מכון ויצמן למדע
WEIZMANN INSTITUTE OF SCIENCE

Machine Learning in Particle Theory
- MITP Summer School 2023

Eilam Gross

Particle Flow with Deep Learning

✅Lecture 1: GNN+Attention

✅Lecture 2: Transformers + Set Generation
(with the help of **N. Kakati** and **N. Soybelman**)

✓Lecture 3: Hyper Graphs + TSPN Particle Flow
(with the help of **N. Kakati, Etienne Dreyer**)


Syllabus

✅ Graph Neural Nets

- ✅ Set to Graph

✅ Attention is all you need

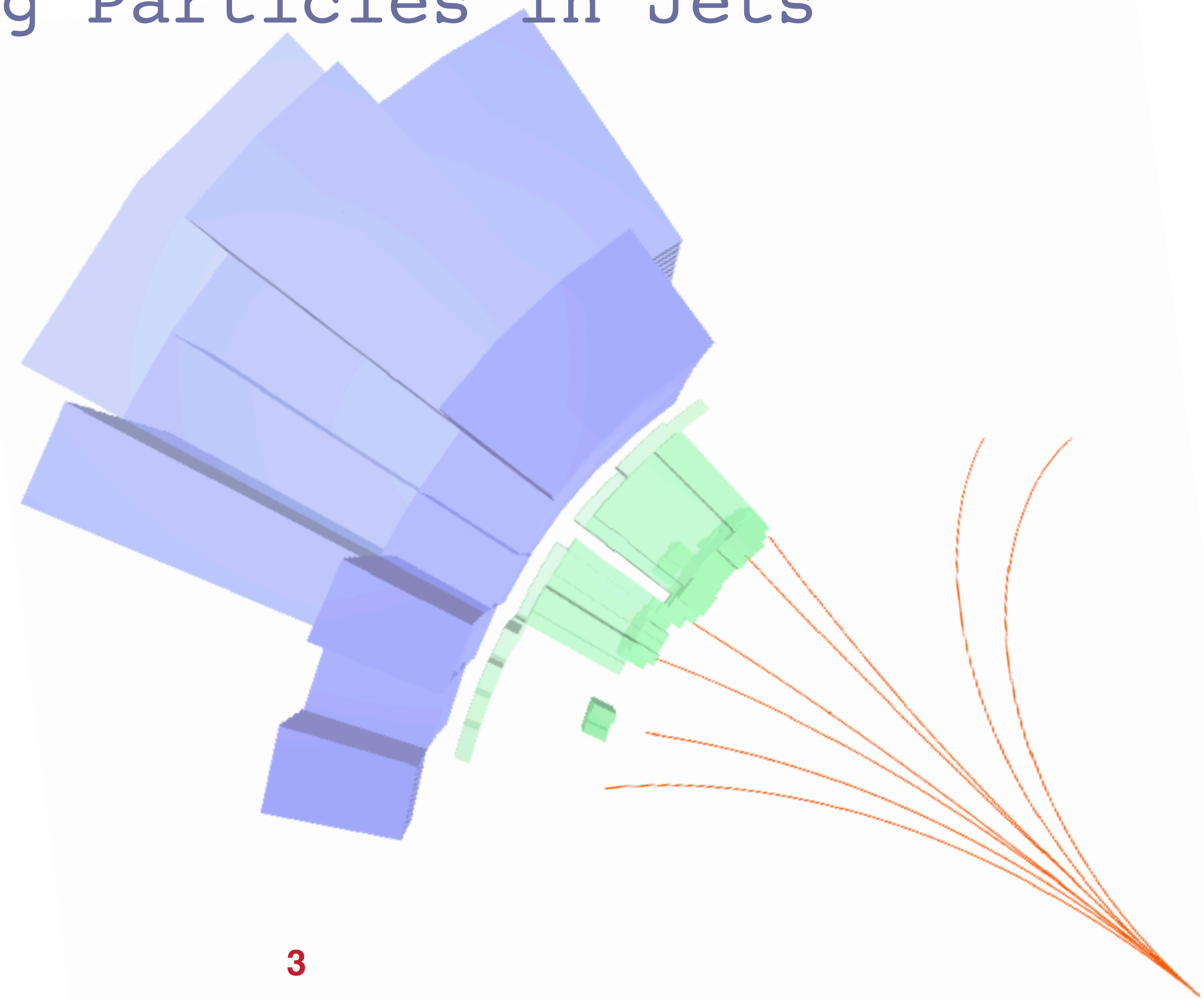
- ✅ Transformers, ✅ Slot Attention (SA)
- ✅ Set Prediction Networks with a Transformer and SA (TSPN-SA)

✅ Constrained Variational Auto Encoder (cVAE)

✔ Particle Flow
(Reconstructing Particles in Jets using TSPN-SA,
Hyper-Graph PFlow [HGPflow])

✅ Simulation of PF Objects (Using TSPN-SA, cVAE)

Towards Computer Vision Particle Flow
or
Reconstructing Particles in Jets



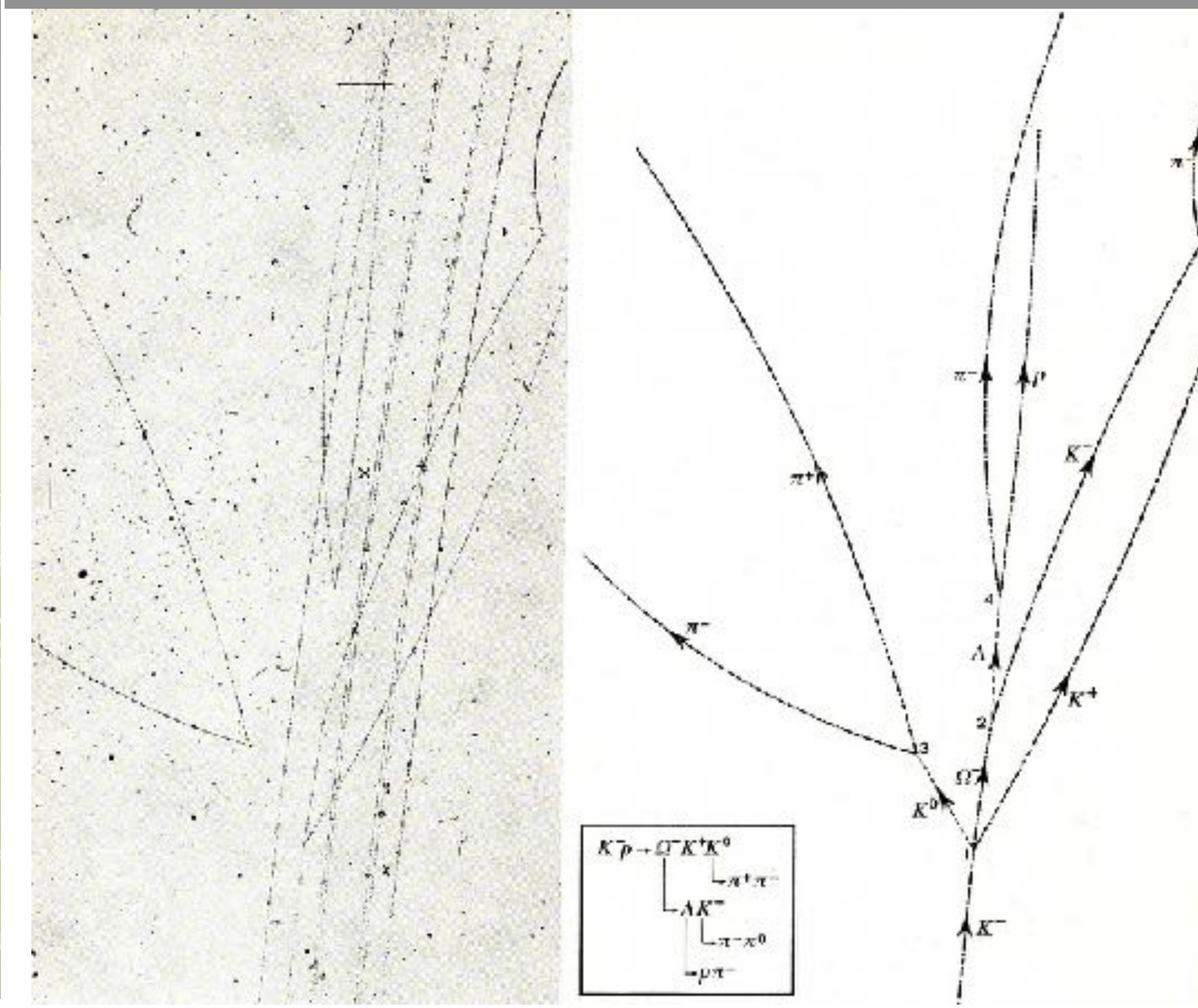
Bubble Chamber

1964

Omega Minus Discovery

Piecing together particles

Einstein: imagination is more important than knowledge.

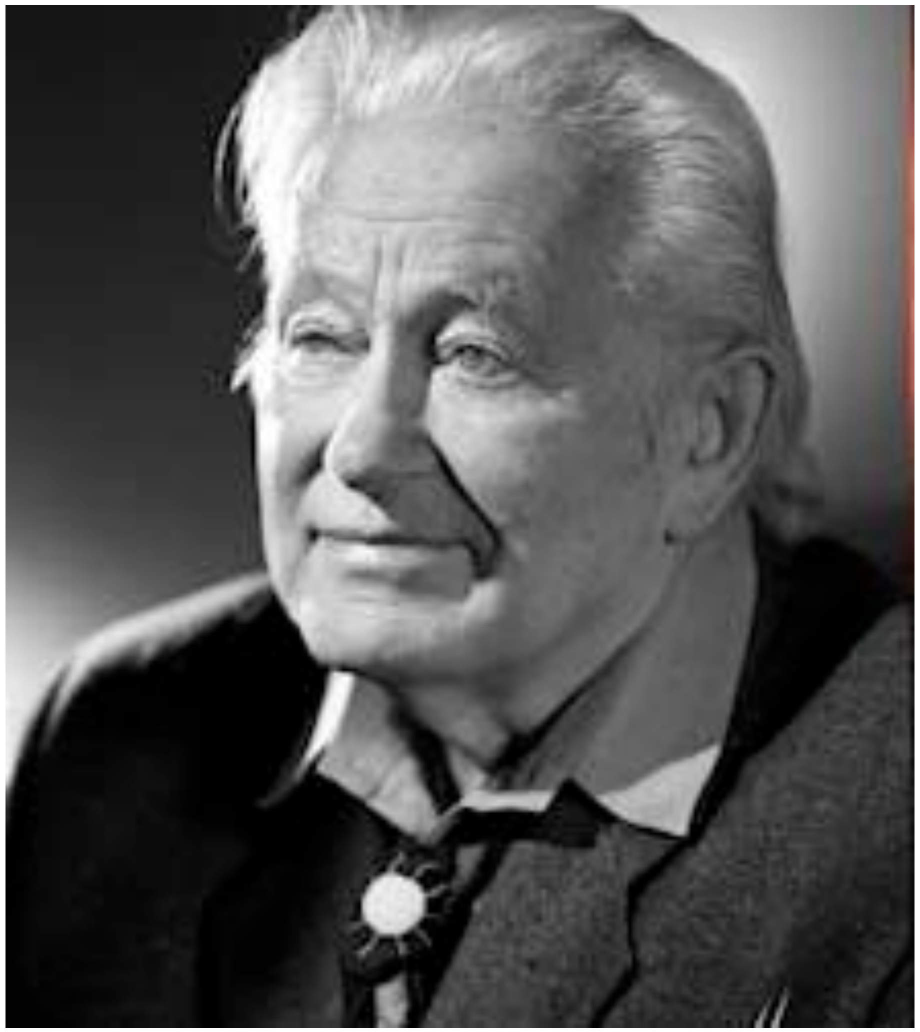


1968 Mutiwire Proportional Chamber

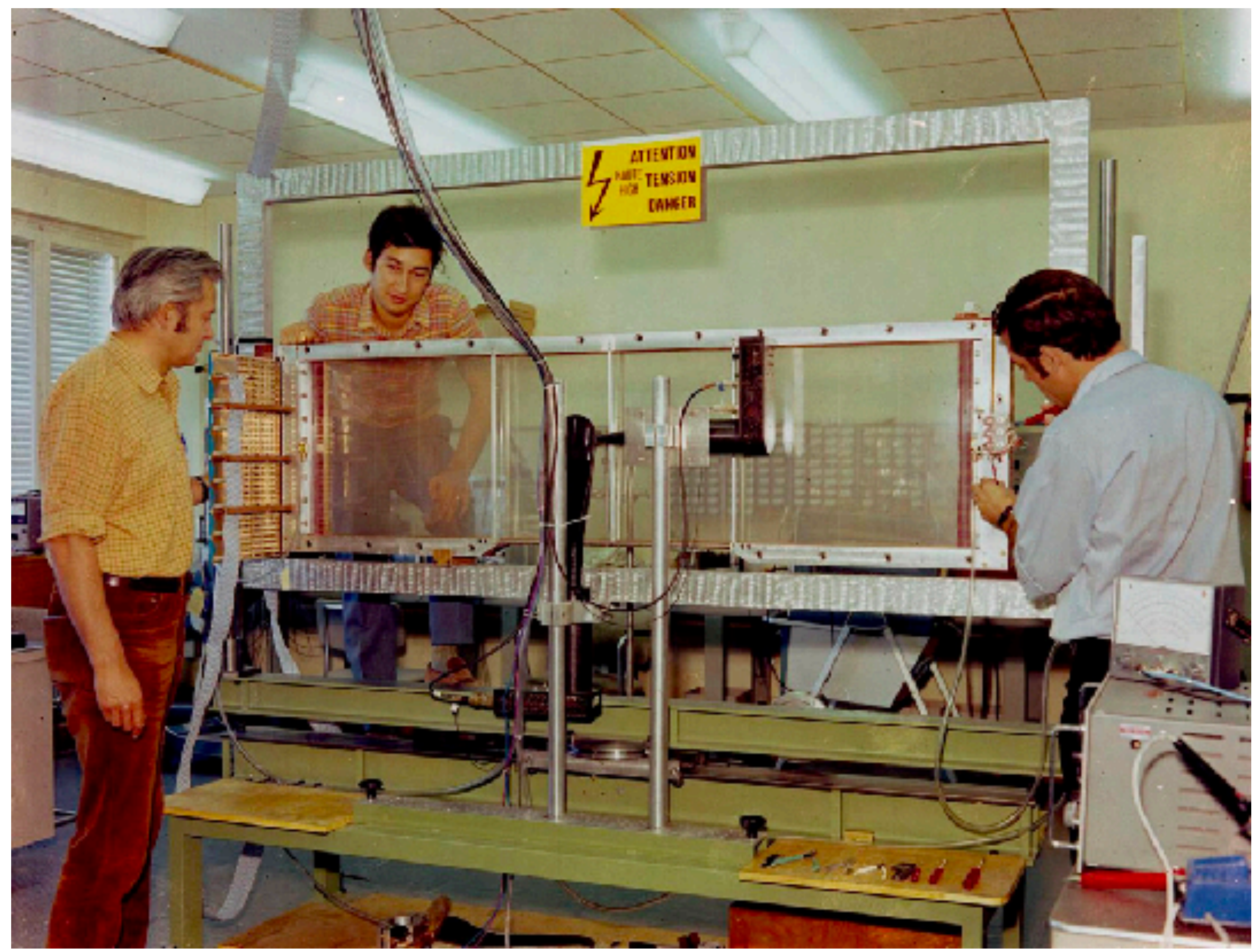
1992

Georges Charpak

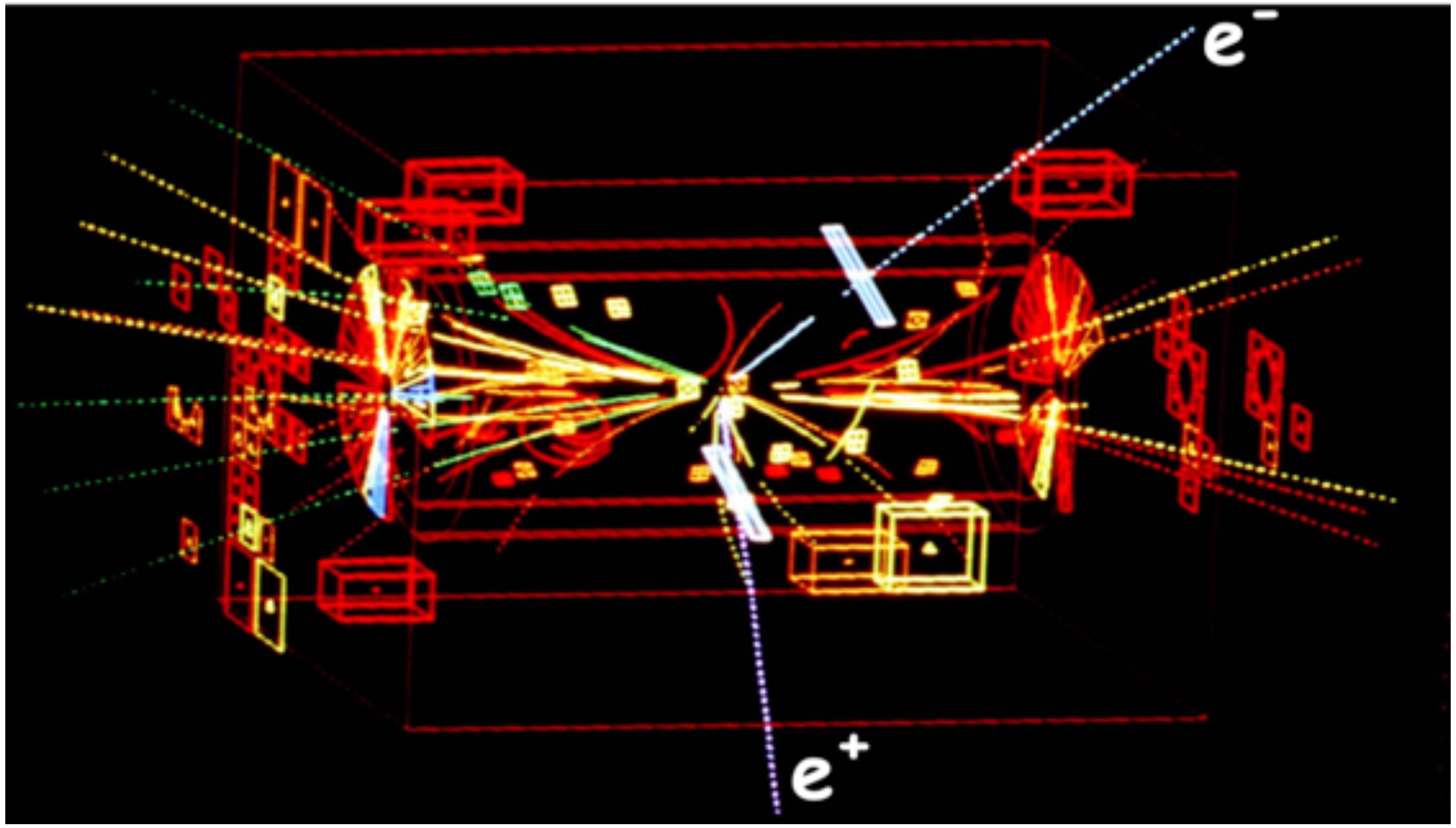
Piecing together particles



1968 multiwire proportional chamber



Piecing together particles



UA1

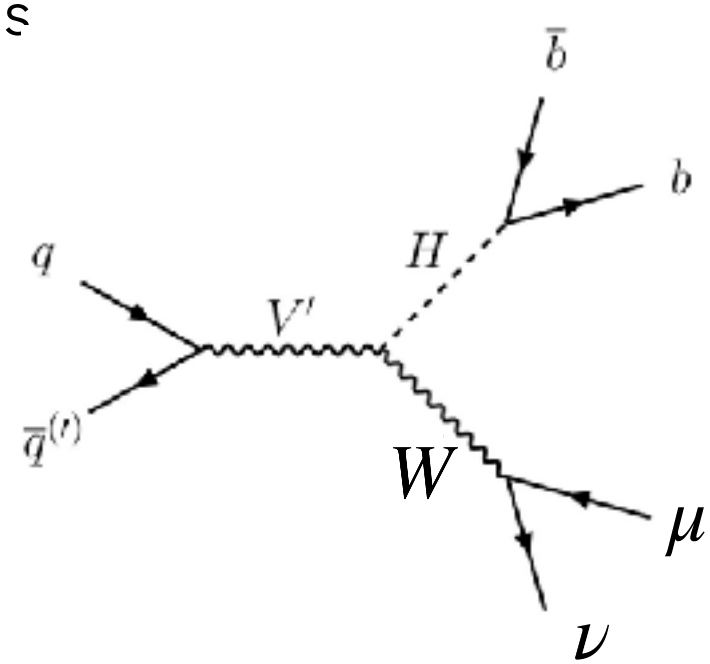
1984

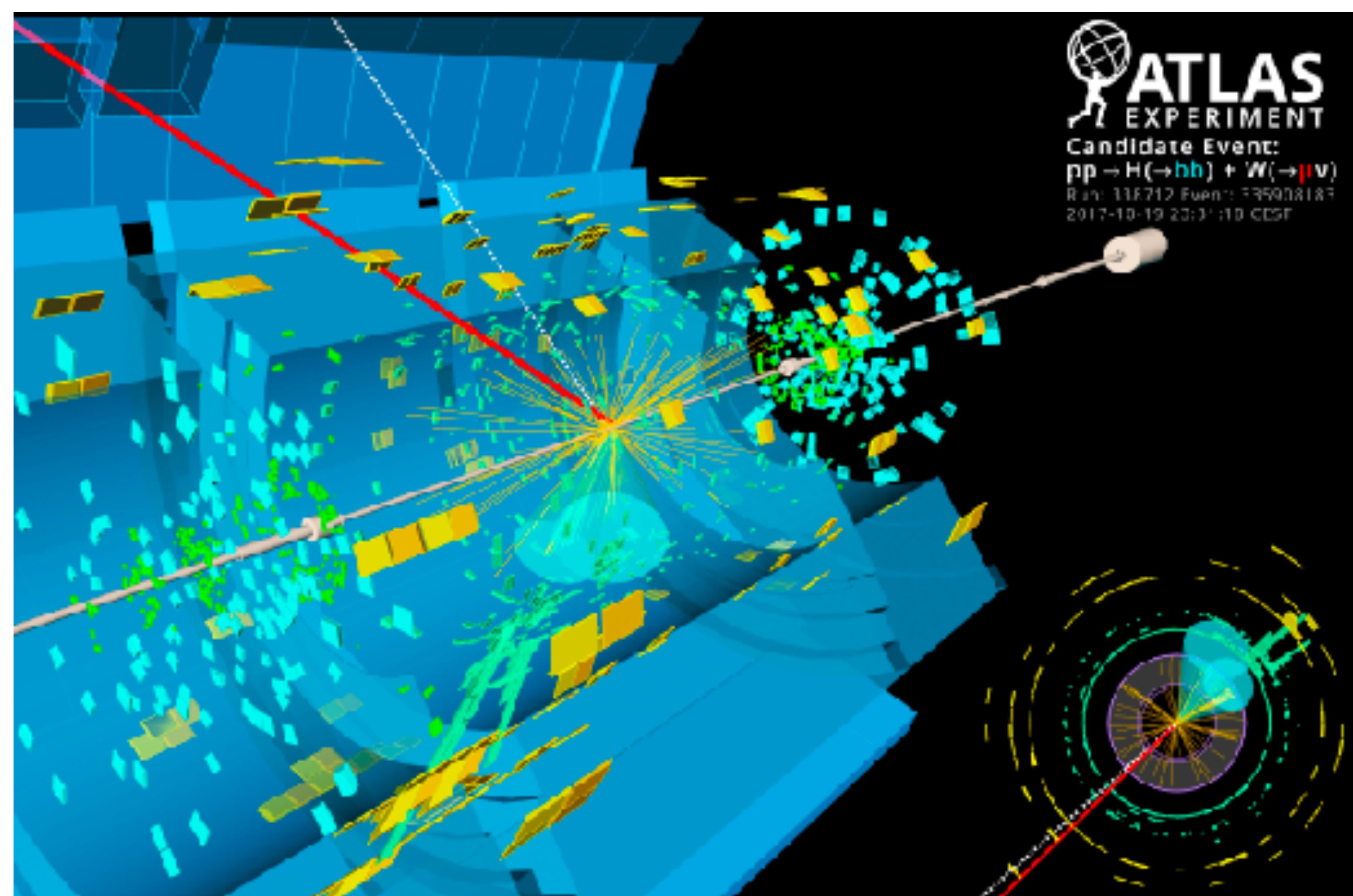
W, Z bosons

ATLAS & CMS

2013

Higgs boson





A Particle Detector

Piecing together particles

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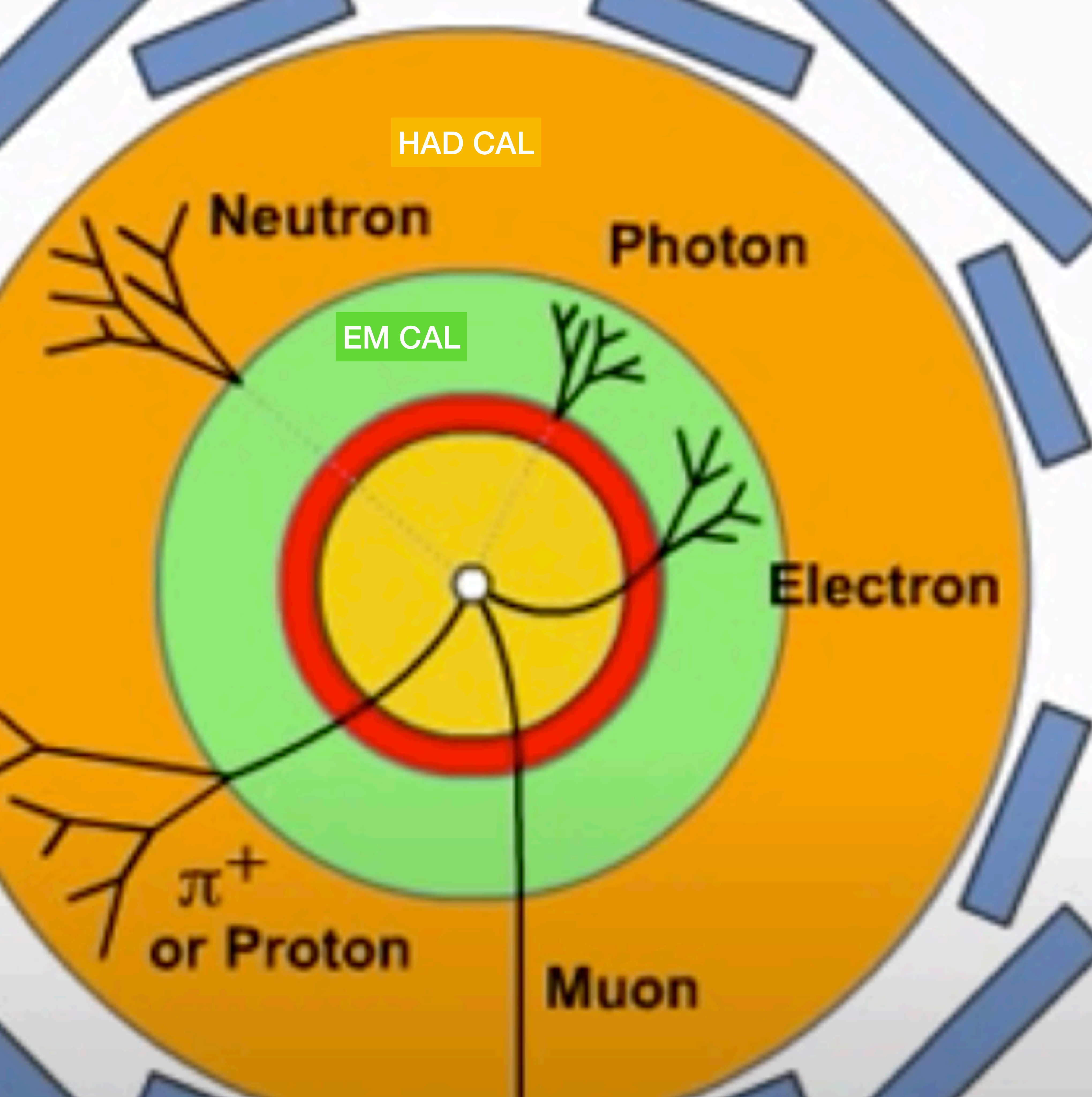
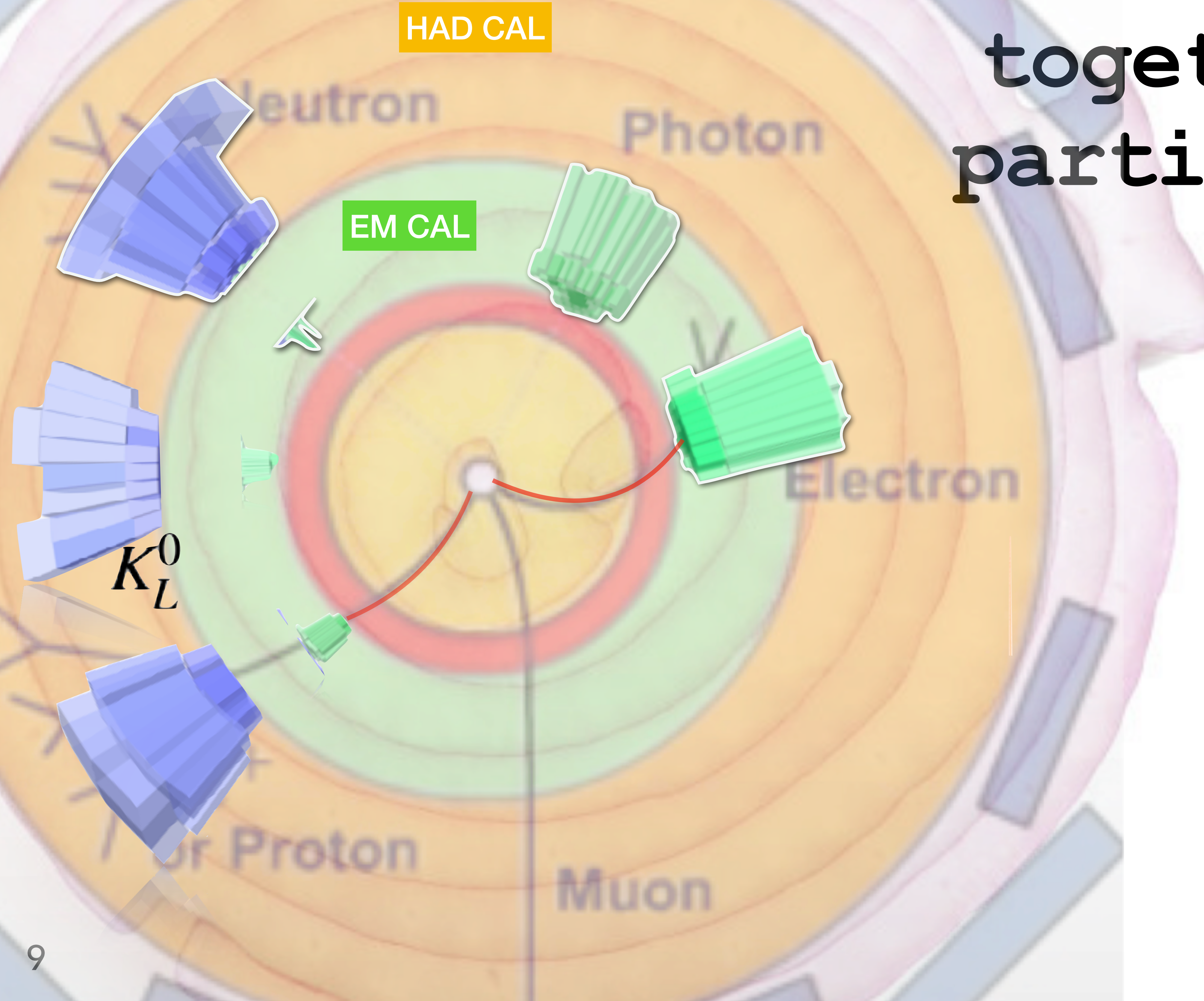
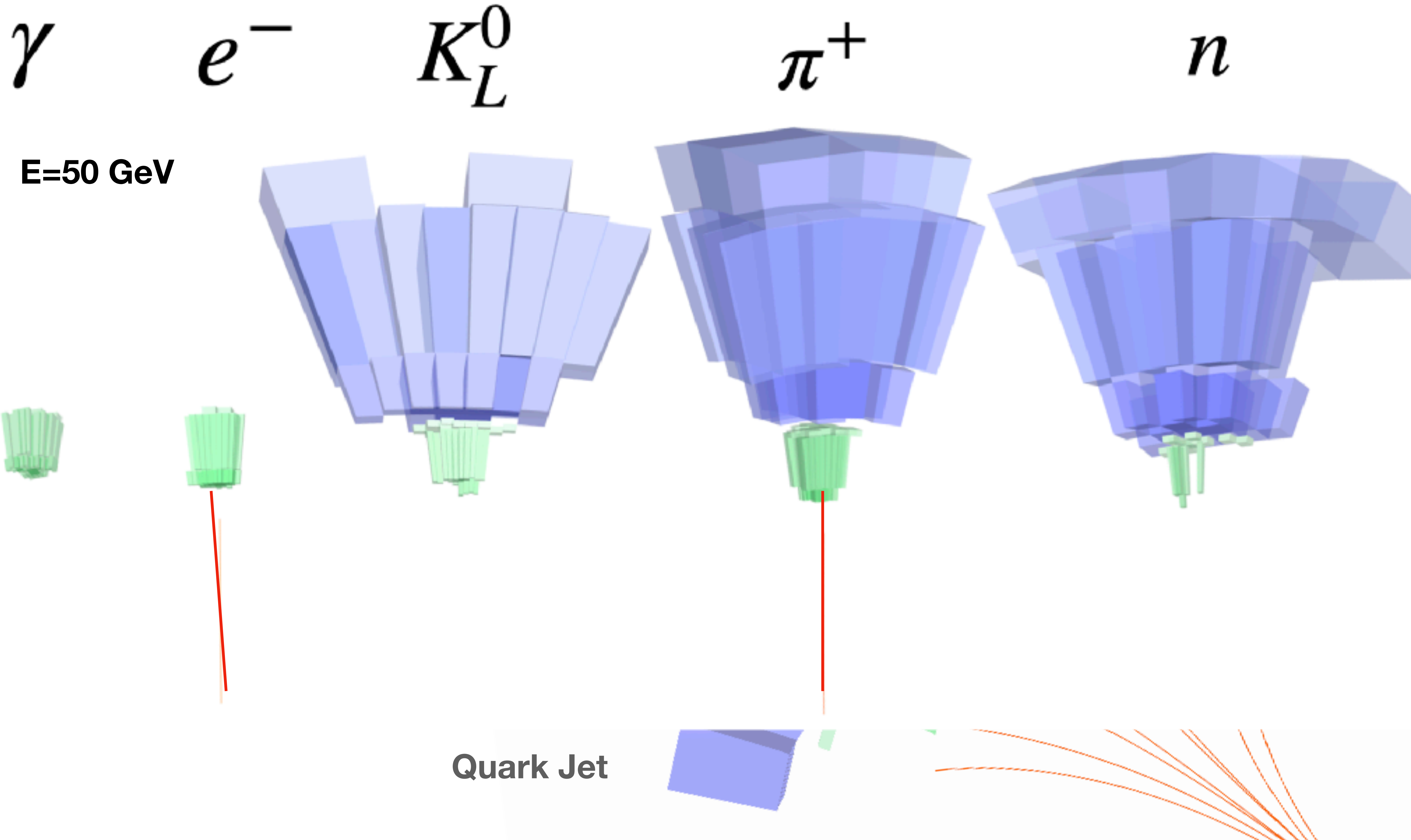
ether
ticles



