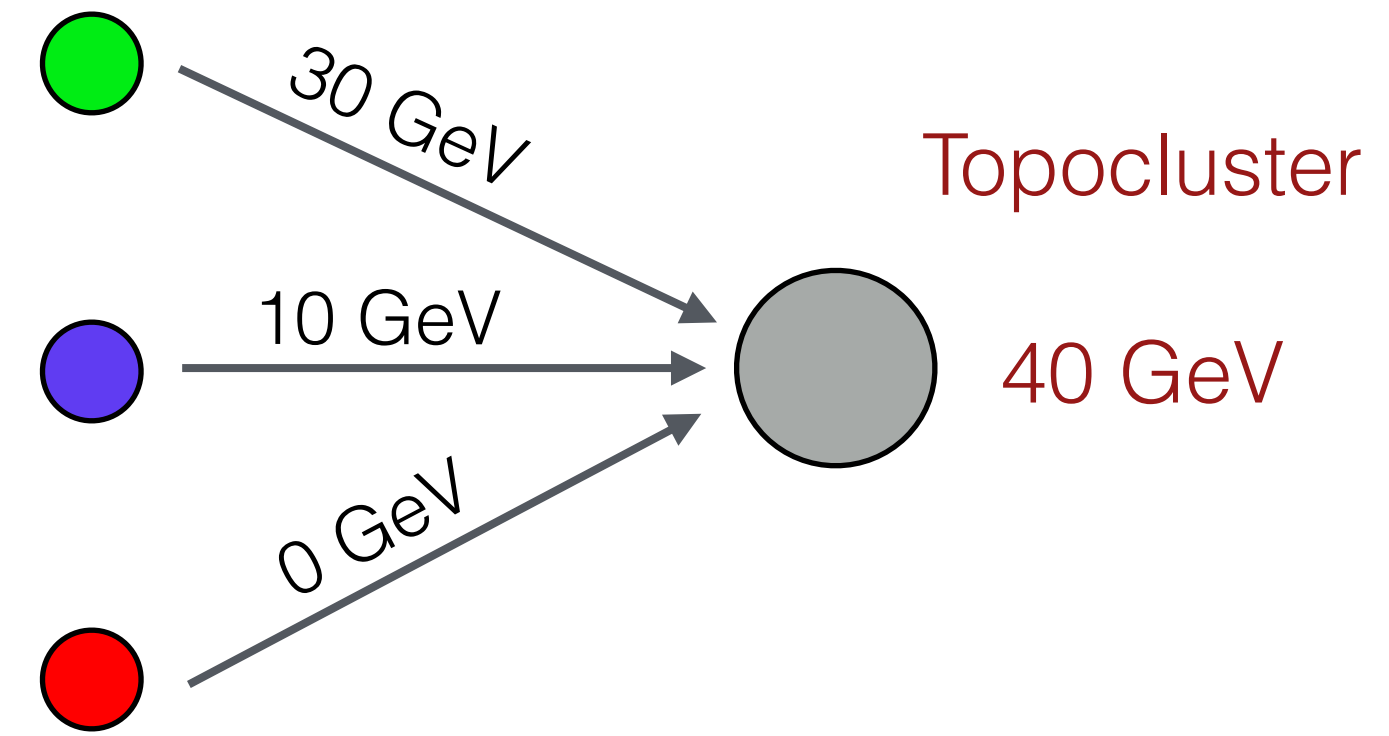


# Incidence matrix

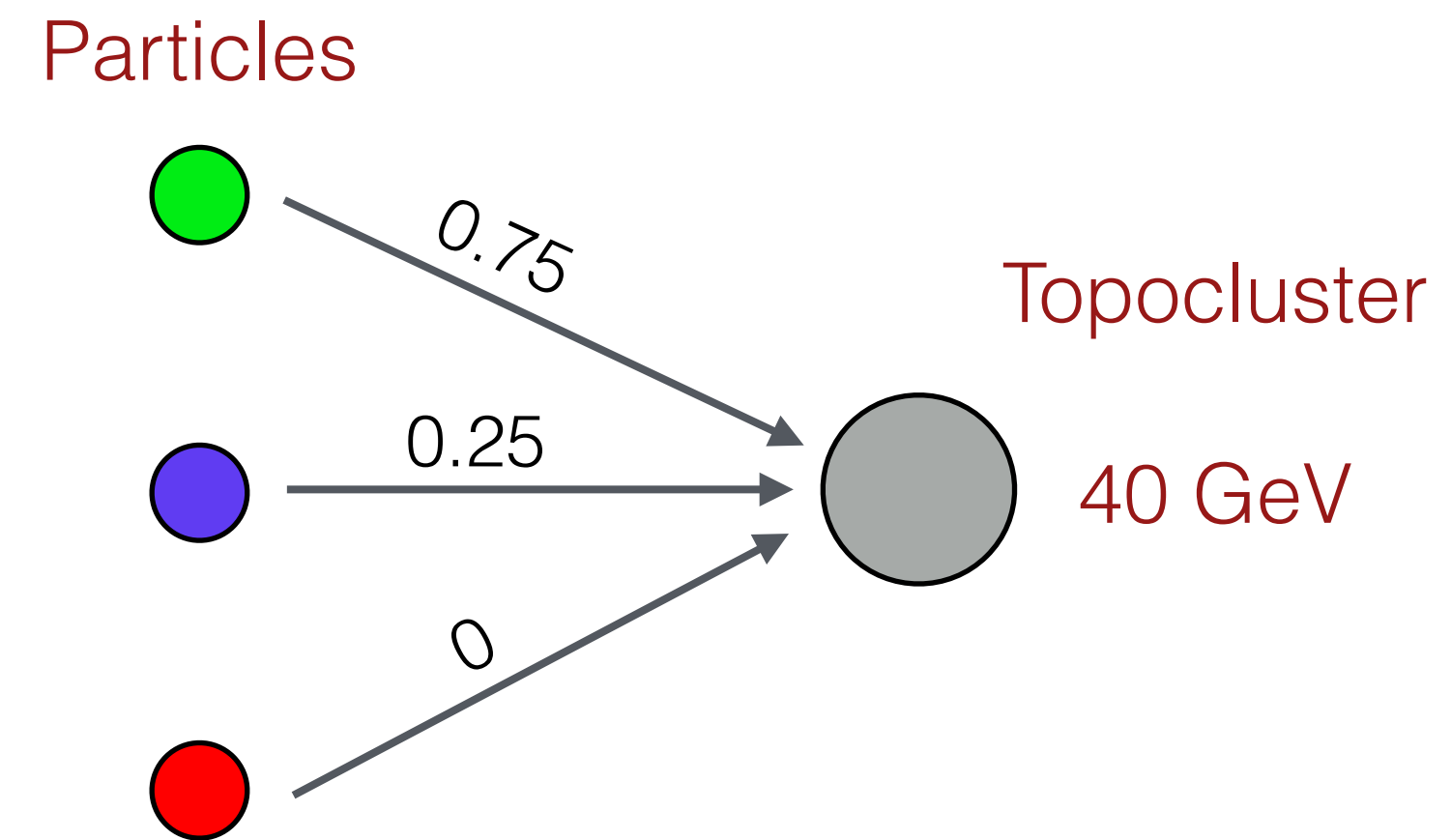
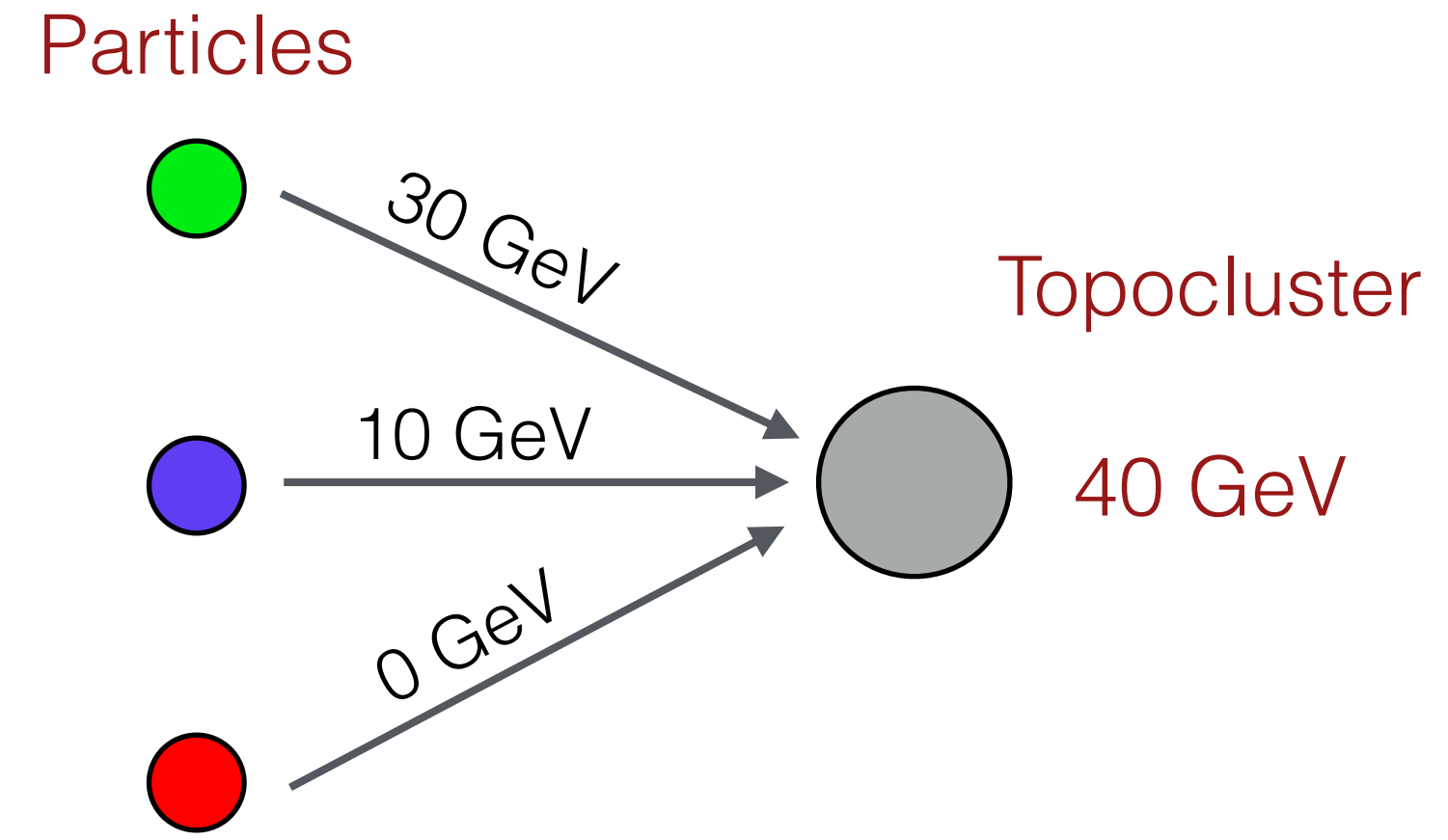
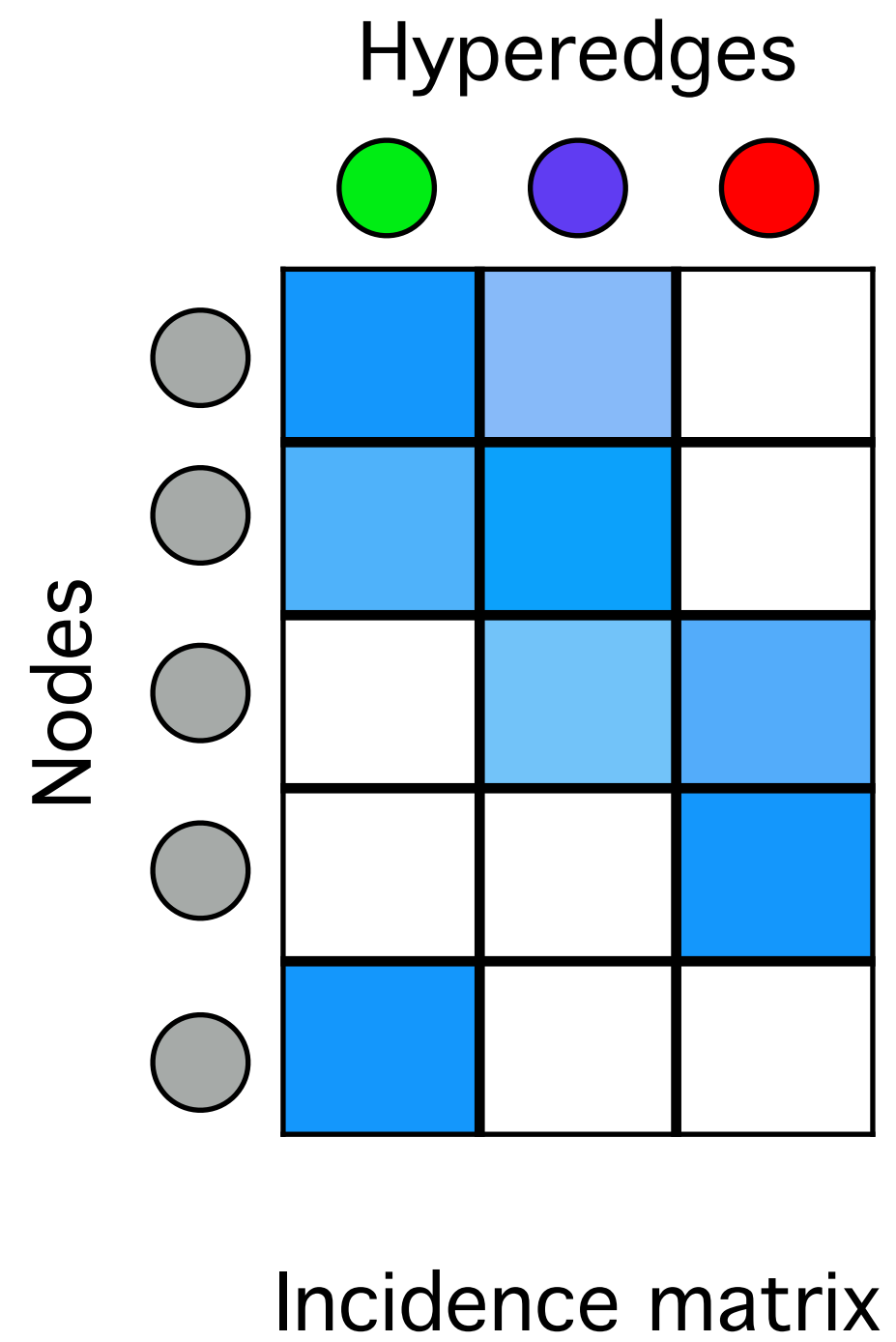


Incidence matrix

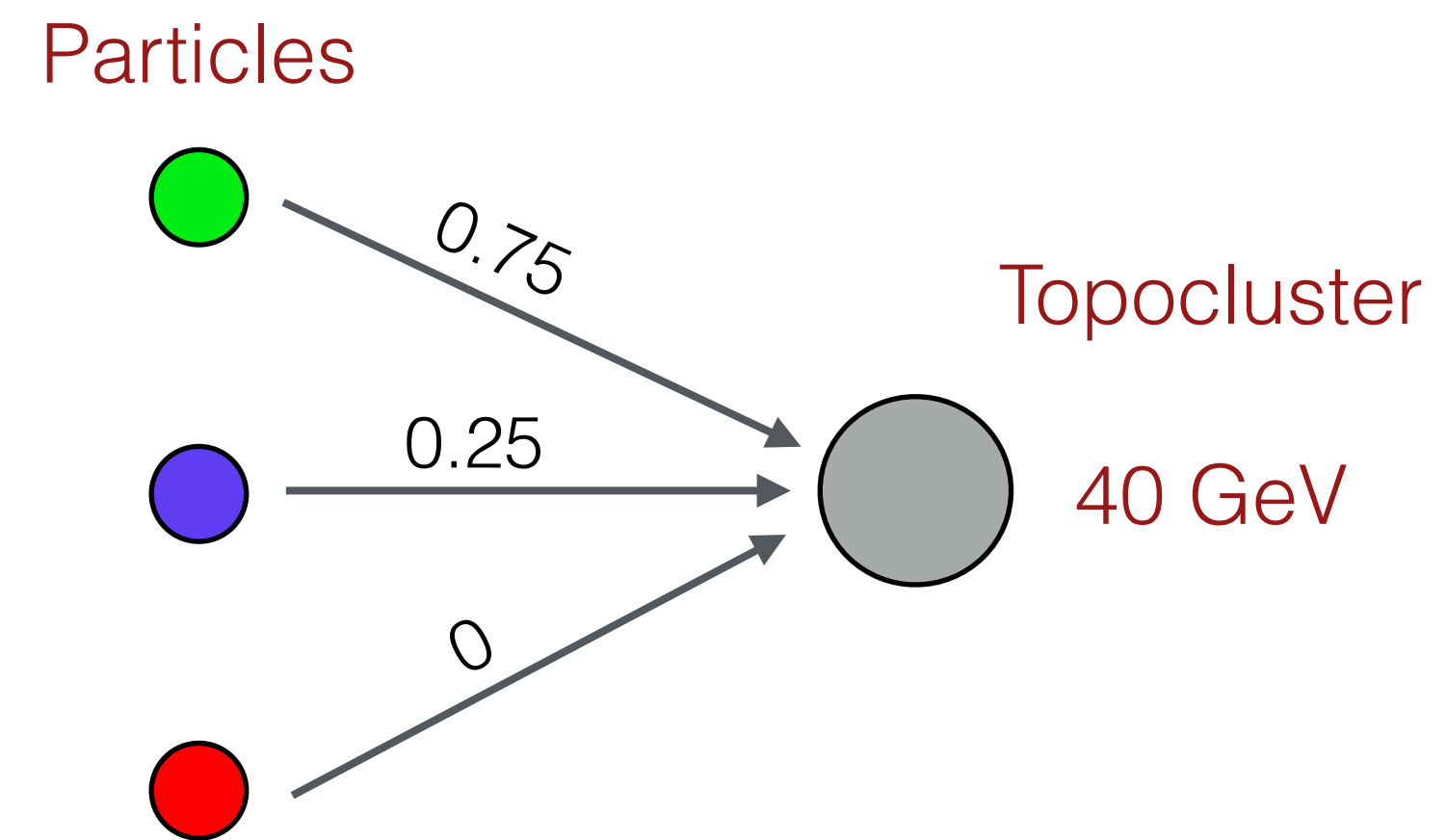
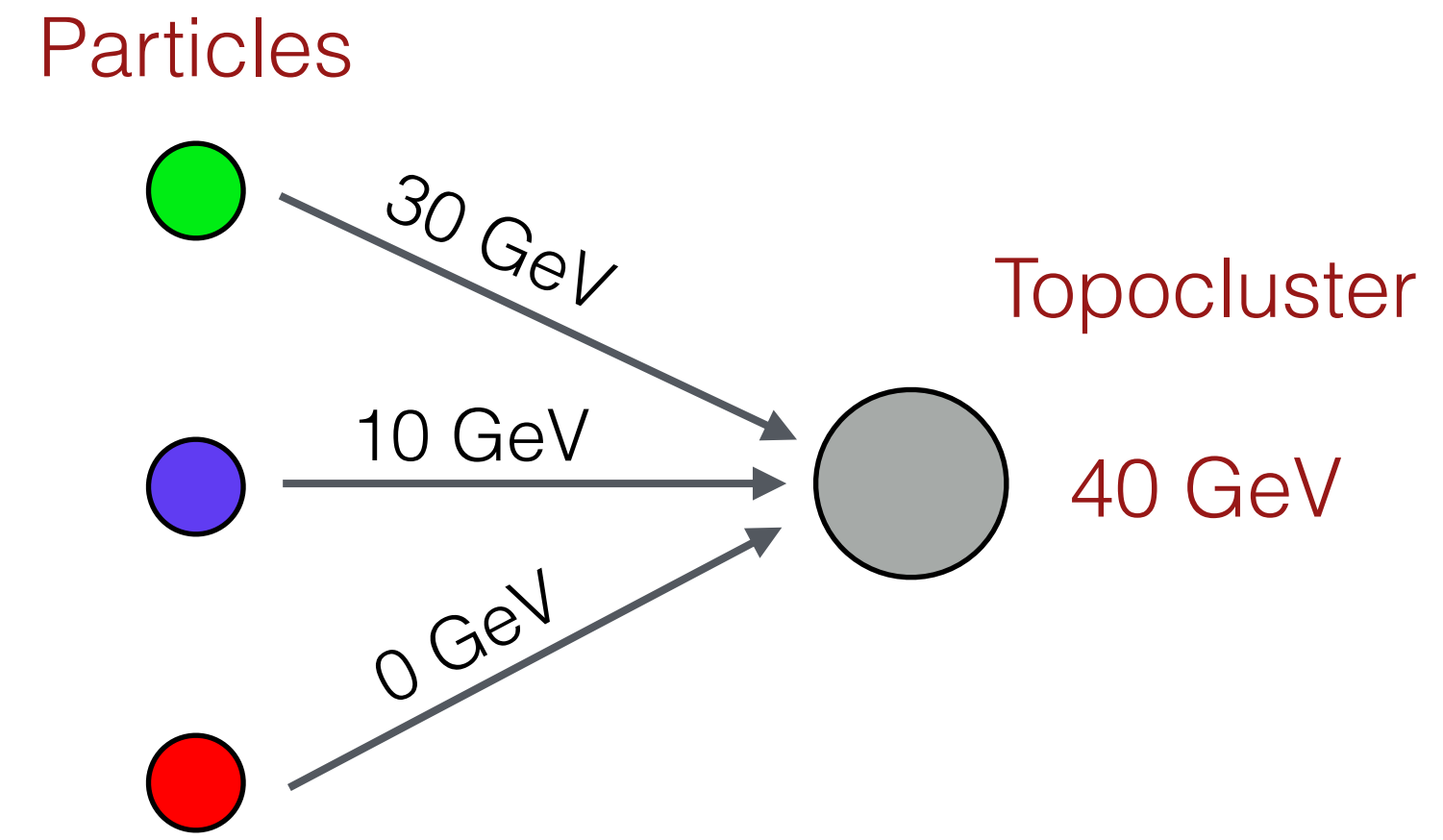
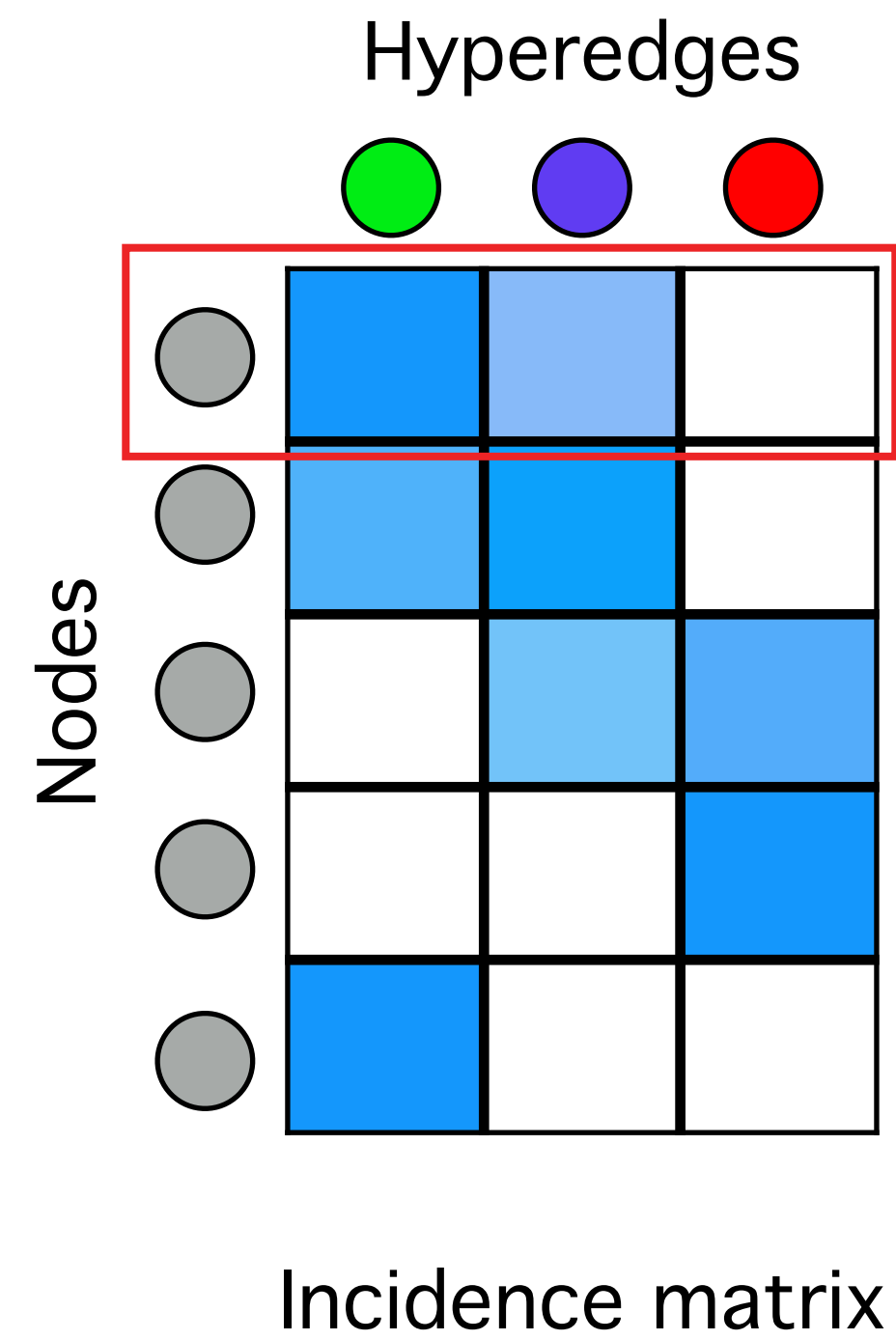
Particles



# Incidence matrix

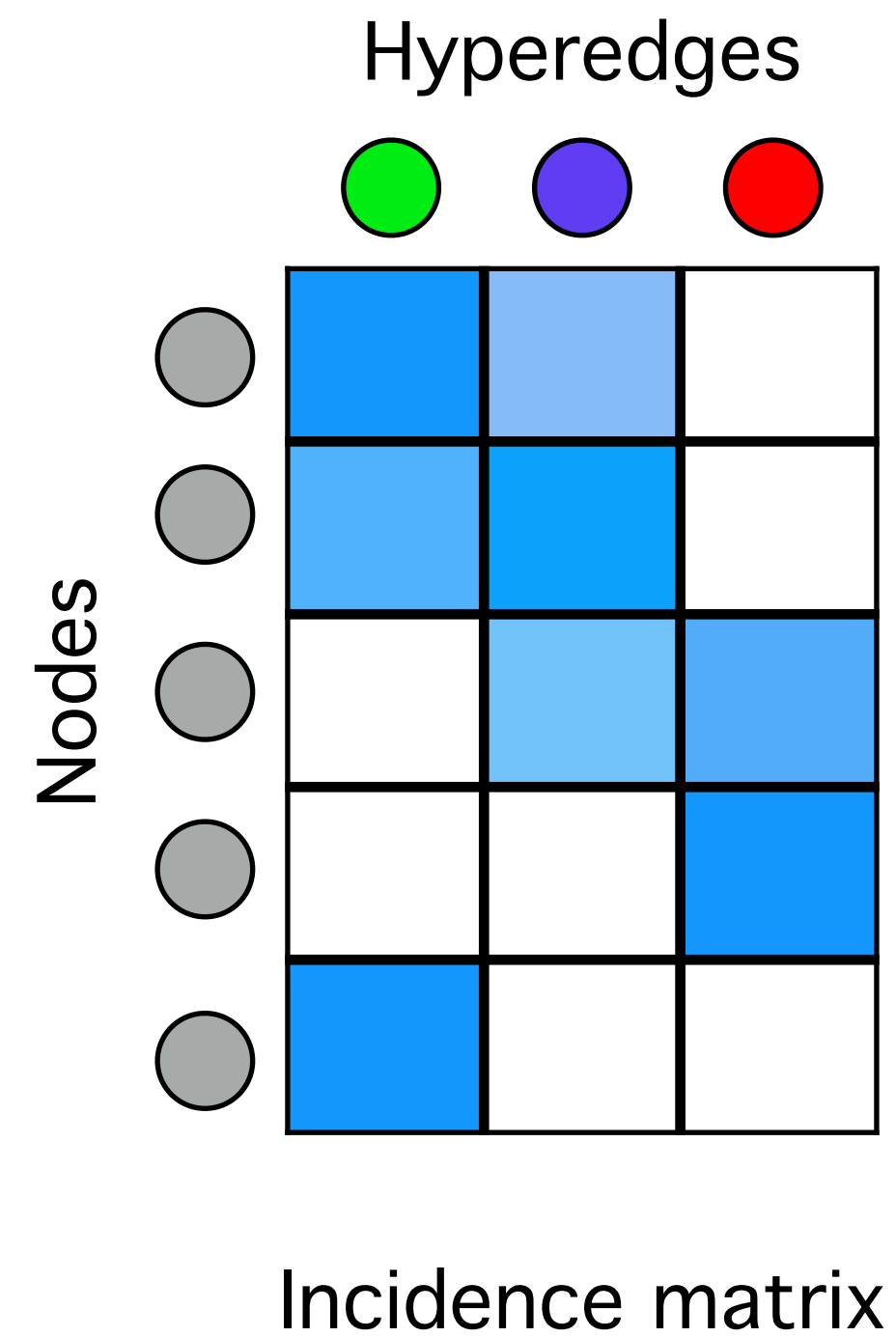


# Incidence matrix

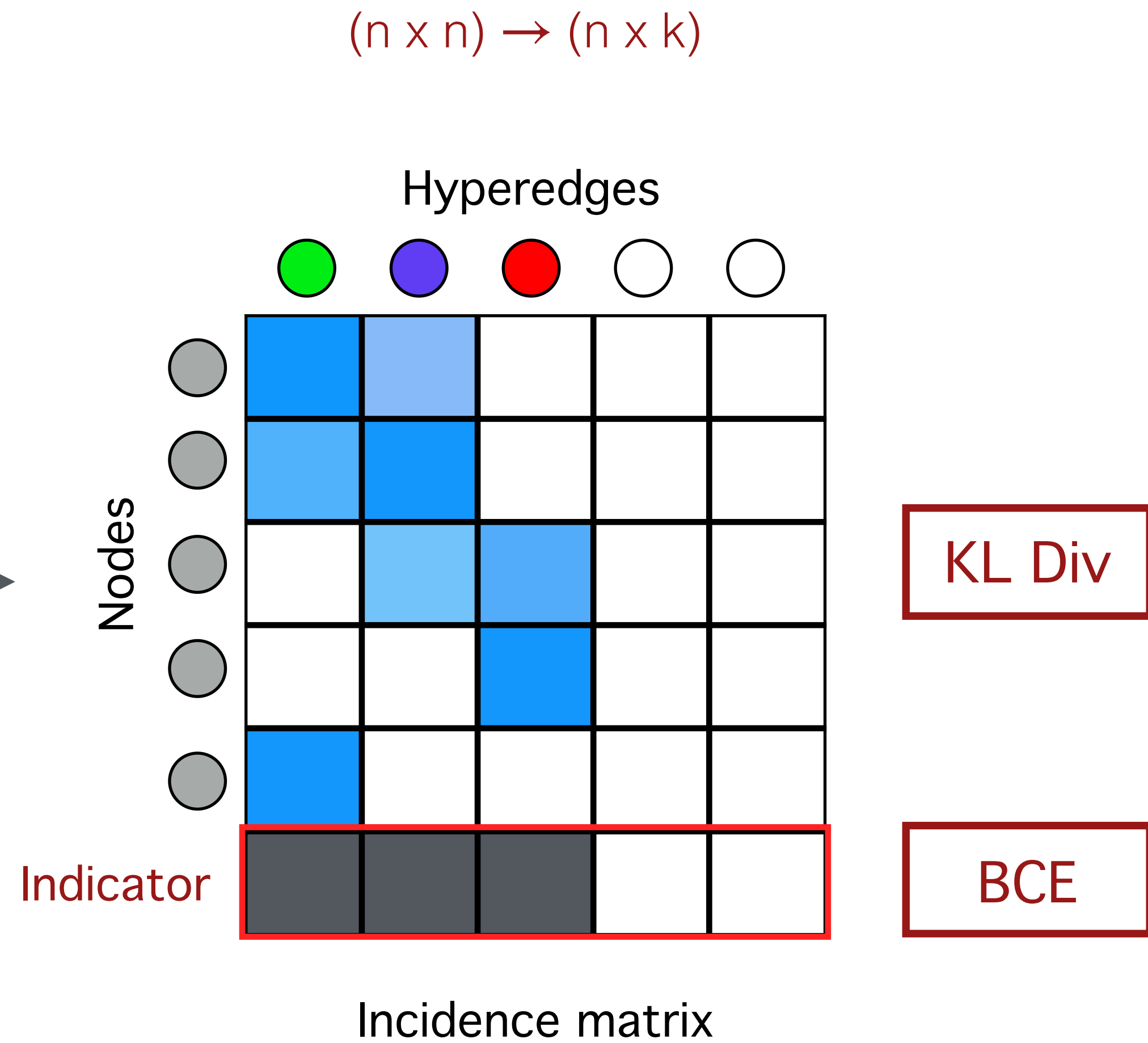


# Indicator

- Variable number of particles
- Indicator to the rescue!



Always  $k$  particles  
Indicator



# Learning the Hypergraph

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## Recurrently Predicting Hypergraphs

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**Gertjan J. Burghouts**  
TNO  
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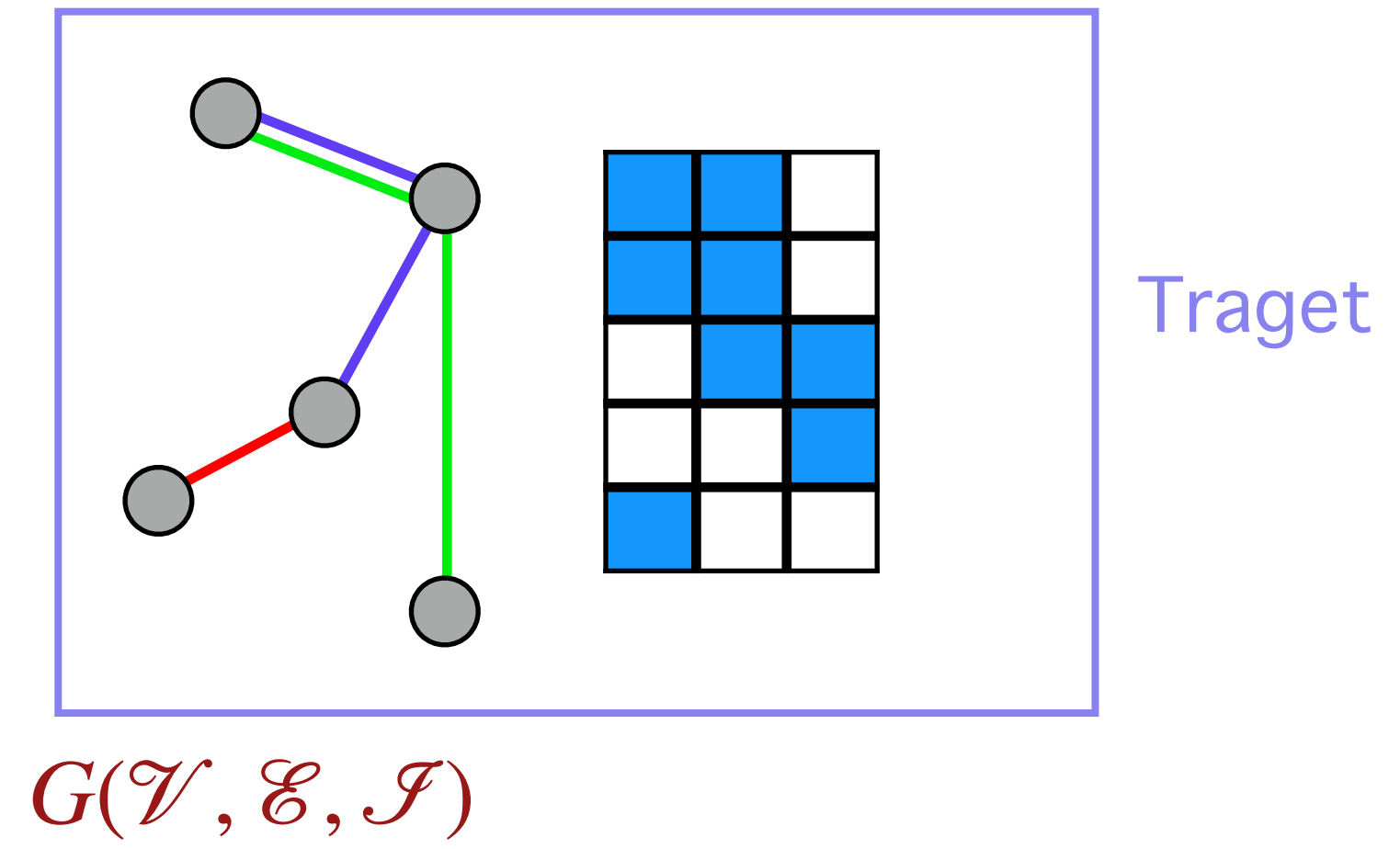
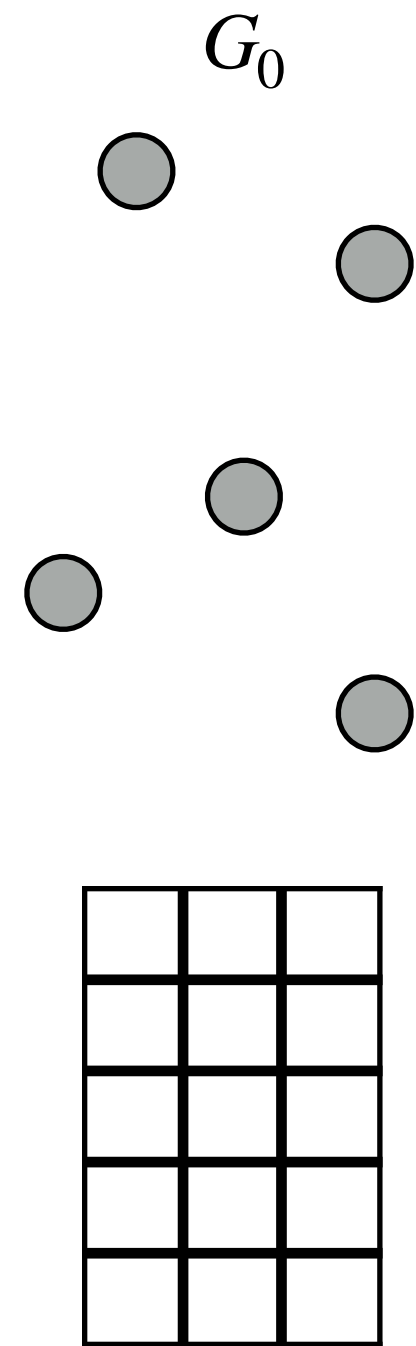
**Cees G. M. Snoek**  
University of Amsterdam  
cgmsnoek@uva.nl

Aligns well with our Physics motivations

<https://arxiv.org/pdf/2106.13919.pdf>

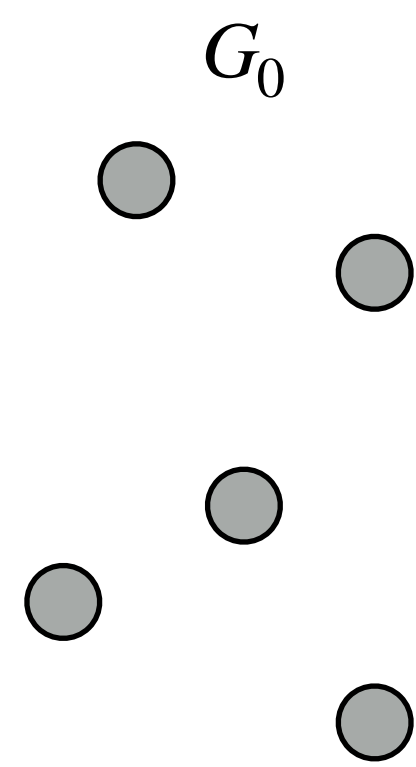
# Recurrently learning Hypergraph

Recurrence! (X16)

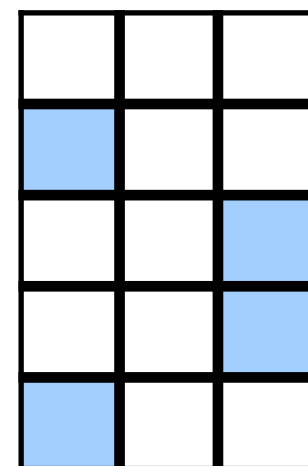
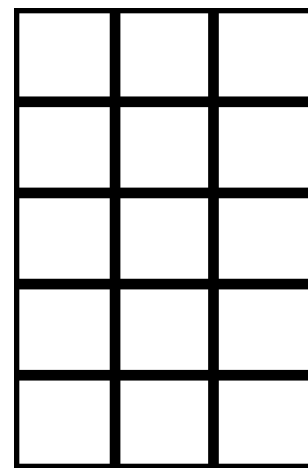
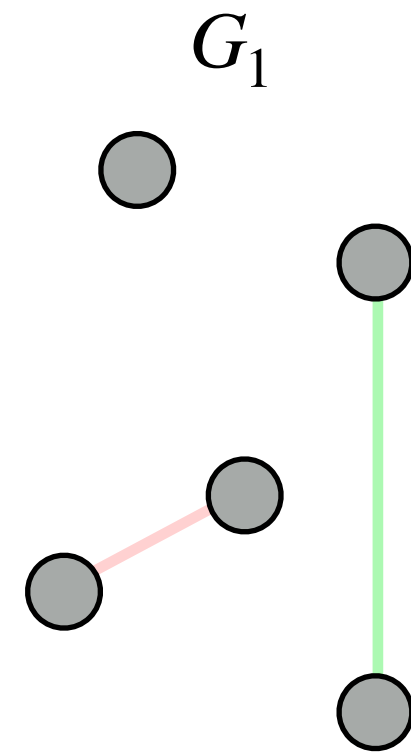