A Particle Detector

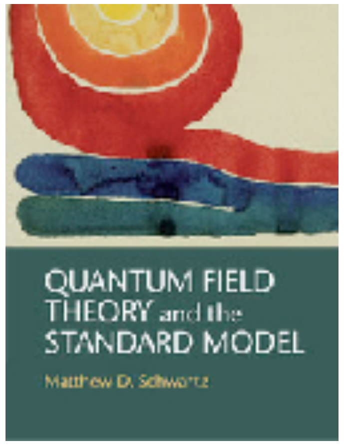
Piecing together particles

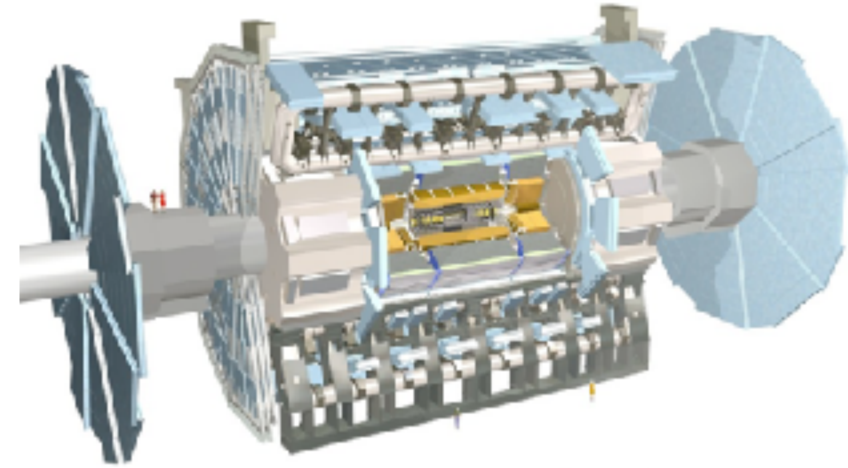


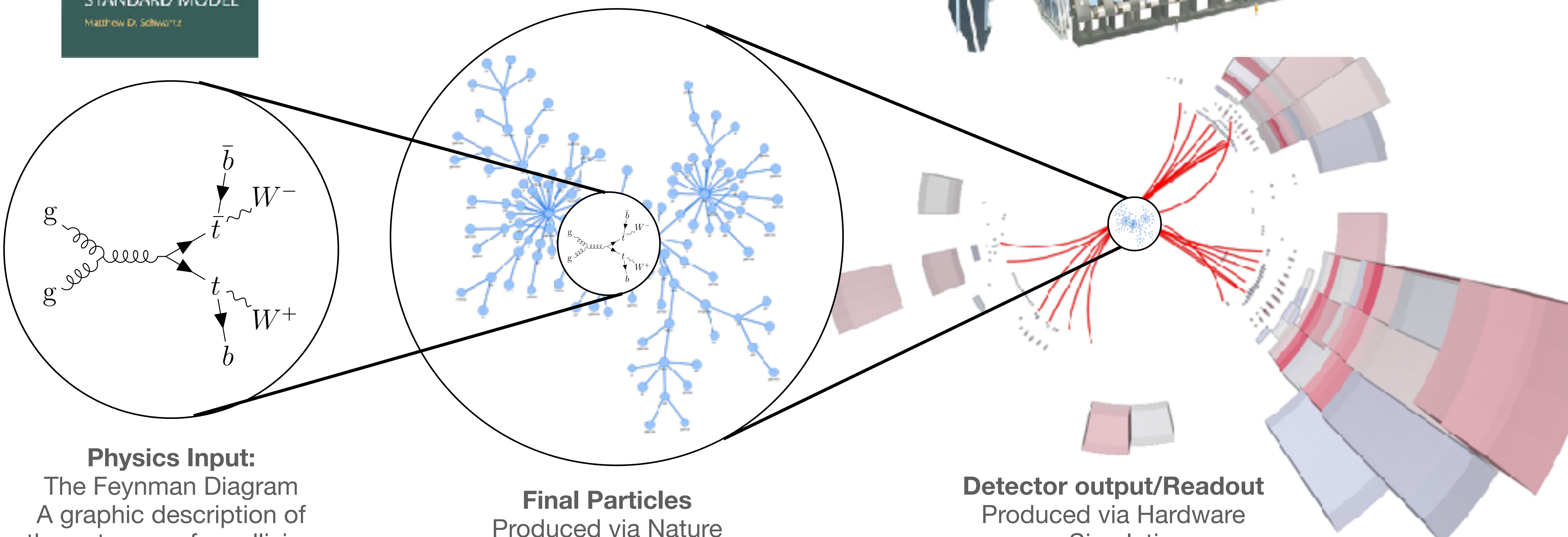


Most Neutral Hadrons below 5 GeV release their Energy in Ecal only

In a Nut Shell:
From Reconstruction to Particles







Physics Input:
The Feynman Diagram
A graphic description of
the outcome of a collision
(Produced by a real Collision
or a simulated collision)

Final Particles
Produced via Nature
or Simulation

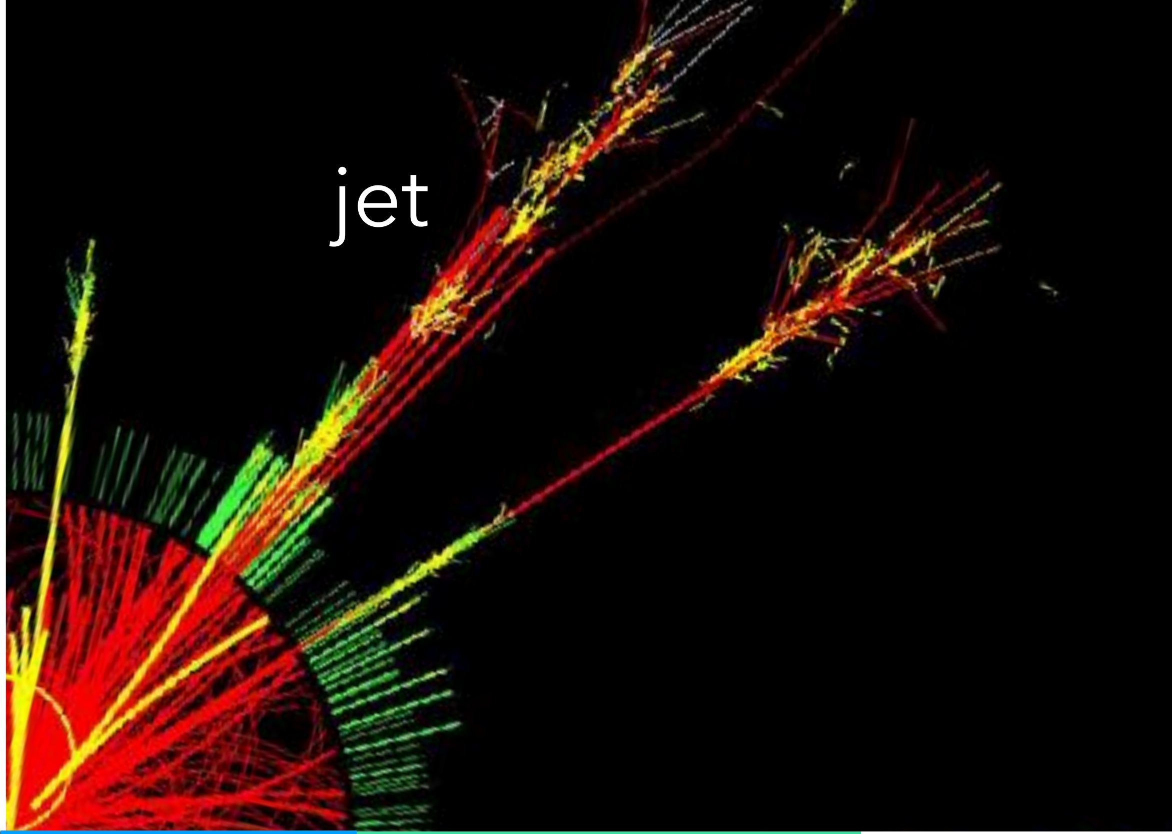
Detector output/Readout
Produced via Hardware
or Simulation

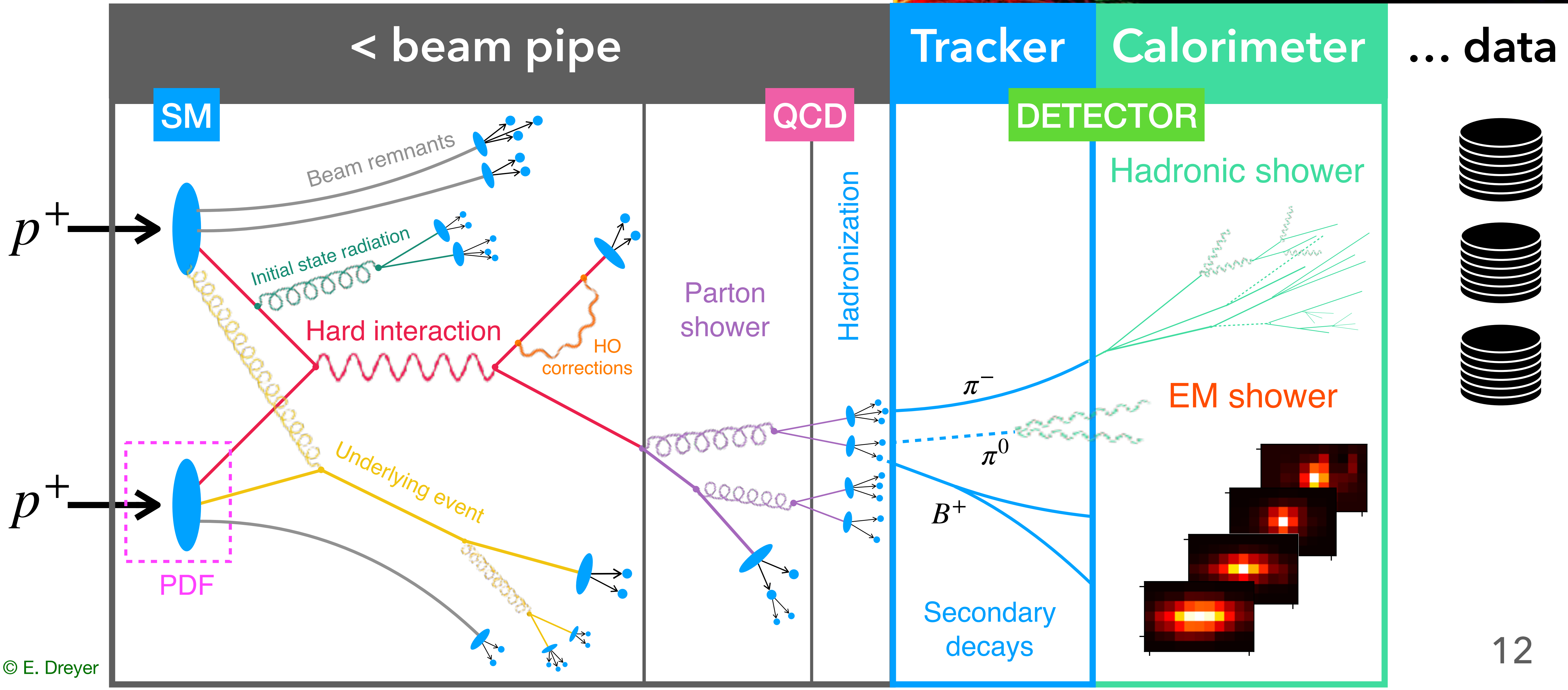
The Goal: Reconstruct the stable outgoing particles from the detector readout.

Information flow in p^+p^+ collisions

Soft QCD dynamics

$\Longrightarrow$ collimated jets of hadrons





The inverse problem

Event classification

Reconstruction

Clustering

Regression

momentum

p_T ($10^0 - 10^3$ GeV)

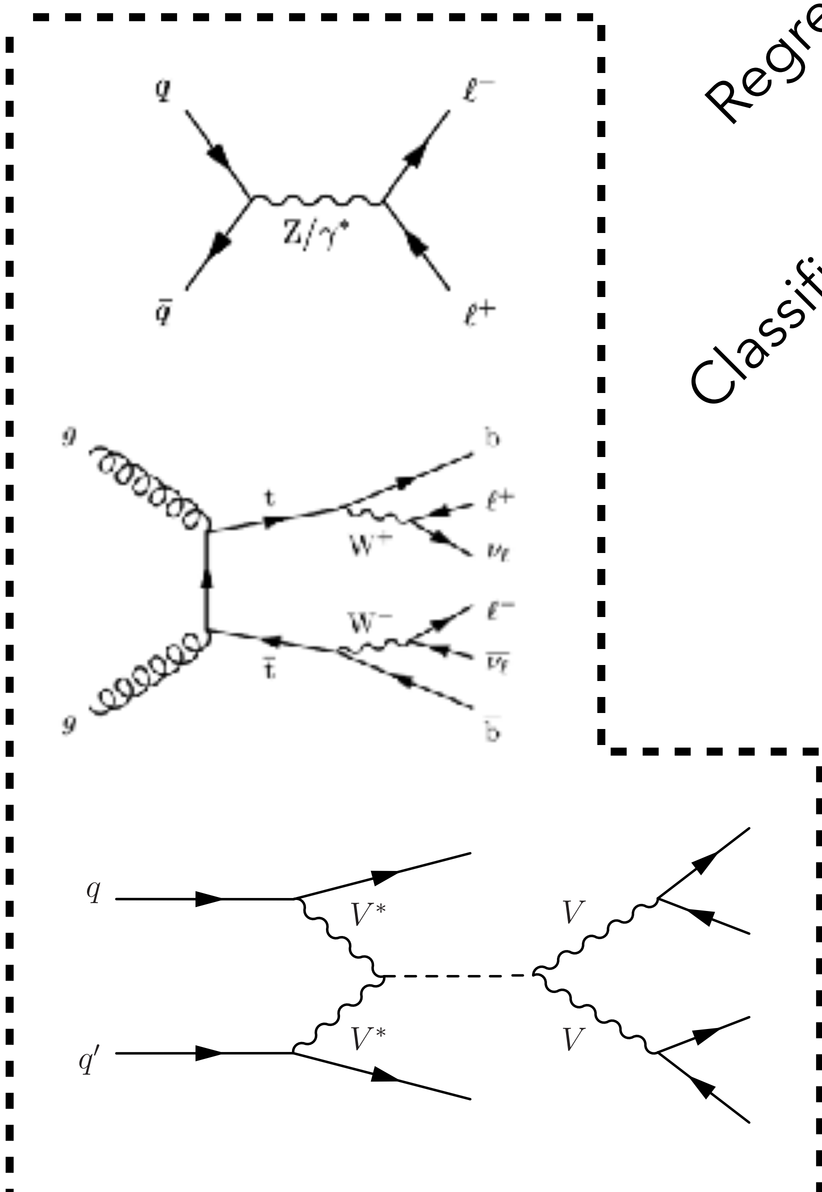
Classification

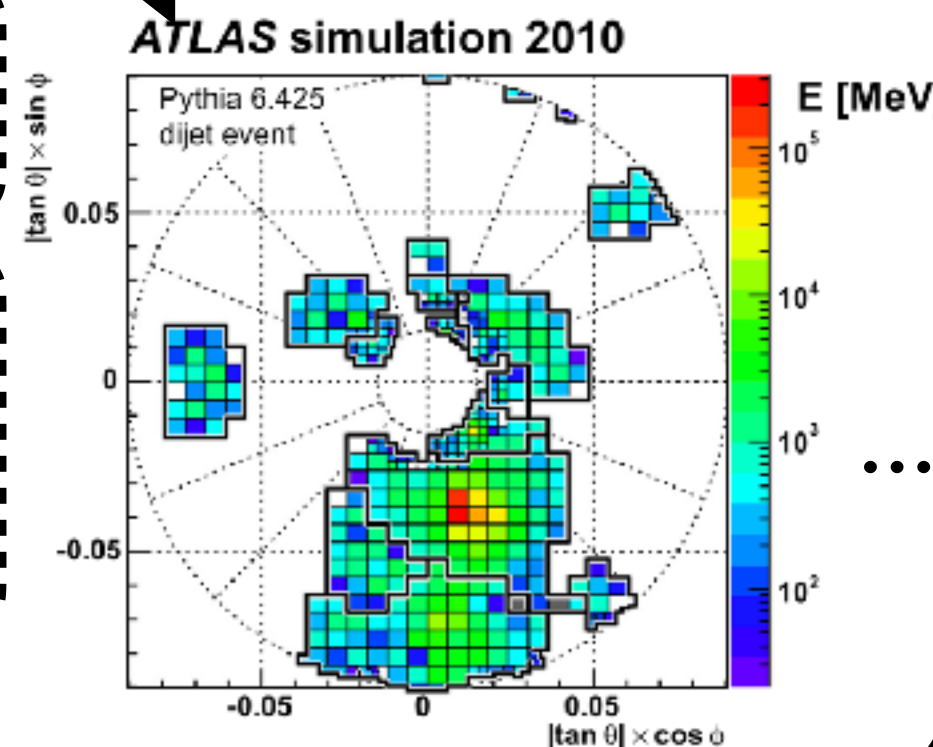
γ

e, μ, τ

ν (E_T^{miss})

hadrons (jets)

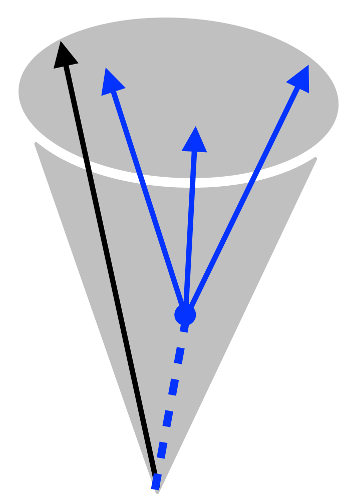


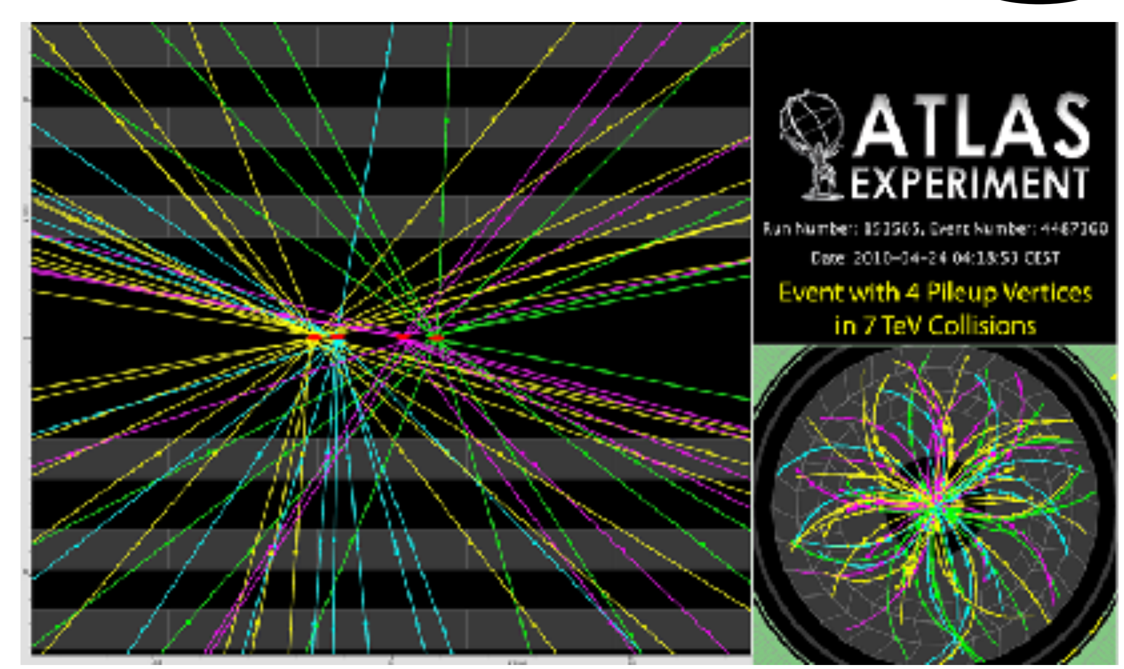


... data

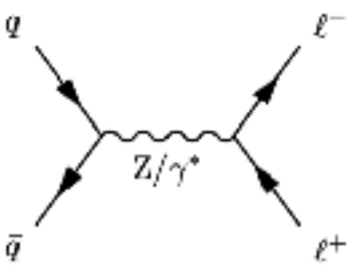
Tracking

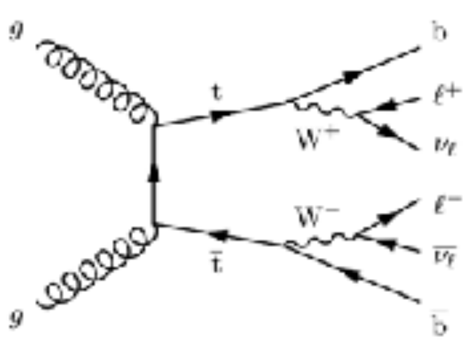
Jet tagging

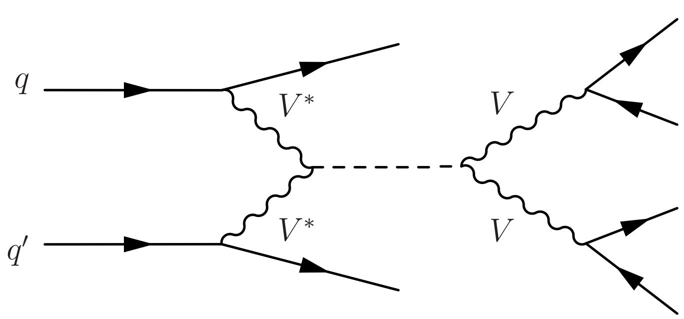


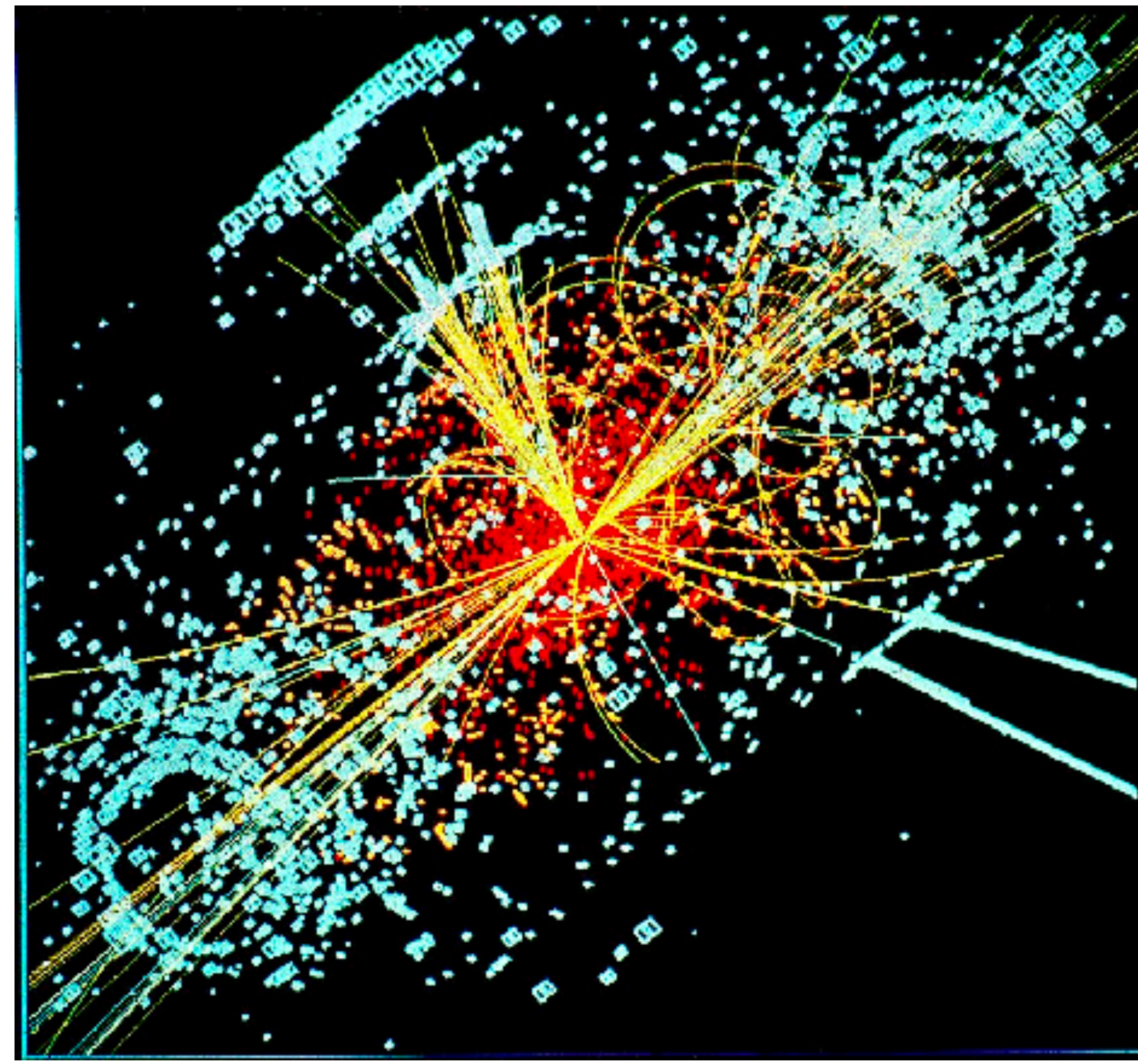


The Holy Grail of Particle Physics









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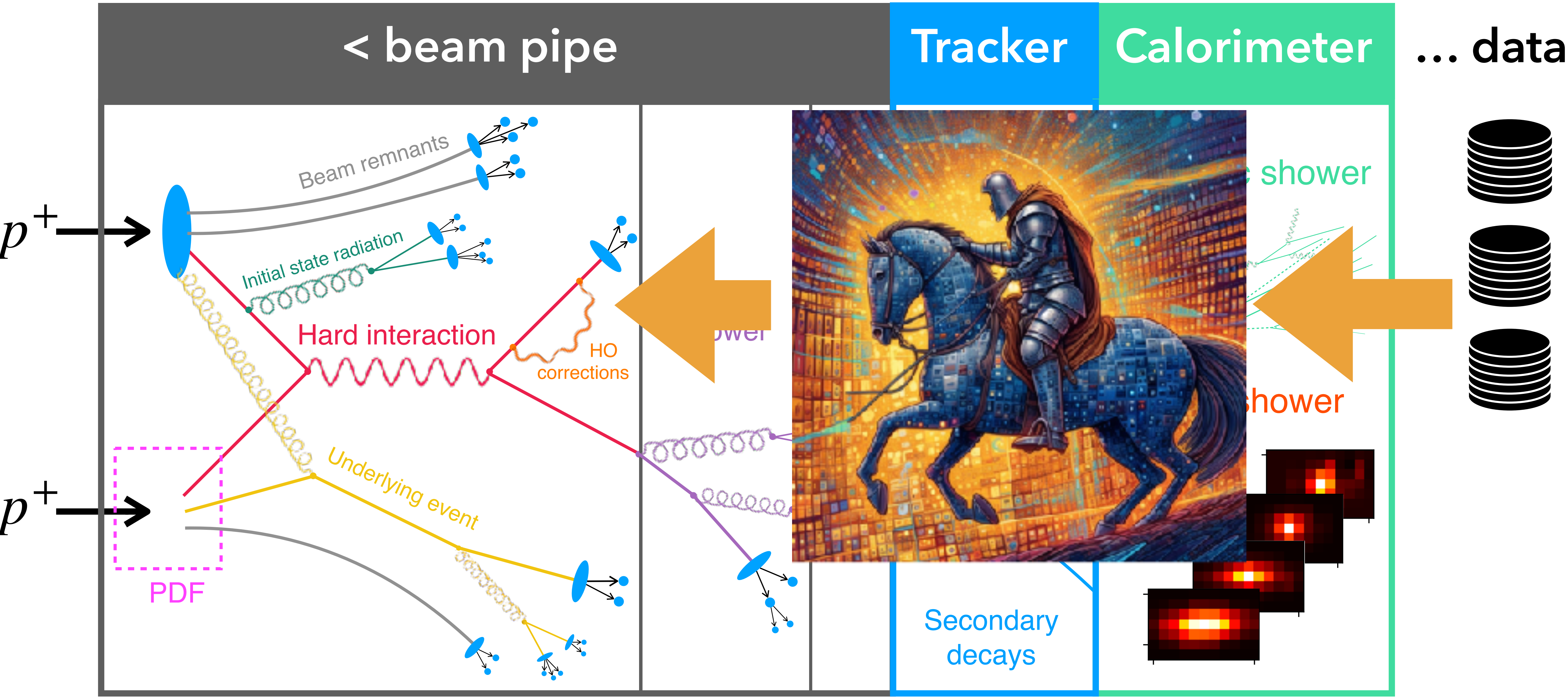
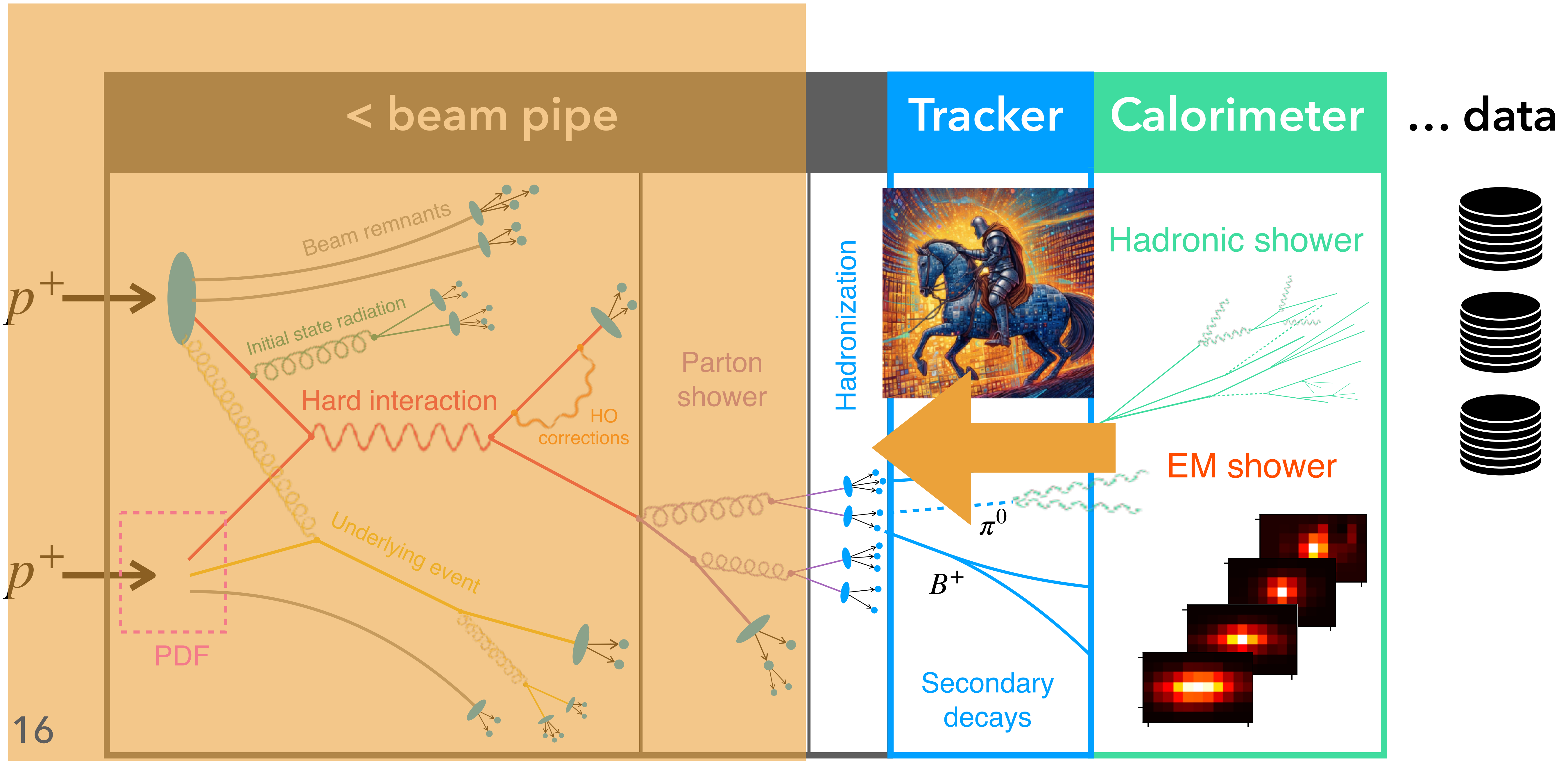