# Recurrently learning Hypergraph

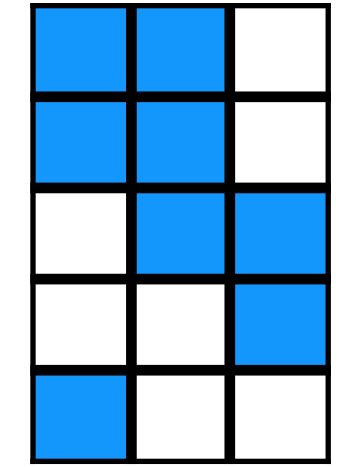
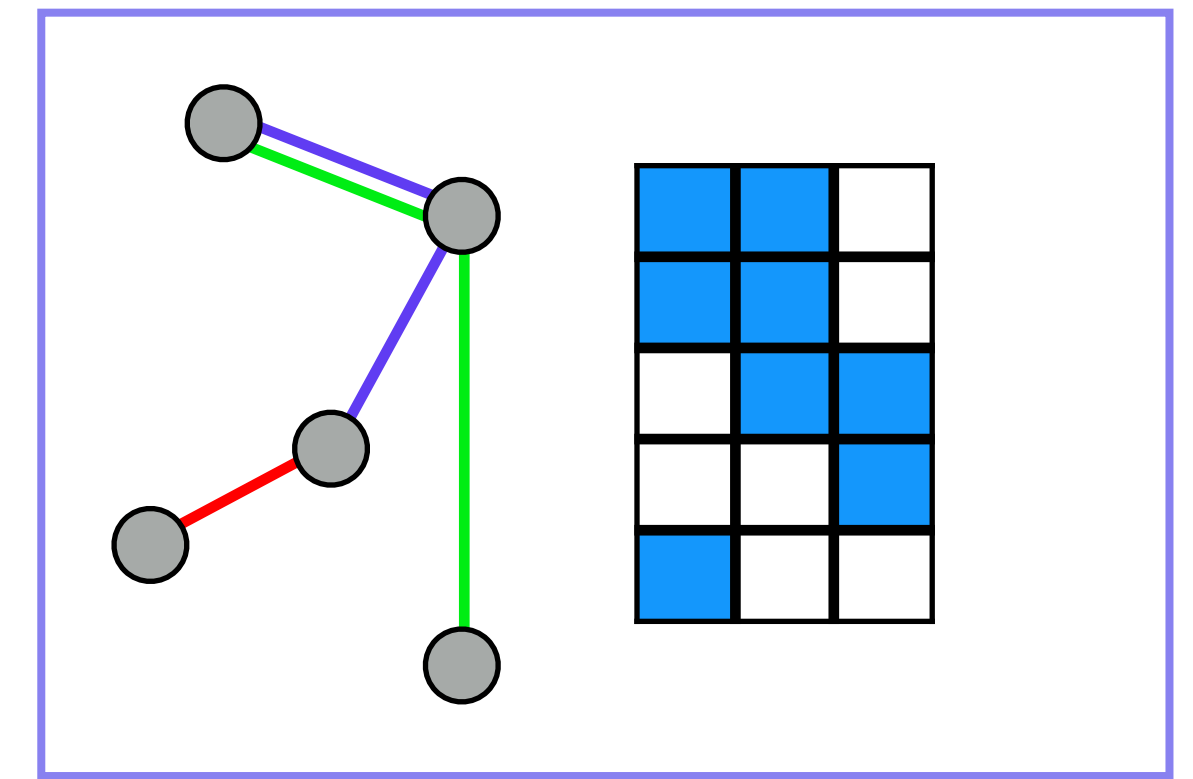
Recurrence! (X16)



GNN



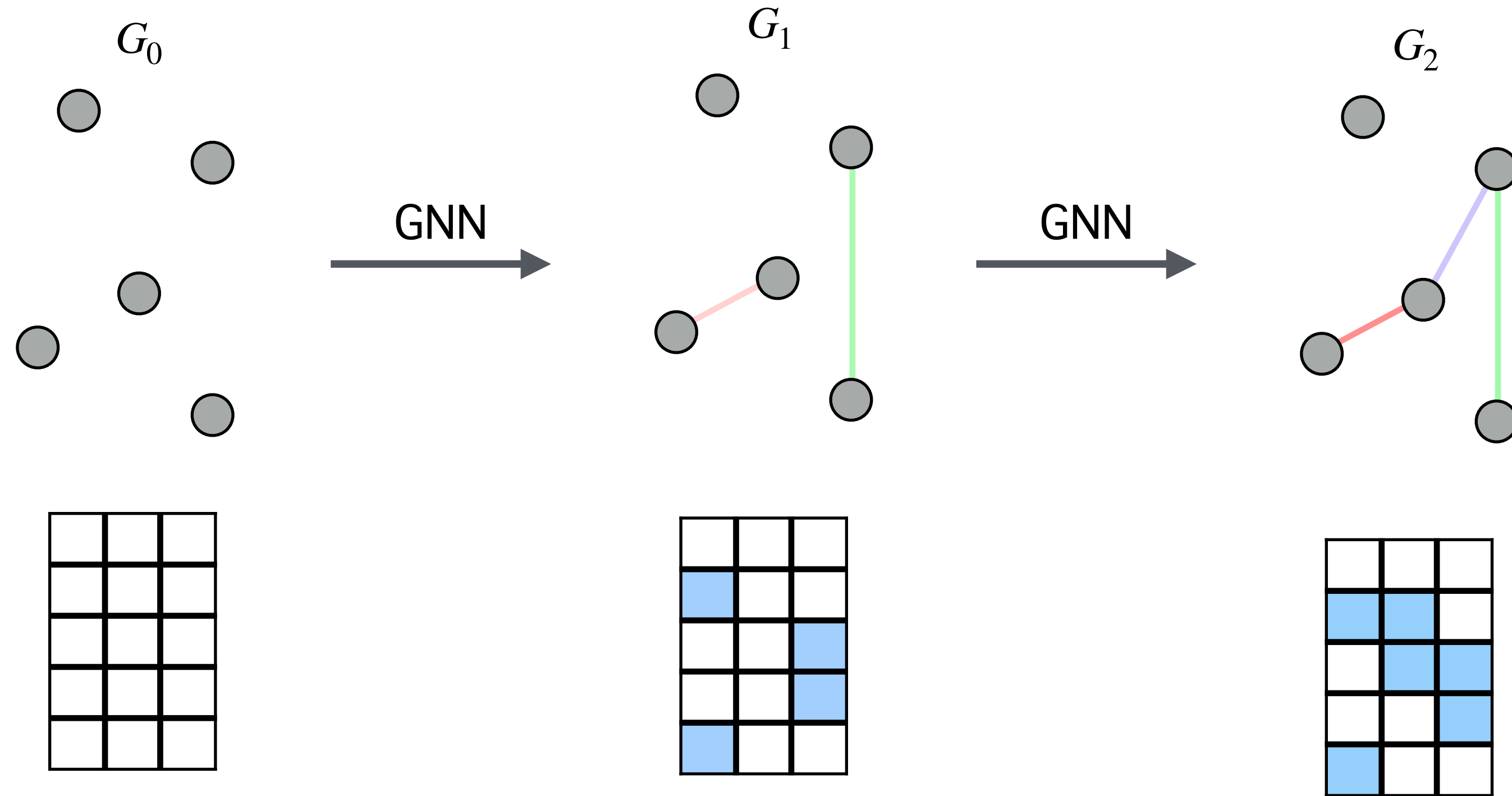
$G(\mathcal{V}, \mathcal{E}, \mathcal{F})$



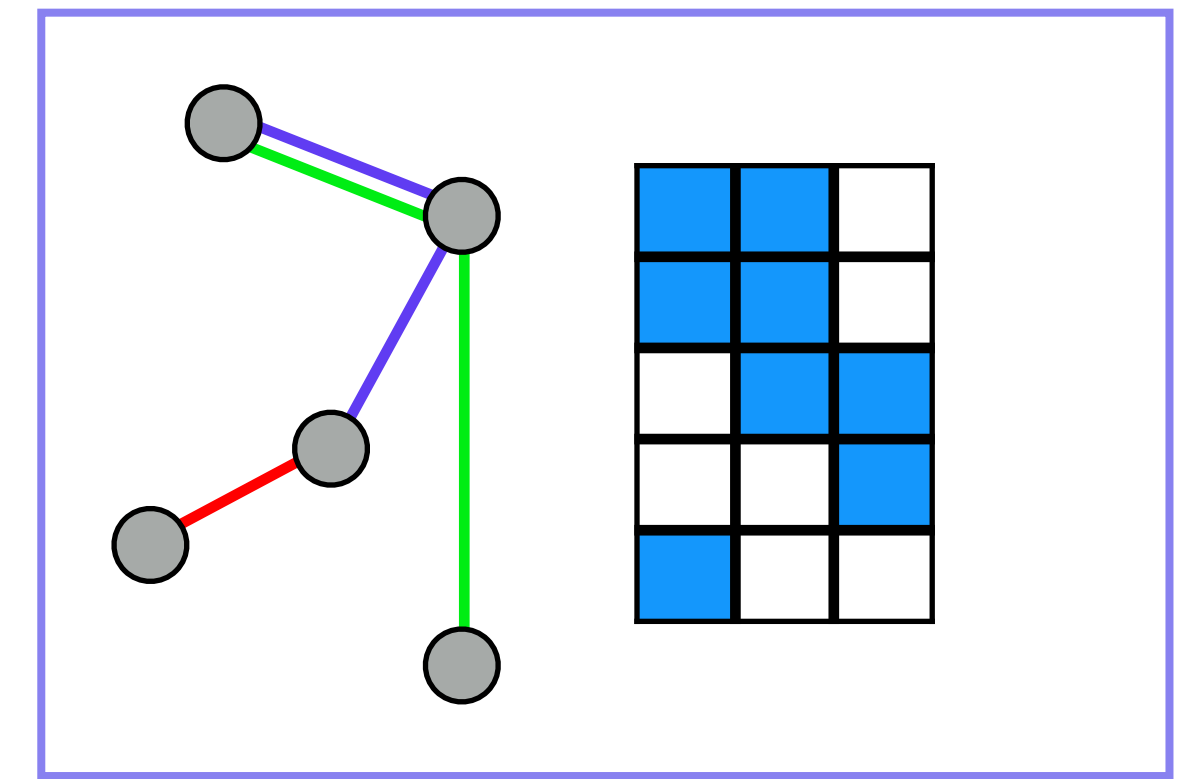
Traget

# Recurrently learning Hypergraph

Recurrence! (X16)



$G(\mathcal{V}, \mathcal{E}, \mathcal{F})$

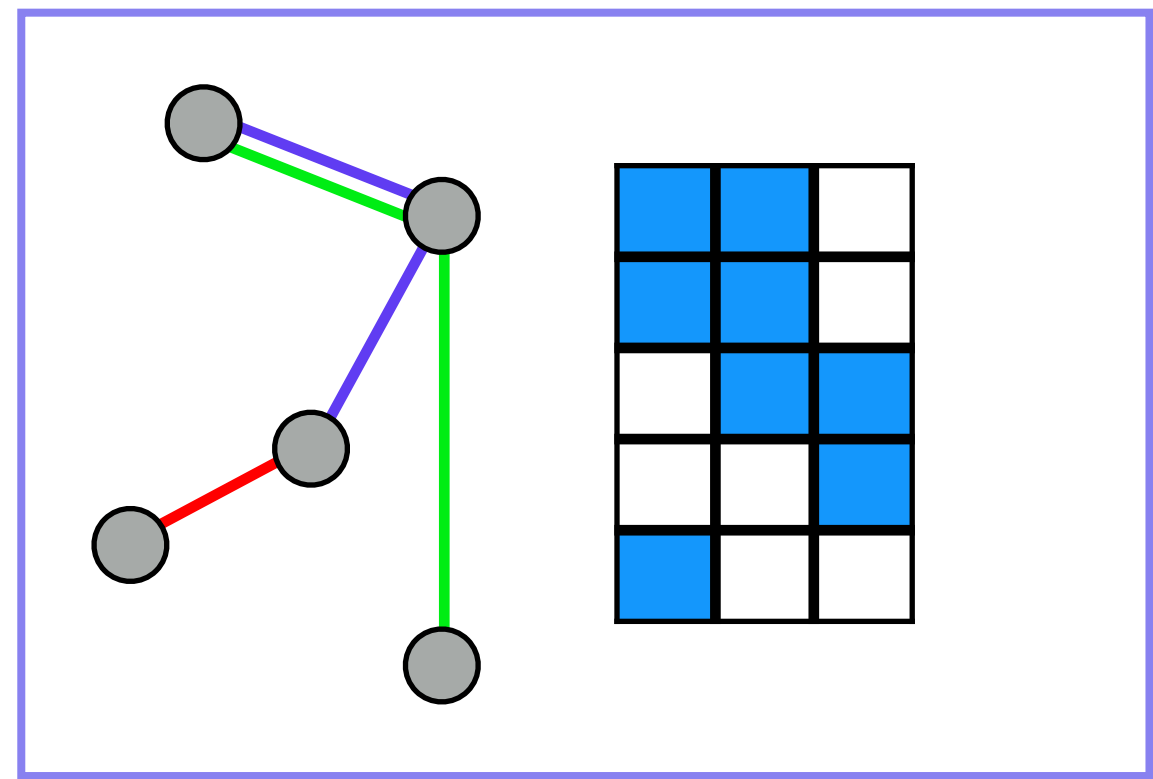


Traget



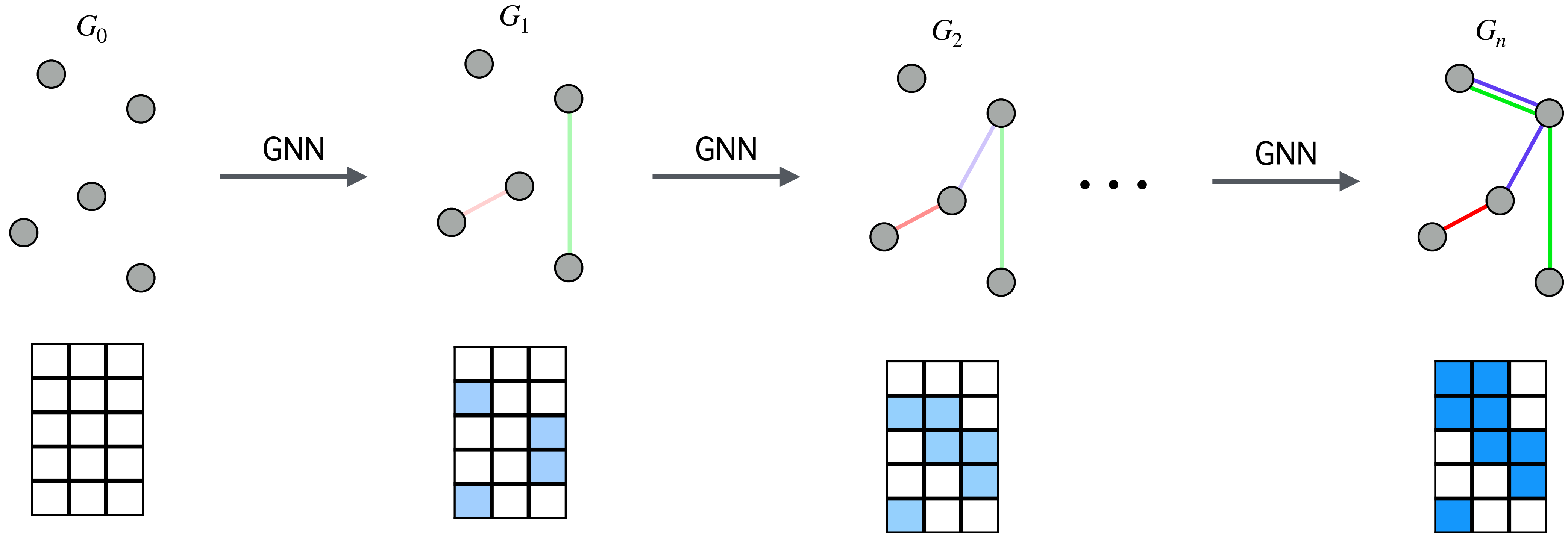
# Recurrently learning Hypergraph

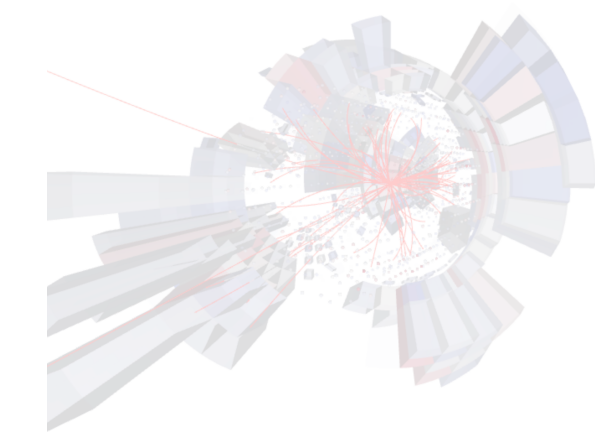
Recurrence! (X16)



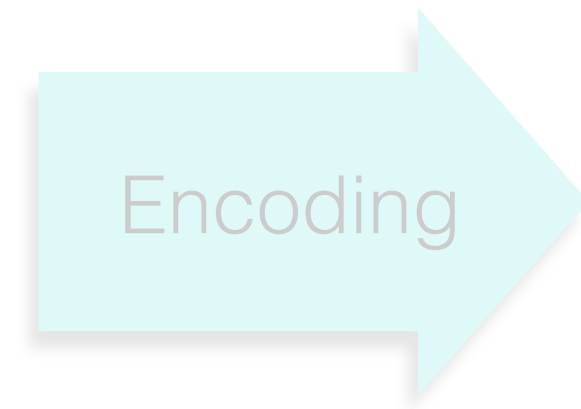
Traget

$G(\mathcal{V}, \mathcal{E}, \mathcal{F})$

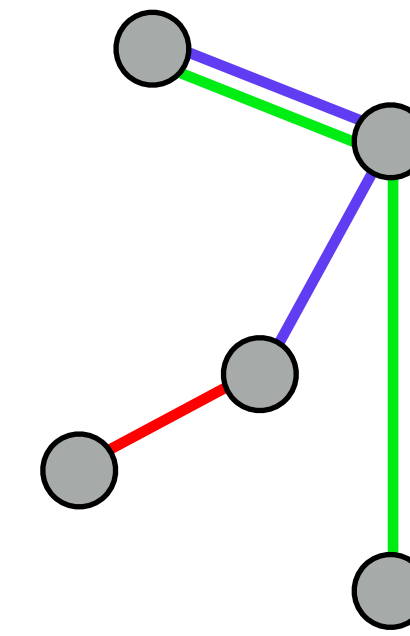




Detector data  
(Tracks, cells)