The Holy Grail of Particle Physics

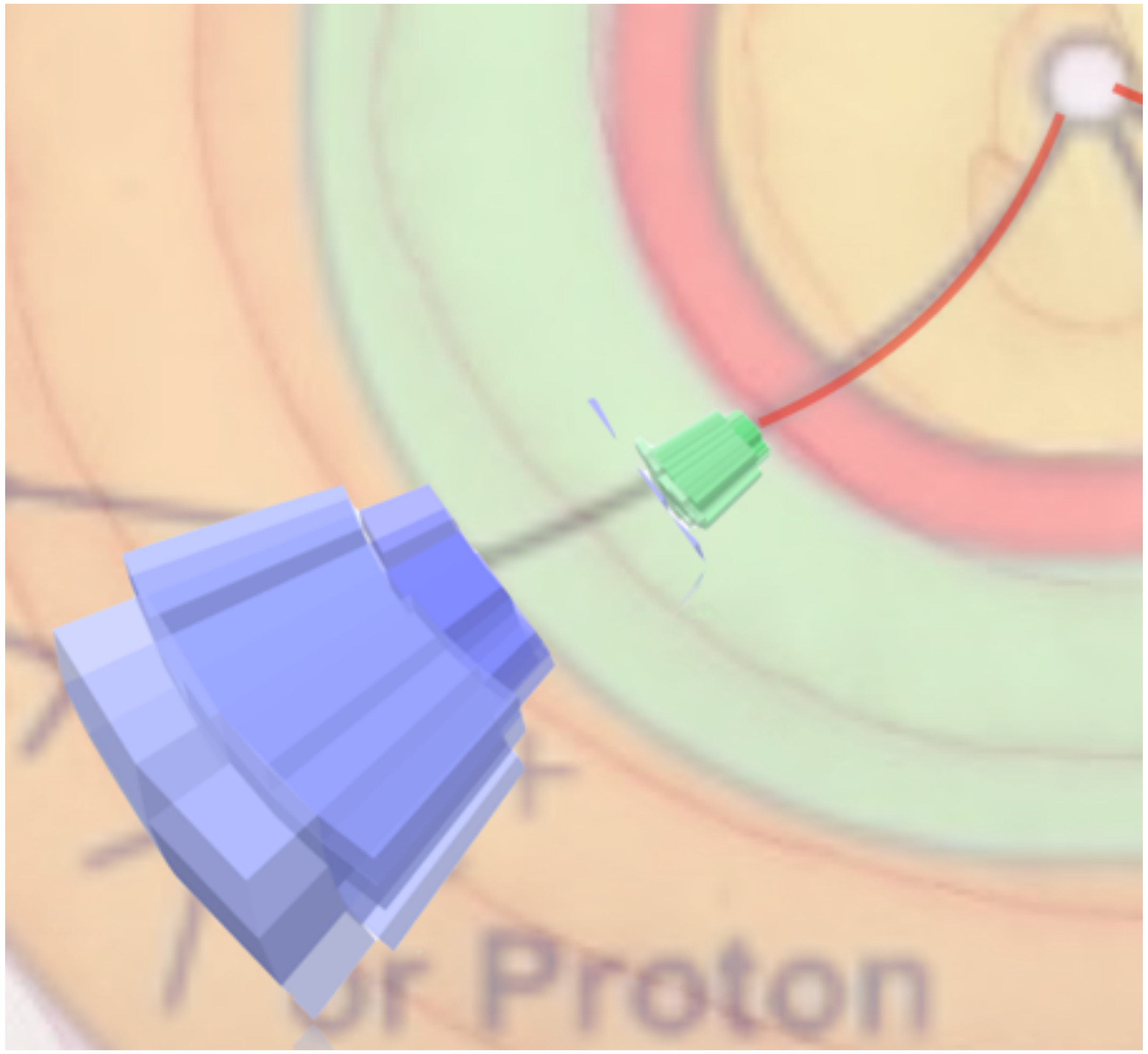
Still a way to go…

From Reconstruction to Particles



Particle Flow

- Combine track and calorimeter information in a complementary way while avoiding double counting

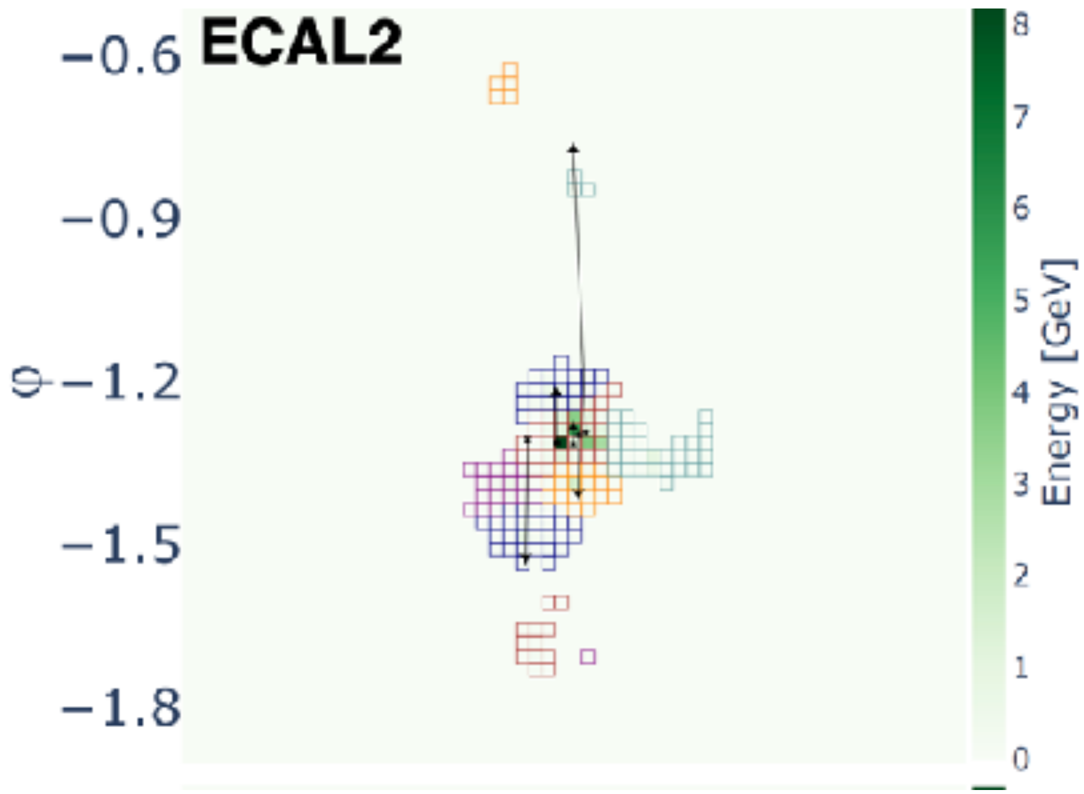


Classical ATLAS "Particle flow" paradigm

Problem: Double counting of Tracks and Energy deposit

Traditional recipe [1]

1. Cluster groups of cells which are adjacent and have high energy significance around some seed $\left(\frac{E}{\sigma_E} > 4.6\right)$ ->**TOPOCLUSTERS**
2. Find associated tracks
3. Decide whether to merge with additional topoclusters
4. Subtract expected E from track to infer contribution from neutral particles

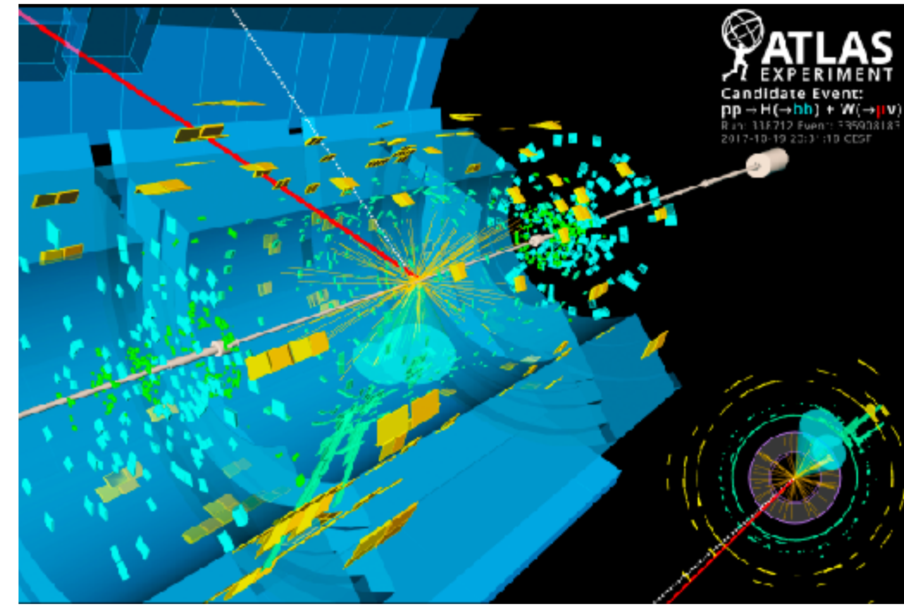


Can we approach this as a machine learning task?

[1] ATLAS Collaboration. Jet reconstruction and performance using particle flow with the ATLAS Detector. Eur. Phys. J. C 77 (2017)

The Work Plan

- In order to learn you need a detailed realistic detector simulation ala ATLAS, CMS etc… Including Tracks & Cells



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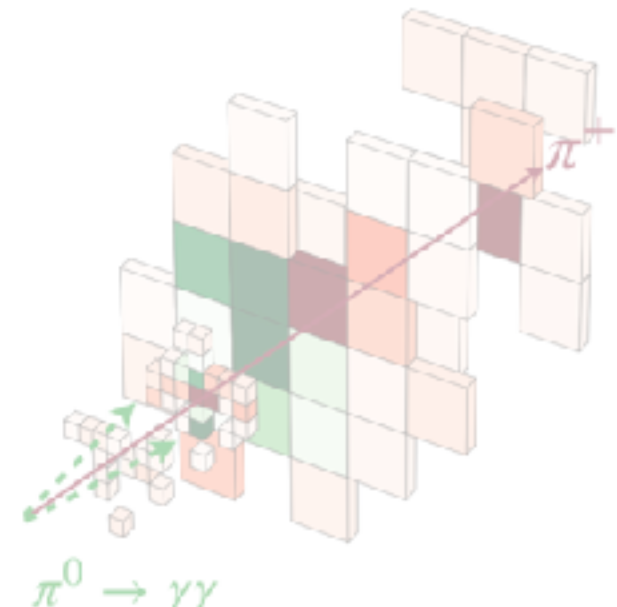

- Can you reconstruct a whole Jet?

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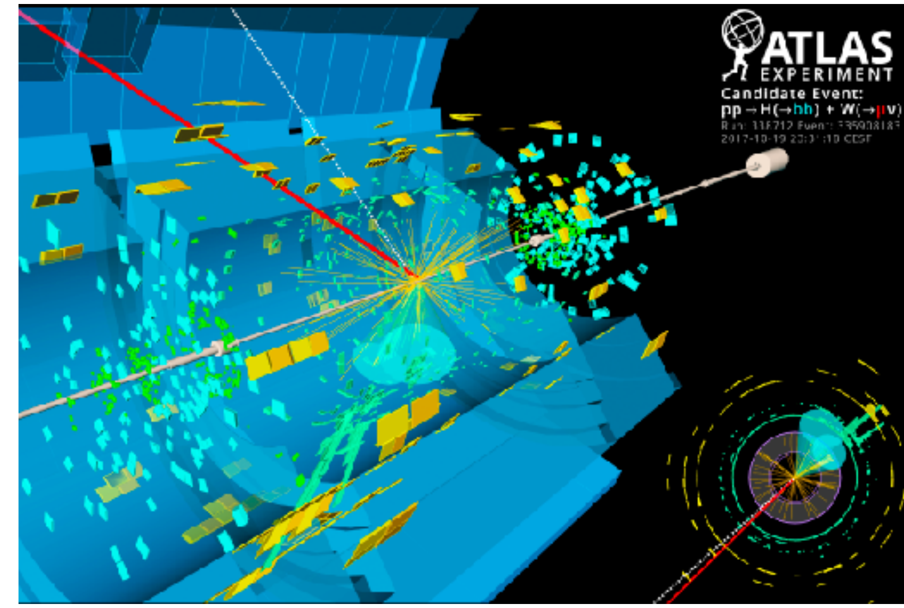

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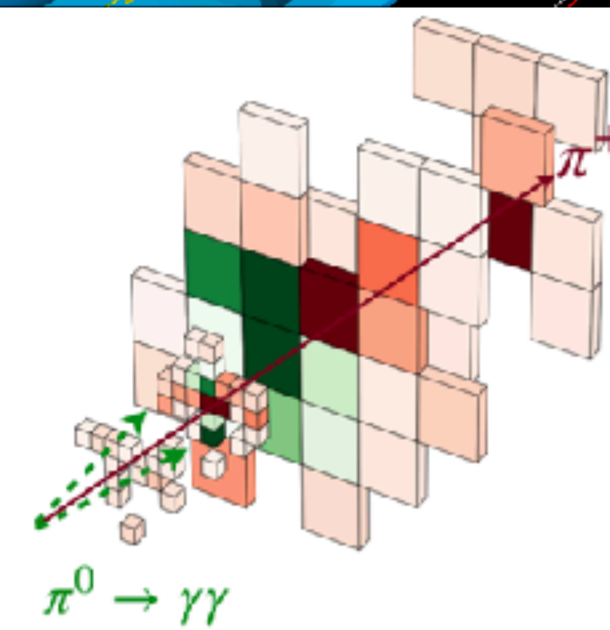

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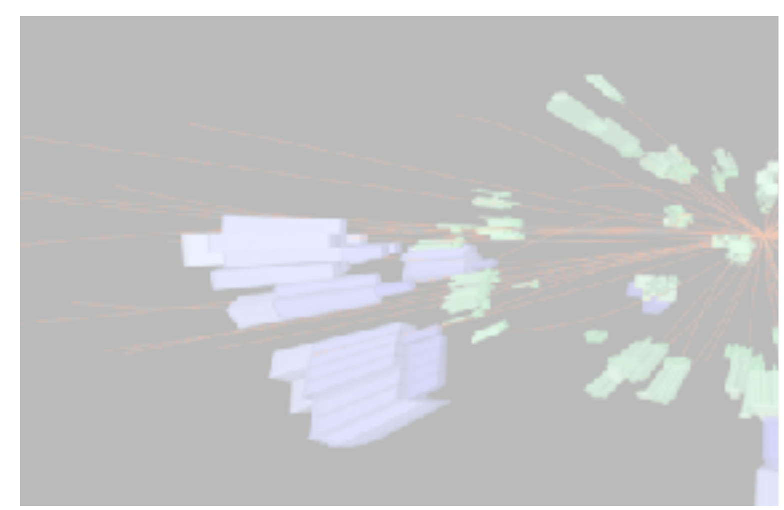

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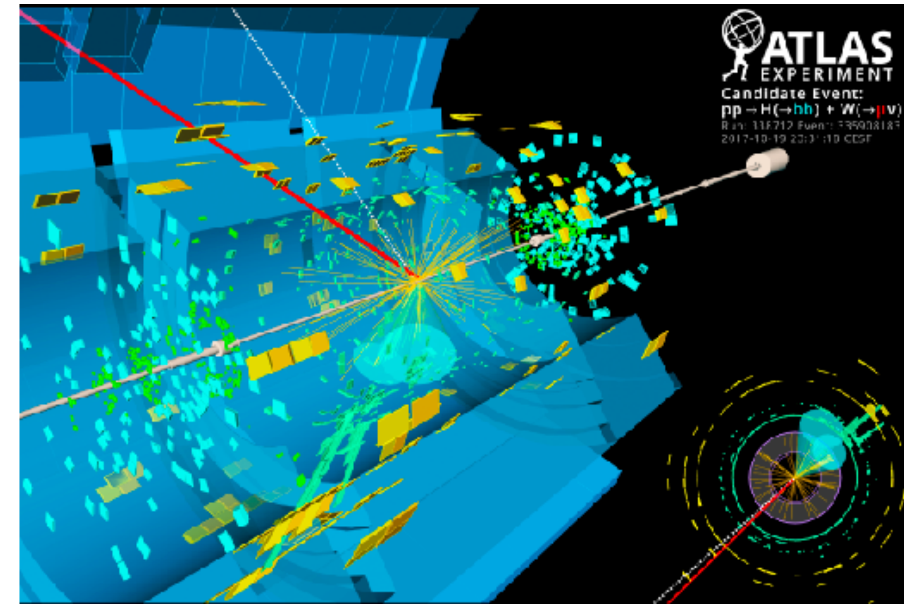

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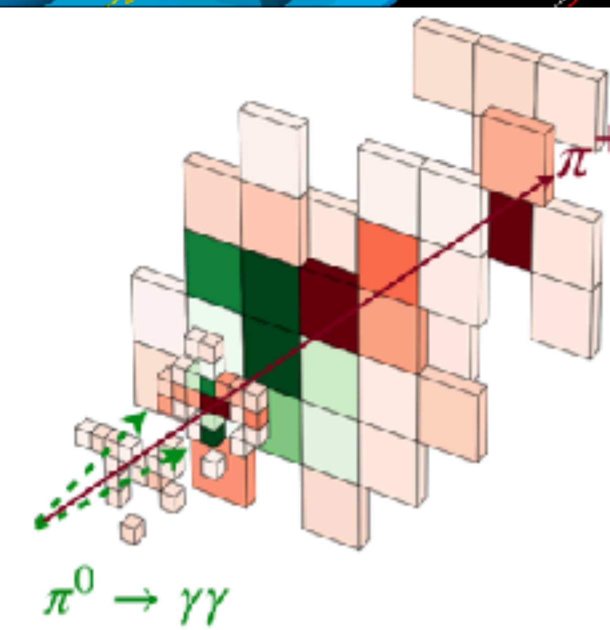

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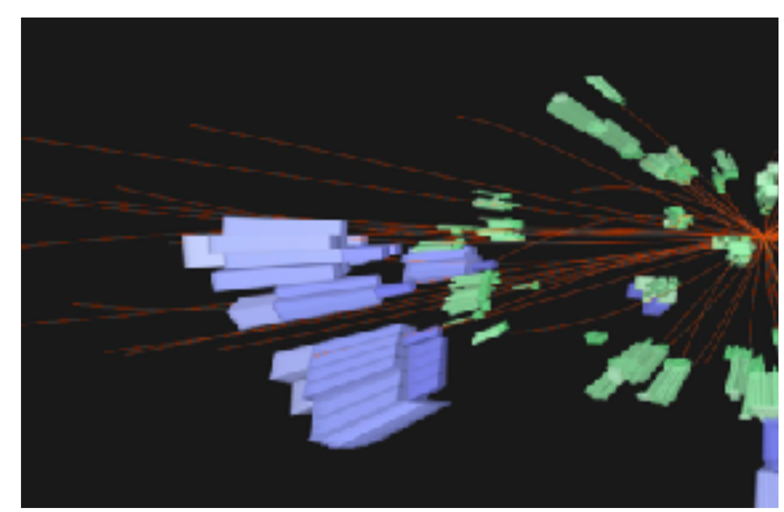
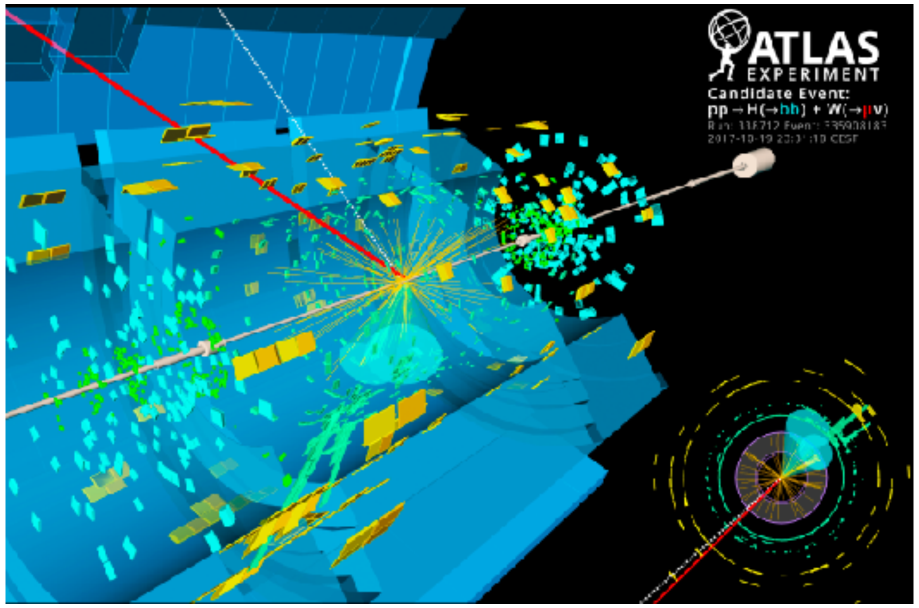


The (Talk) Work Plan



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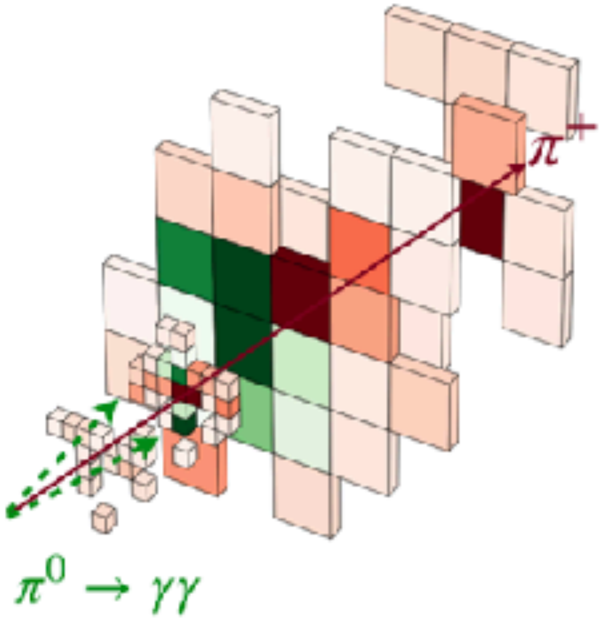

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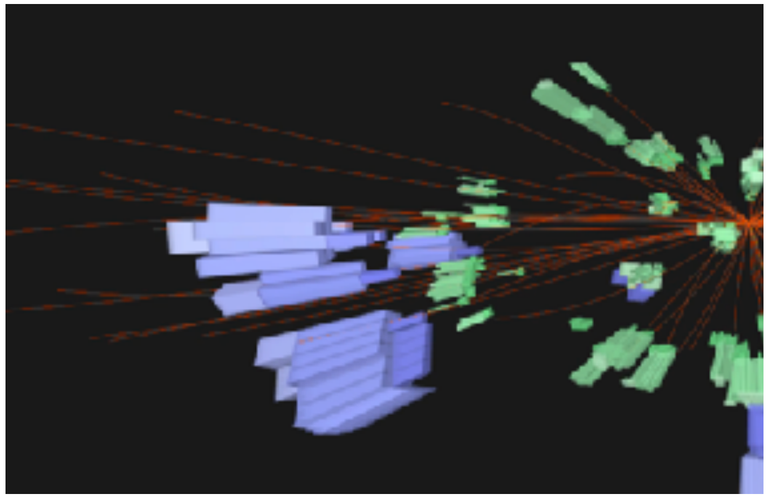

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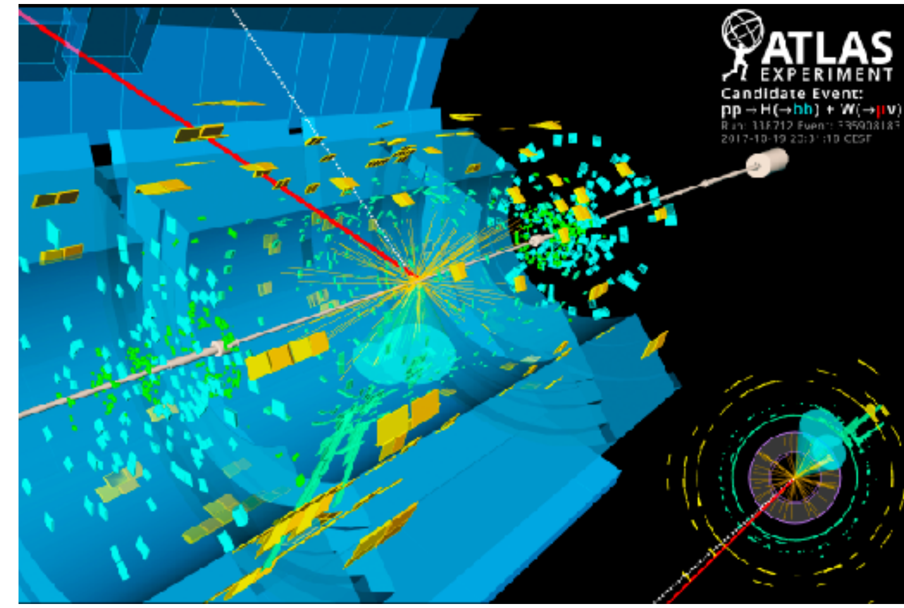

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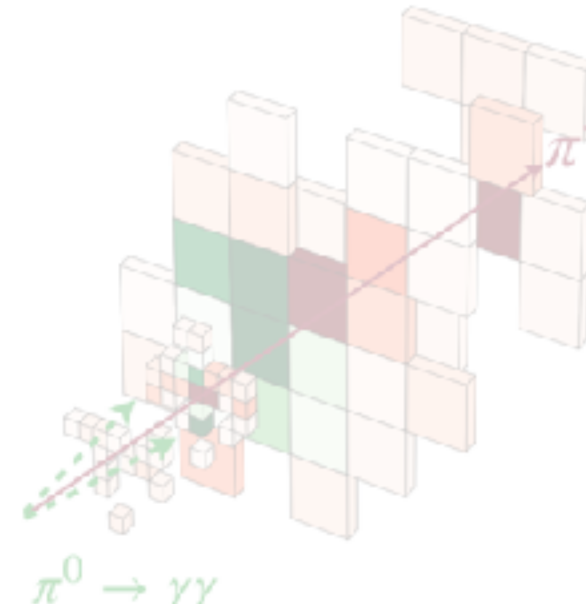

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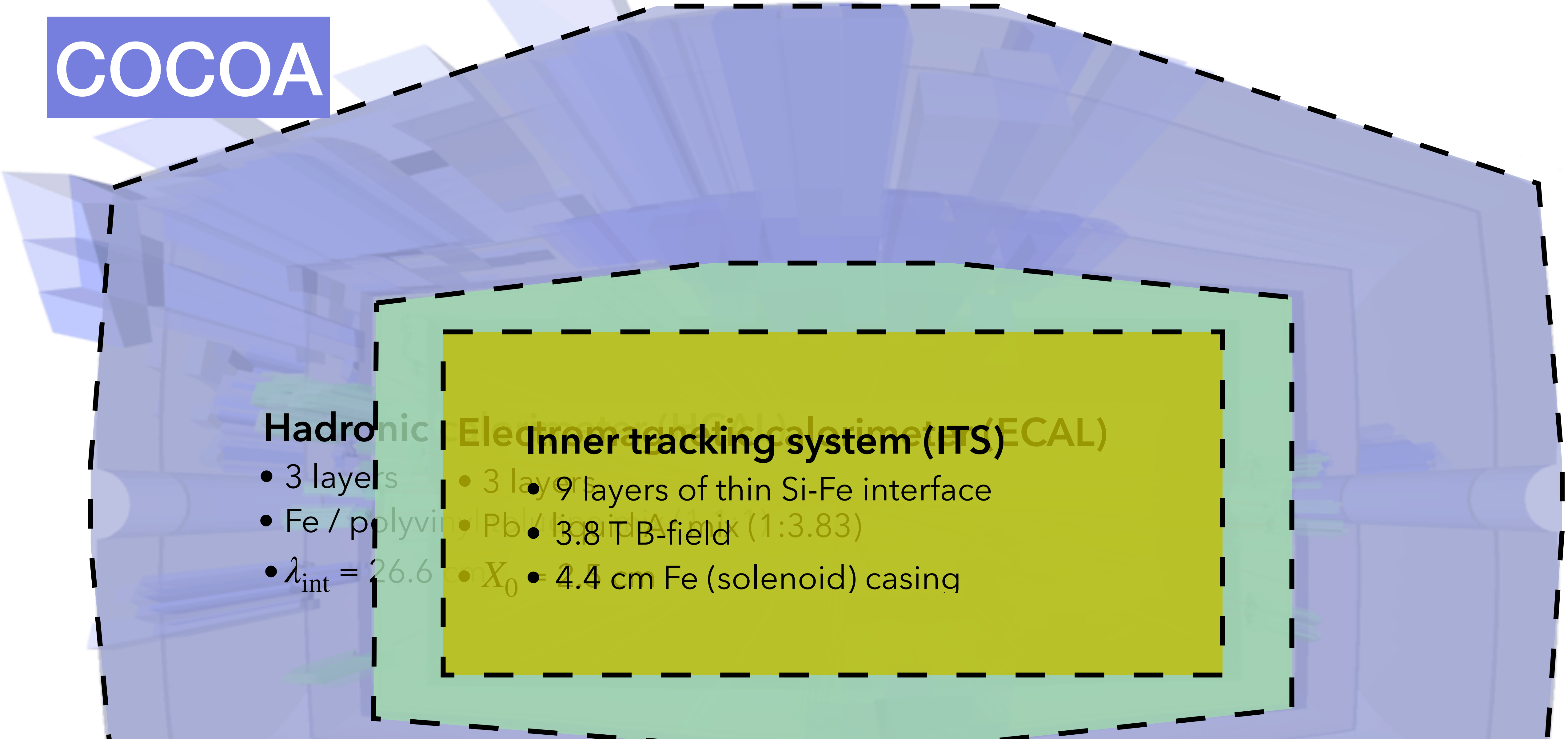
Configurable Calorimeter simulation for AI

COCOA



ATLAS-like calorimeter simulation

- 3 ECAL + 3 HCAL concentric calorimeter layers (GEANT 4)
- Interfaced to an event Monte Carlo generator (Pythia8)
- Tracking emulation in 3.8T magnetic field

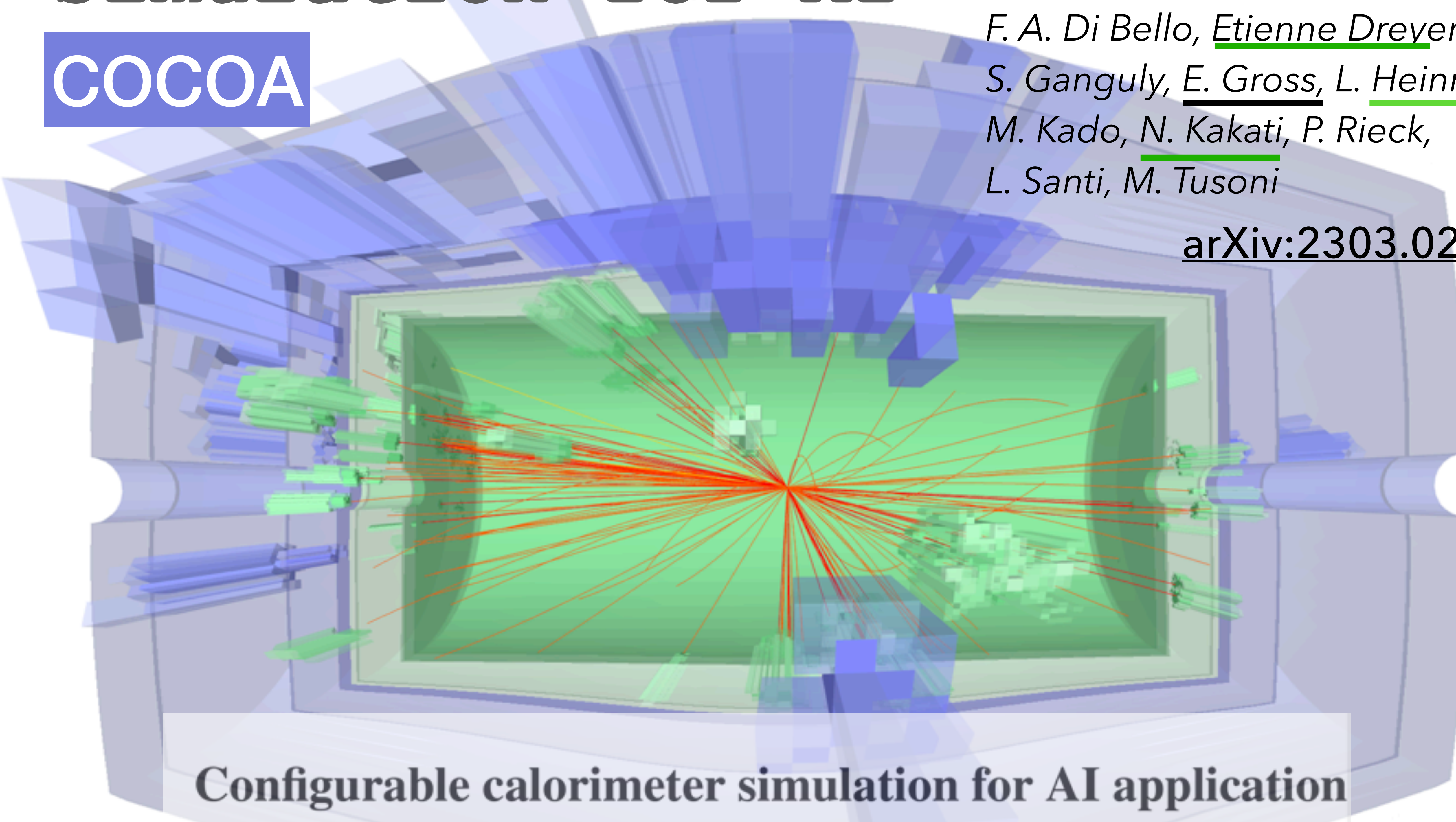
© E. Drenyer

Configurable Calorimeter simulation for AI

COCOA

A. Charkin-Gorbulin, K. Cranmer, F. A. Di Bello, Etienne Dreyer, S. Ganguly, E. Gross, L. Heinrich, M. Kado, N. Kakati, P. Rieck, L. Santi, M. Tusoni

arXiv:2303.02101



Configurable calorimeter simulation for AI application

Francesco Armando Di Bello [1], Anton Charkin-Gorbulin [2], Kyle Cranmer [4,5], Etienne Dreyer [3,c], Sanmay Ganguly [6,a], Eilam Gross [3], Lukas Heinrich [7], Lorenzo Santi [9], Marumi Kado [8,9], Nilotpal Kakati [3], Patrick Rieck [4,b], Matteo Tusoni [9]

COCOA Event Display

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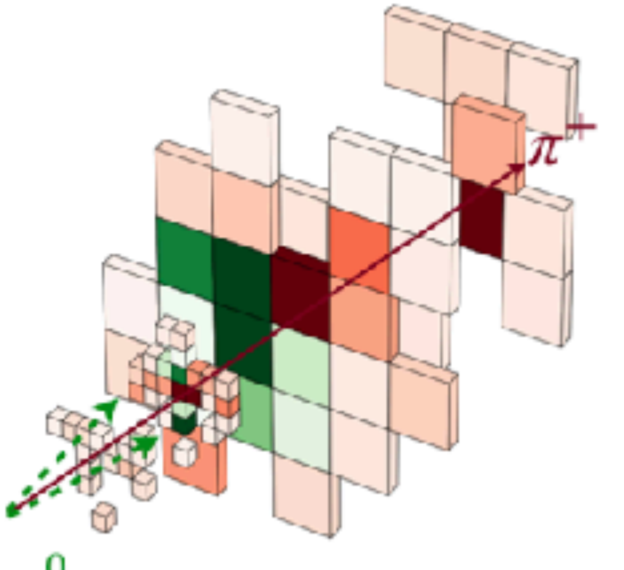

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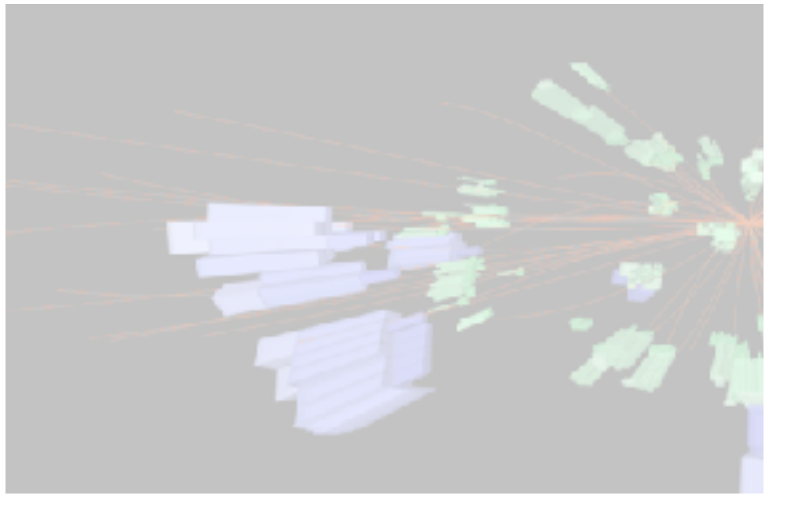
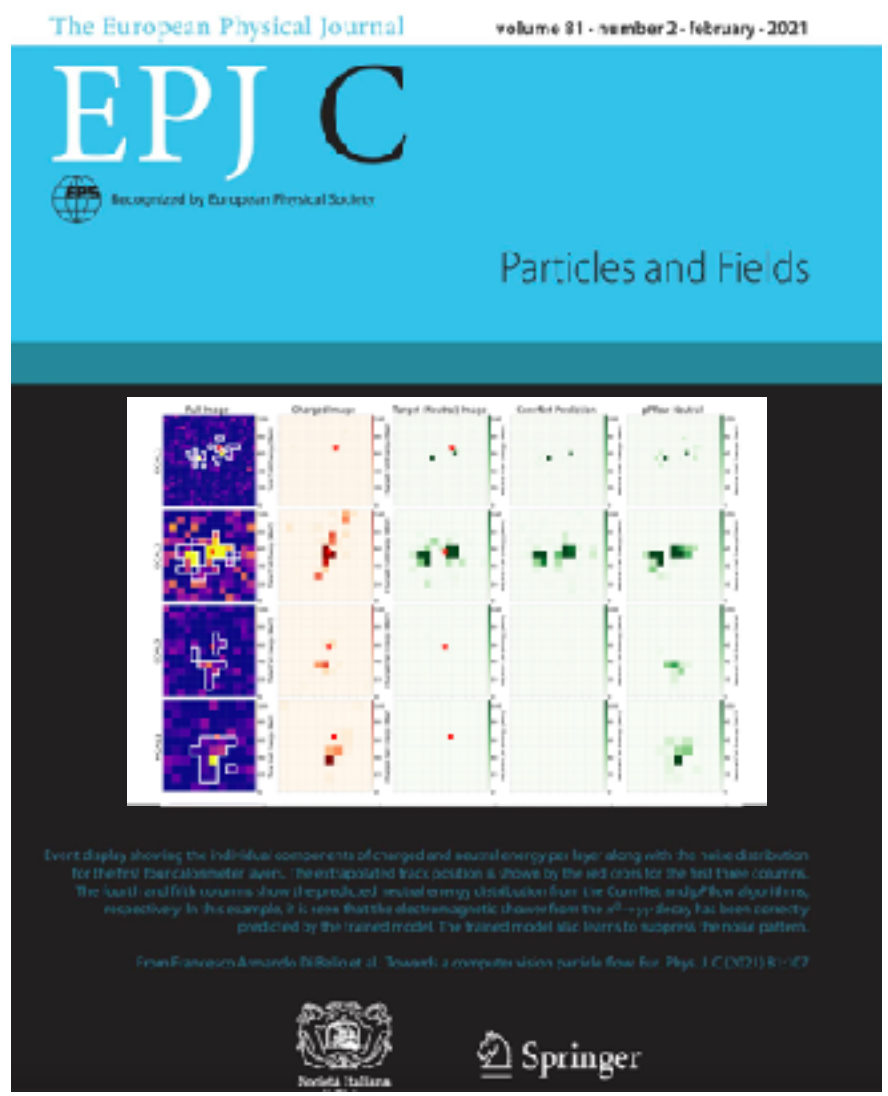


Proof of Concept (Convolutional NN)

Towards a Computer Vision Particle Flow *

Francesco Armando Di Bello[a,3], Sanmay Ganguly[b,1], Eilam Gross[1], Marumi Kado[3,4], Michael Pitt[2], Lorenzo Santi [3], Jonathan Shlomi[1]

https://arxiv.org/pdf/2003.08863.pdf



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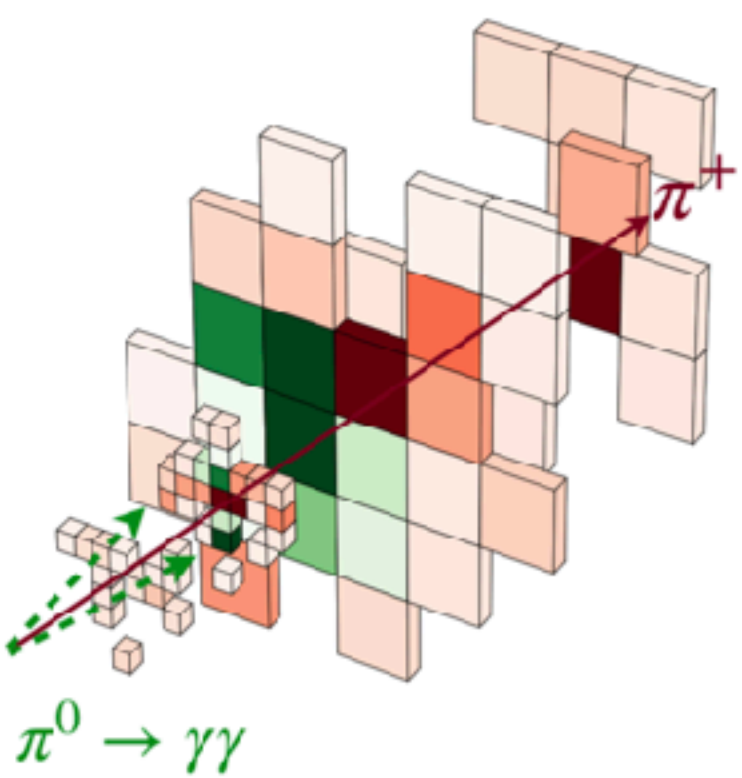
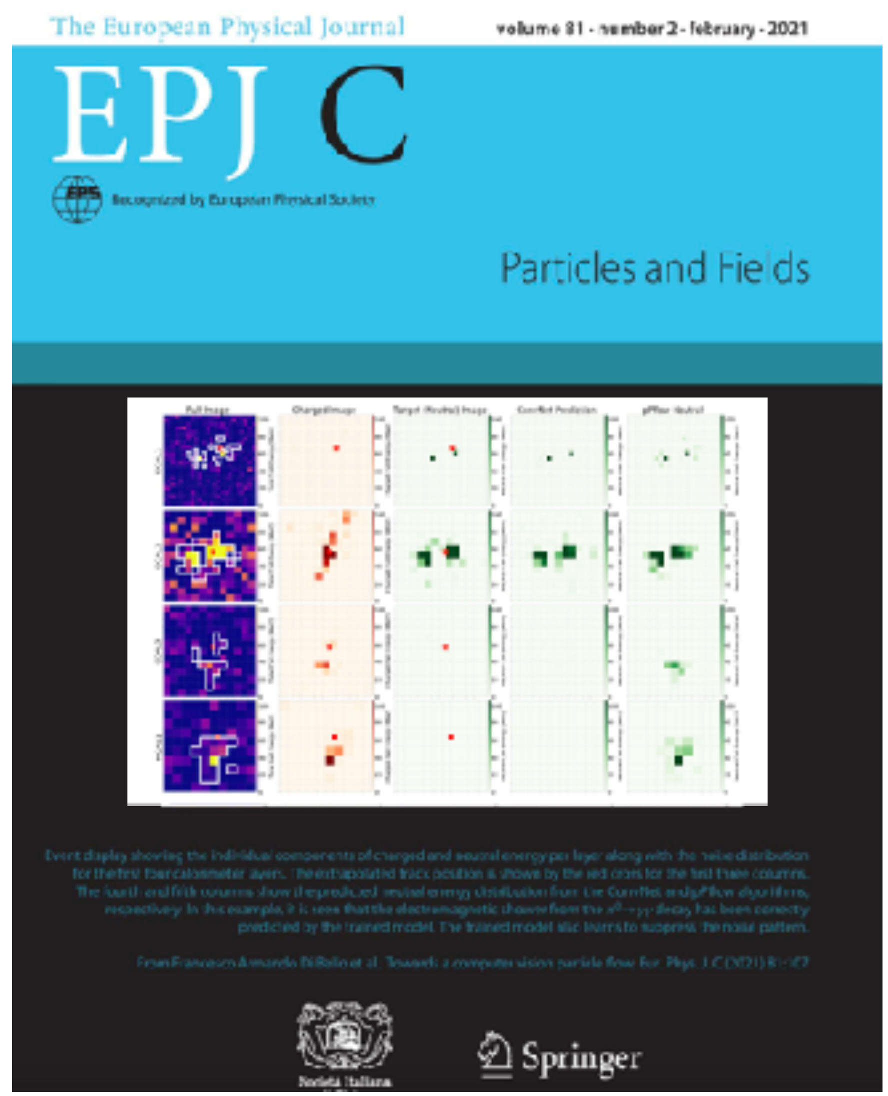
Overlapping $\pi^+$and $\pi^0(\rightarrow \gamma\gamma)$





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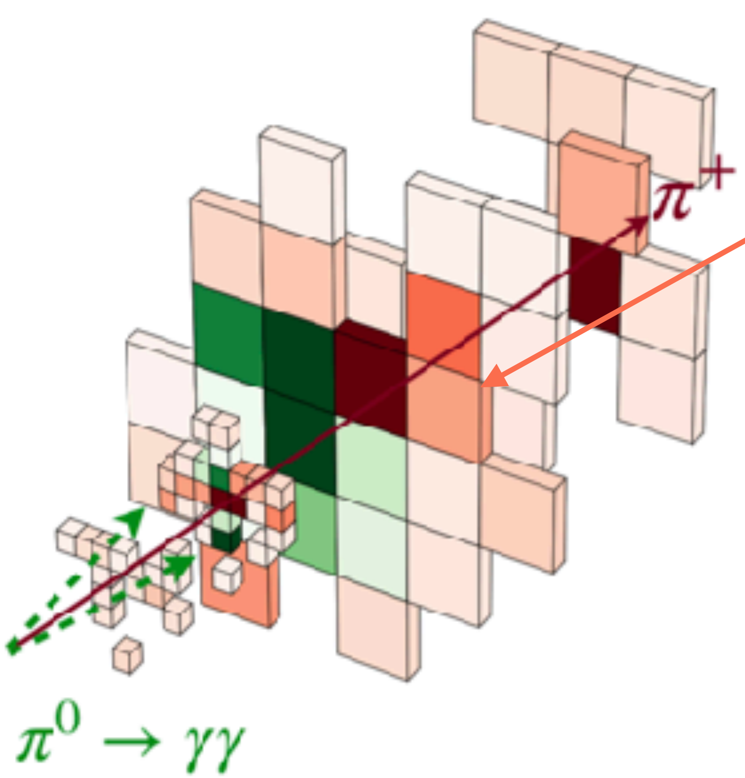

The Good'n old Parametrized Pflow
PPflow

Combining tracks and clusters lead to double counting

1. Parametrize the energy deposit of charged particles in the calorimeter
2. Subtract it from the total calorimeter deposited energy to get the Neutral Energy deposit

Proof of Concept (Convolutional NN)

Towards a Computer Vision Particle Flow *

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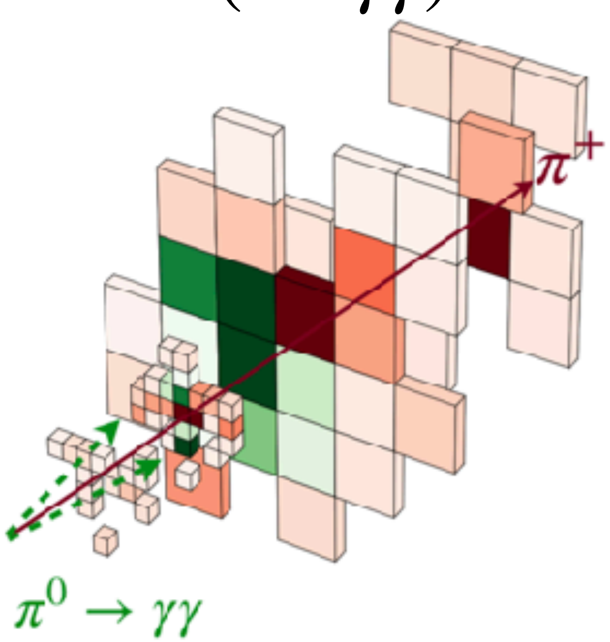
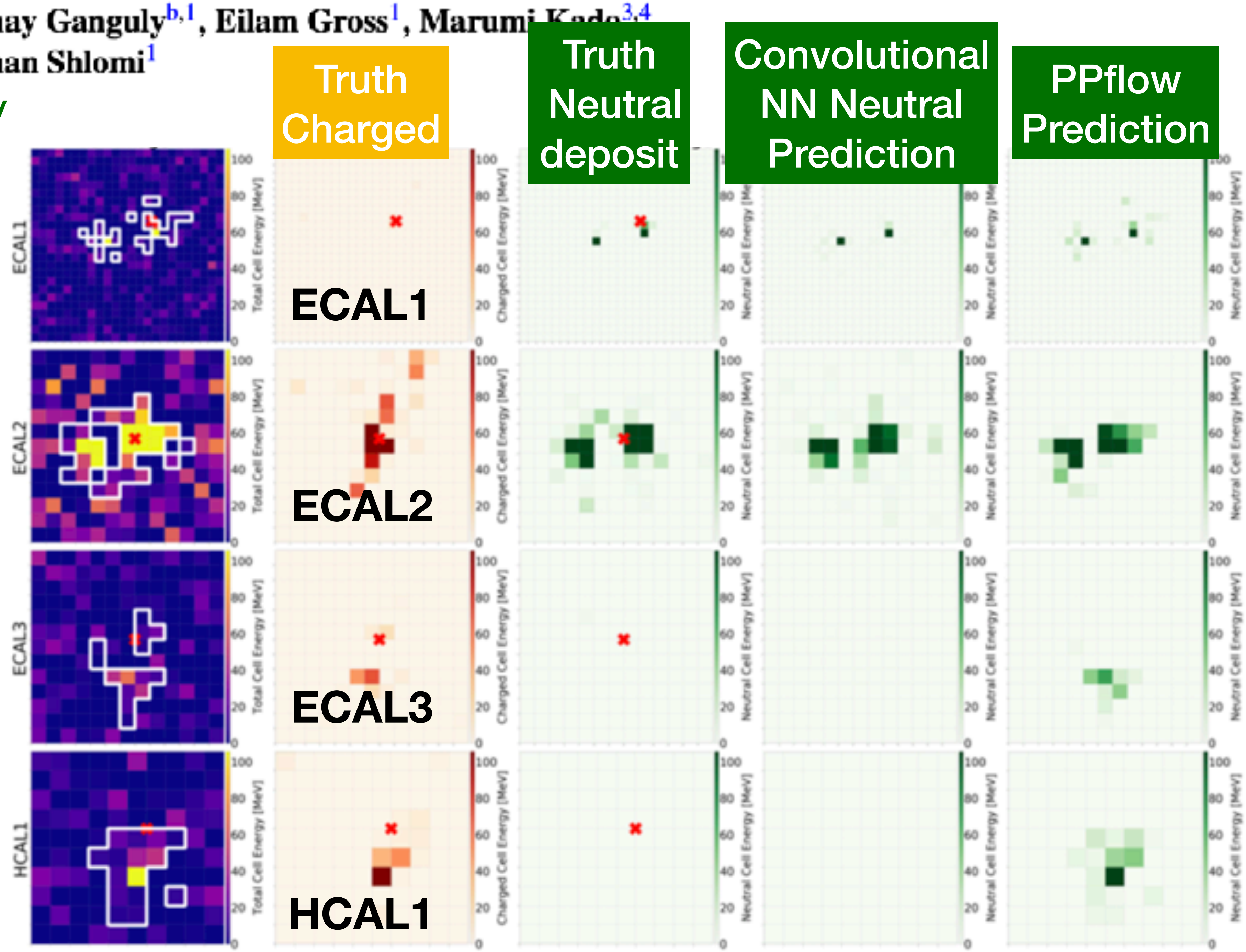
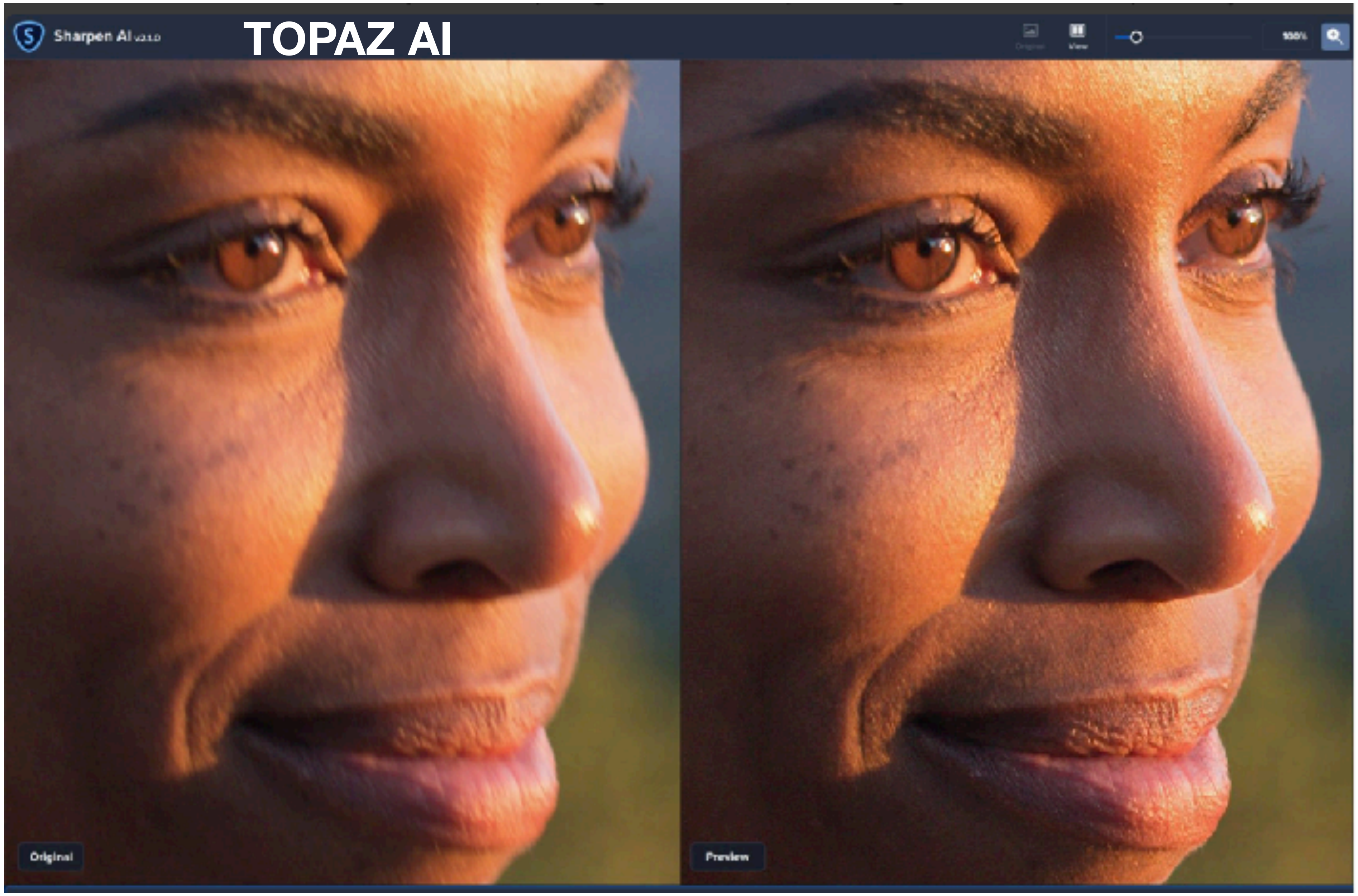




A Byproduct: Super Resolution

Train the net to match low resolution to high resolution photograph.



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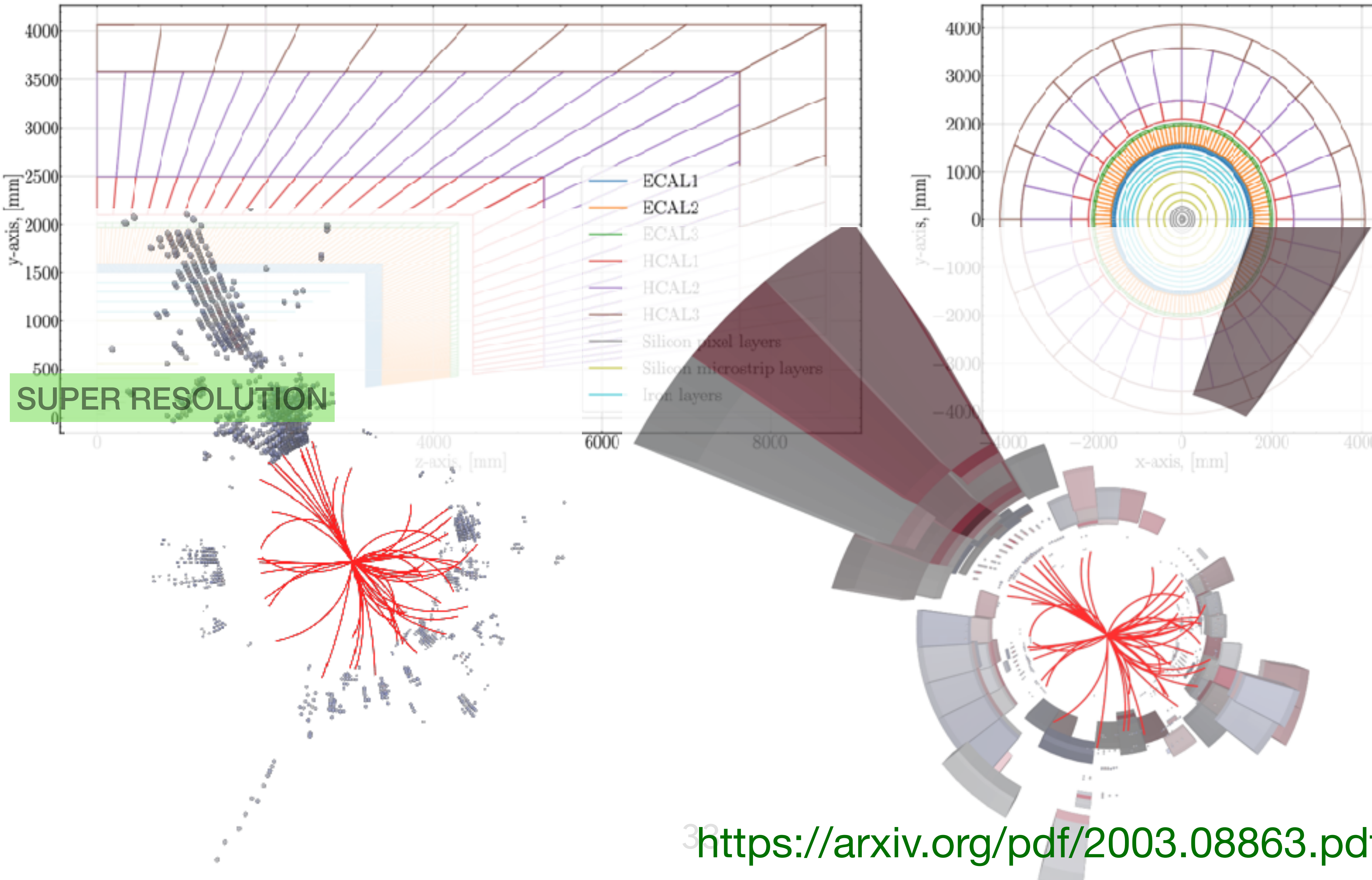
Train the net to match low resolution to high resolution detector readout.
Do an inverse inference to predict the final particles.