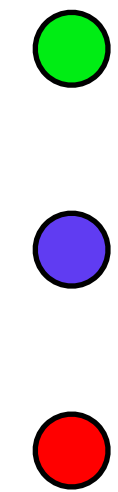


Encoded data



Hypergraph

## Step 3



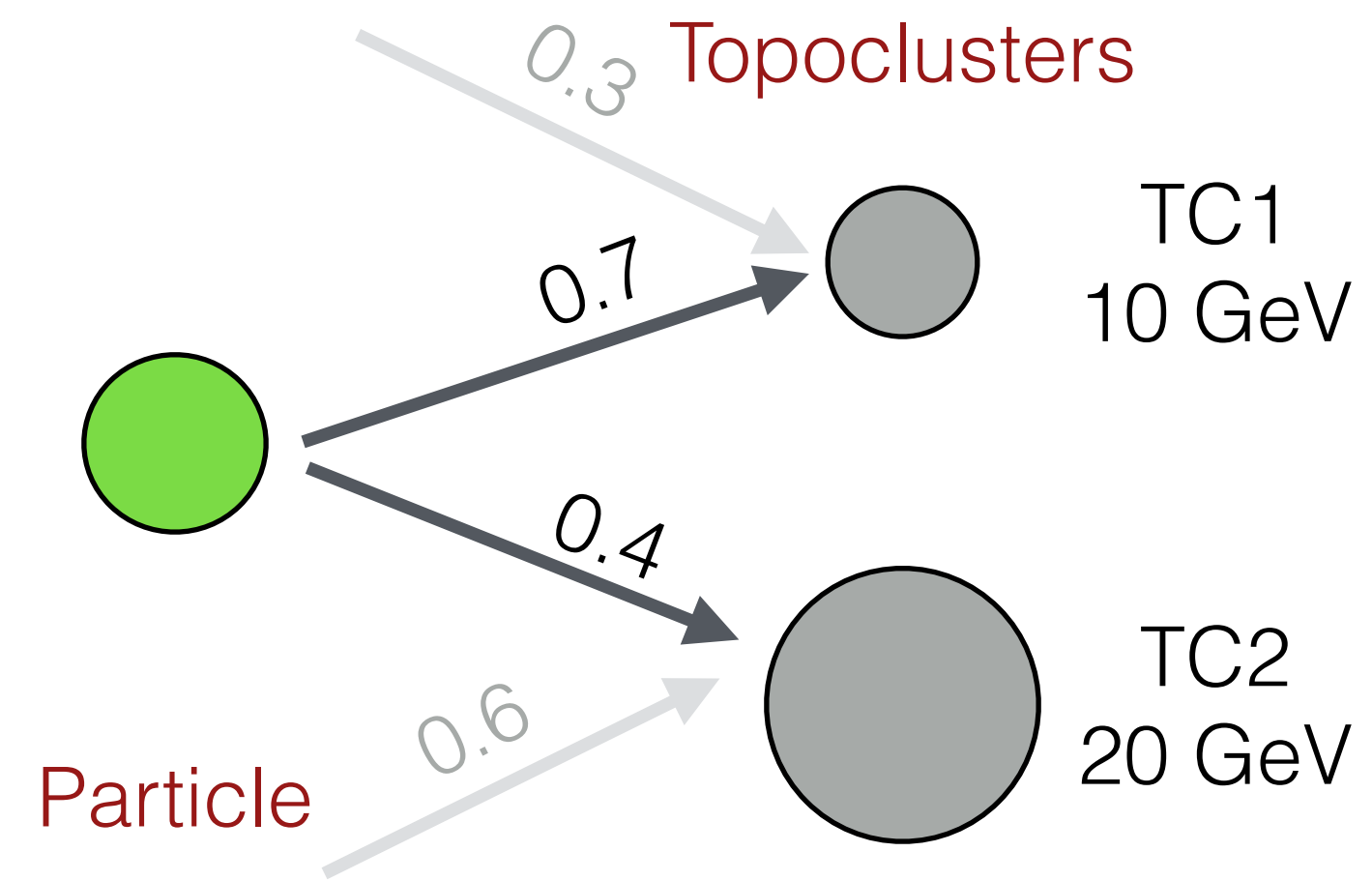
Particles

# Proxy properties

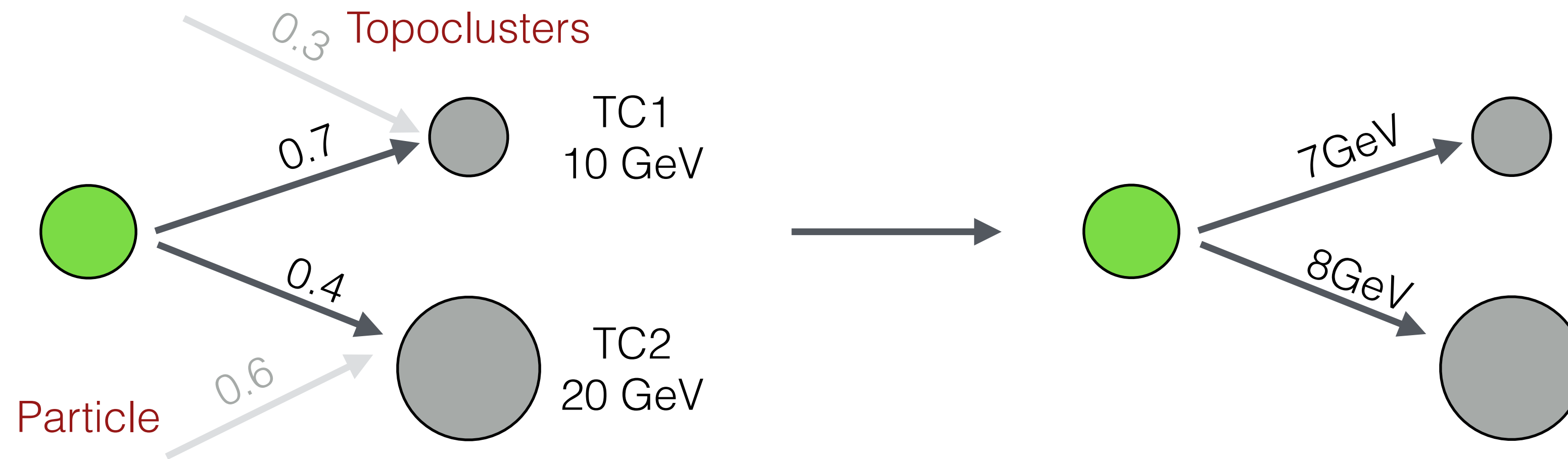
- With the incidence matrix, we already know a lot about the particles!
- For charged particles,
  - The tracks are a good (but not perfect) representation of the particles
  - Let's use it and improve over it

# Proxy properties (neutral)

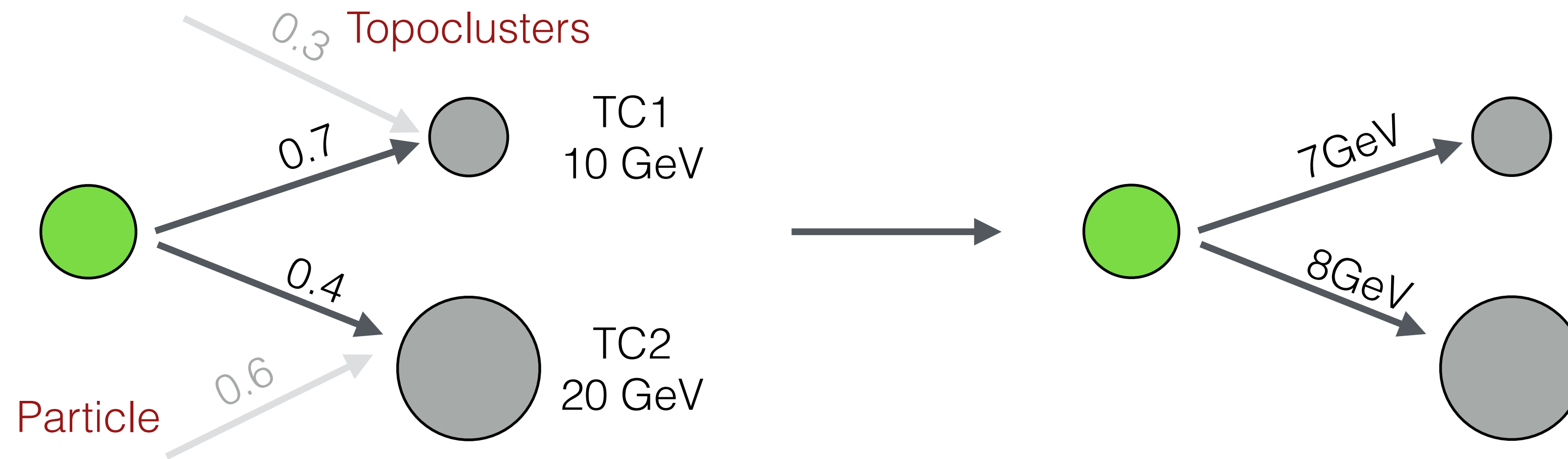
# Proxy properties (neutral)



# Proxy properties (neutral)

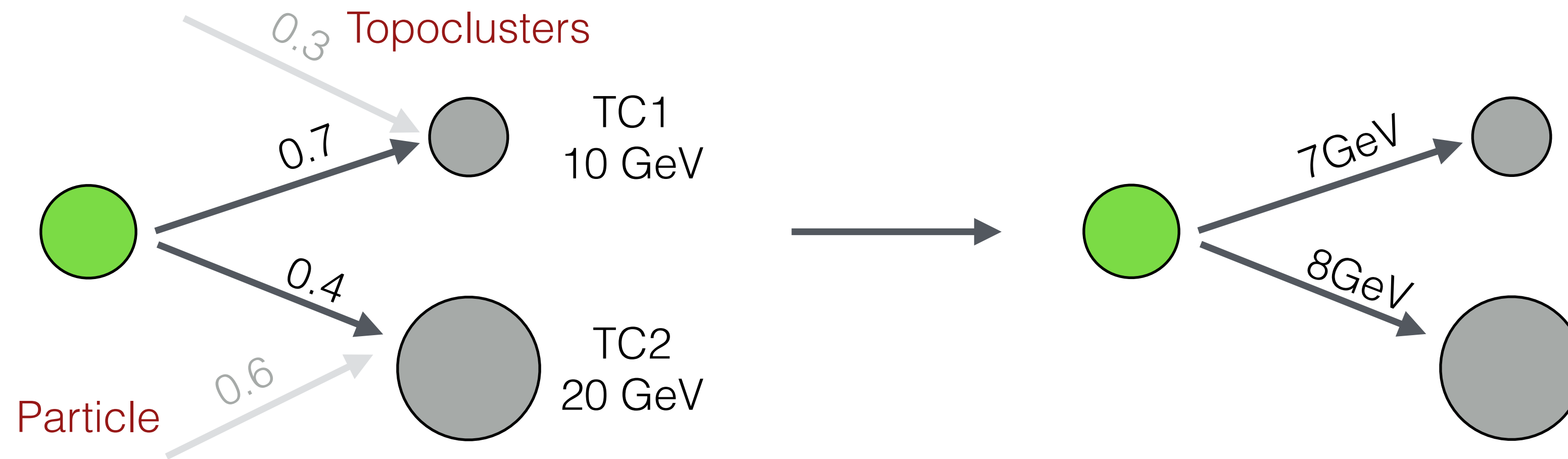


# Proxy properties (neutral)



Proxy properties of 

# Proxy properties (neutral)

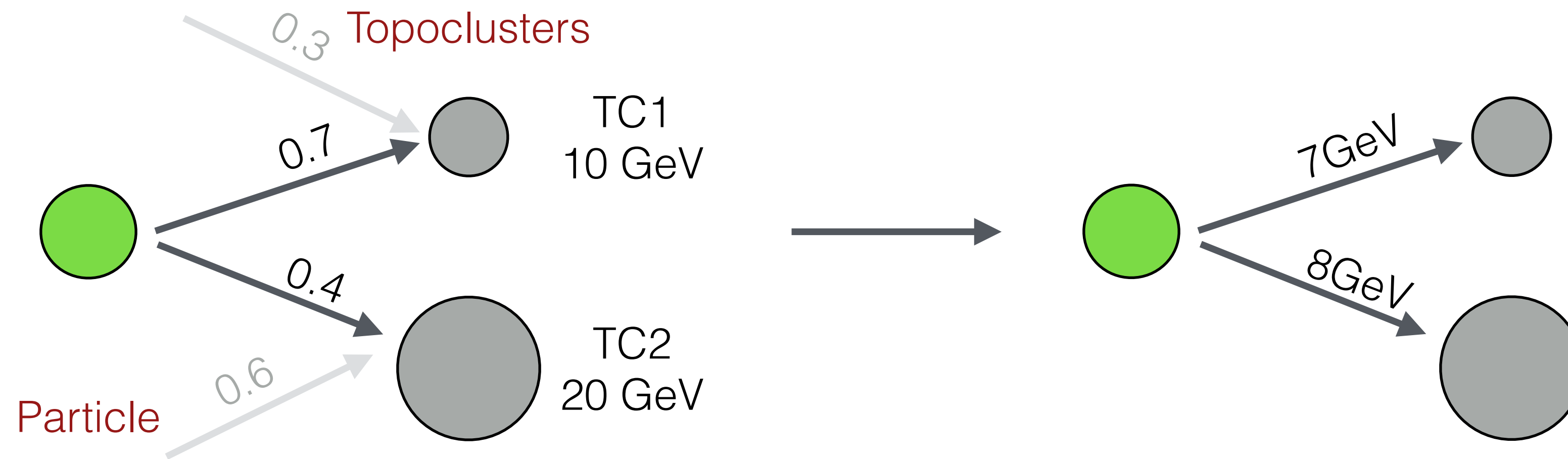


Proxy properties of 

- $E = E1 + E2 = 15\text{GeV}$



# Proxy properties (neutral)

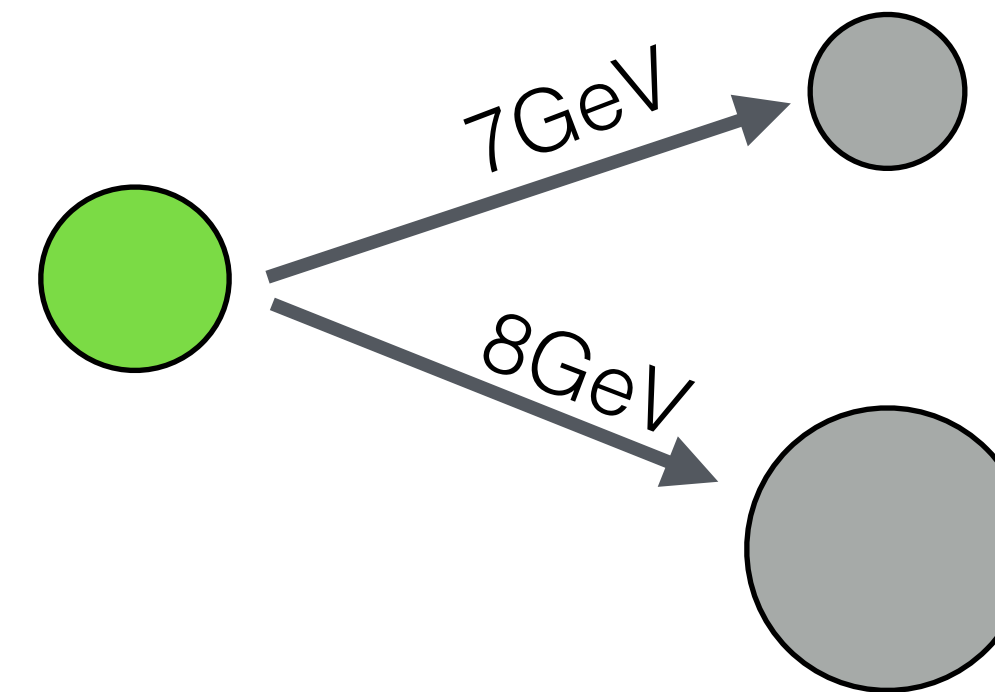
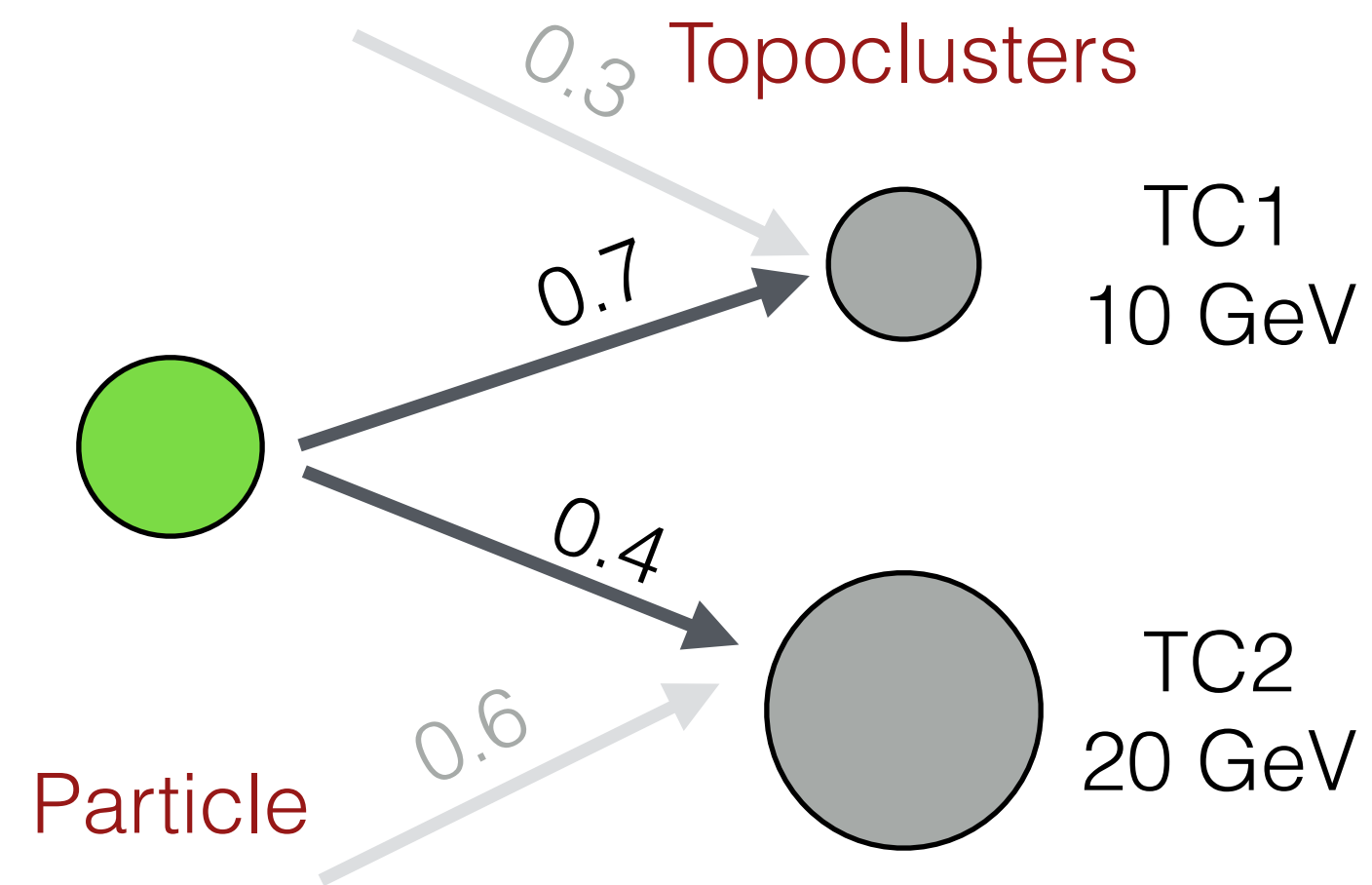


Proxy properties of 

- $E = E_1 + E_2 = 15\text{GeV}$

- $\eta = \frac{7\eta_1 + 8\eta_2}{15}$

# Proxy properties (neutral)



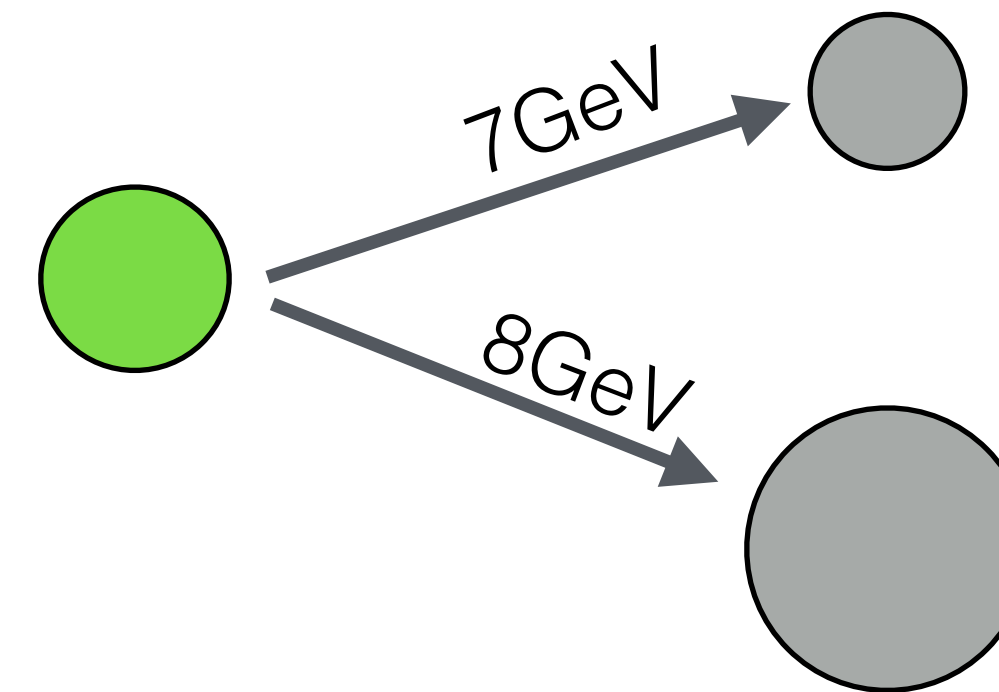
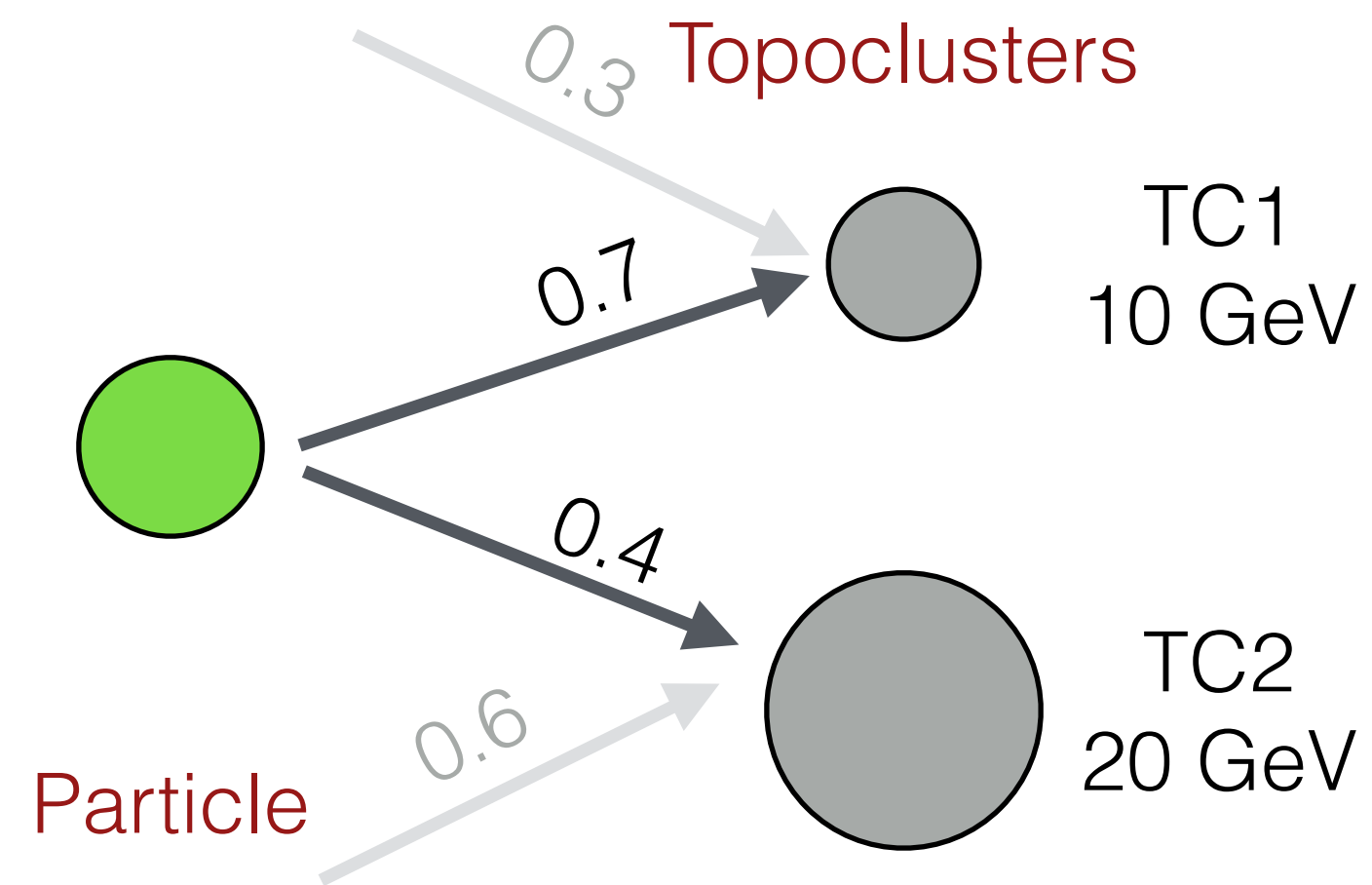
Proxy properties of 