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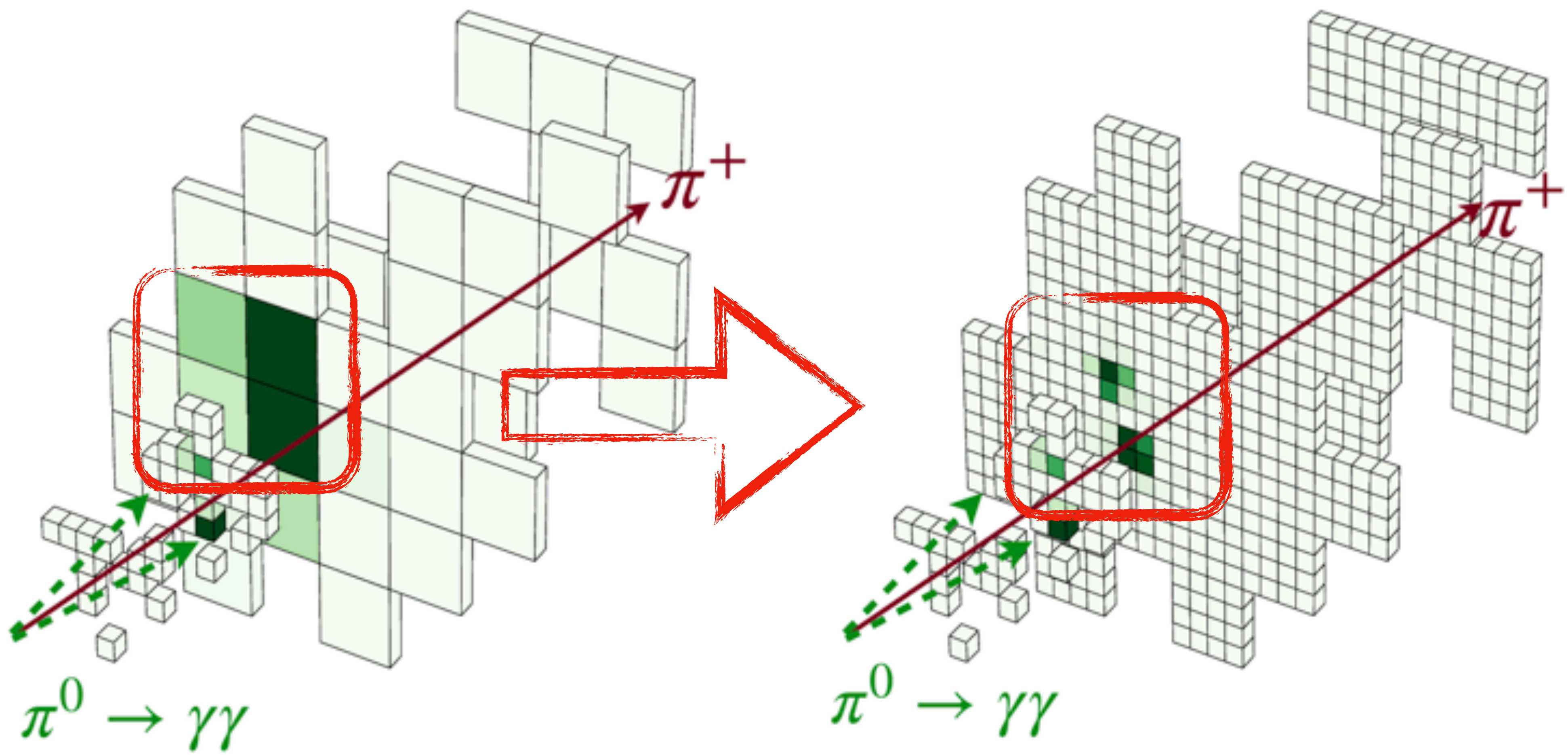

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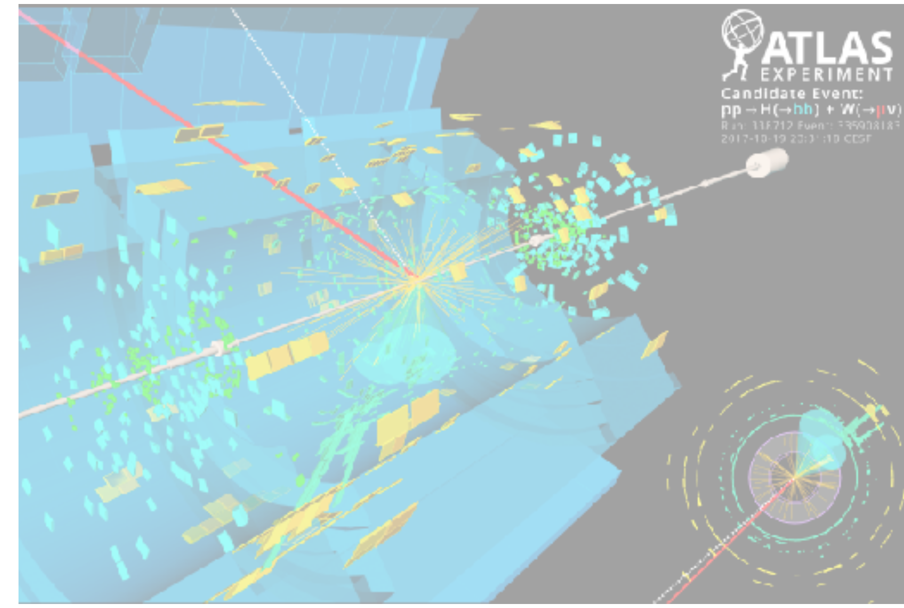
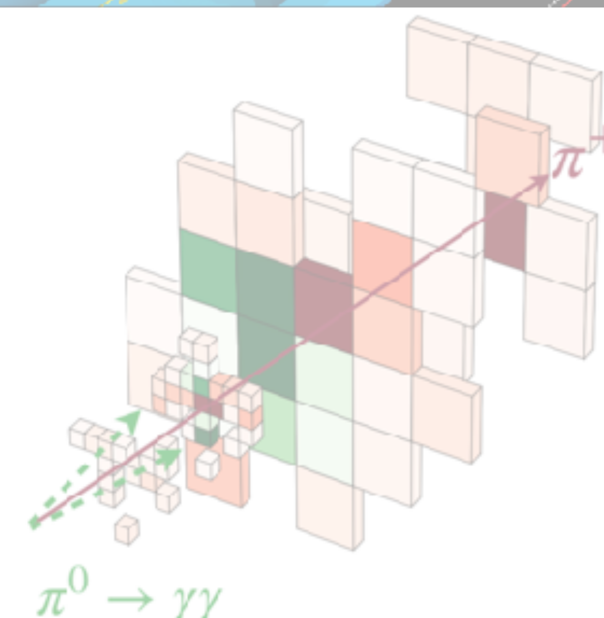
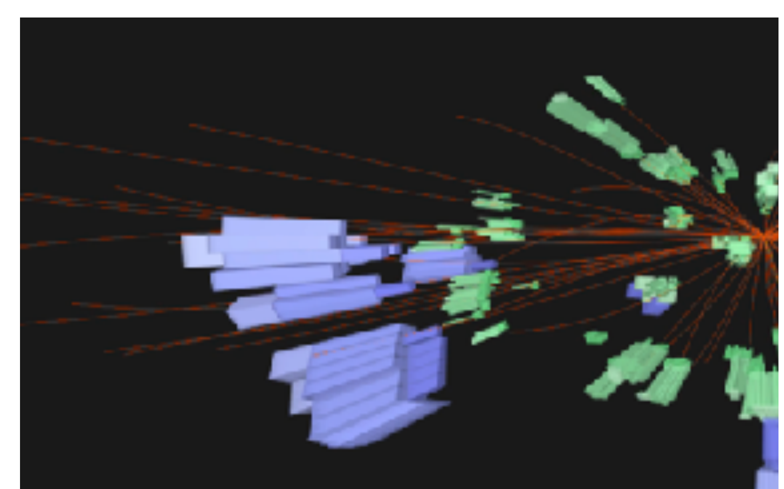


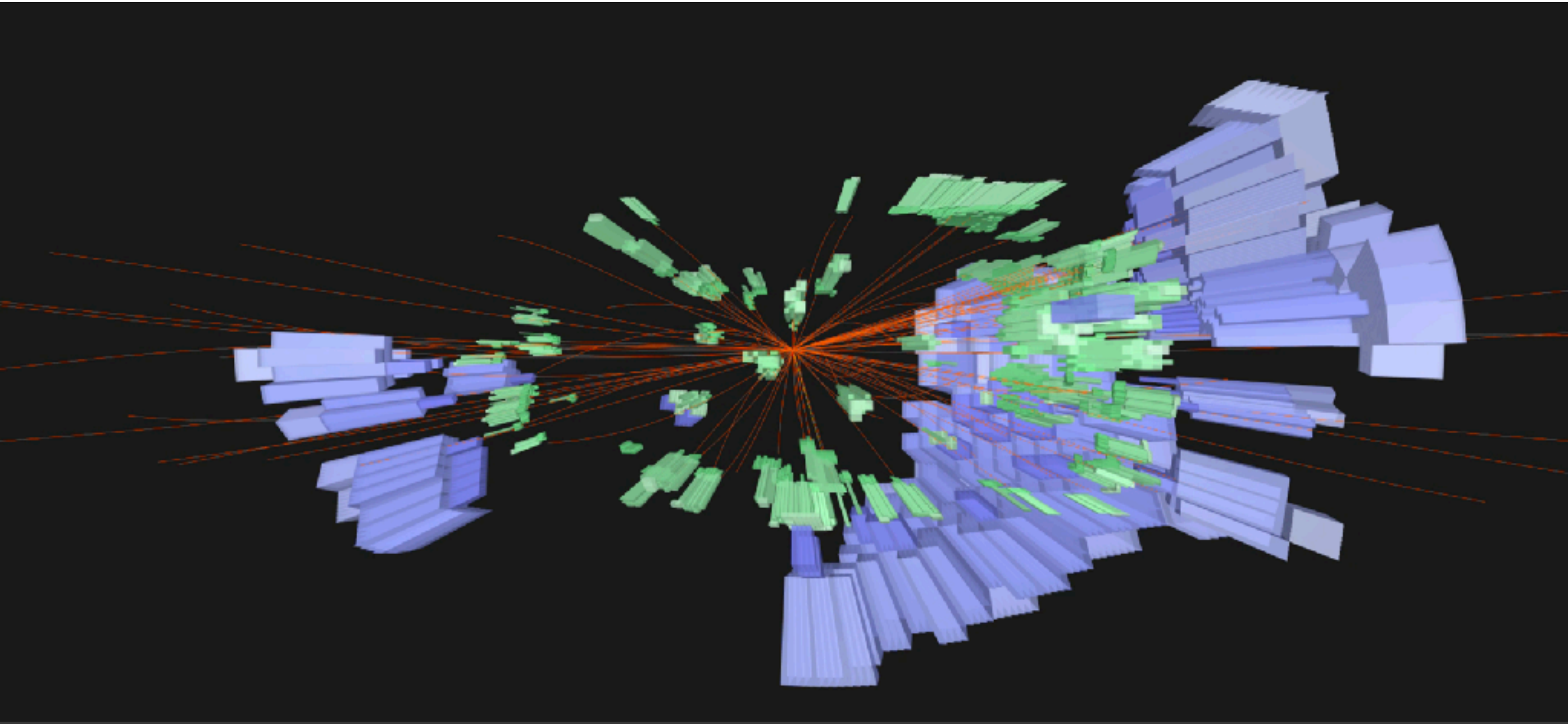
- Proof of Concept, can you tell a Neutral Hadron (e.g. $\pi^0 \to \gamma\gamma$) from an overlapping Charged Hadron (e.g. π^+)



- Can you reconstruct a whole Jet?



THE CHALLENGE:
Reconstruct a Whole Jet



Reconstructing particles in jets using set transformer and hypergrap prediction networks

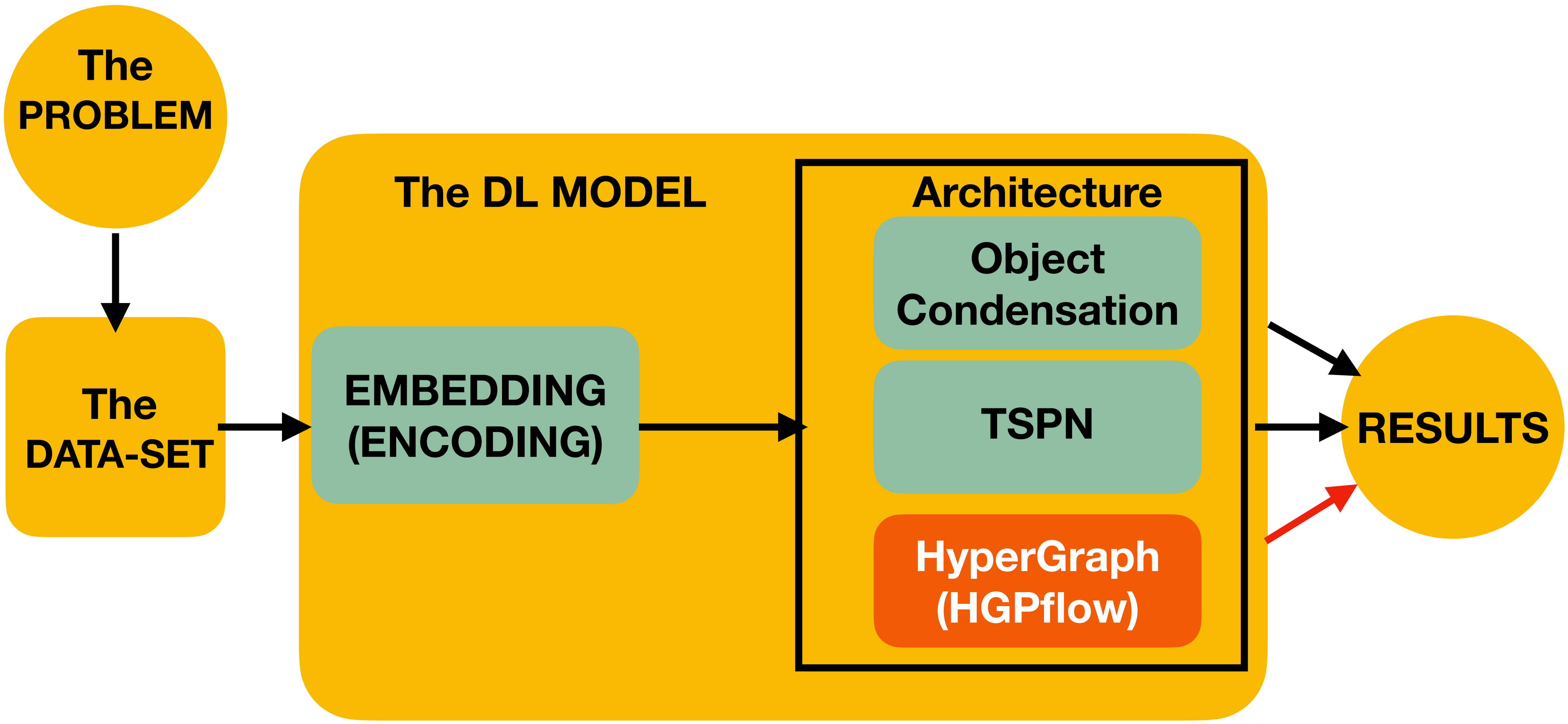
Francesco Armando Di Bello [1,a], Etienne Dreyer [2,b], Sanmay Ganguly [3], Eilam Gross [2], Lukas Heinrich [4], Anna Ivina [2], Marumi Kado [5,6], Nilotpal Kakati [2,c], Lorenzo Santi [6], Jonathan Shlomi [2], Matteo Tusoni [6]

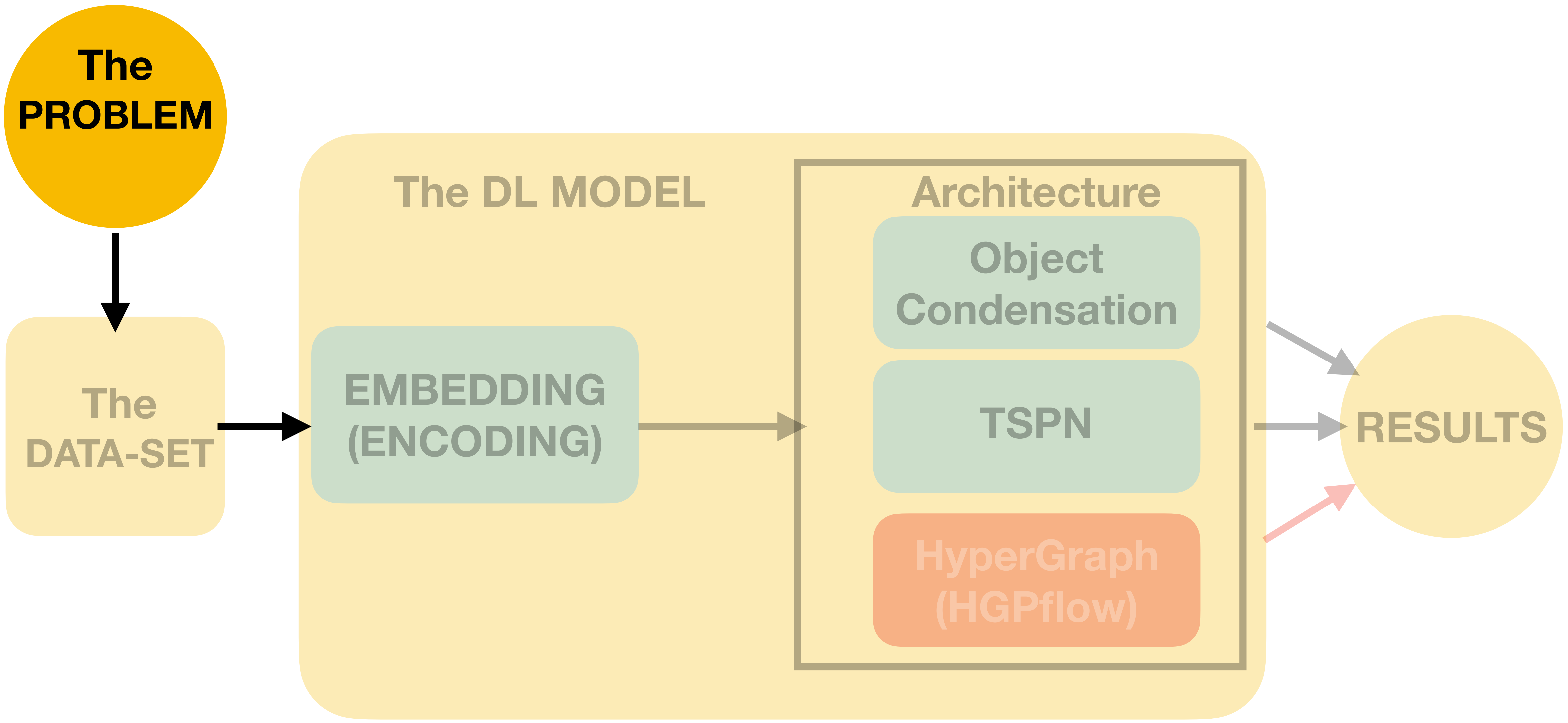
[1] INFN and University of Genova
[2]Weizmann Institue of Science
[3]ICEPP, University of Tokyo
[4]Technical University of Munich
[5]Max Planck Institute for Physics
[6]INFN and Sapienza University of Rome

Received: date / Accepted: date

https://arxiv.org/abs/2212.01328

Accepted for Publication in EPJC

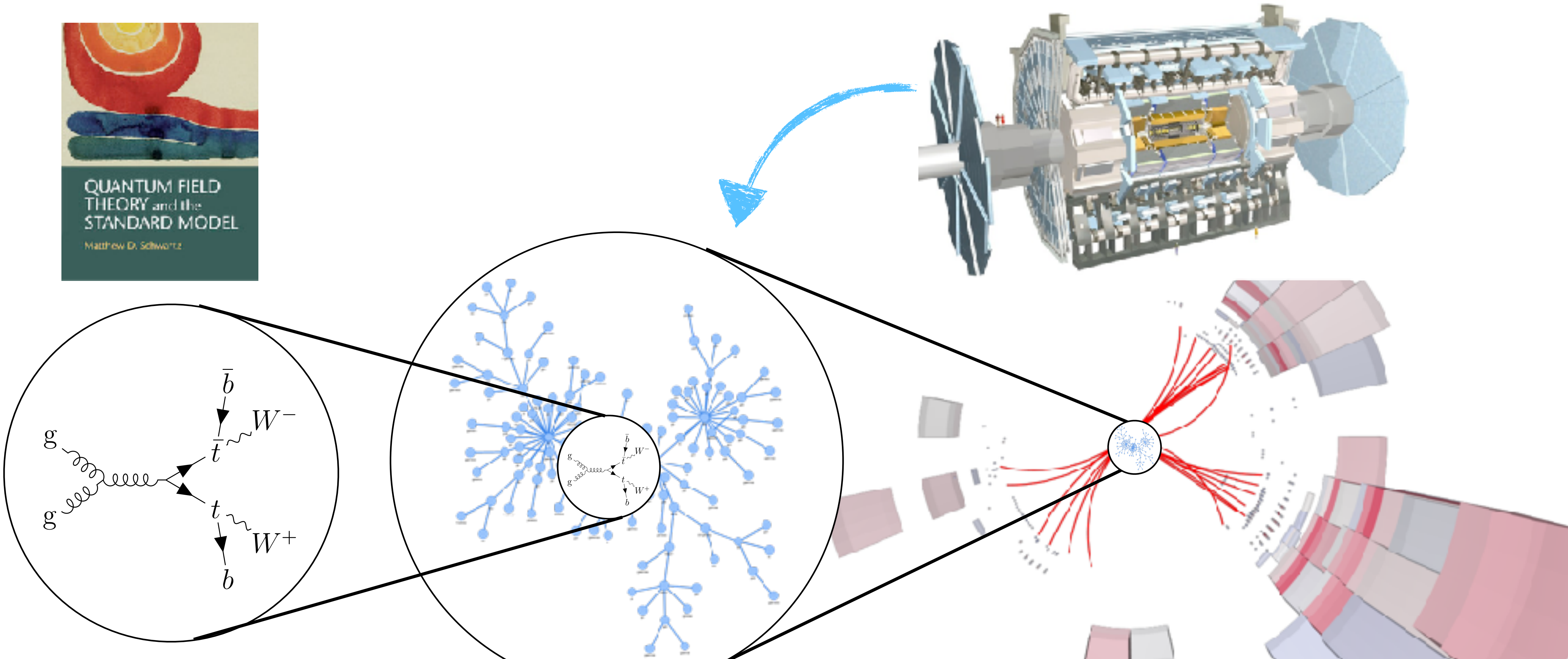

The PROBLEM
The DATA-SET
The DL MODEL
EMBEDDING (ENCODING)
Architecture
Object Condensation
TSPN
HyperGraph (HGPflow)
RESULTS



The PROBLEM
The DATA-SET
The DL MODEL
EMBEDDING (ENCODING)
Architecture
Object Condensation
TSPN
HyperGraph (HGPflow)
RESULTS

In a Nut Shell:
From Reconstruction to Particles

The Goal: Reconstruct the stable outgoing particles from the detector readout.

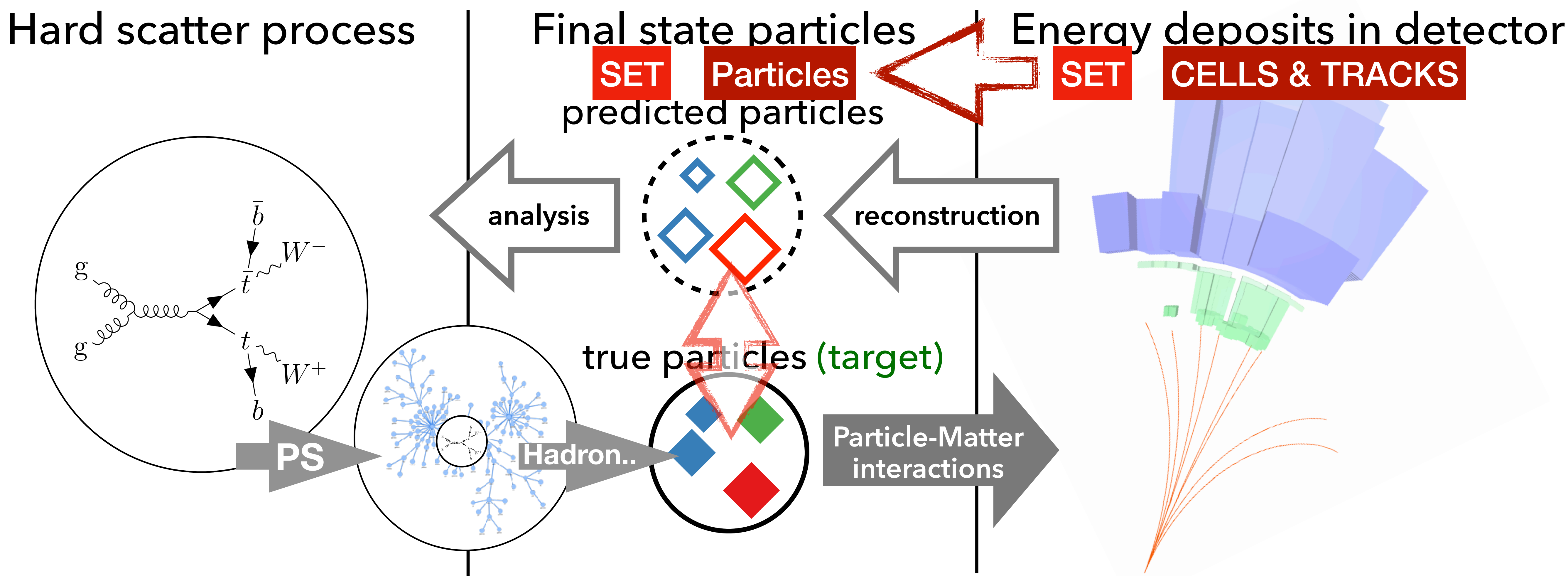


Physics Input:
The Feynman Diagram
A graphic description of
the outcome of a collision
(Produced by a real Collision
or a simulated collision)

Final Particles
Produced via Nature
or Simulation

Detector output/Readout
Produced via Hardware
or Simulation

Particle reconstruction

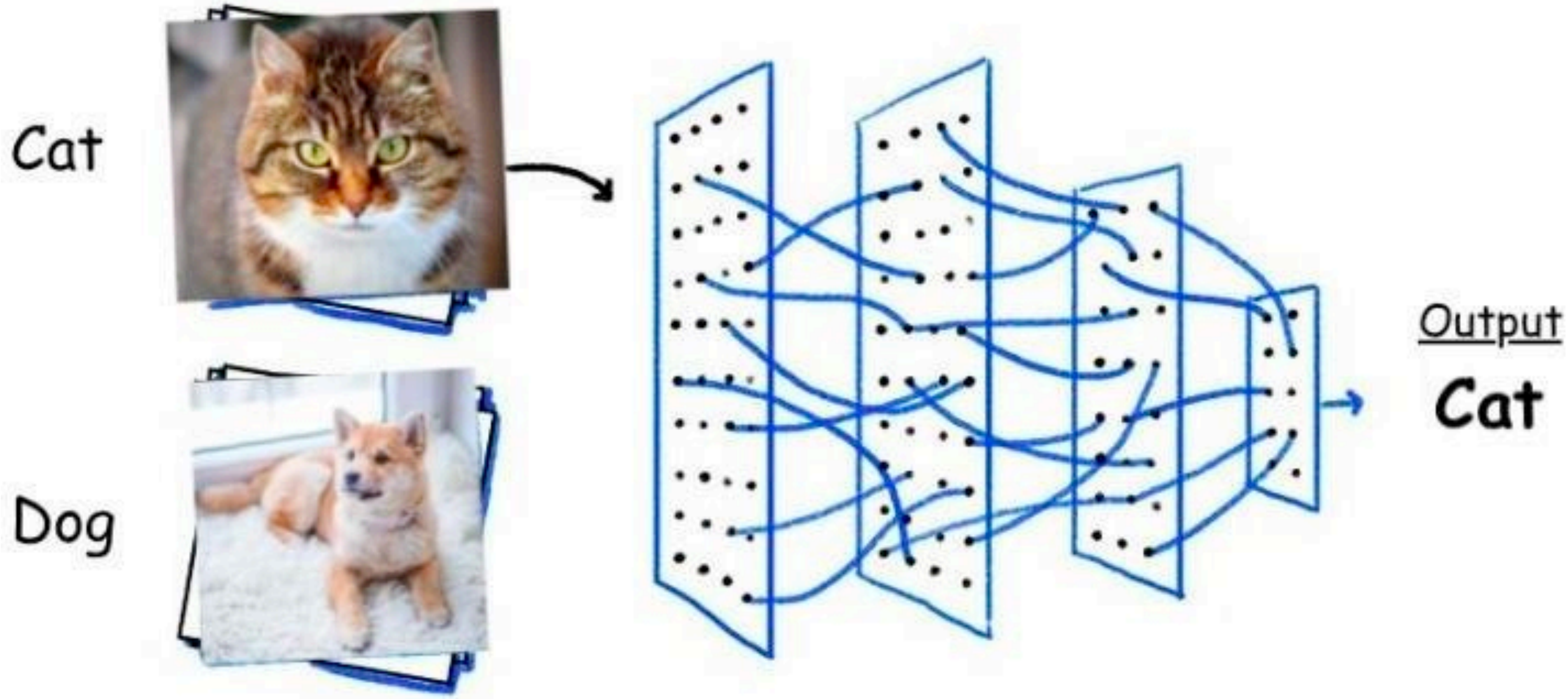


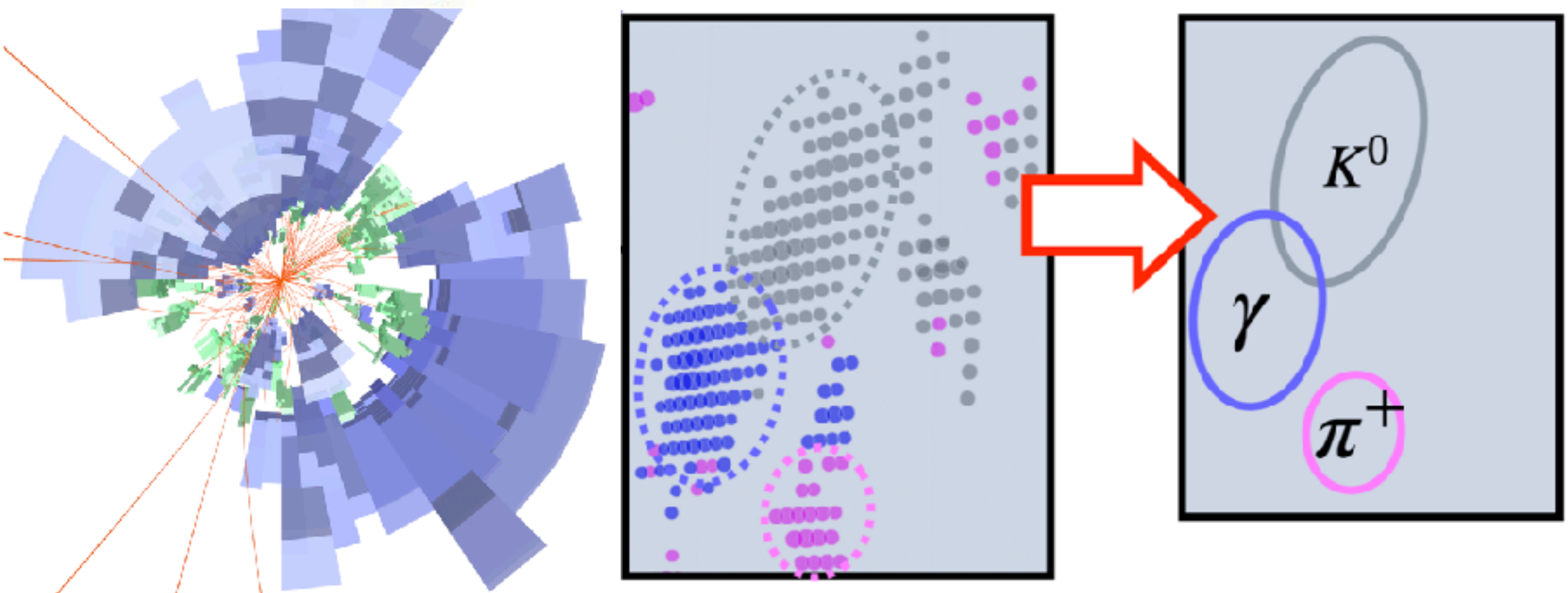
Infer the **set** of particles (reconstructed output) which produced the **set** of energy deposits in detector (cells and tracks)

Challenges:

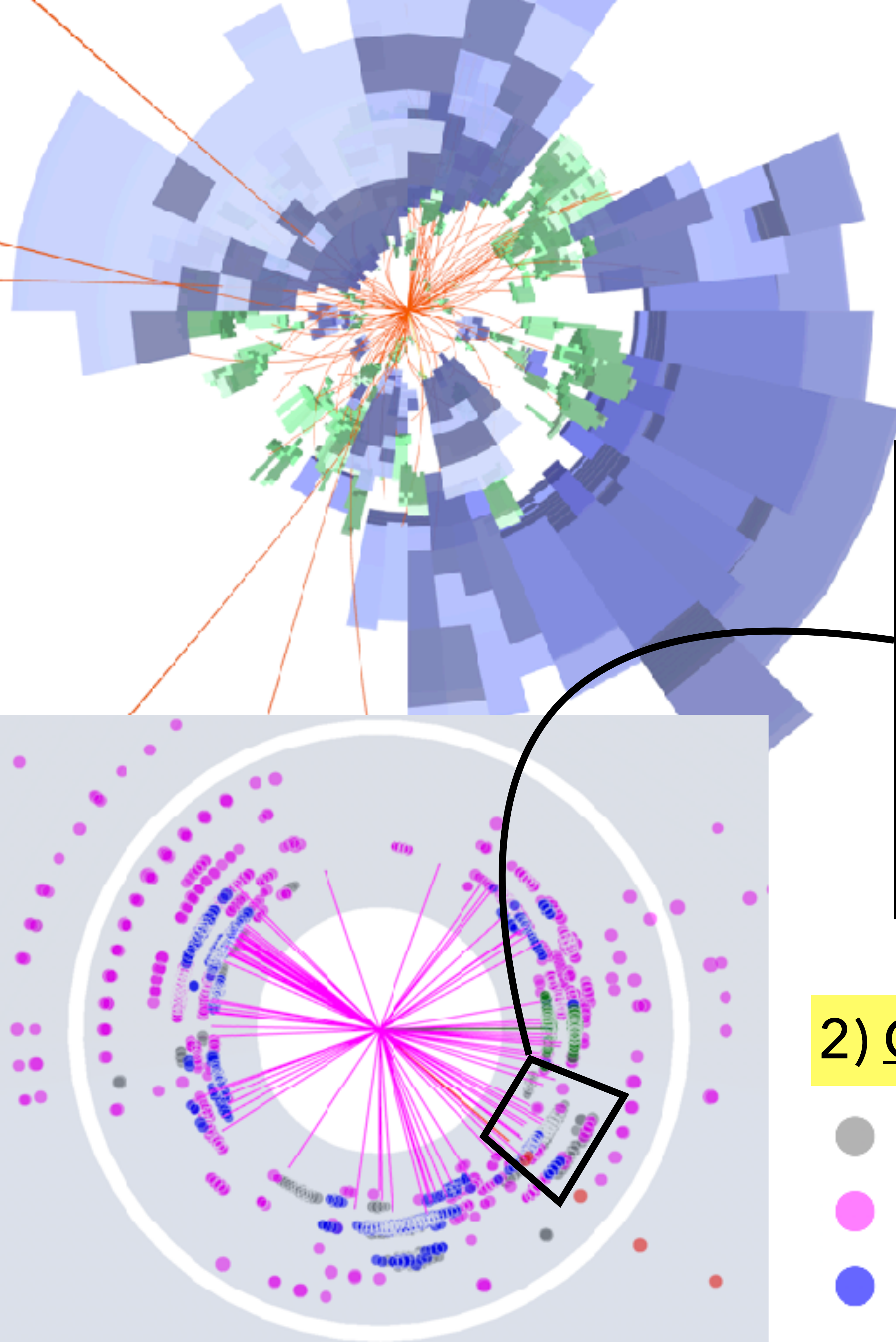
- Physical overlap (due to collimated particles and pileup)
- Feature overlap between different particle signatures (e.g. energy deposits)
- Dimensionality of data and complexity of 3D spatial correlations

Cats & Dogs Classification is a Piece of Cake

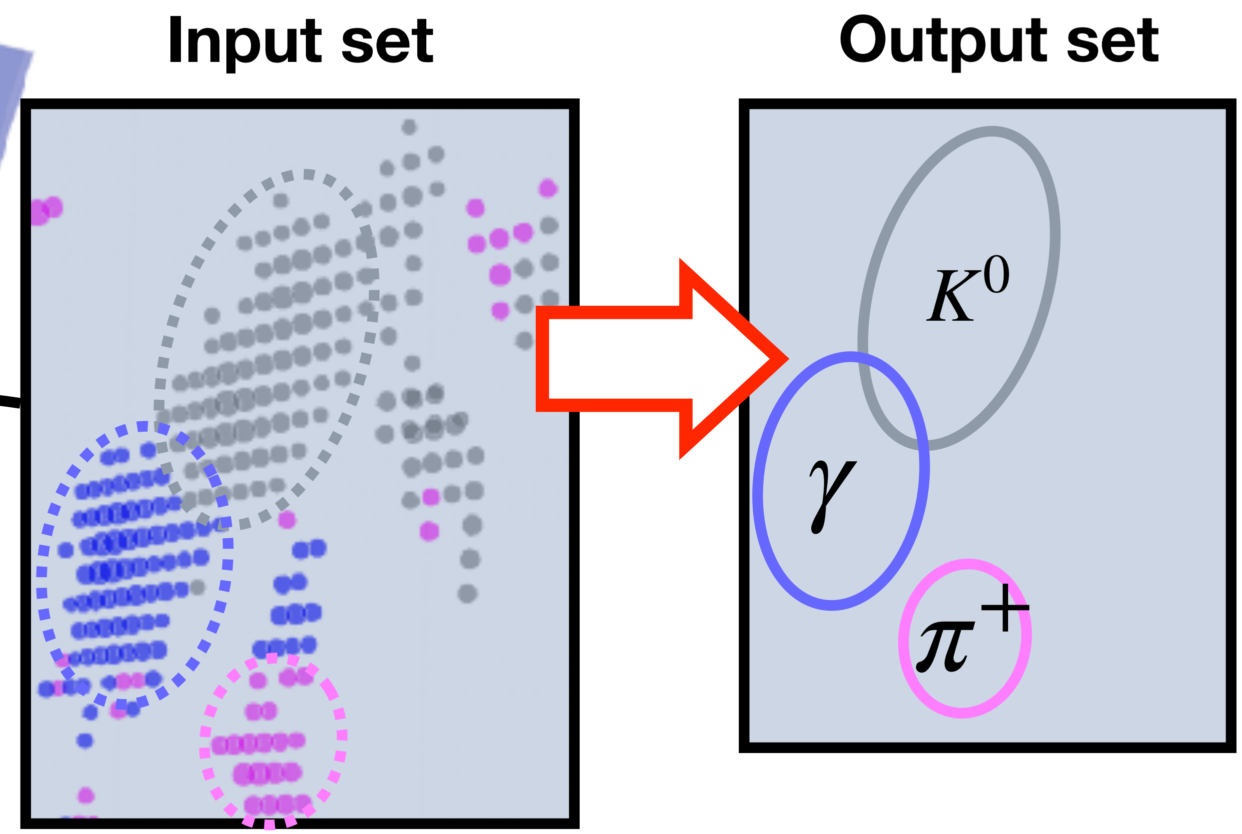




Particle reco. set-to-set task



1) Reconstruct particles (cardinality)

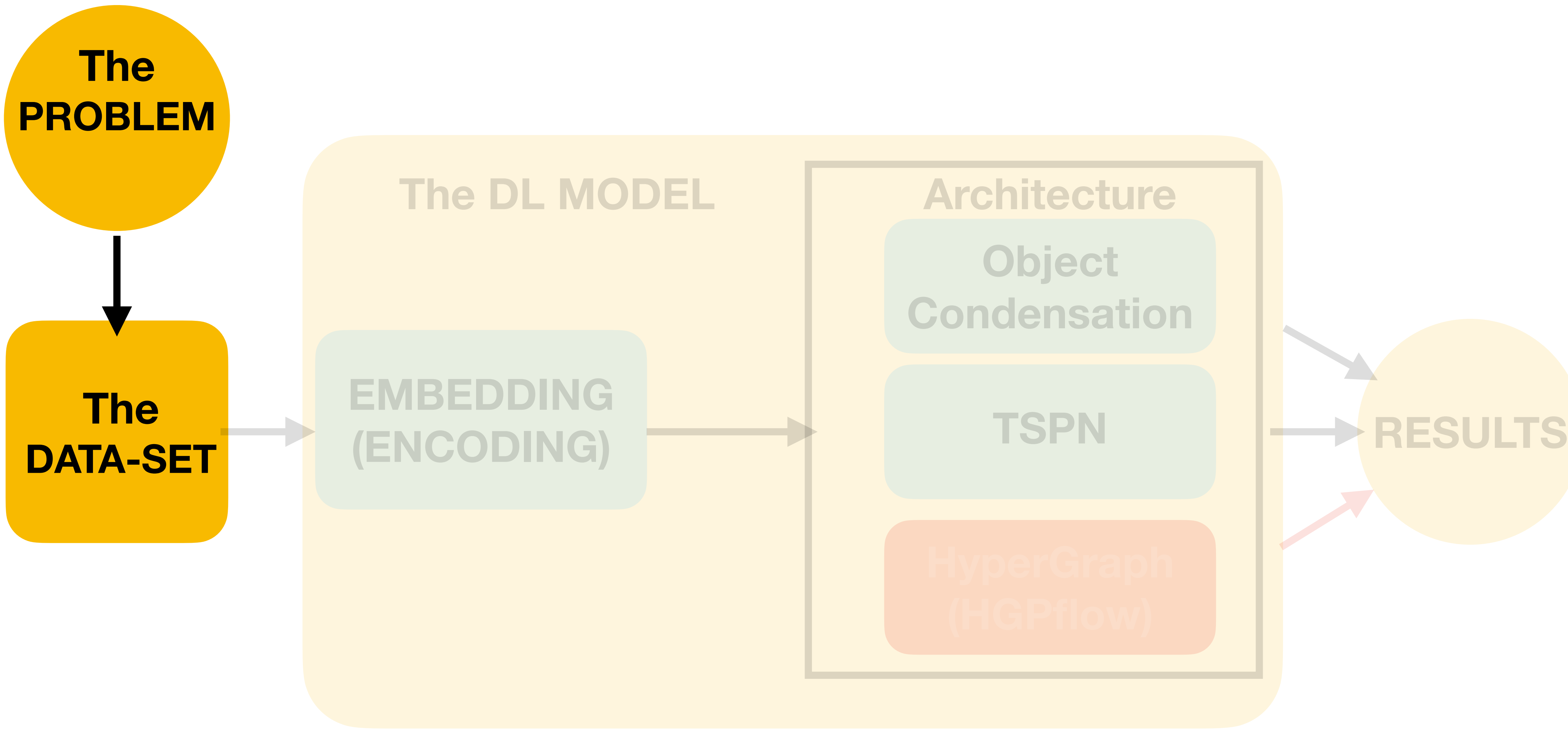


2) Classify them

- neutral had.,
- charged had.,
- photon,

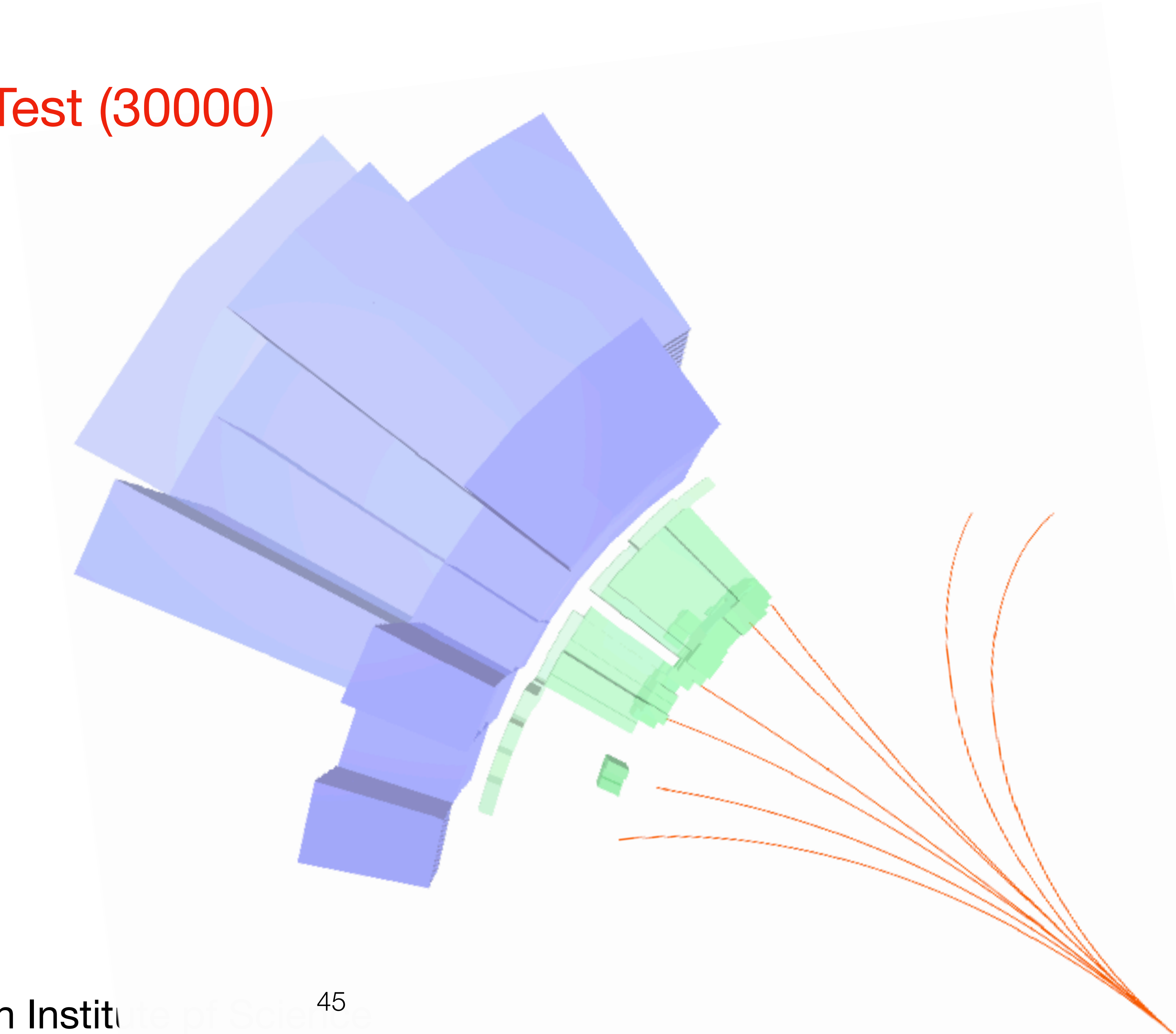
3) Regress their properties

- ✓ Direction (η, ϕ)
- ✓ Momentum (p_{T})


The PROBLEM
The DATA-SET
The DL MODEL
EMBEDDING (ENCODING)
Architecture
Object Condensation
TSPN
HyperGraph (HGPflow)
RESULTS

The Data Set

- Single Light Jets
- Train (50000) Test (30000)



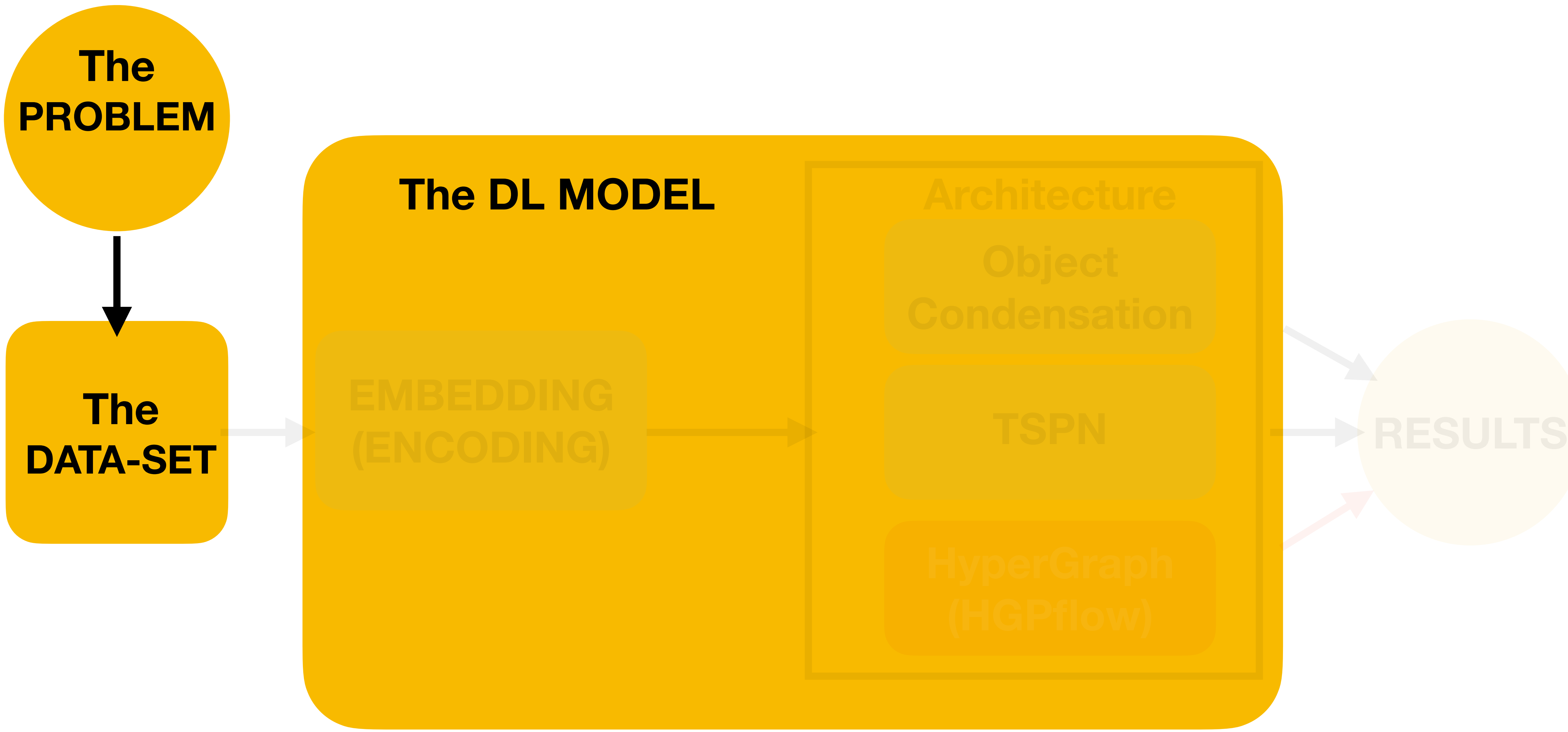
Diving into Deep Learning

The PROBLEM

The DATA-SET

RESULTS

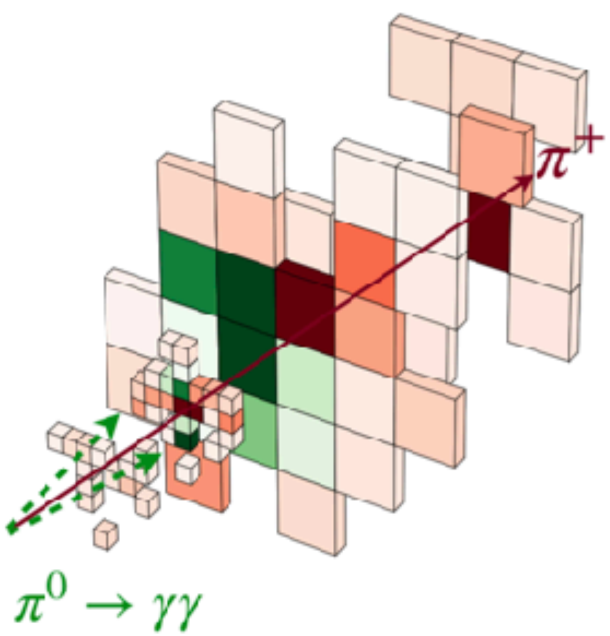
Diving into Deep Learning

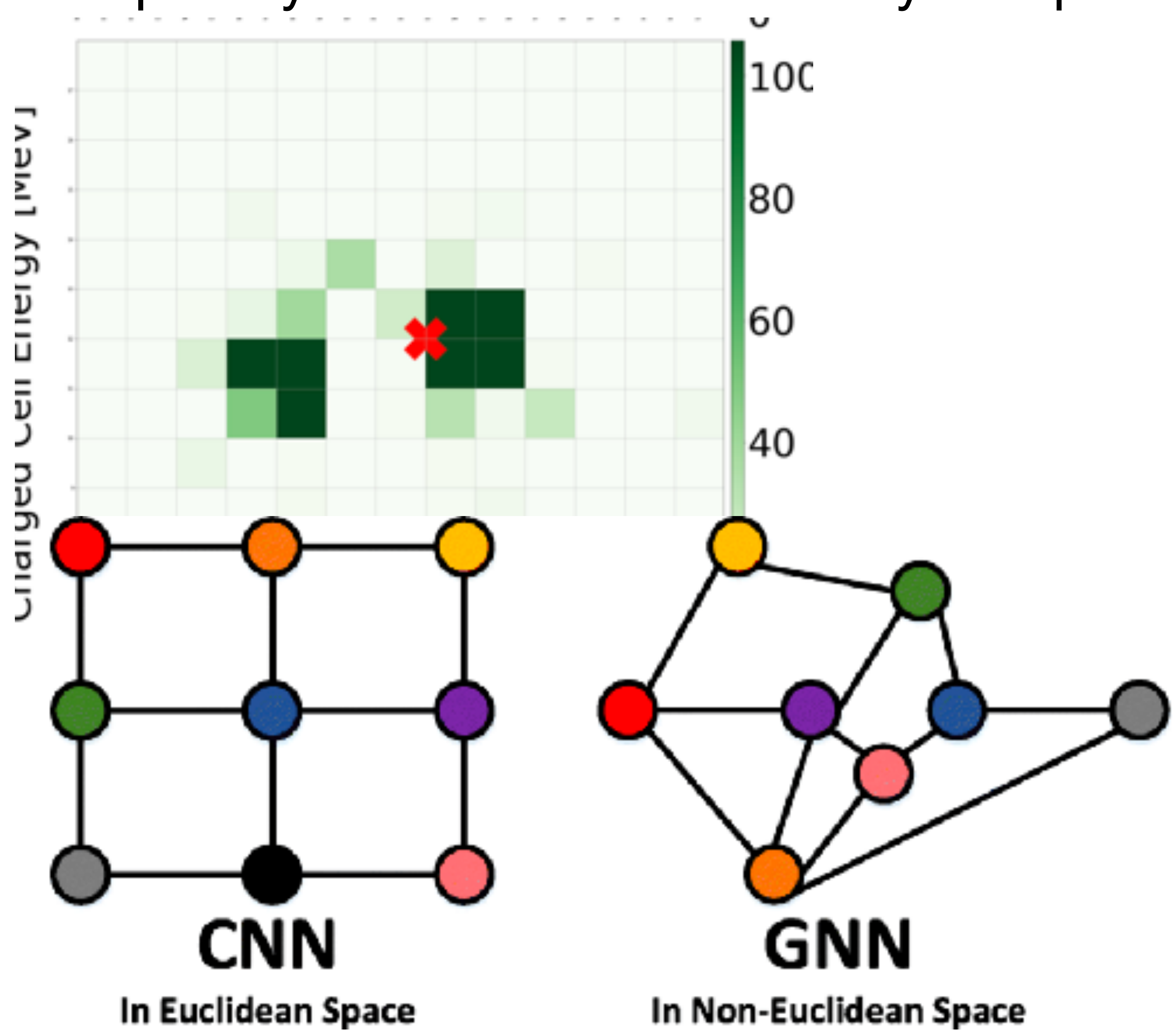


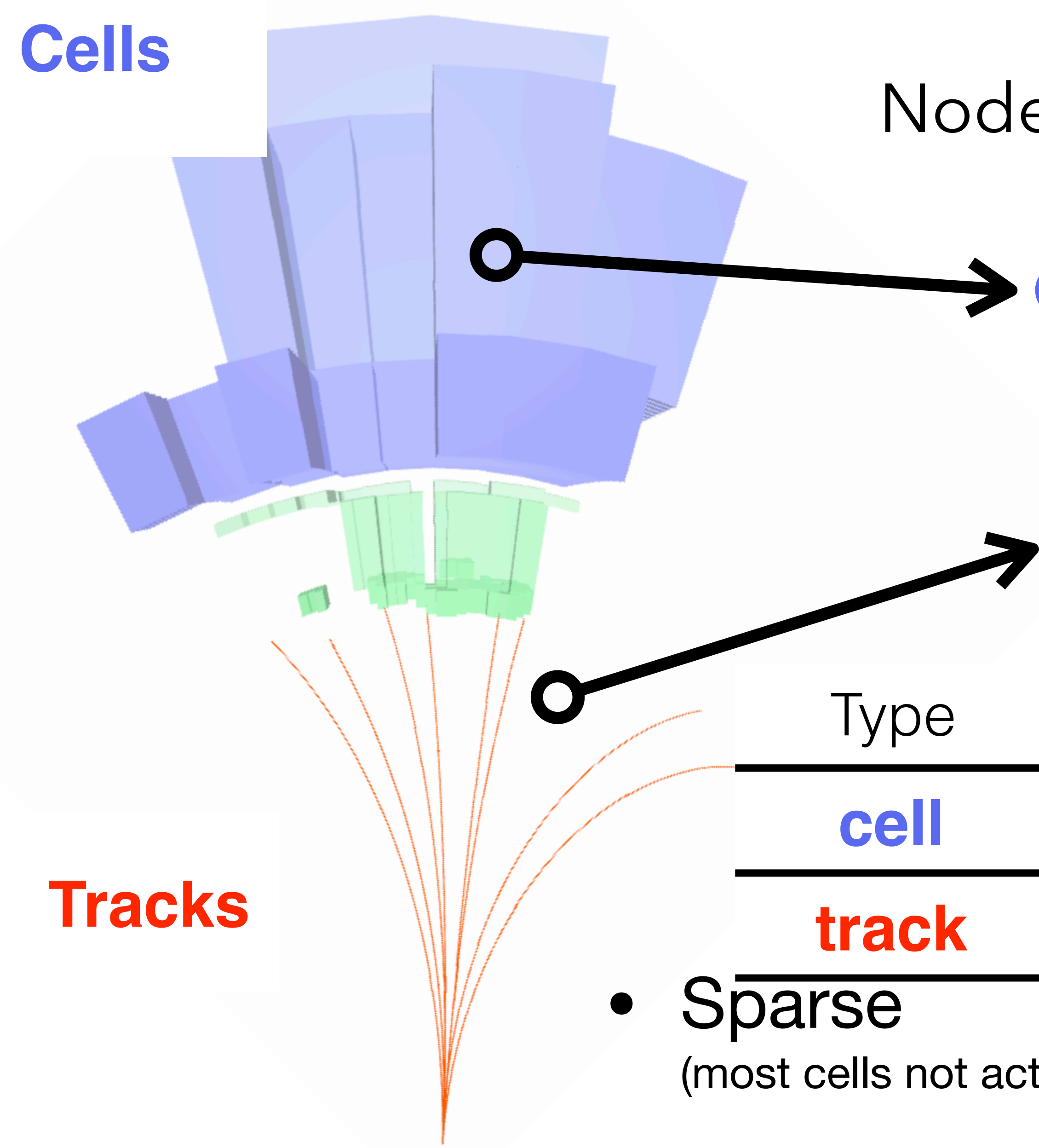
Graph vs Convolutional NN

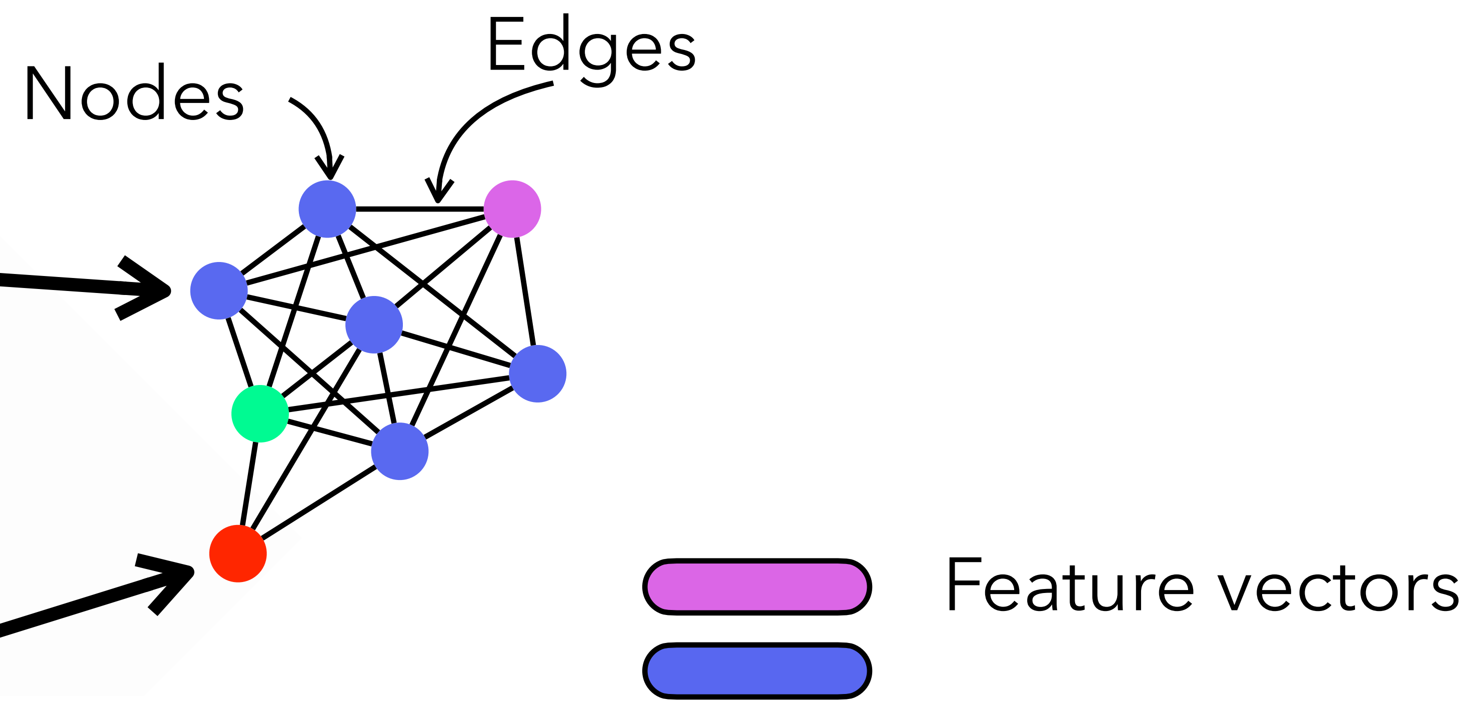
- CNNs are specially built to operate on regular (Euclidean) structured data, while in GNNs the numbers of nodes connections vary and the nodes are unordered.

- Graphs capture spatial correlations encoded in irregular detector geometry and well suited to the sparsity and variable cardinality of input set.