- $E = E_1 + E_2 = 15\text{GeV}$

- $\eta = \frac{7\eta_1 + 8\eta_2}{15}$

- $\phi = \frac{7\phi_1 + 8\phi_2}{15}$

# Proxy properties (neutral)



Proxy properties of 

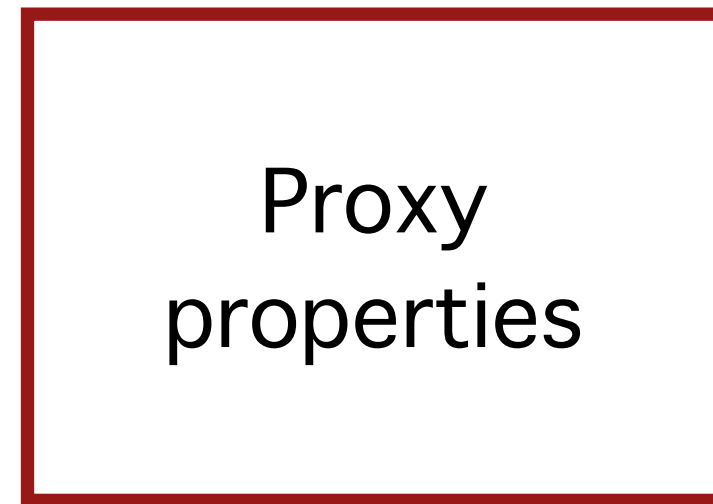
- $E = E_1 + E_2 = 15\text{GeV}$

- $p_T = \frac{E}{\cosh(\eta)}$

- $\eta = \frac{7\eta_1 + 8\eta_2}{15}$

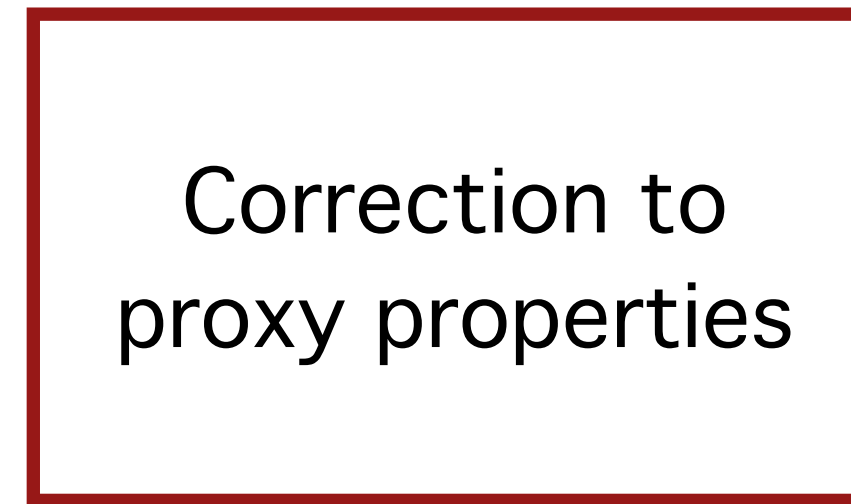
- $\phi = \frac{7\phi_1 + 8\phi_2}{15}$

# Additional network



$p_T$

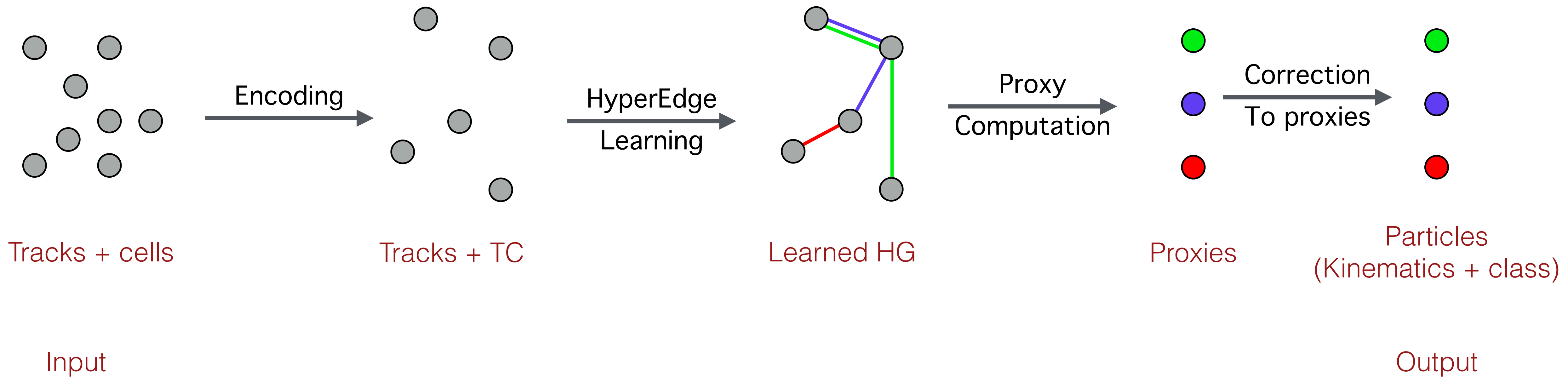
Neural Network  
→



$\Delta p_T$

$$\text{Particle } p_T = p_T + \Delta p_T$$

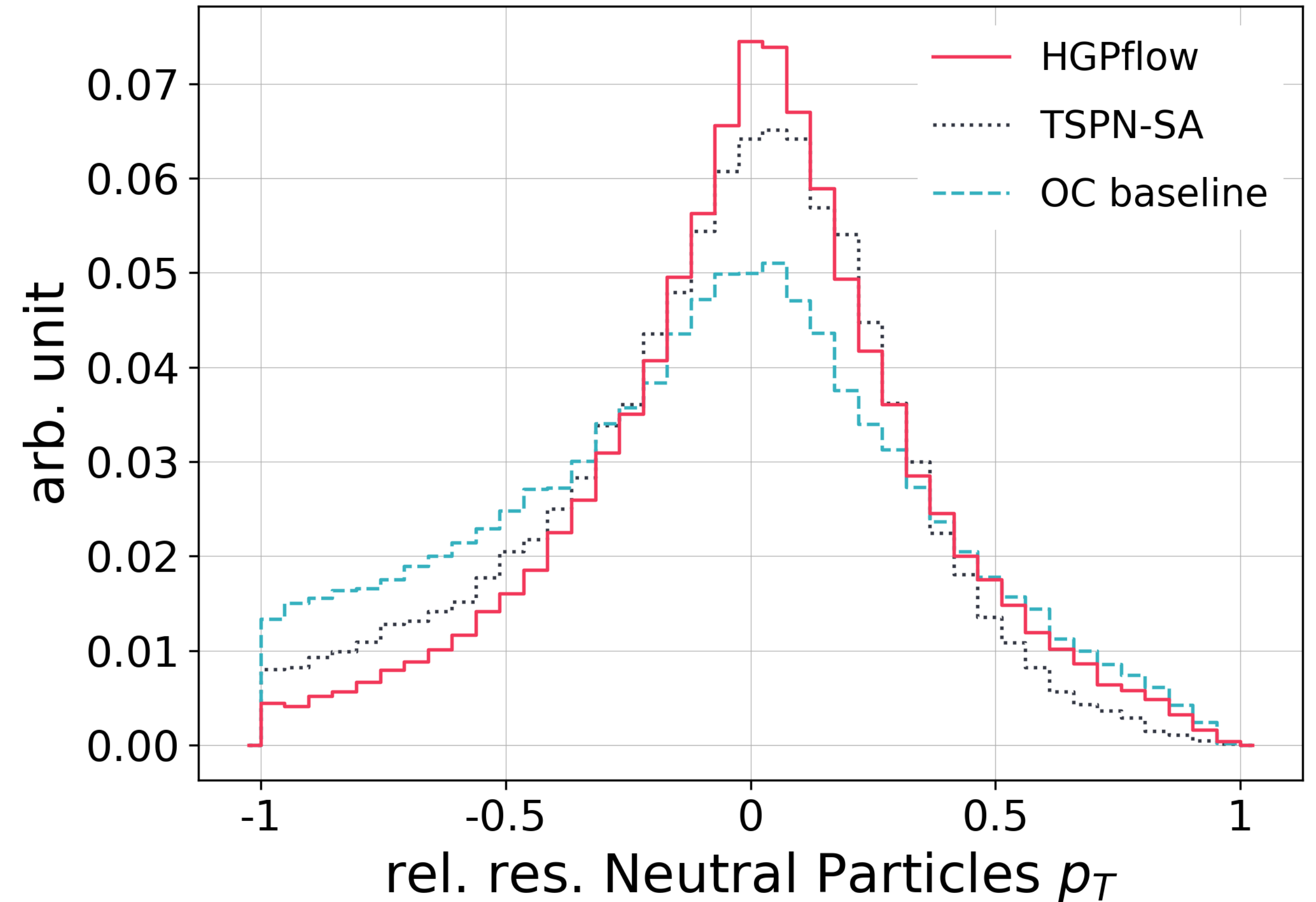
# Overall architecture



**So, does it work?**

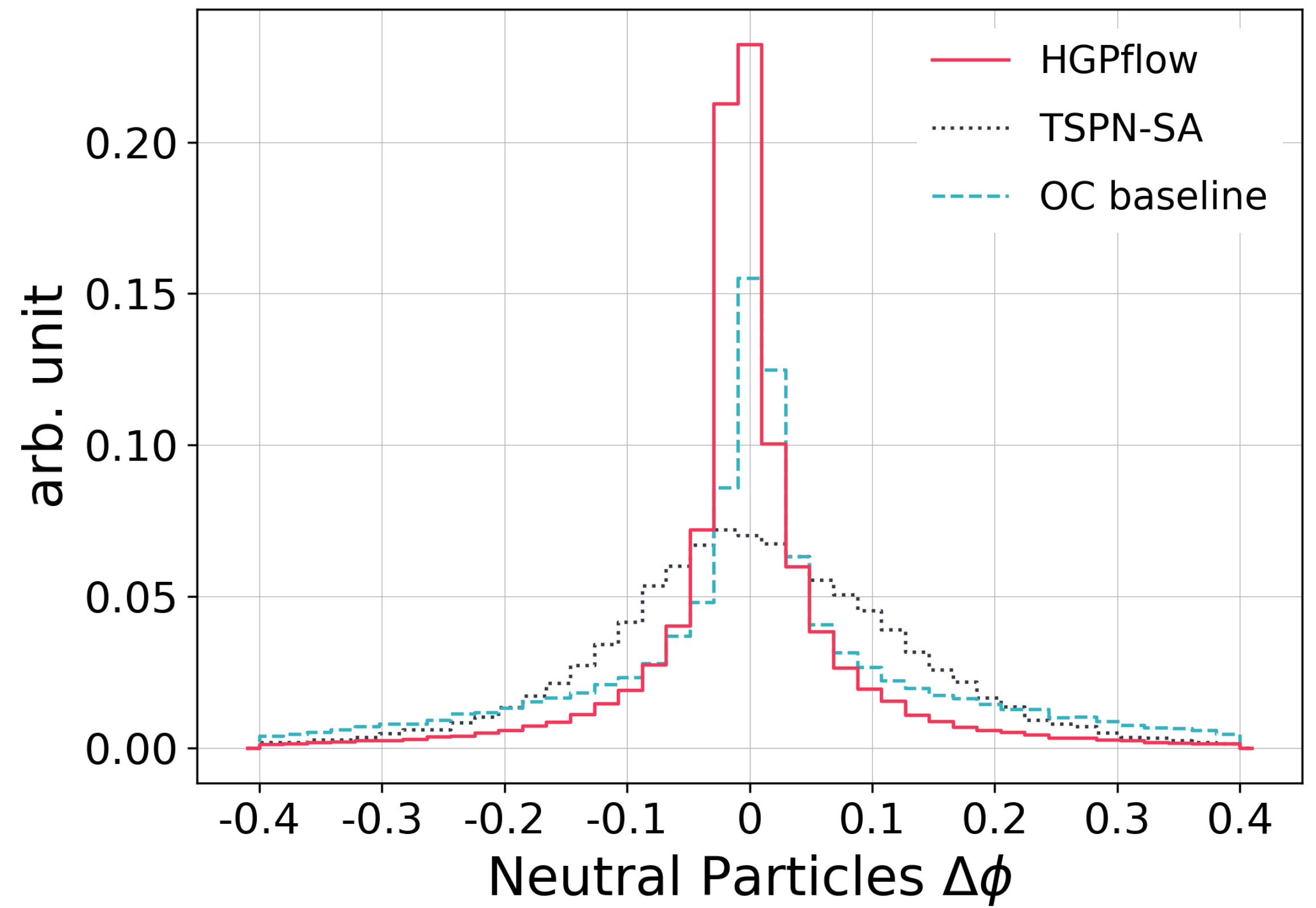
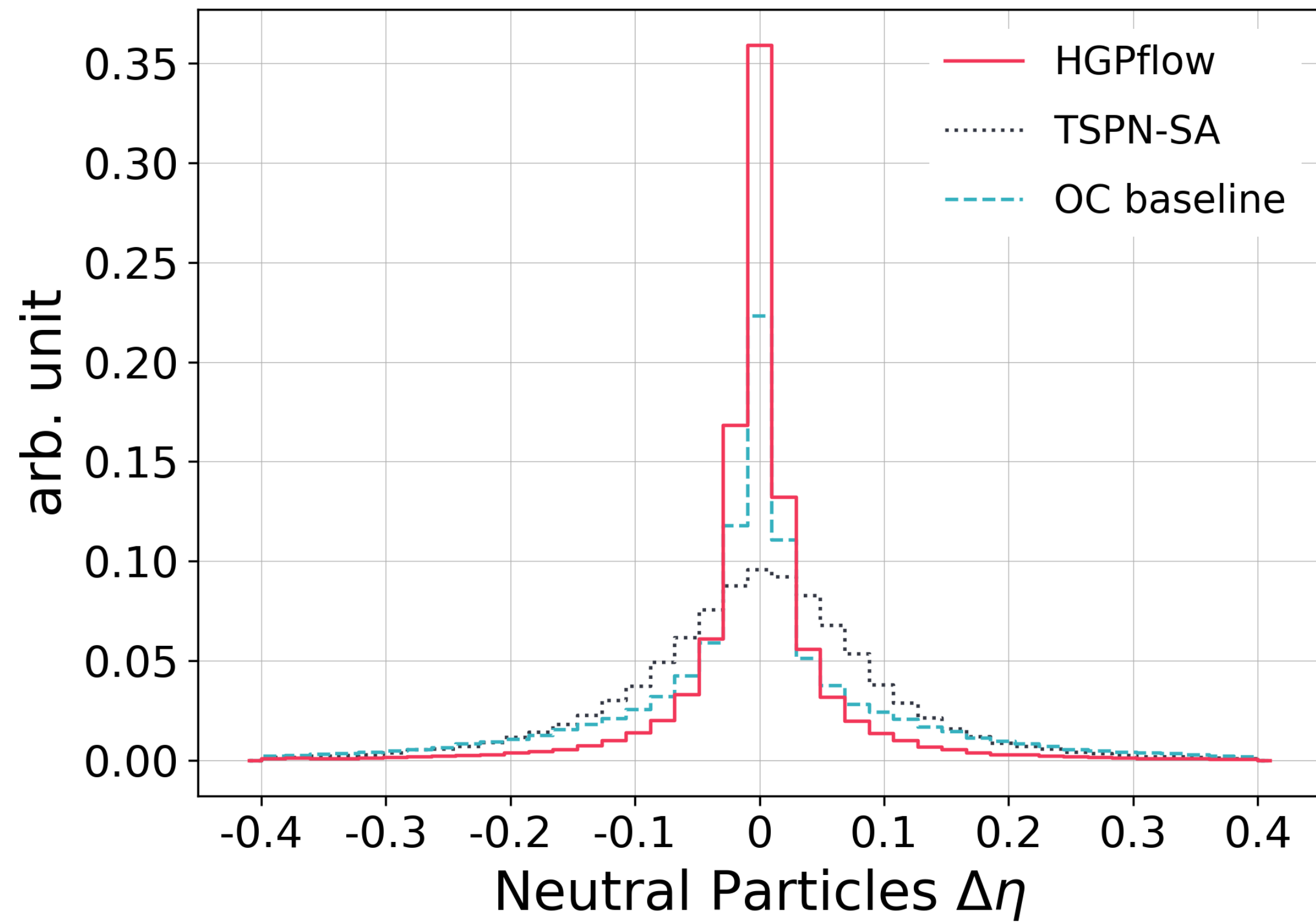
# Neutral particles

- HG can understand overlapping showers more precisely
- Helps in better reconstruction



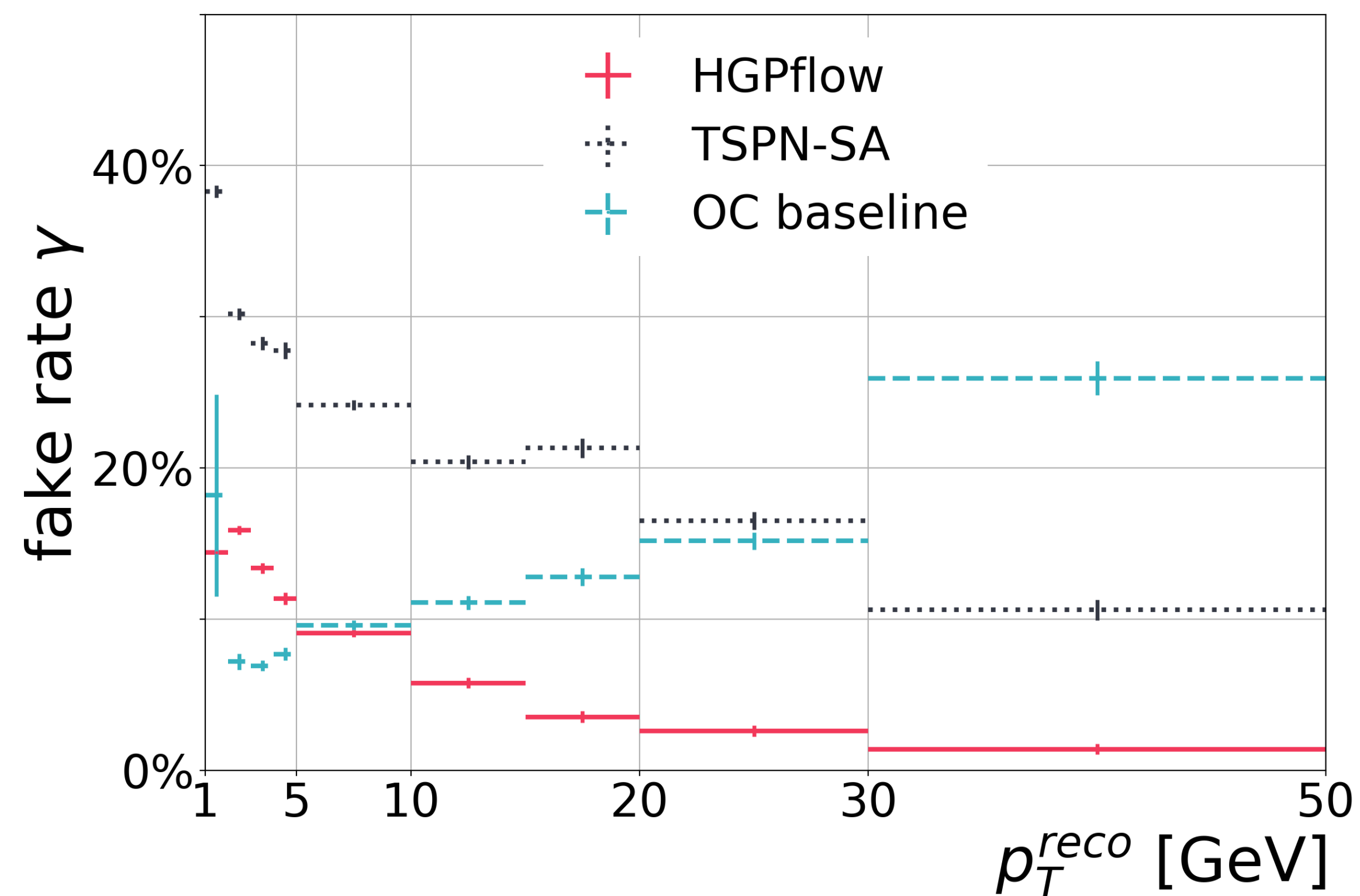
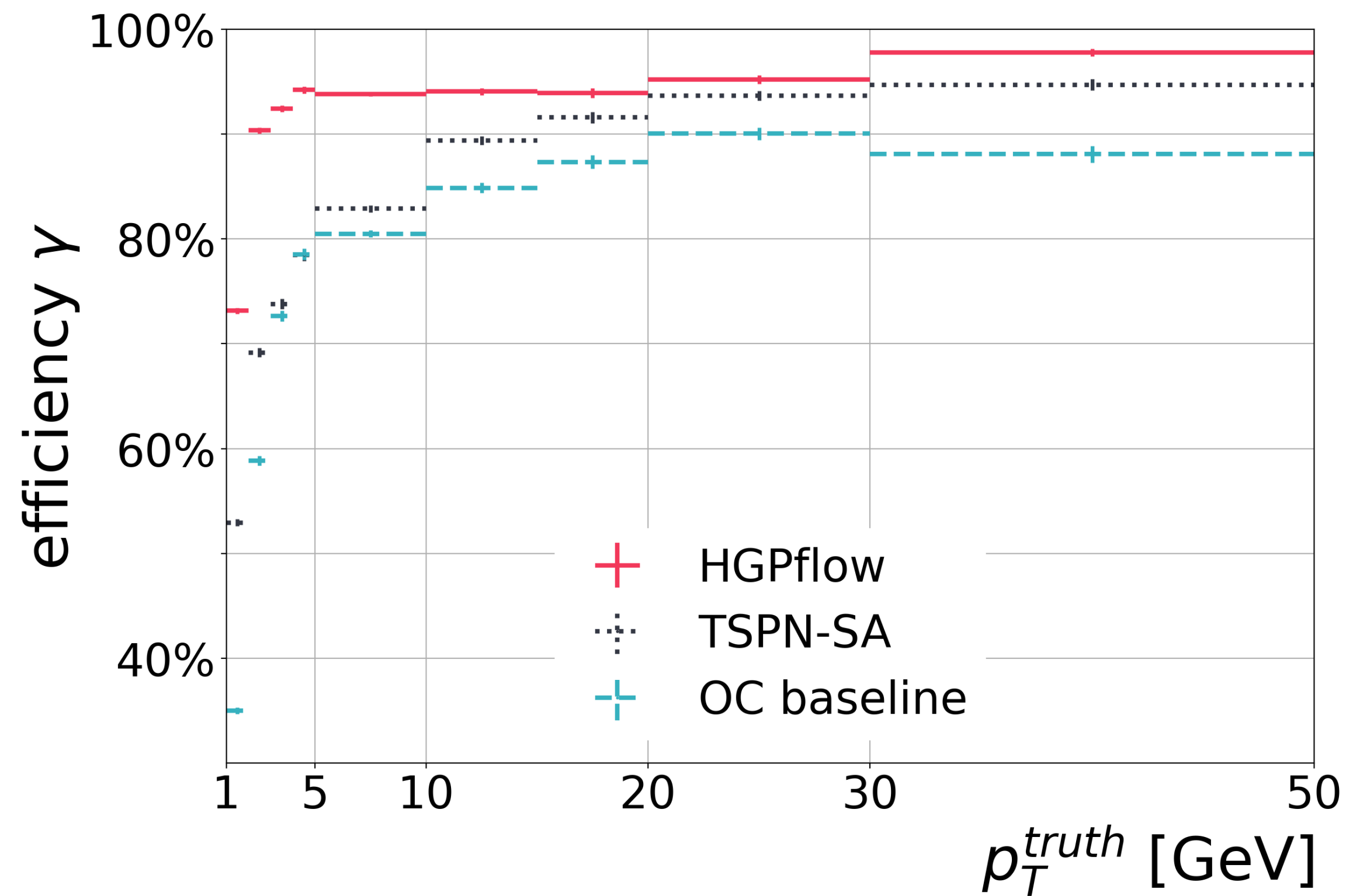
$$\frac{\text{Truth} - \text{predicted}}{\text{Truth}}$$

# Neutral particles

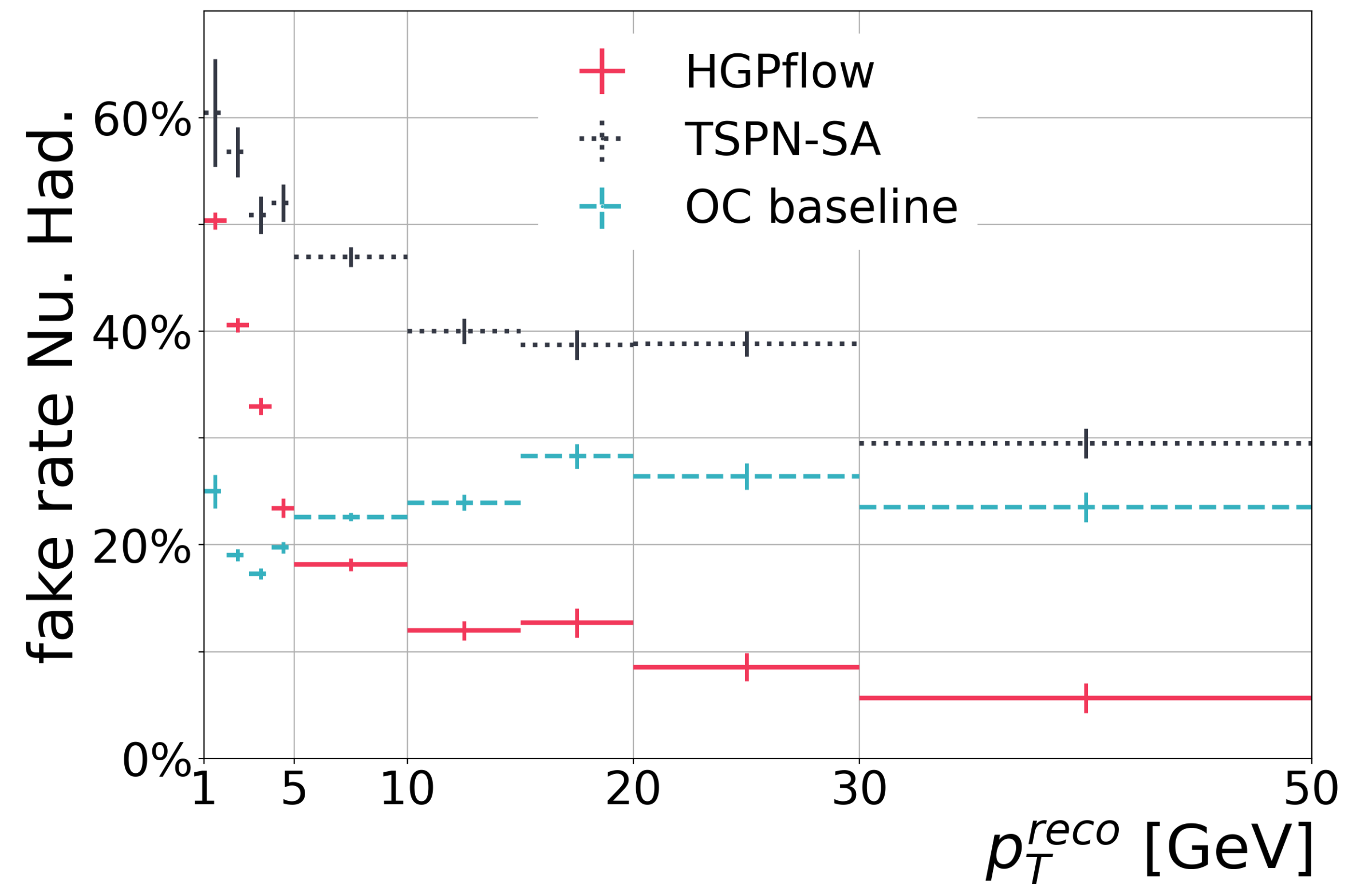
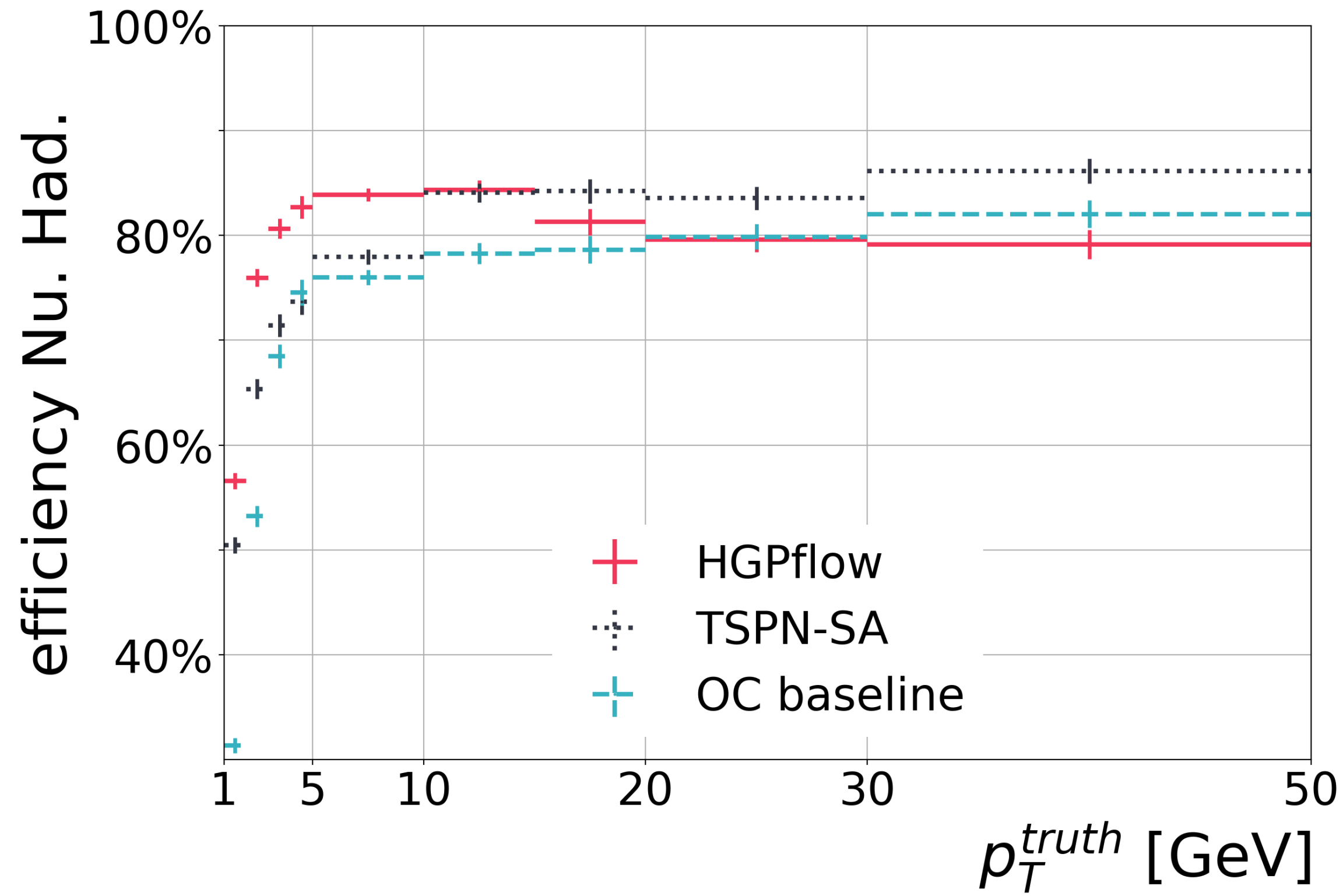




# Neutral particles (photons)



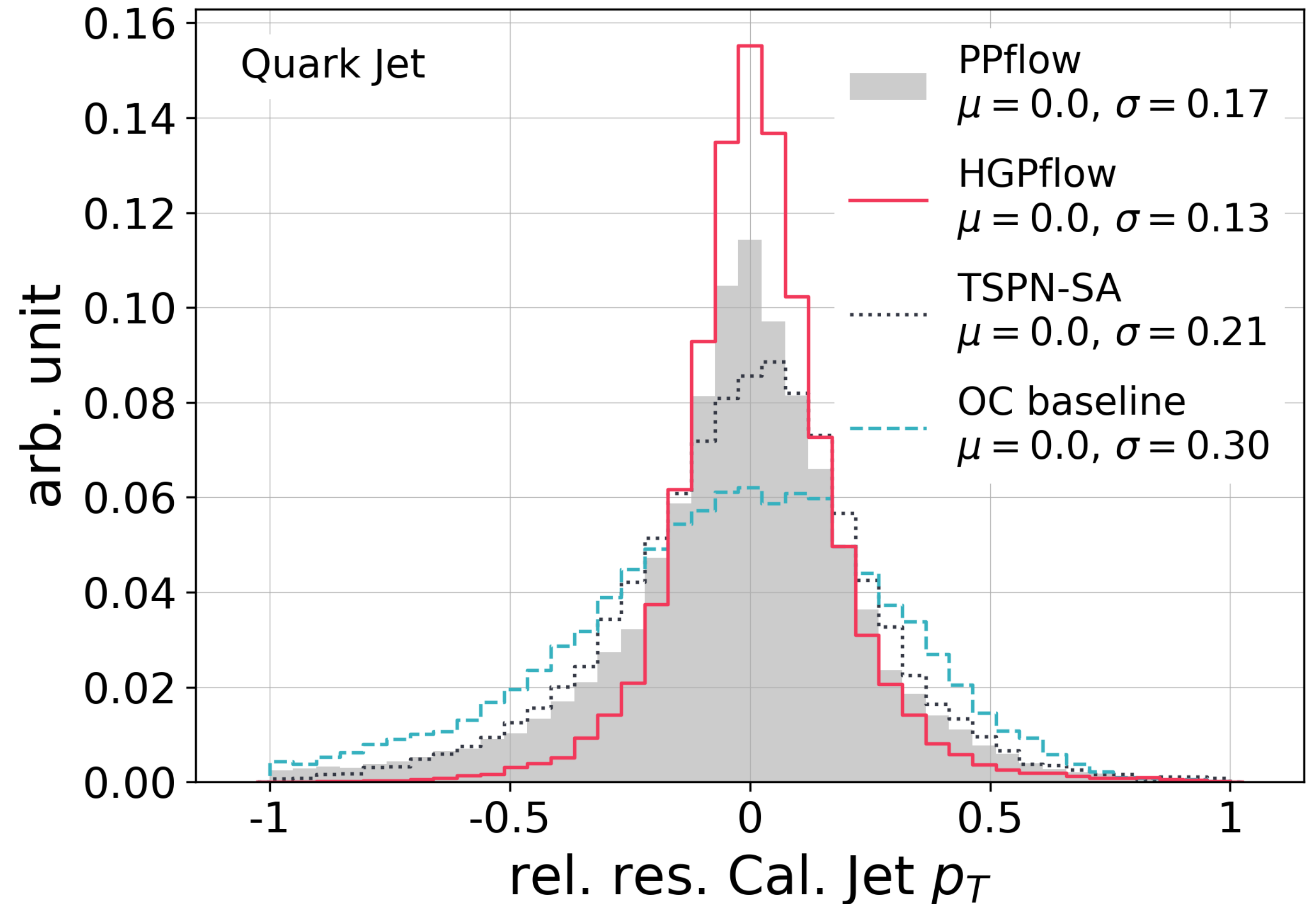
# Neutral particles (neutral hadrons)



# Jets

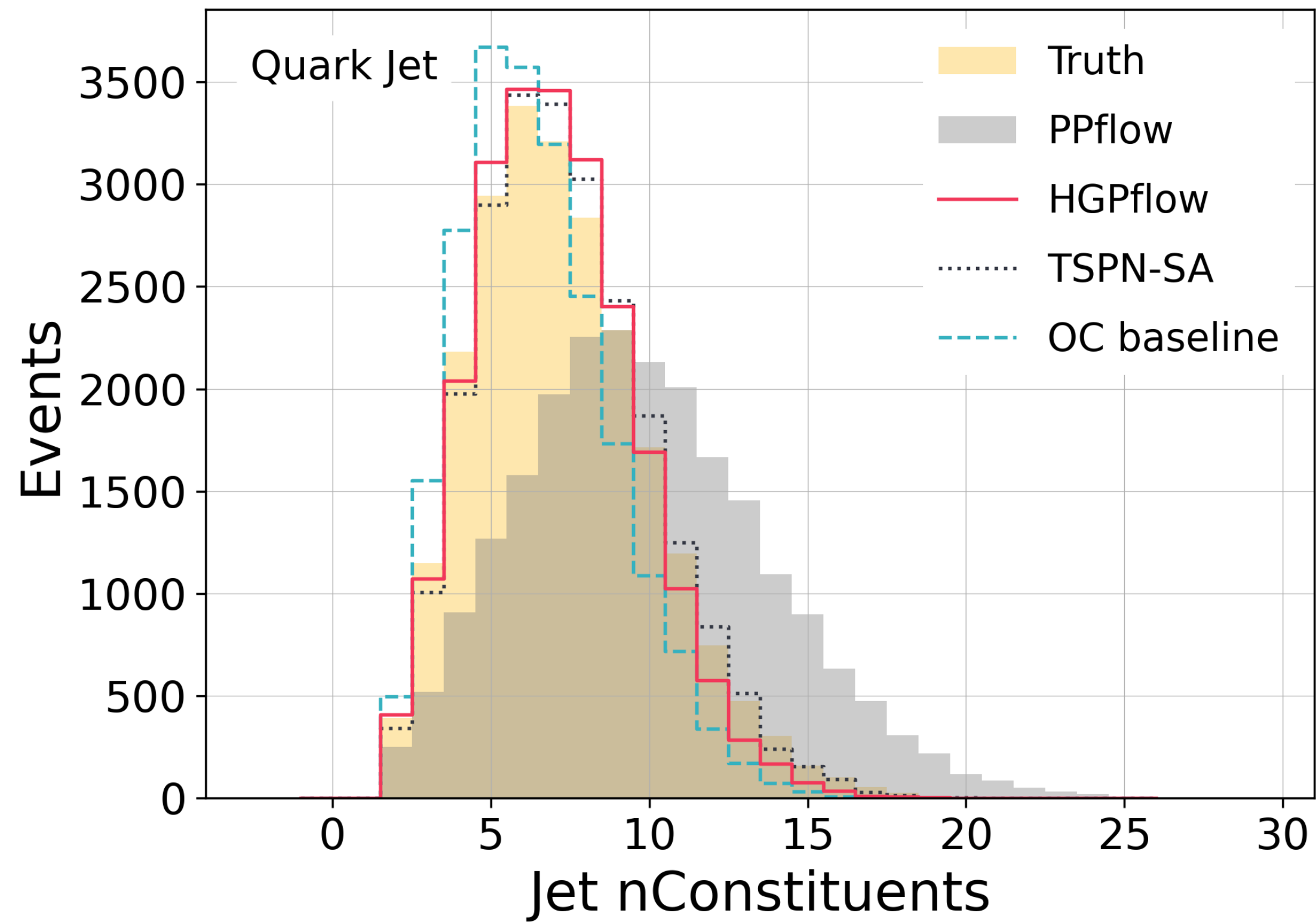
- PPflow is optimized for jet resolution,
- ML algos were not trained on this objective

Improved Resolution!