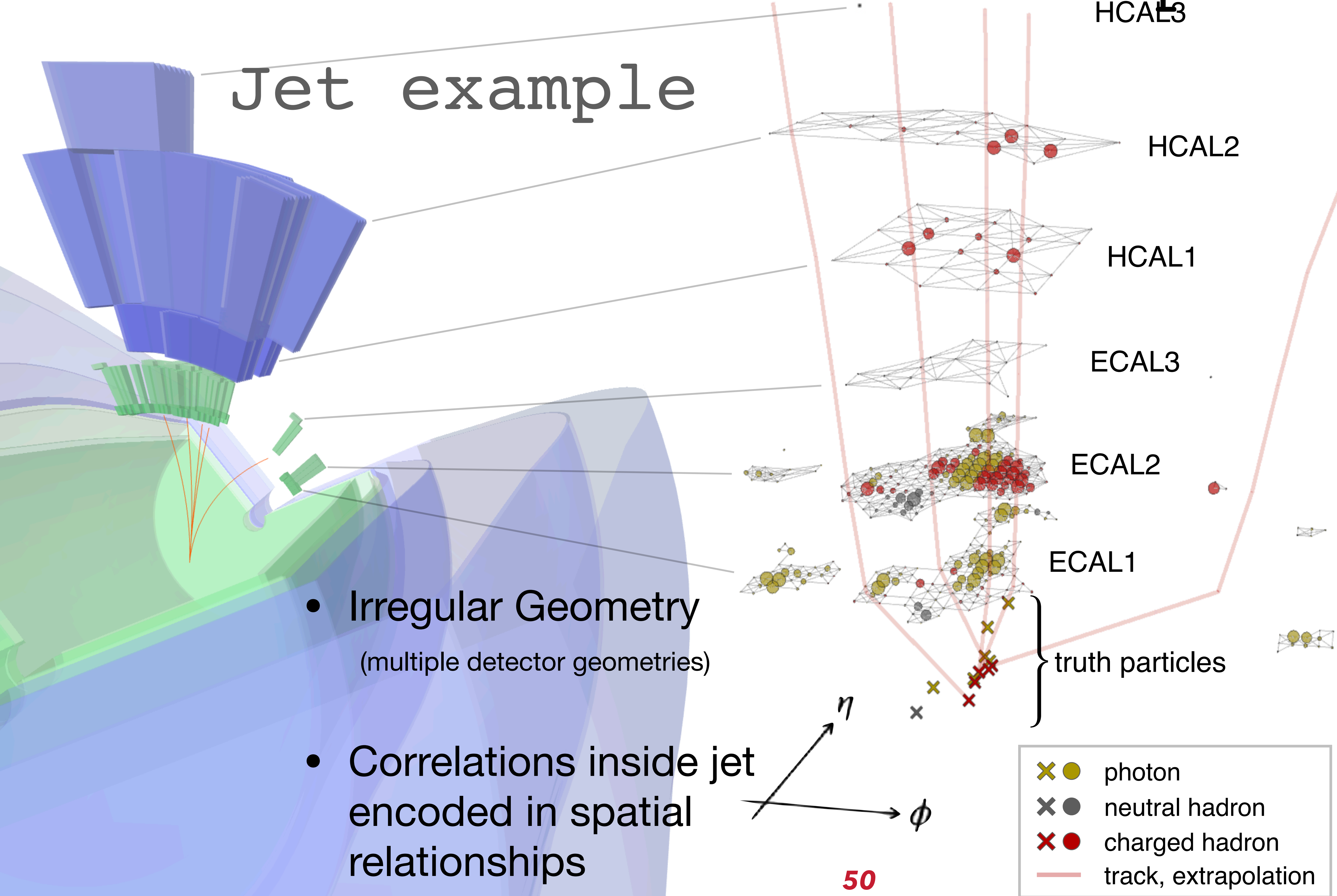


Type	Spatial	Kinematic
cell	x, y, z, η, ϕ, layer	E
track	$d_0, z_0, \{\eta, \phi\}_{\text{pv,extrapolated}}$	$p_T, q/p$

- Sparse
  (most cells not activated)
- Set-to-Set
  (reconstructed-to-particles)
- Equivariant
  (permute input nodes should not affect the conclusion)

Detector Readout as a Graph

Jet example

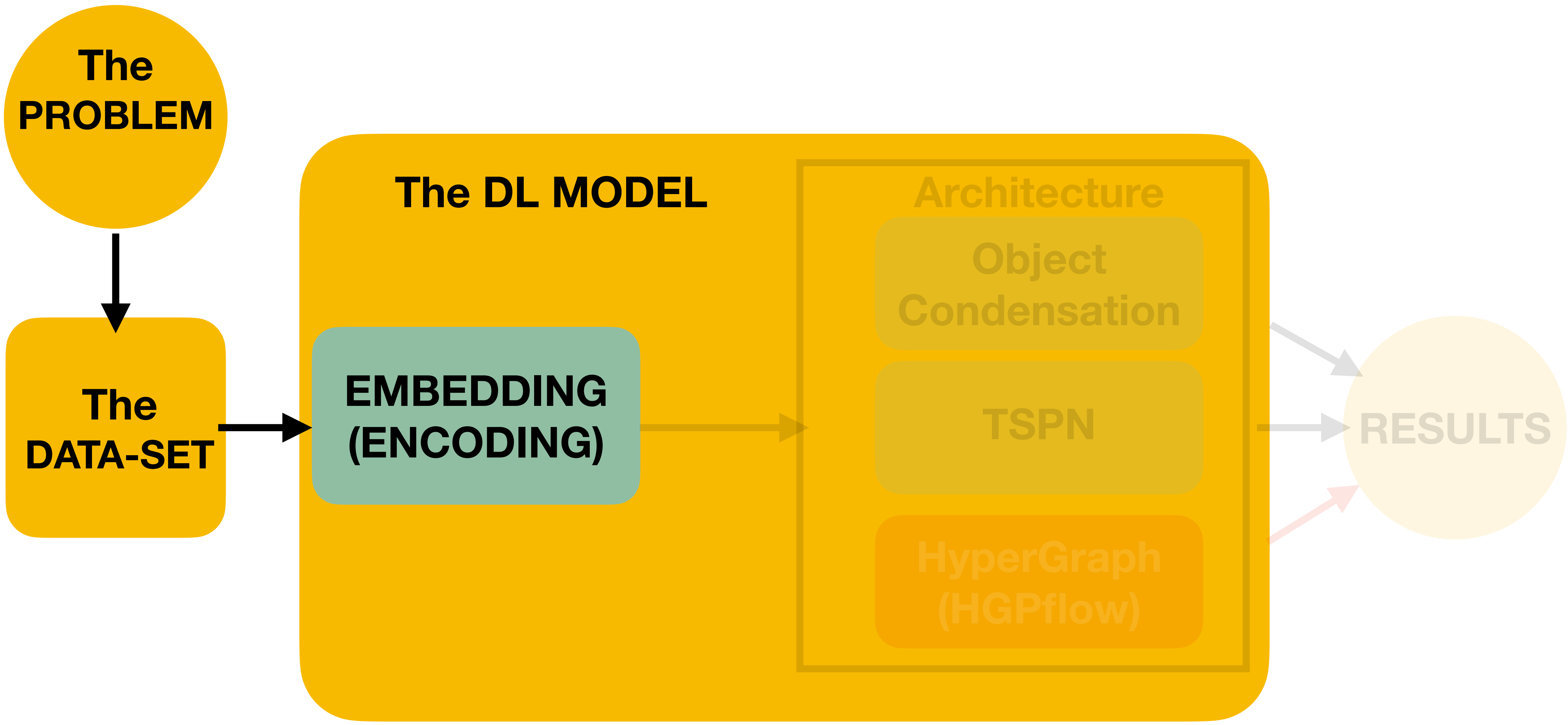


- Irregular Geometry

  (multiple detector geometries)

- Correlations inside jet encoded in spatial relationships

Diving into Deep Learning

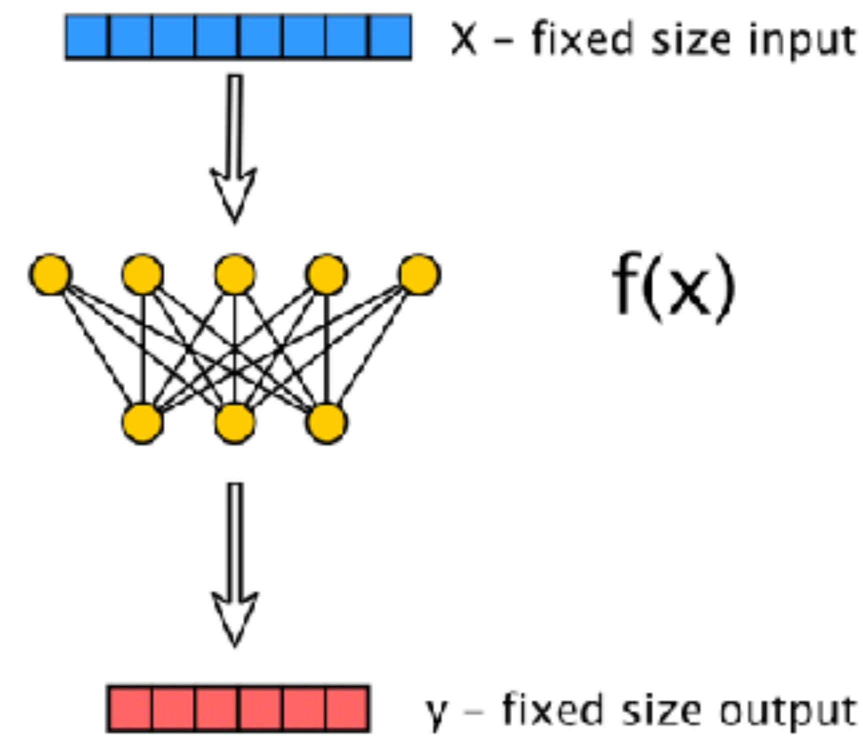


GRAPH NN 101

- MLP (Multi Layer Perceptron) [NN] is the basic building block which encodes features into the Deep Learning language

- It has a fixed-size of input and output

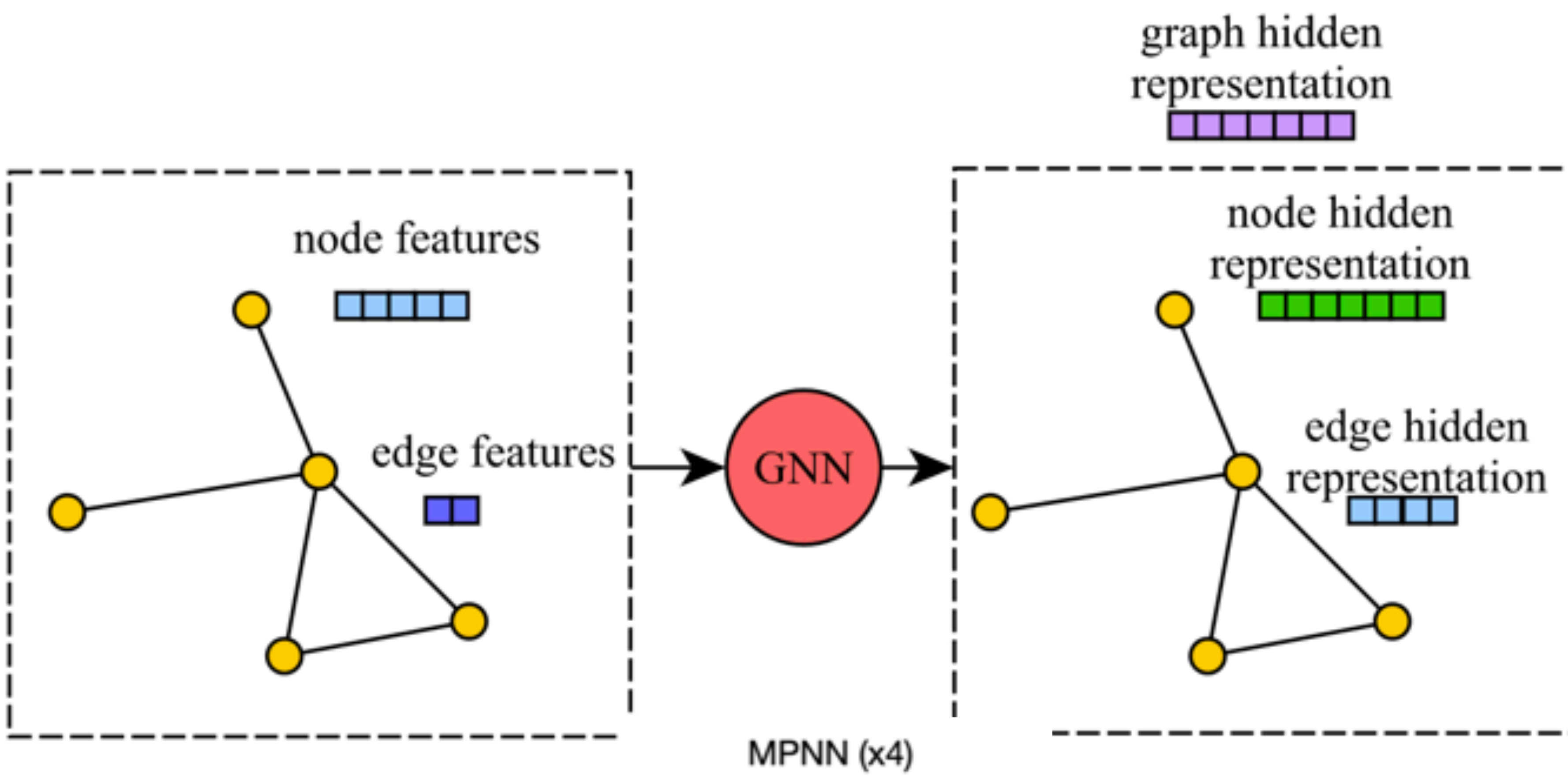
- This structure can, in theory, learn to approximate any function



GRAPH NN 101

- MLP (Multi Layer Perceptron) [NN] is the basic into t
- It has input
- This appr

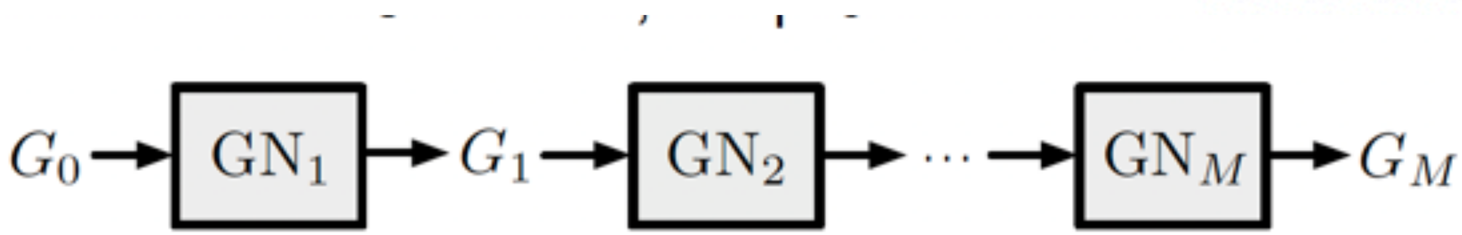
X – fixed size input

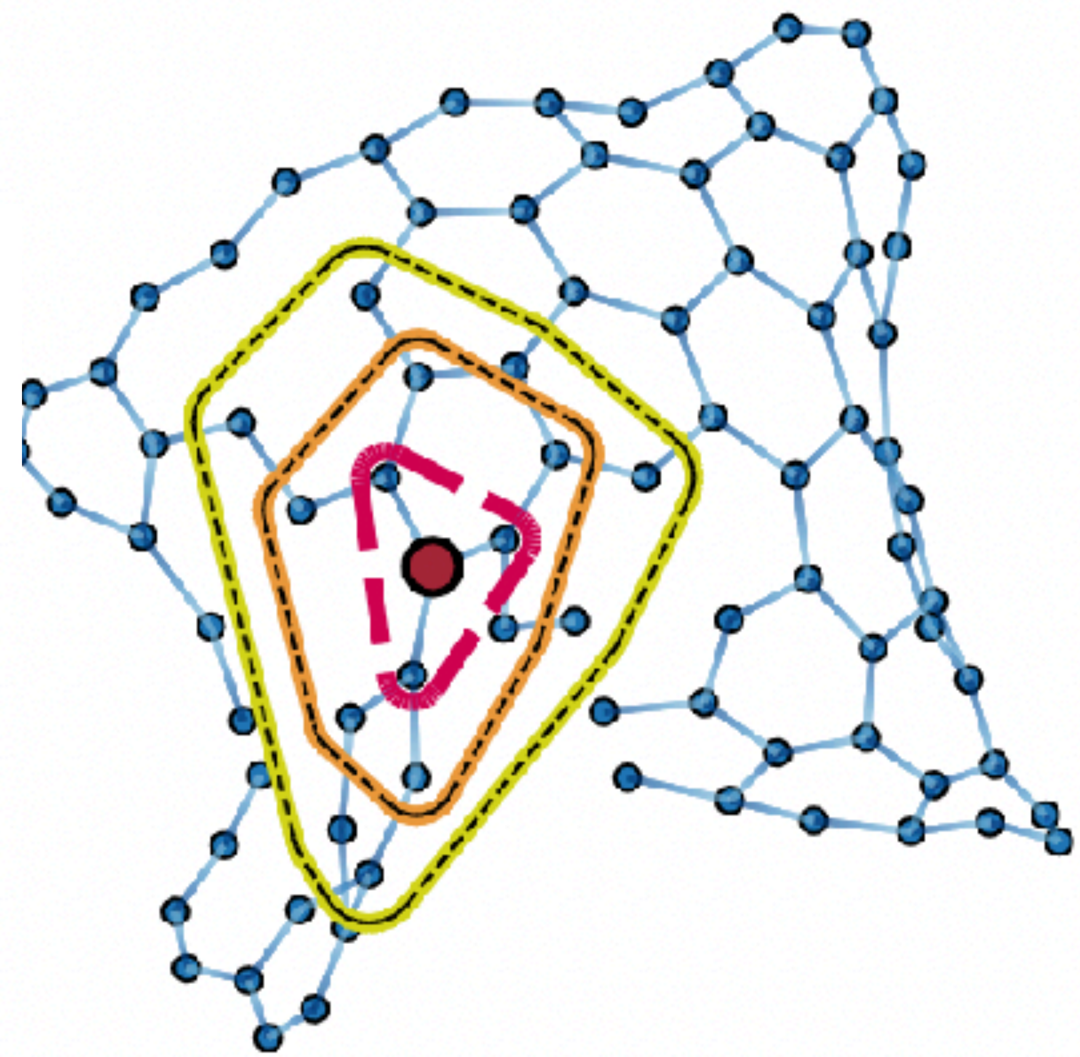


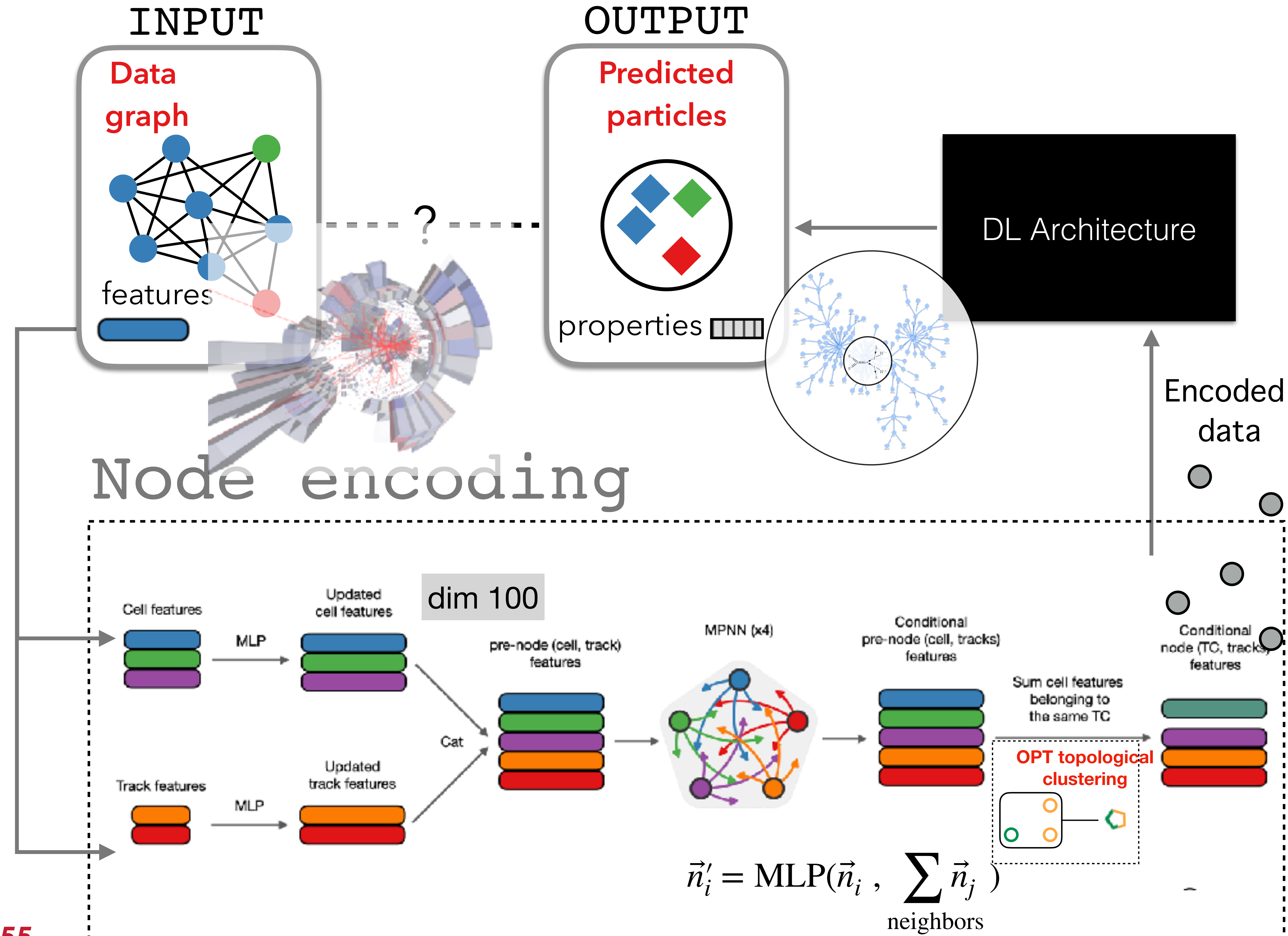
$$\vec{n}_i' = \mathrm{MLP}(\vec{n}_i\ ,\ \sum_{\text{neighbors}} \vec{n}_j\ )$$

Increasing the Receptive Field

- Stacking GN Blocks increases the receptive field of a node
- Each iteration communicates with a remoter circle of neighbors

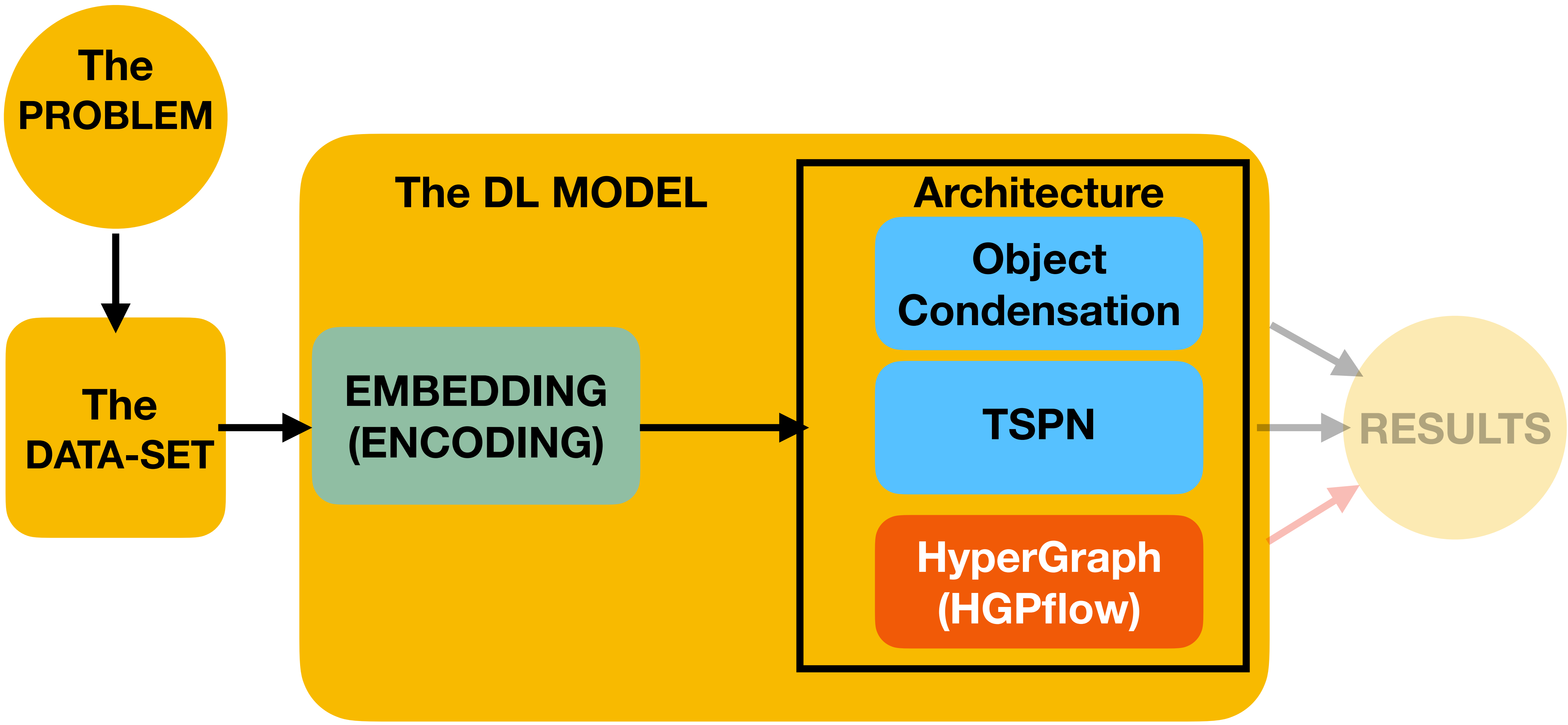




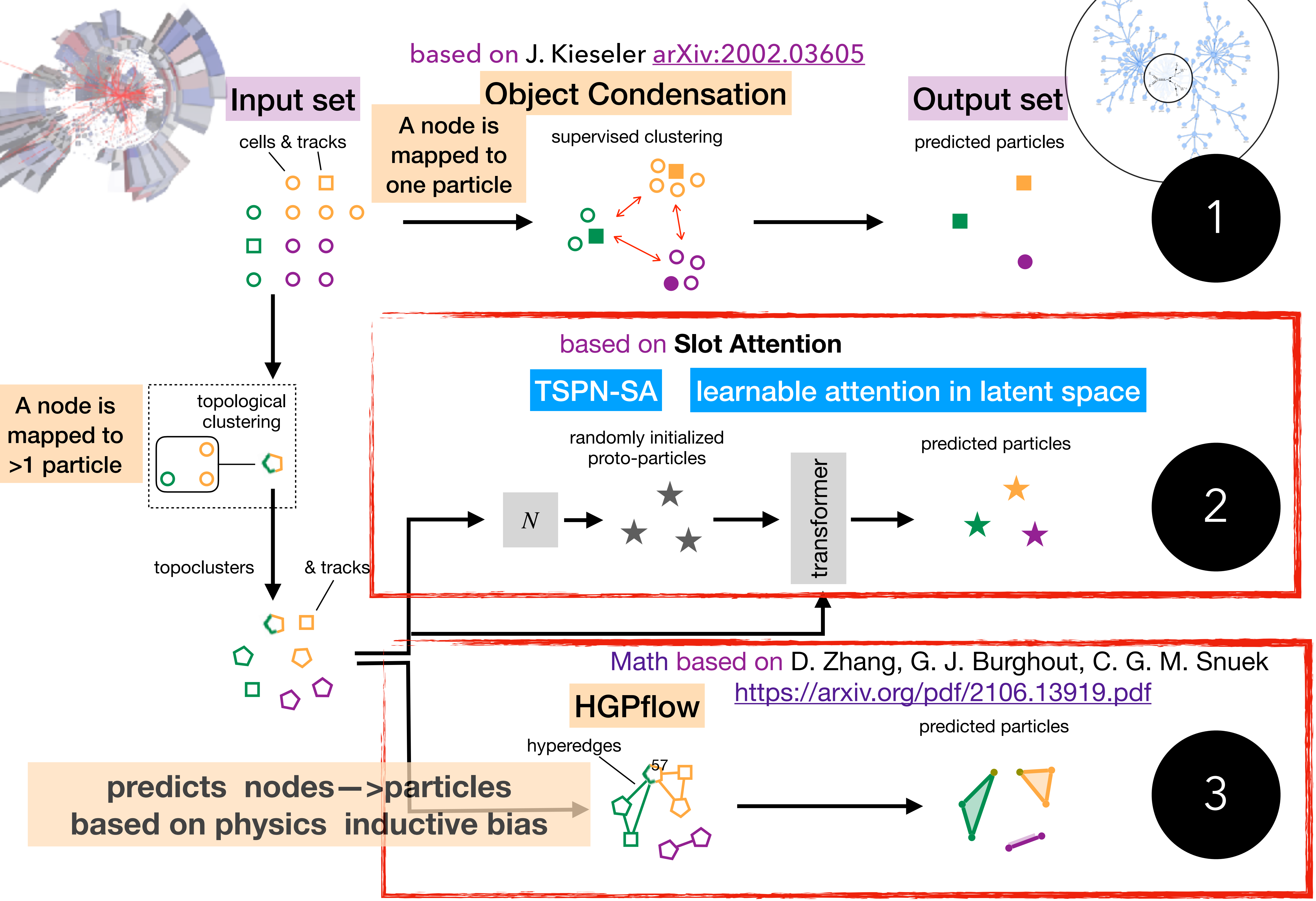


INPUT
Data graph
features
?
OUTPUT
Predicted particles
properties
DL Architecture
Encoded data
Node encoding
Cell features
MLP
Updated cell features
dim 100
Track features
MLP
Updated track features
Cat
pre-node (cell, track) features
MPNN (x4)
Conditional pre-node (cell, tracks) features
Sum cell features belonging to the same TC
OPT topological clustering
Conditional node (TC, tracks) features
$\vec{n}_i' = \mathrm{MLP}(\vec{n}_i\ ,\ \sum_{\text{neighbors}} \vec{n}_j\ )$

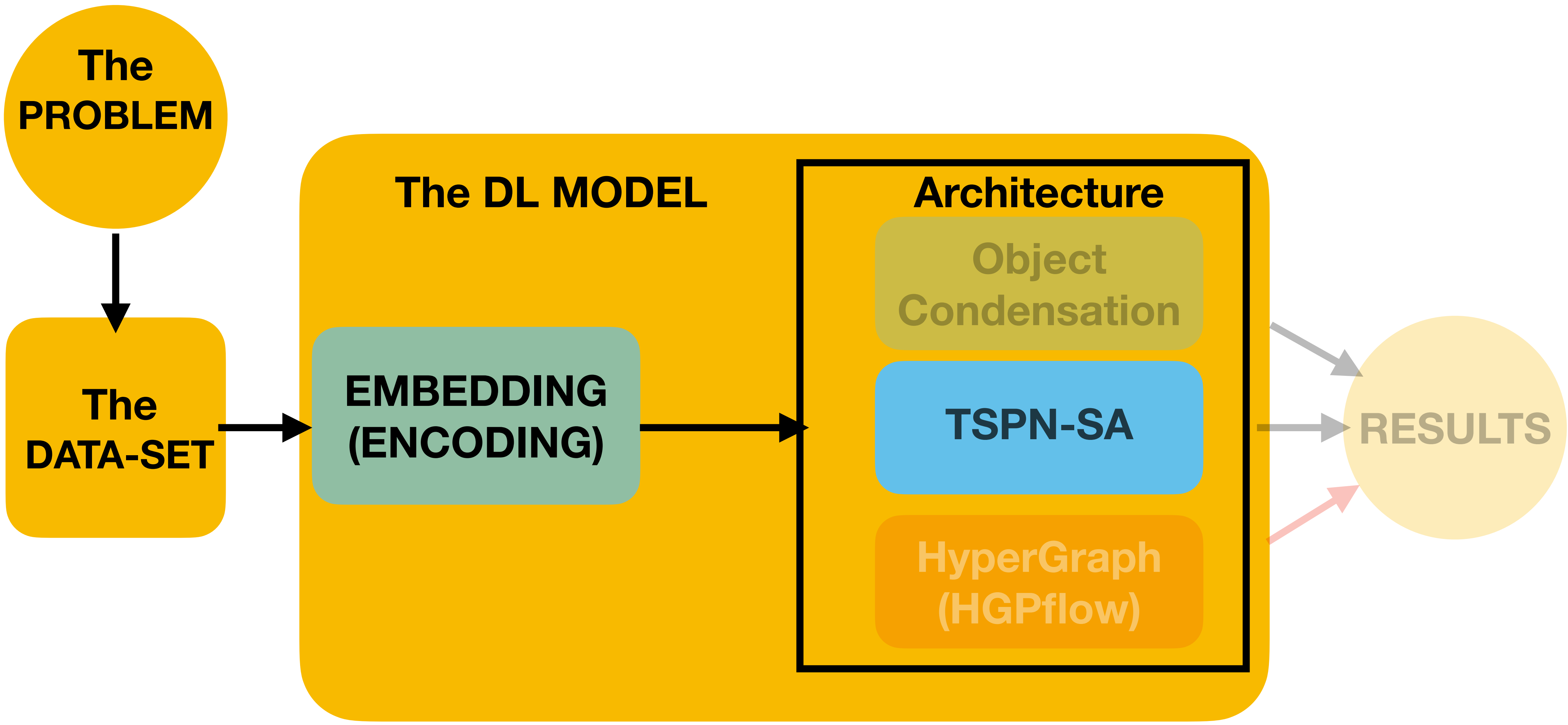
Diving into Deep Learning



Going from (many) nodes to (few) particles

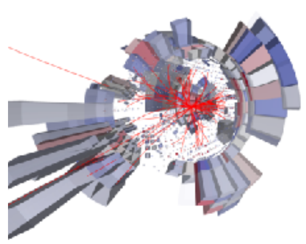


Diving into Deep Learning

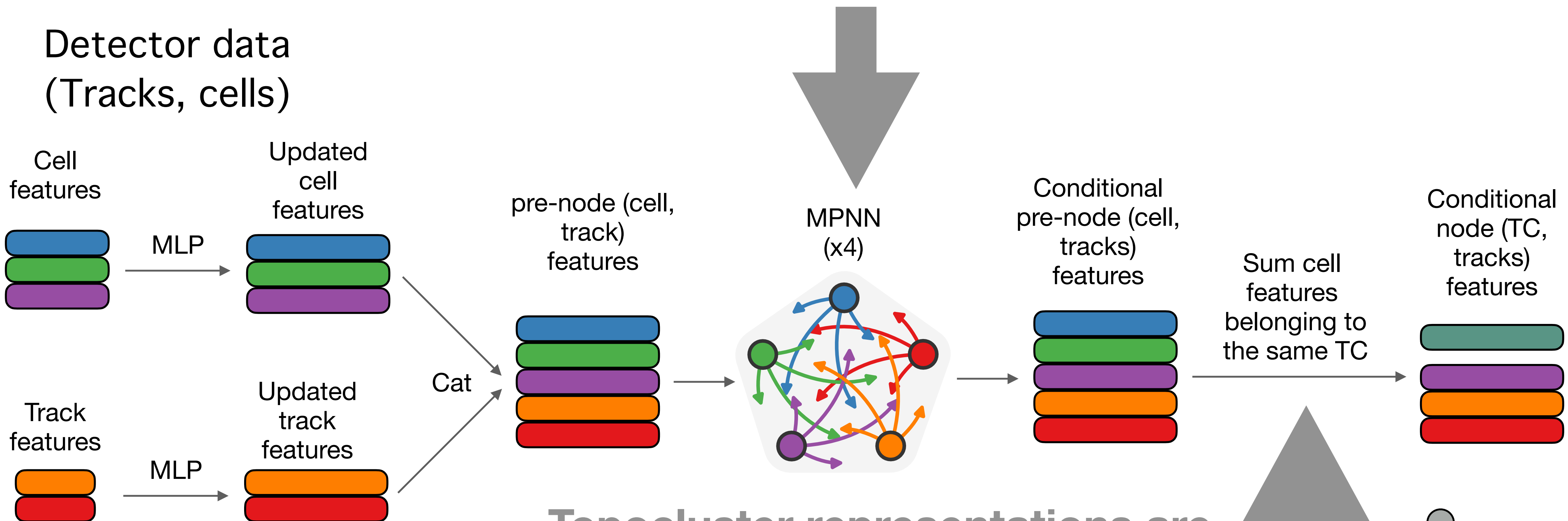


Embedding the DATA

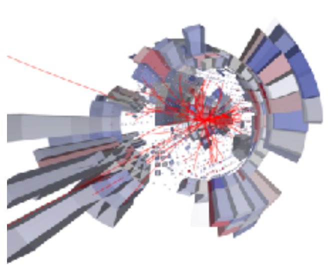
The node encodings are updated to incorporate the graph relational structure via 4 successive blocks of message passing along edges.