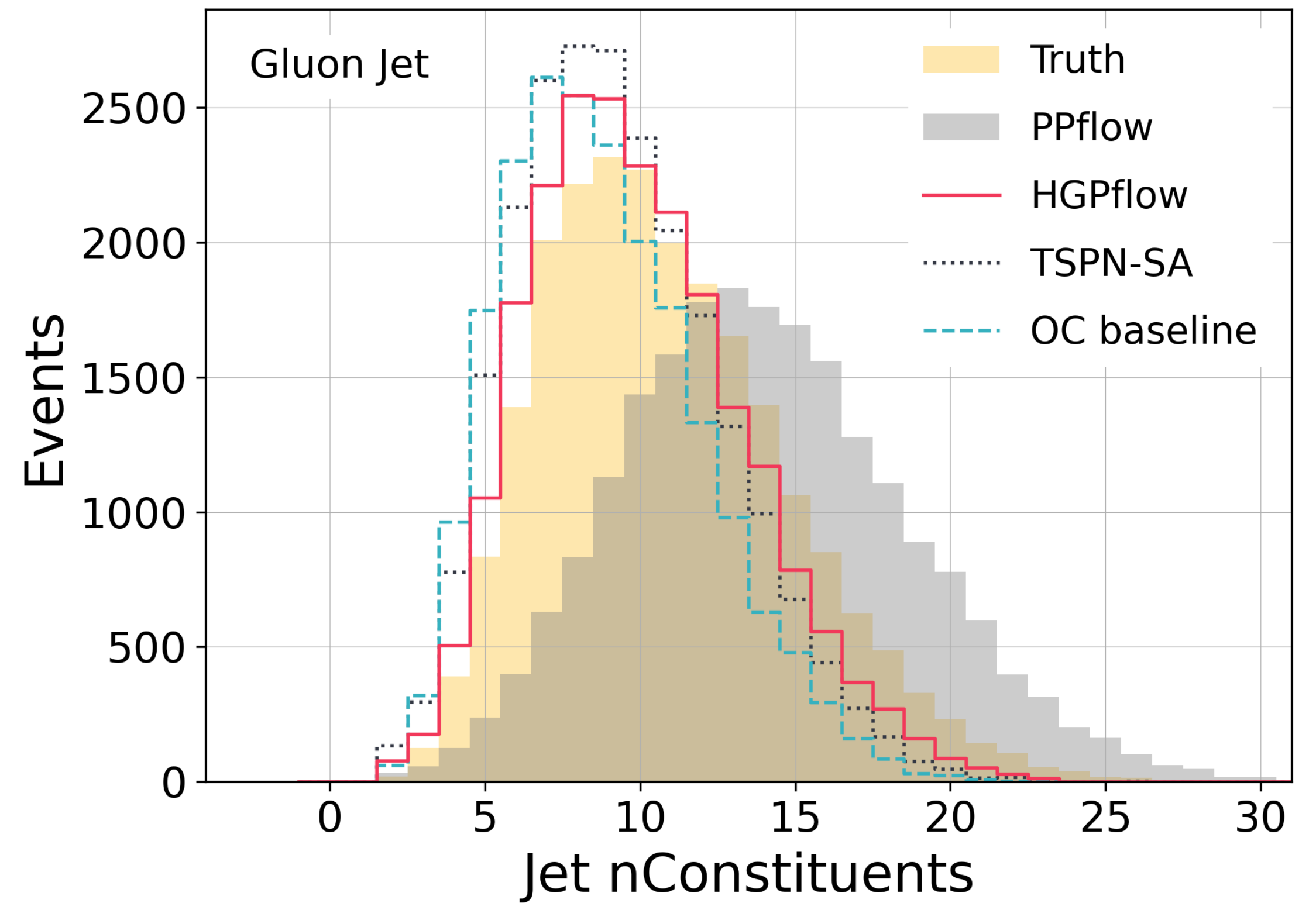
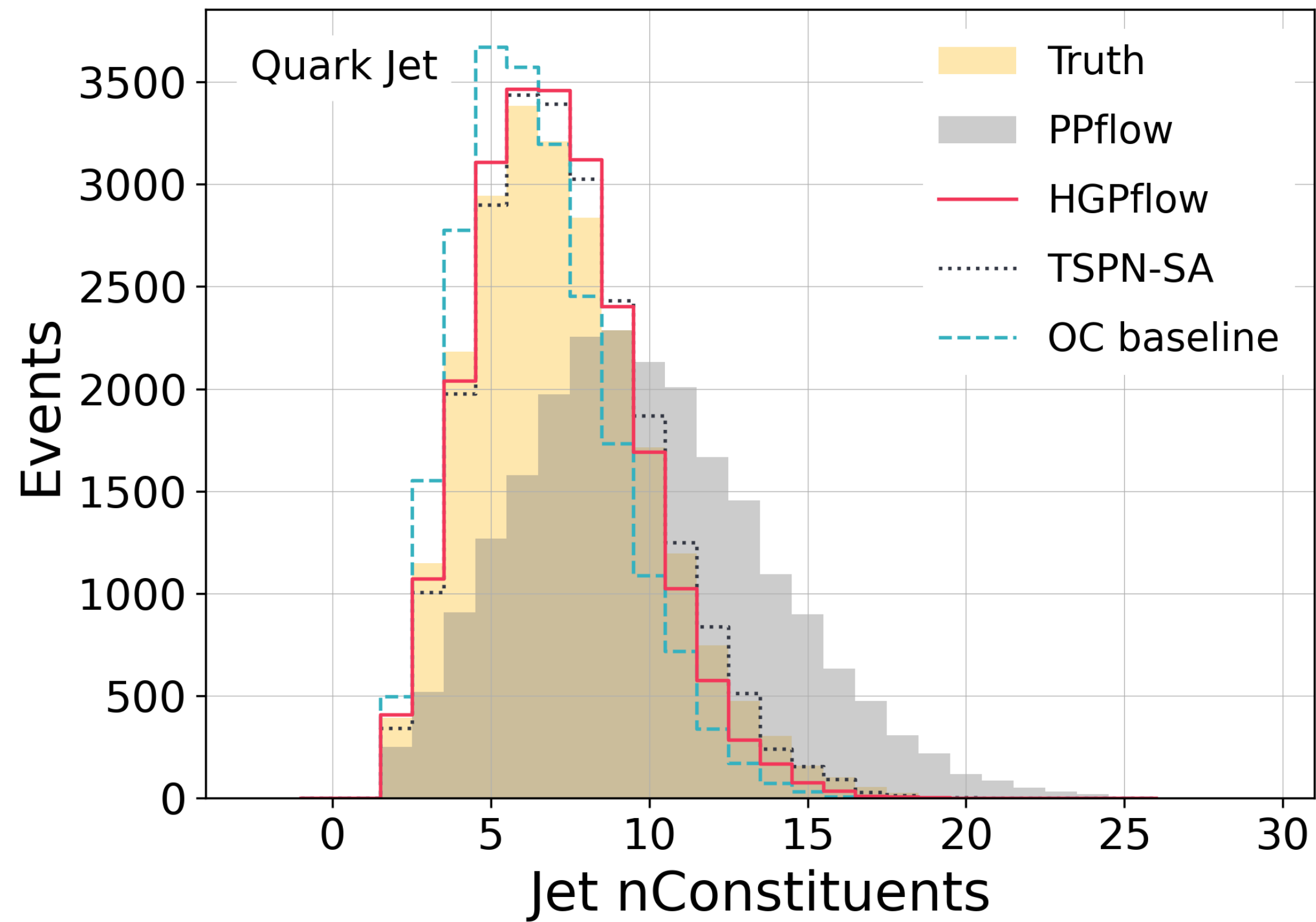


$$\frac{\text{Truth} - \text{predicted}}{\text{Truth}}$$

# Jet constituent

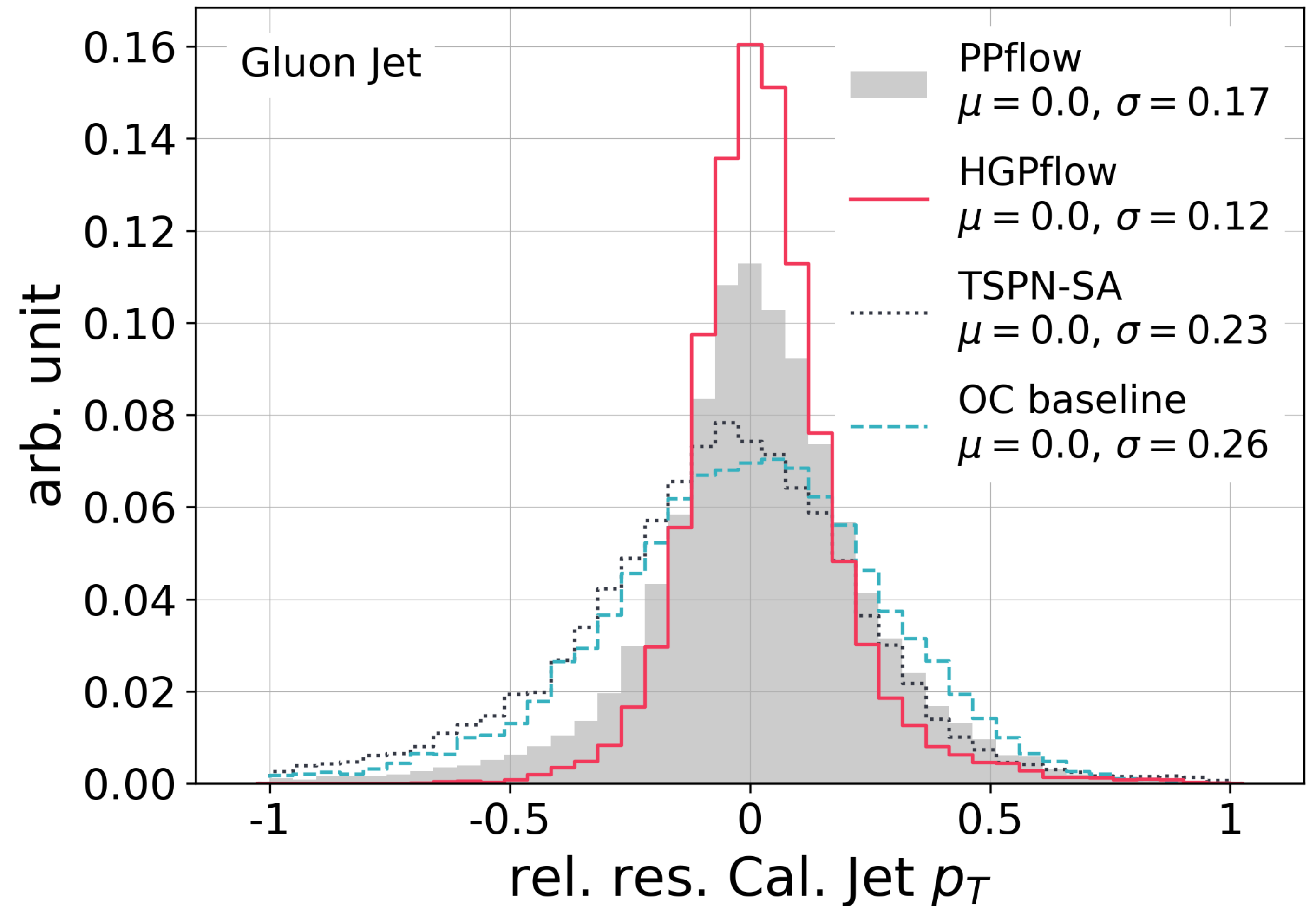


# Jet constituent



# Generalization (gluon jets)

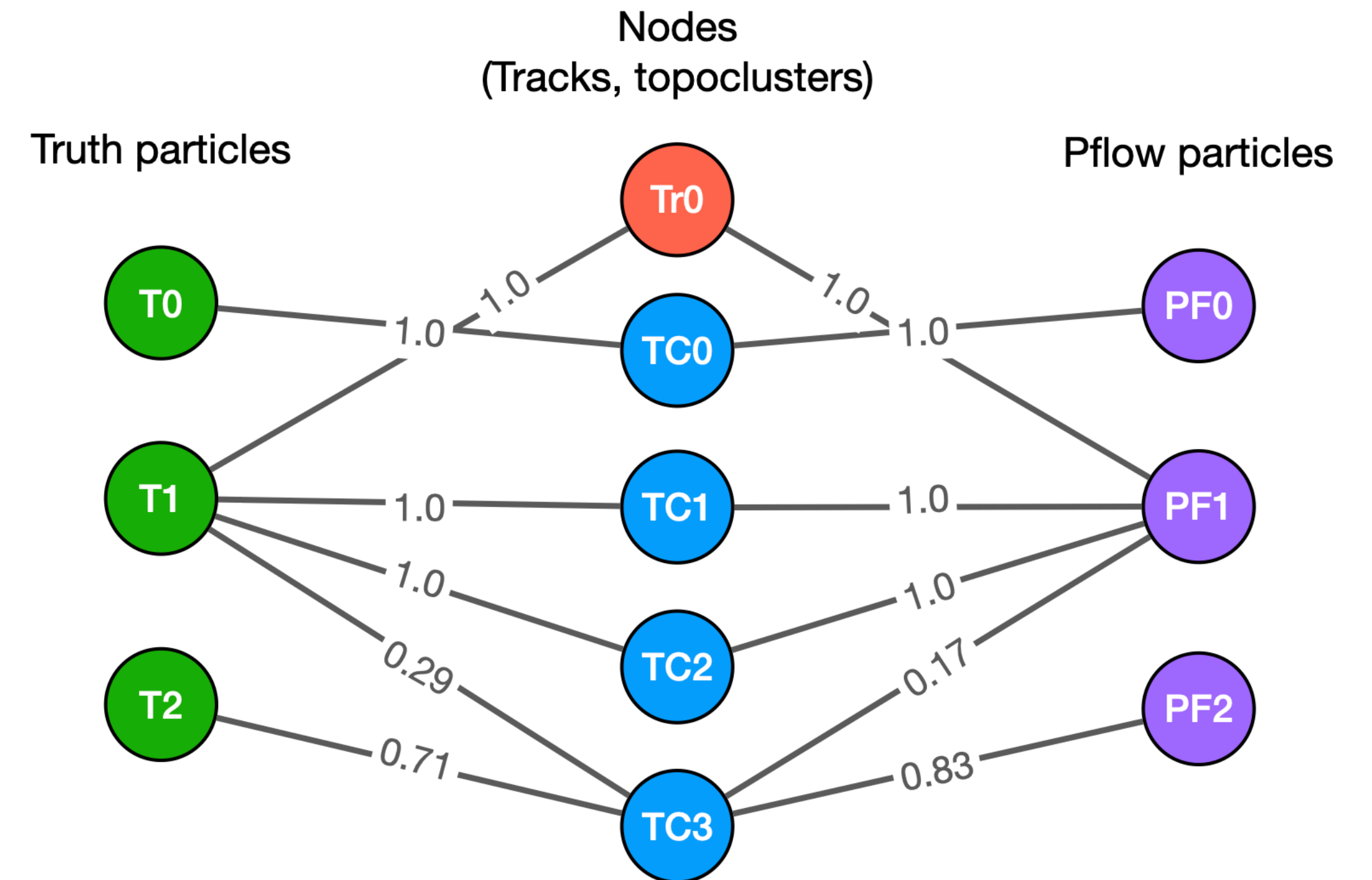
- Similar story as before
- HGPflow generalizes pretty well to the gluon jets as well!



$$\frac{\text{Truth} - \text{predicted}}{\text{Truth}}$$

# Interpretability

- Advantages of learning energy-based incidence matrix
- Inductive-bias towards energy conservation (softmax)
- Proxies
- Interpretable fake, inefficiency
- Supervised links b/w particle and input nodes



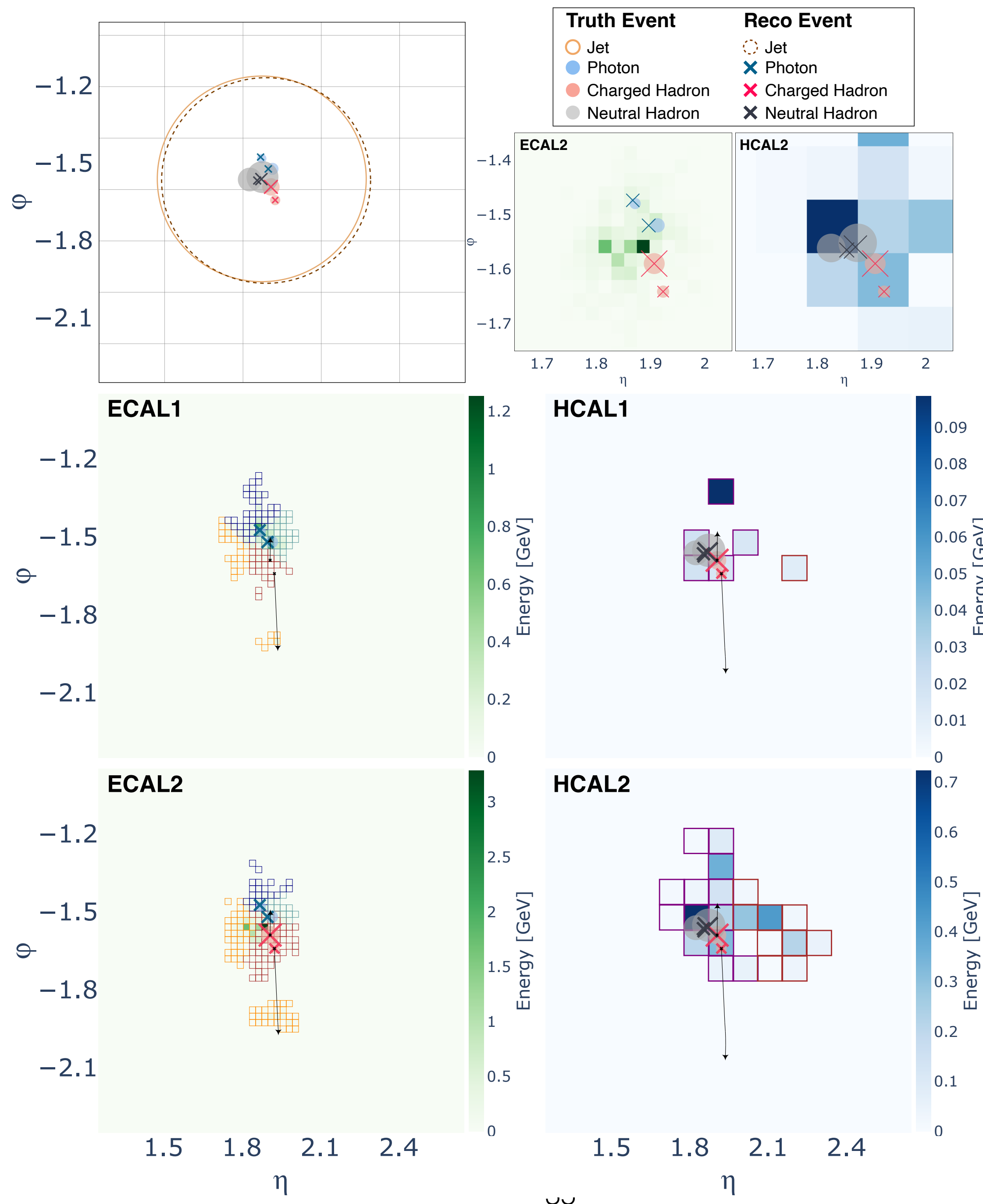
**What's next?**



# What's next?

- Moving onto full event
  - Try training on full events
  - Partition the events and run HGPflow on each partition; combine the output
    - Conserves locality
- Pileup

# Event Display Reconstruction with HGPflow

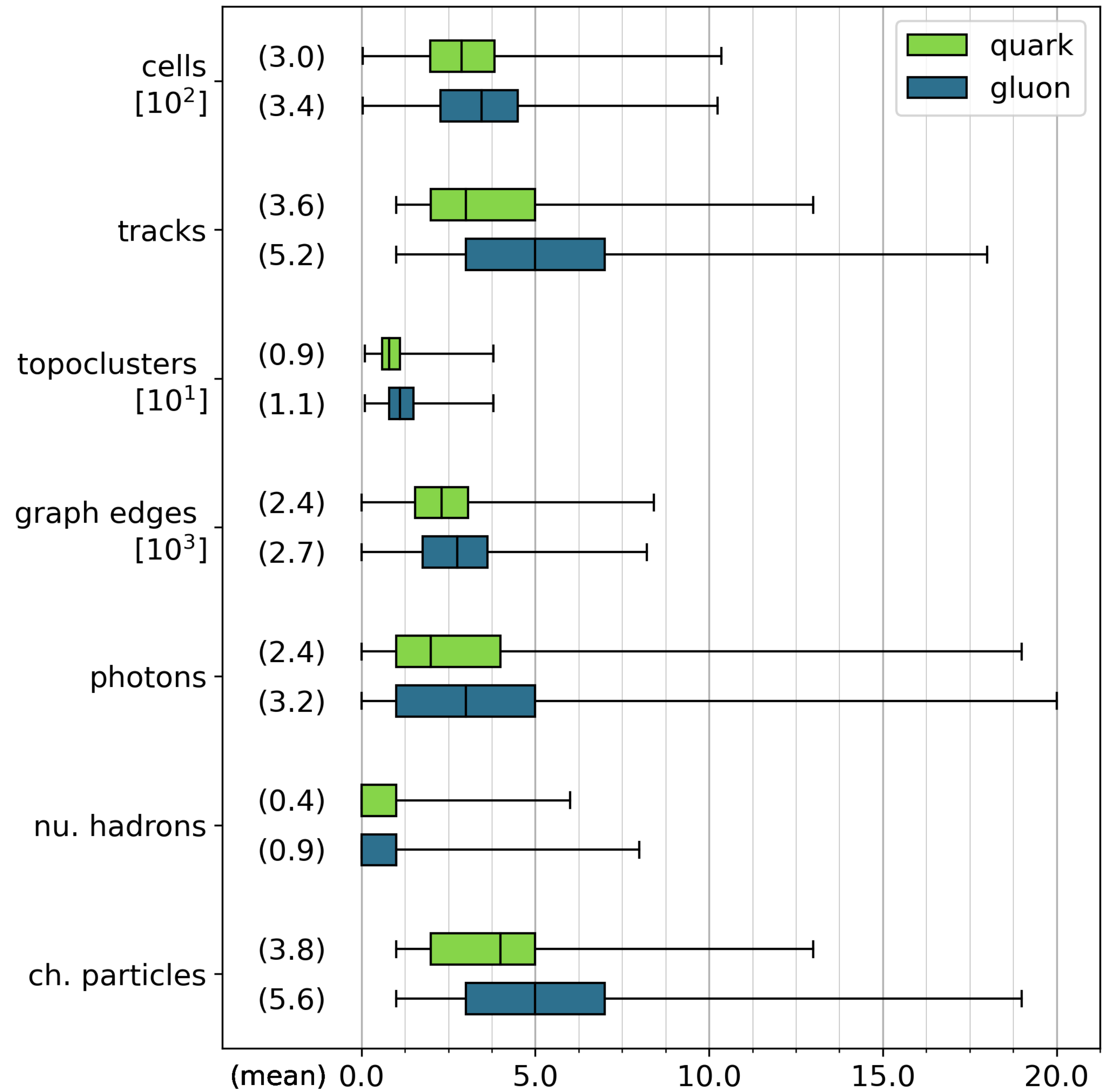


*Thank you...*

**Thank you**

# Data composition

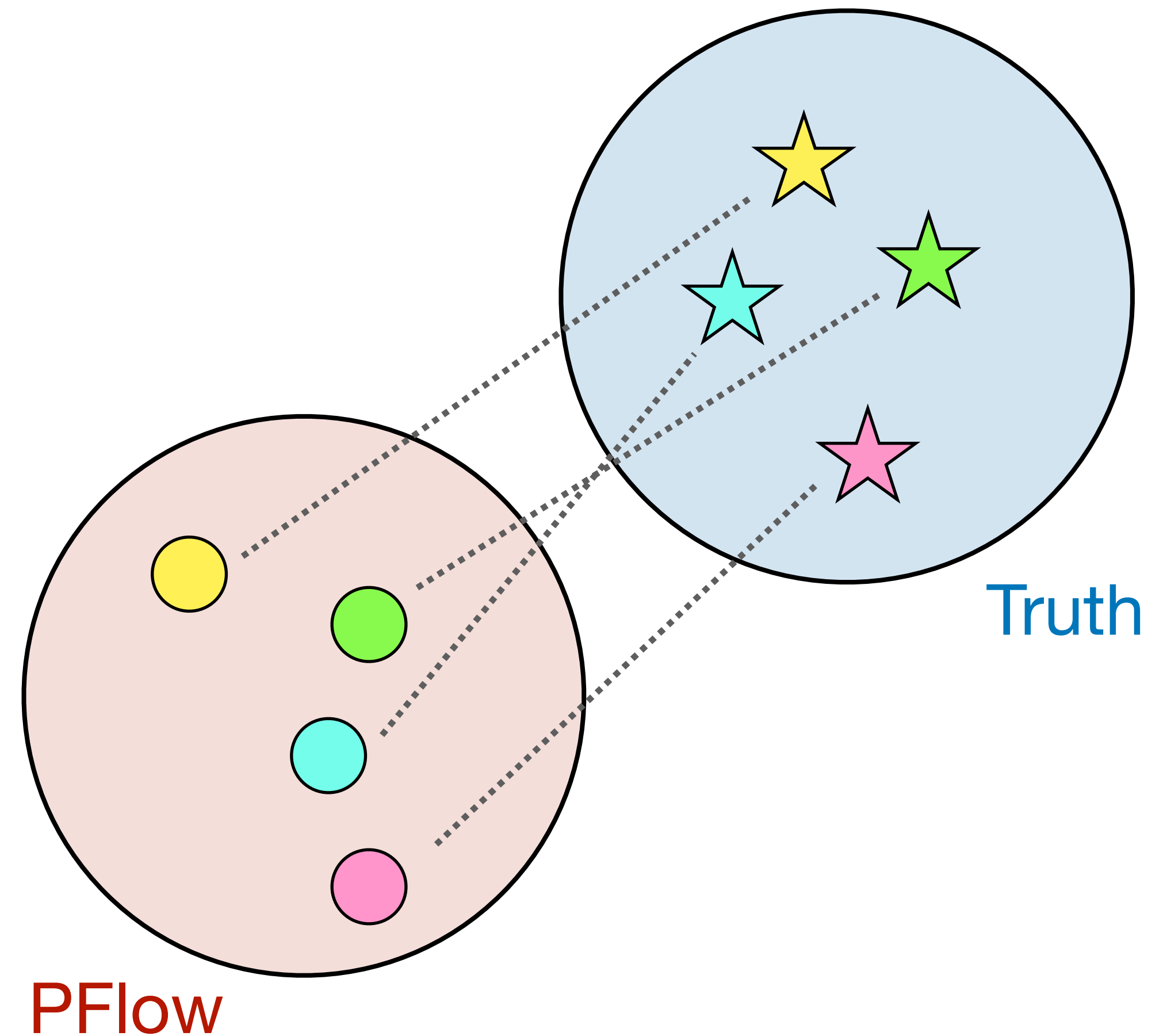
- Cardinality
- Track



# Hungarian matching

- Truth particles and predicted particles are both **sets**
- Need to find matches b/w the two sets of particles
- Hungarian matching with the metric

- $\left(\frac{\Delta p_T}{p_T}\right)^2 + \Delta R^2$



# Initialization of the HG

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Nodes,  $\mathcal{V}_j^{t=0} =$  output of Encoding

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Nodes,  $\mathcal{V}_j^{t=0} =$  output of Encoding

Hyperedges,  $\mathcal{E}_j^{t=0} =$  Random initialization from Gaussian noise

Incidence,  $\mathcal{J}_{i,j}^{t=0} = 0;$  (no connectivity)

# Refinements

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$$G^t(\mathcal{V}^t, \mathcal{E}^t, \mathcal{J}^t)$$


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$$G^t(\mathcal{V}^t, \mathcal{E}^t, \mathcal{J}^t)$$

$$\mathcal{J}_{i,j}^t = \phi_I \left( v_j^{t-1}, e_i^{t-1}, \mathcal{J}_{i,j}^{t-1} \right)$$


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$$\left[ v_j^{t-1}, \rho_{e \rightarrow v}(j, t), v_j^0 \right]$$

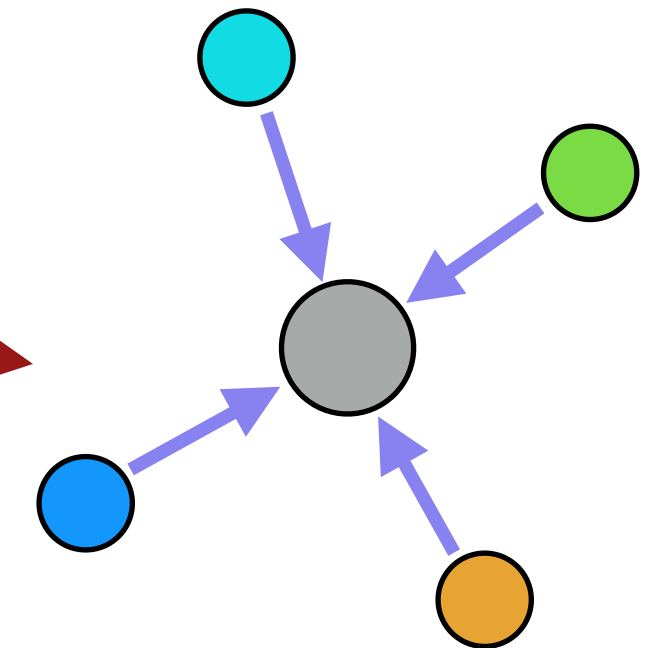
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MLP

$$\left[ v_j^{t-1}, \rho_{e \rightarrow v}(j, t), v_j^0 \right]$$

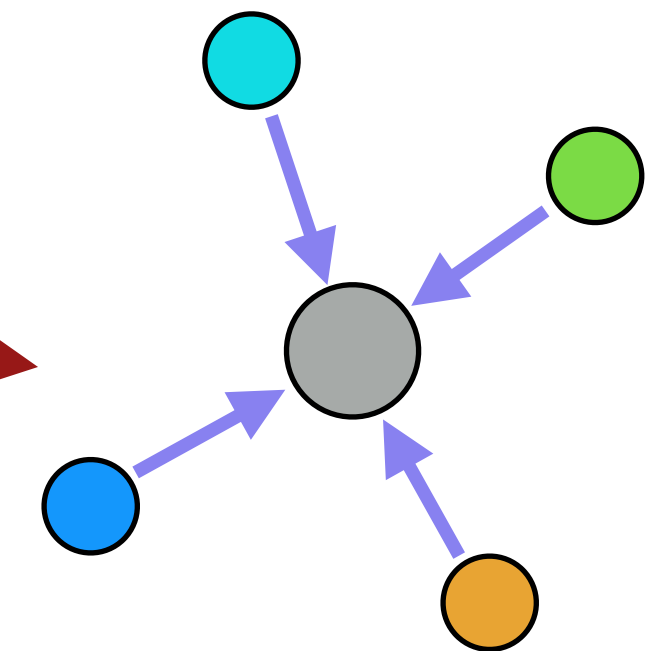


# Refinements

$$G^t(\mathcal{V}^t, \mathcal{E}^t, \mathcal{J}^t)$$

$$\mathcal{J}_{i,j}^t = \phi_I \left( v_j^{t-1}, e_i^{t-1}, \mathcal{J}_{i,j}^{t-1} \right)$$

MLP



$$\left\{ \left[ v_j^{t-1}, \rho_{e \rightarrow v}(j, t), v_j^0 \right] \mid j = 0, 1, 2, \dots \right\}$$



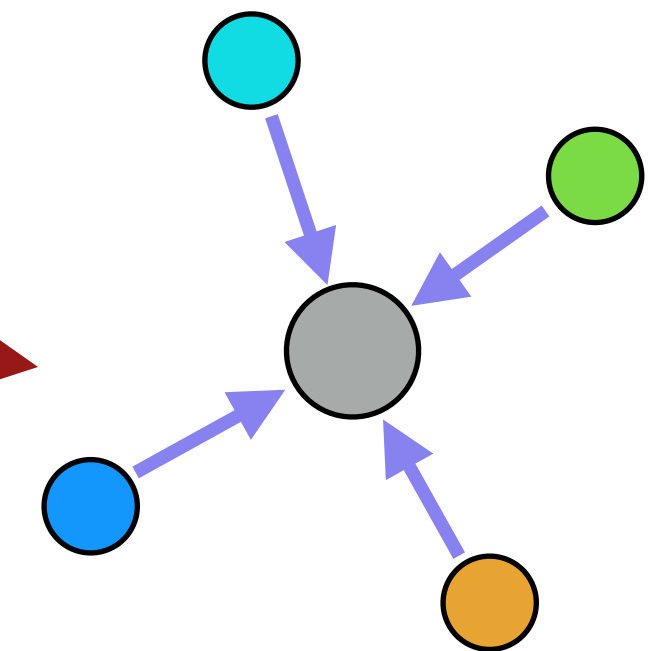
# Refinements

$$G^t(\mathcal{V}^t, \mathcal{E}^t, \mathcal{J}^t)$$

$$\mathcal{J}_{i,j}^t = \phi_I \left( v_j^{t-1}, e_i^{t-1}, \mathcal{J}_{i,j}^{t-1} \right)$$

MLP

$$\mathcal{V}^t = \phi_V \left( \left\{ \left[ v_j^{t-1}, \rho_{e \rightarrow v}(j, t), v_j^0 \right] \mid j = 0, 1, 2, \dots \right\} \right)$$



# Refinements

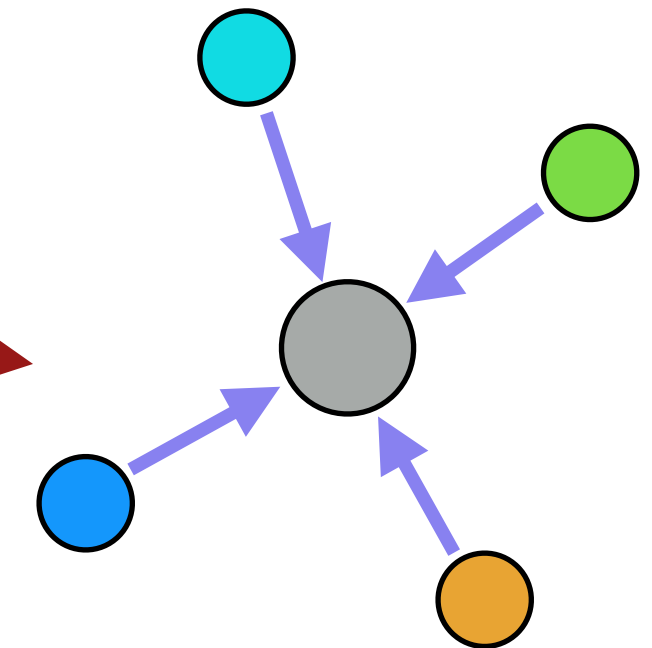
$$G^t(\mathcal{V}^t, \mathcal{E}^t, \mathcal{J}^t)$$

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MLP

$$\mathcal{V}^t = \phi_V \left( \left\{ \left[ v_j^{t-1}, \rho_{e \rightarrow v}(j, t), v_j^0 \right] \mid j = 0, 1, 2, \dots \right\} \right)$$

DeepSet



# Refinements

$$G^t(\mathcal{V}^t, \mathcal{E}^t, \mathcal{J}^t)$$

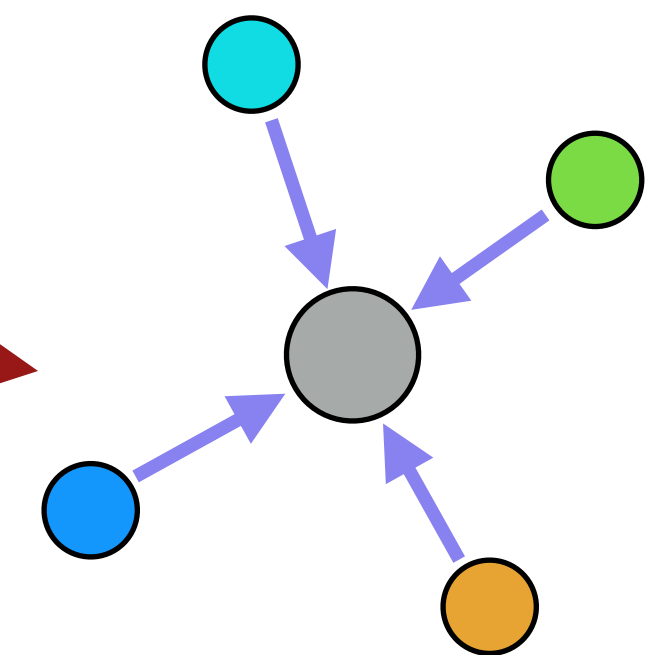
$$\mathcal{J}_{i,j}^t = \phi_I \left( v_j^{t-1}, e_i^{t-1}, \mathcal{J}_{i,j}^{t-1} \right)$$

MLP

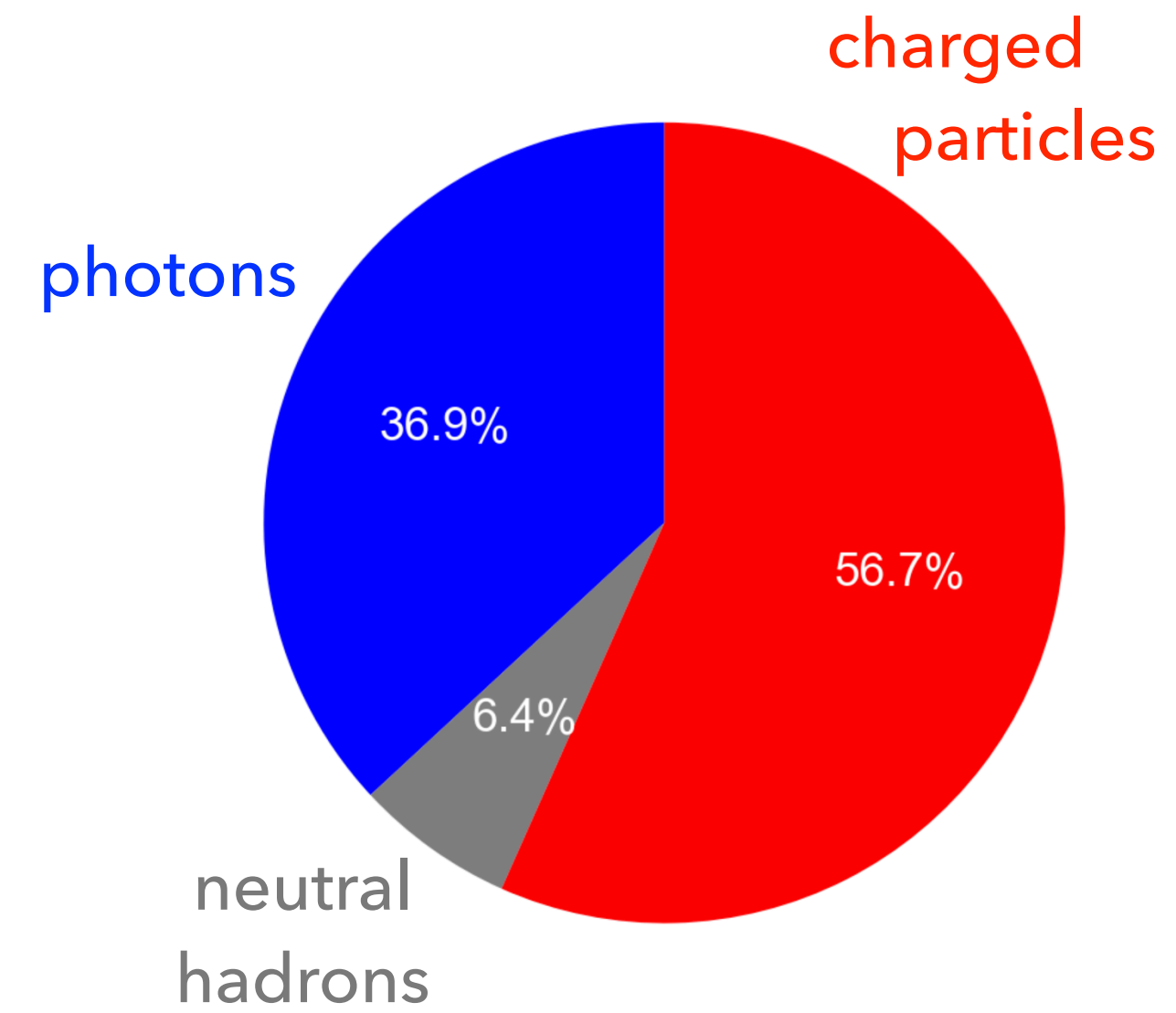
$$\mathcal{V}^t = \phi_V \left( \left\{ \left[ v_j^{t-1}, \rho_{e \rightarrow v}(j, t), v_j^0 \right] \mid j = 0, 1, 2, \dots \right\} \right)$$

DeepSet

$$\mathcal{E}^t = \phi_E \left( \left\{ \left[ e_i^{t-1}, \rho_{e \rightarrow v}(i, t) \right] \mid i = 0, 1, 2, \dots \right\} \right)$$



# Composition



# Charged particle pT resolution

- Improvement in resolution
- Specifically at high pT