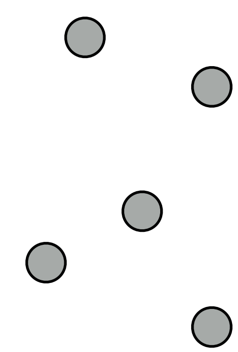
Detector data
(Tracks, cells)



Detector readout

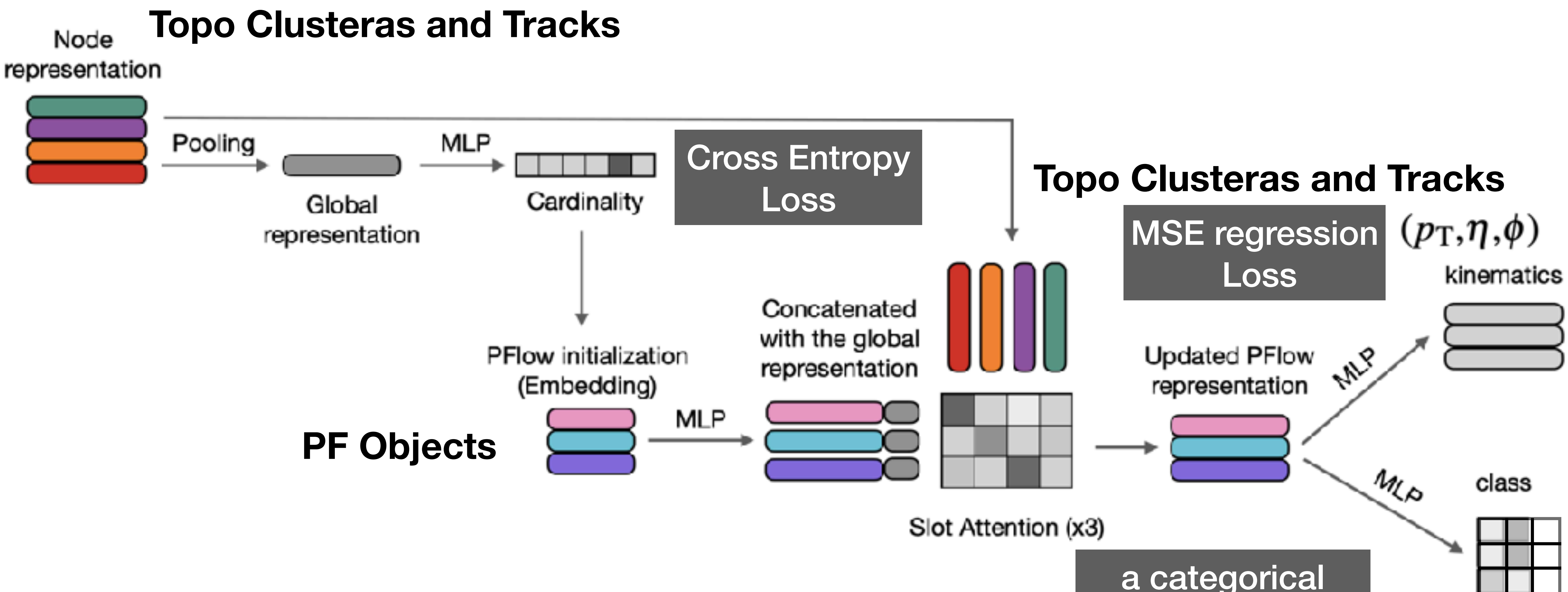


Topocluster representations are computed by the energy-weighted mean of the cell representation vectors belonging to the topocluster.



Encoded data

Slot Attention



a categorical crossentropy (CE) Loss

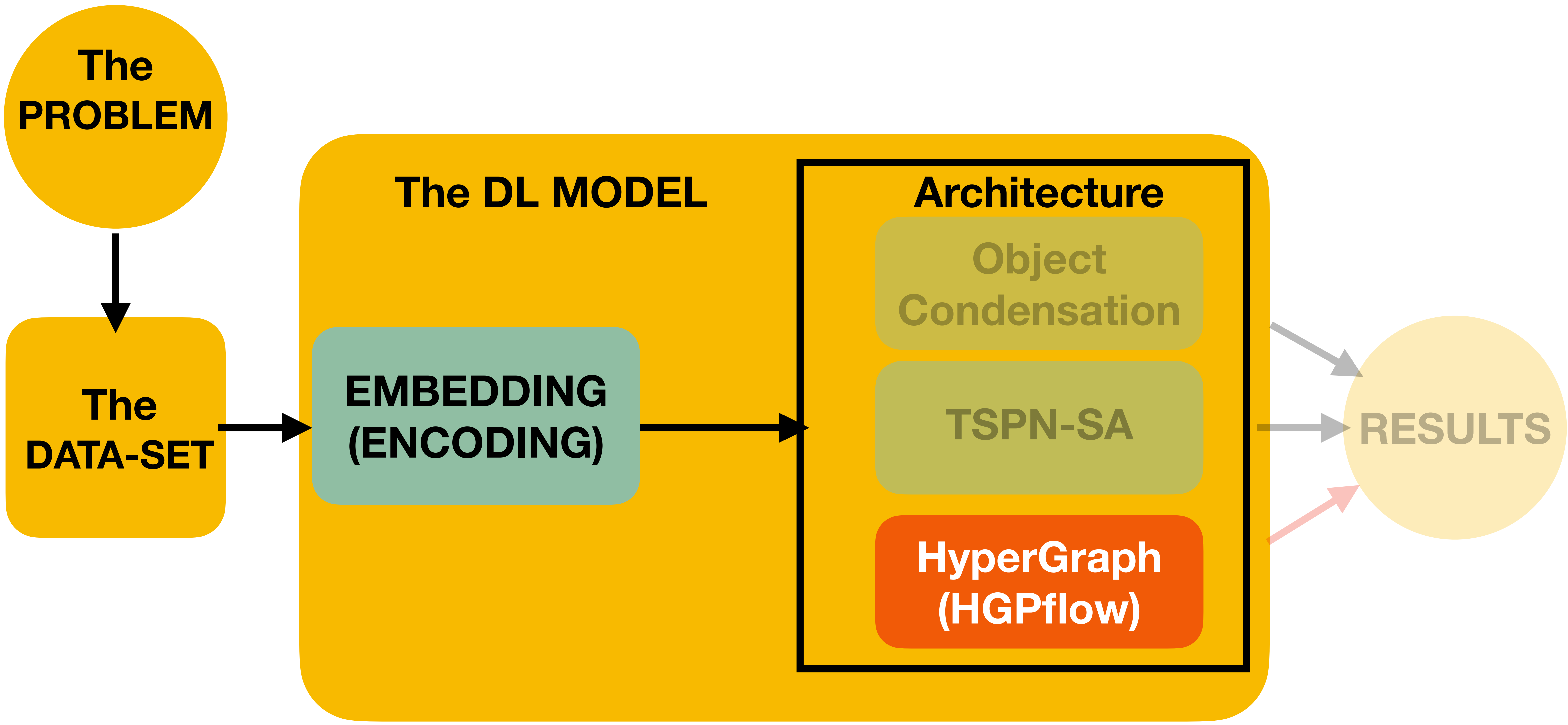
3 Classes:

Charged Particles (e, μ, π^+)
Photons
Neutral Hadrons

easy to tell electrons and muons,
jets contain <5% leptons, mostly pions

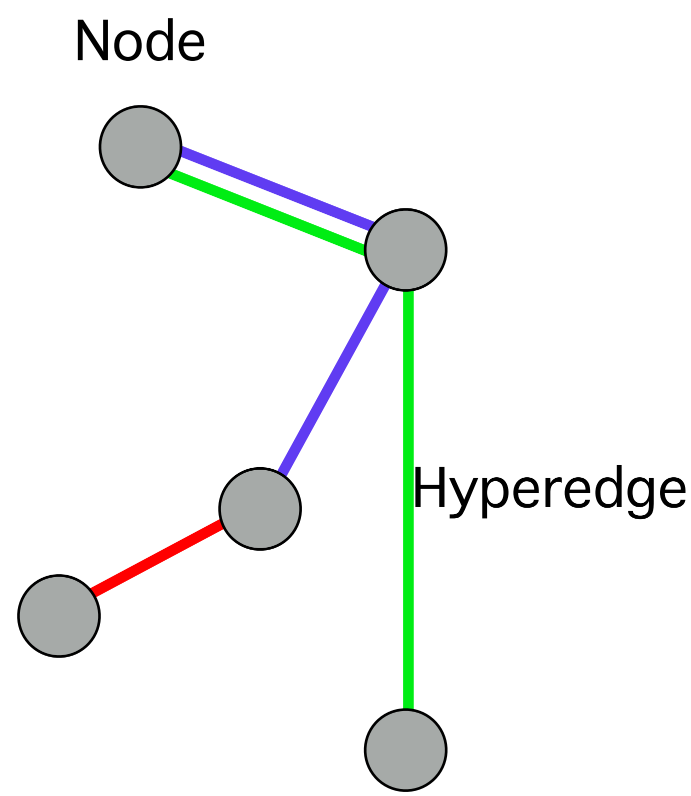
Performance: Later

Diving into Deep Learning



Hypergraph 101

A hypergraph is a generalization of a graph where hyperedges can each connect one, two, or multiple nodes



Hypergraph

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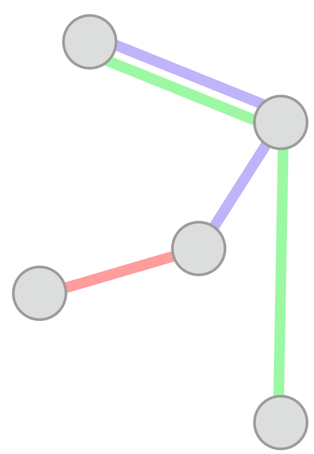
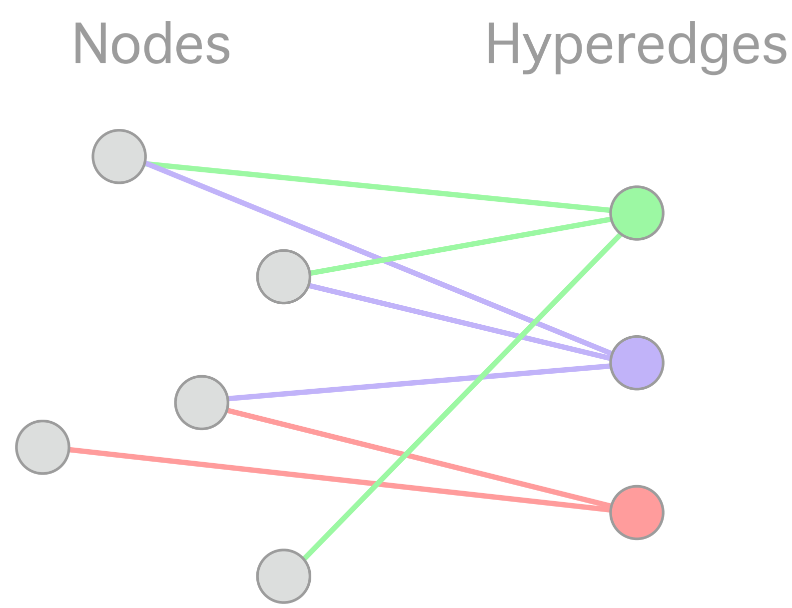
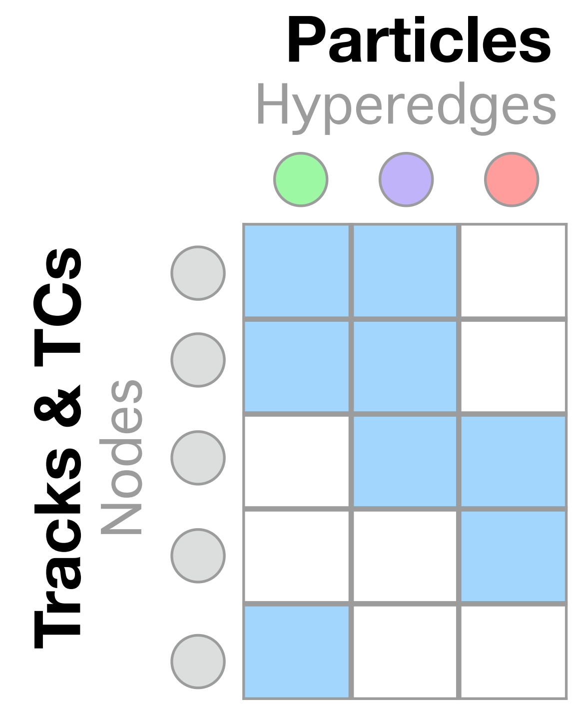
Hypergraph 101



Hypergraph



Bipartite graph



Incidence matrix

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

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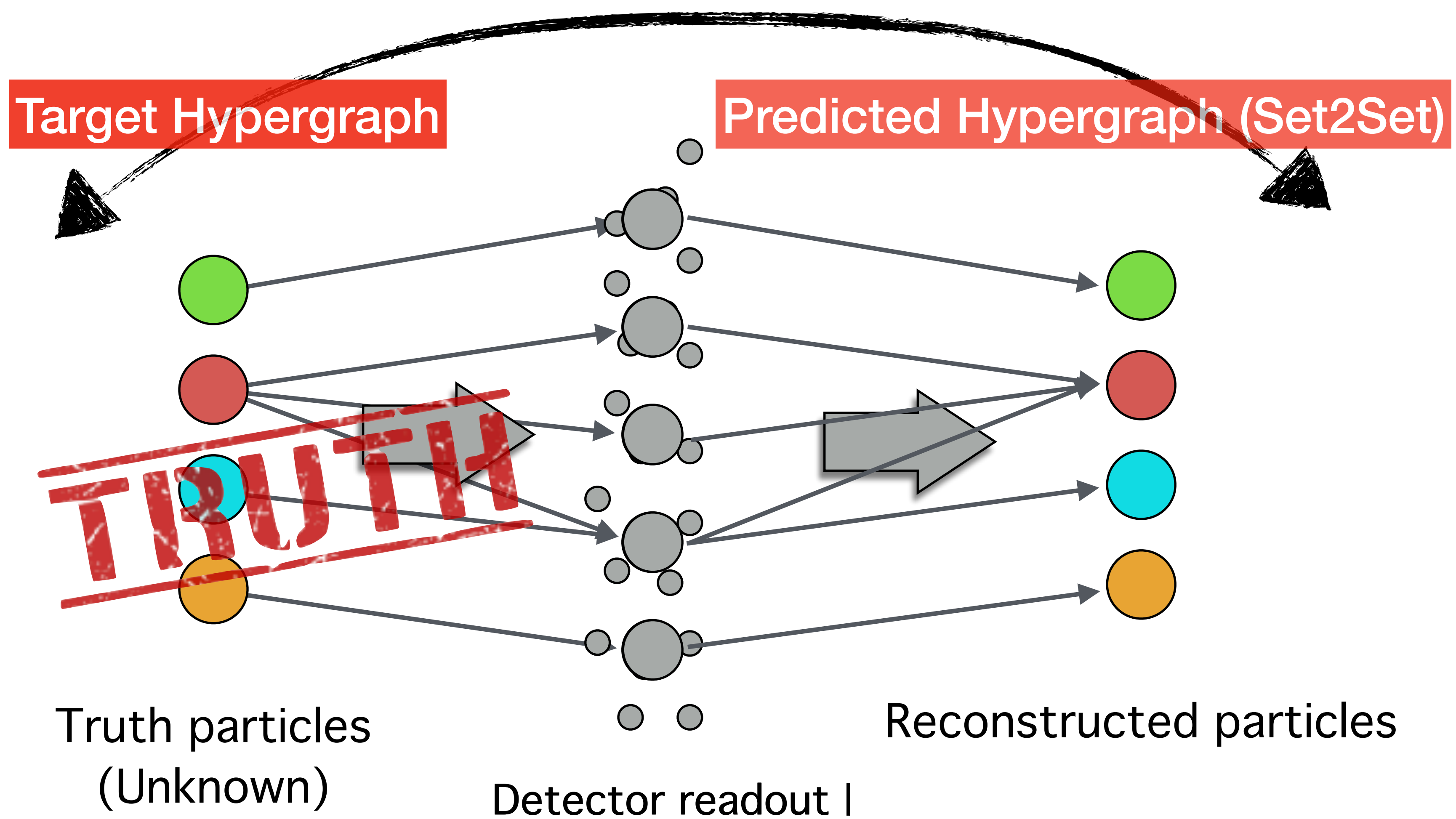
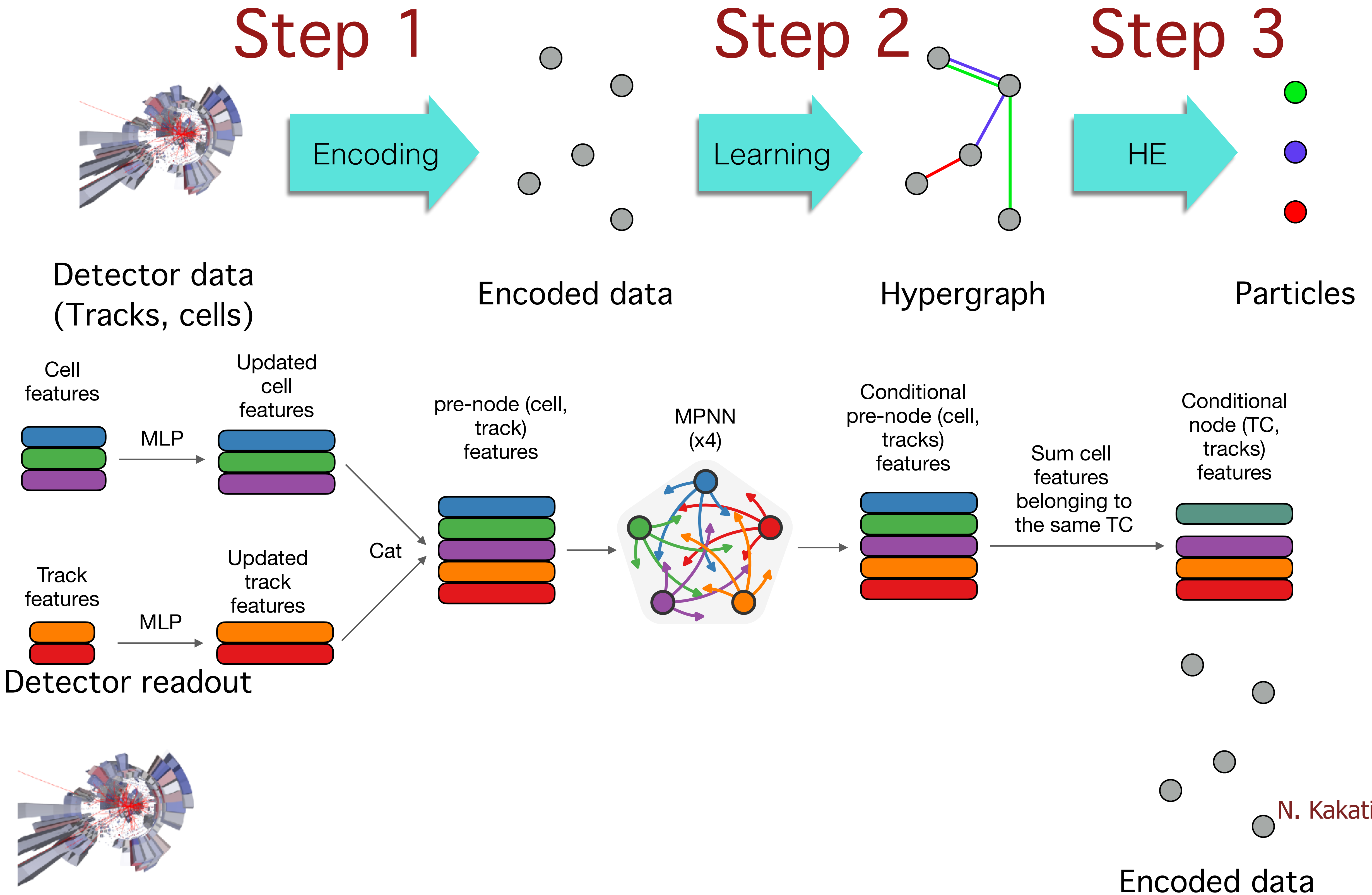
Why HypergGraphs

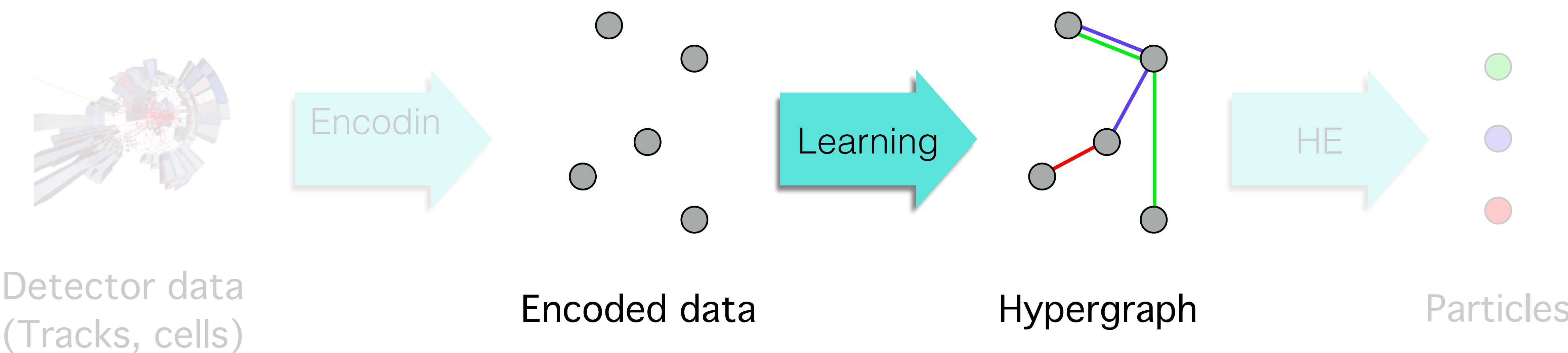
- Particle Flow = Learning a Hypergraph
- Physics Interpretability (next)



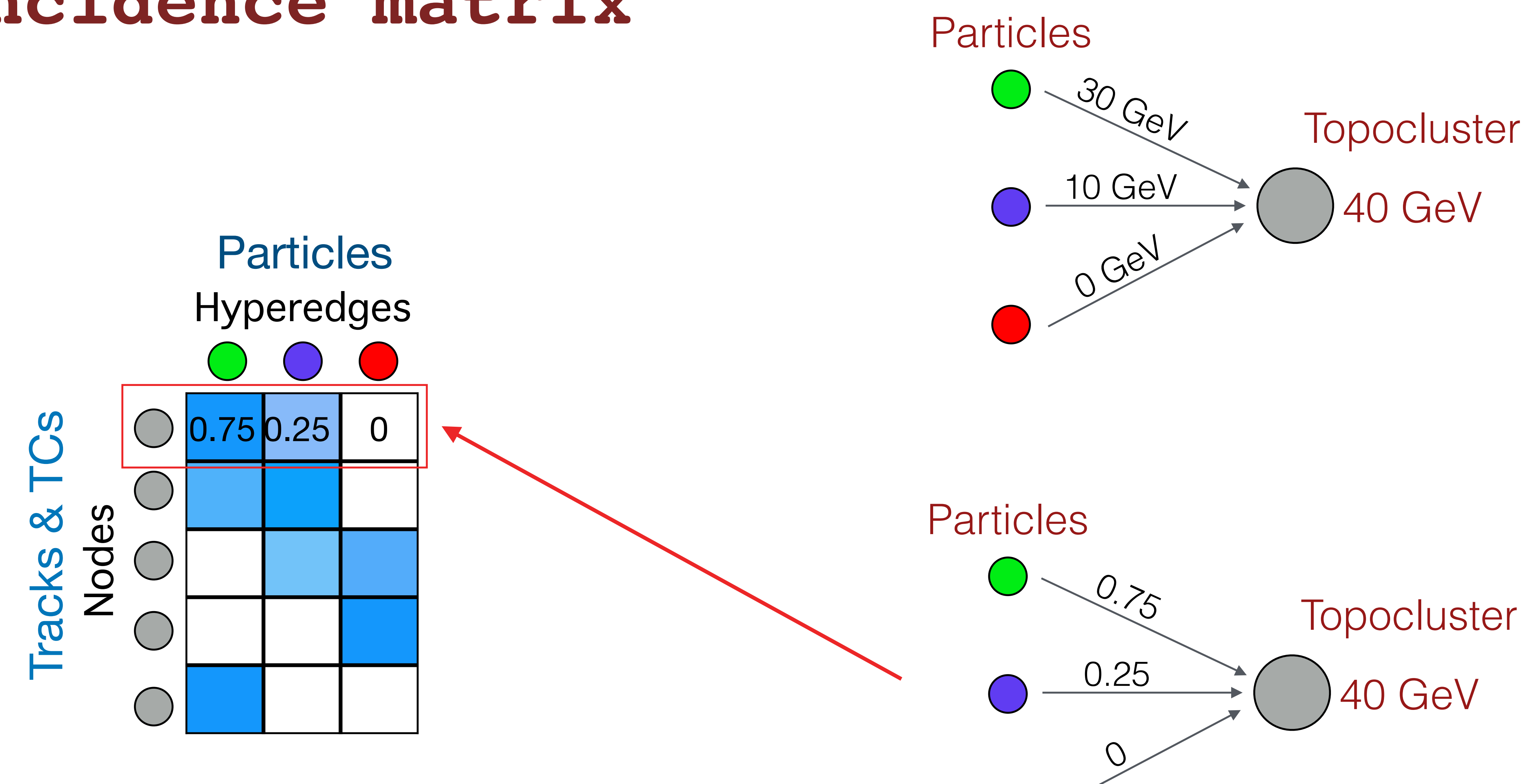
The overall plan



Step 2


Encodin
Learning
HE
Detector data (Tracks, cells)
Encoded data
Hypergraph
Particles

Incidence matrix



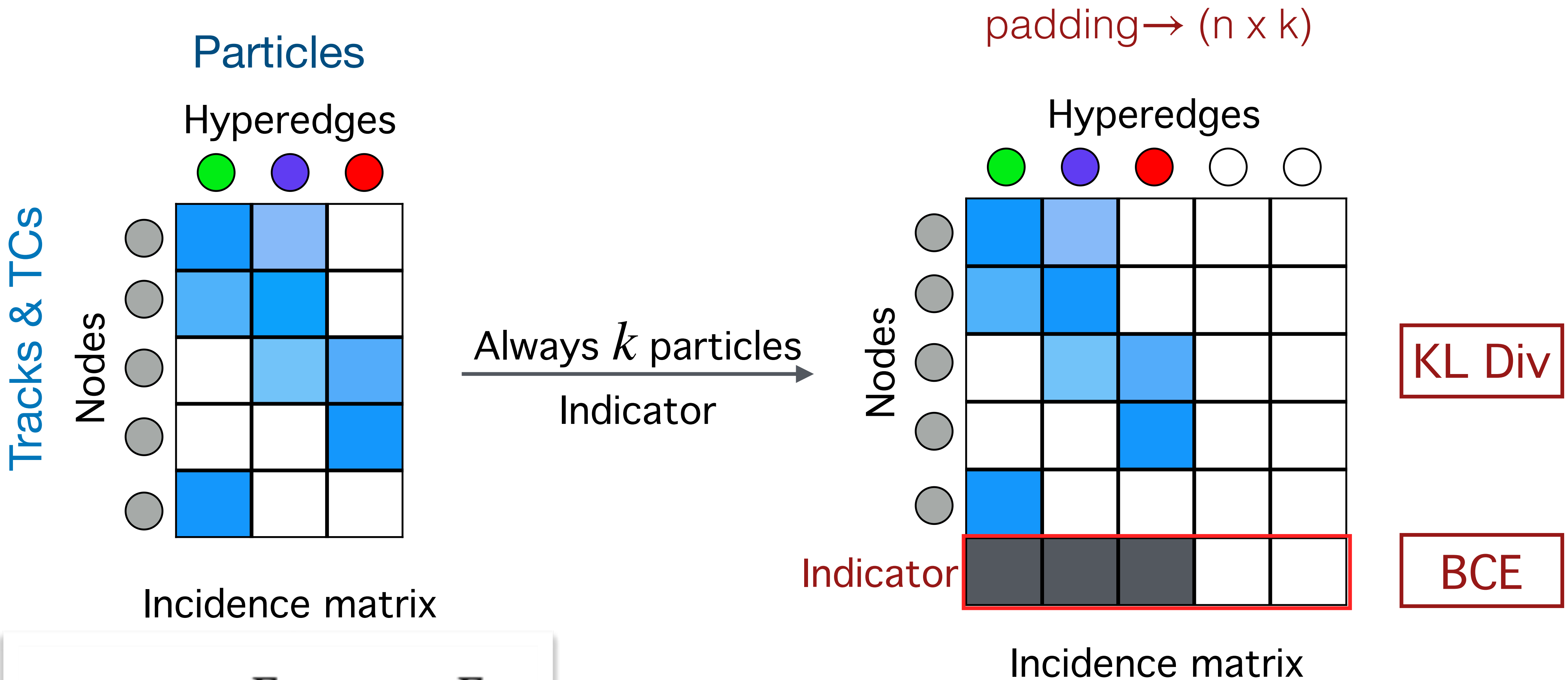
Incidence matrix

Inductive Bias

- ✳ Biased toward E conservation
- ✳ Can approx. particle energy as incidence-weighted sum of node energies

Indicator

- Variable number of particles
- Indicator to the rescue!
- Indicator predicts the cardinality



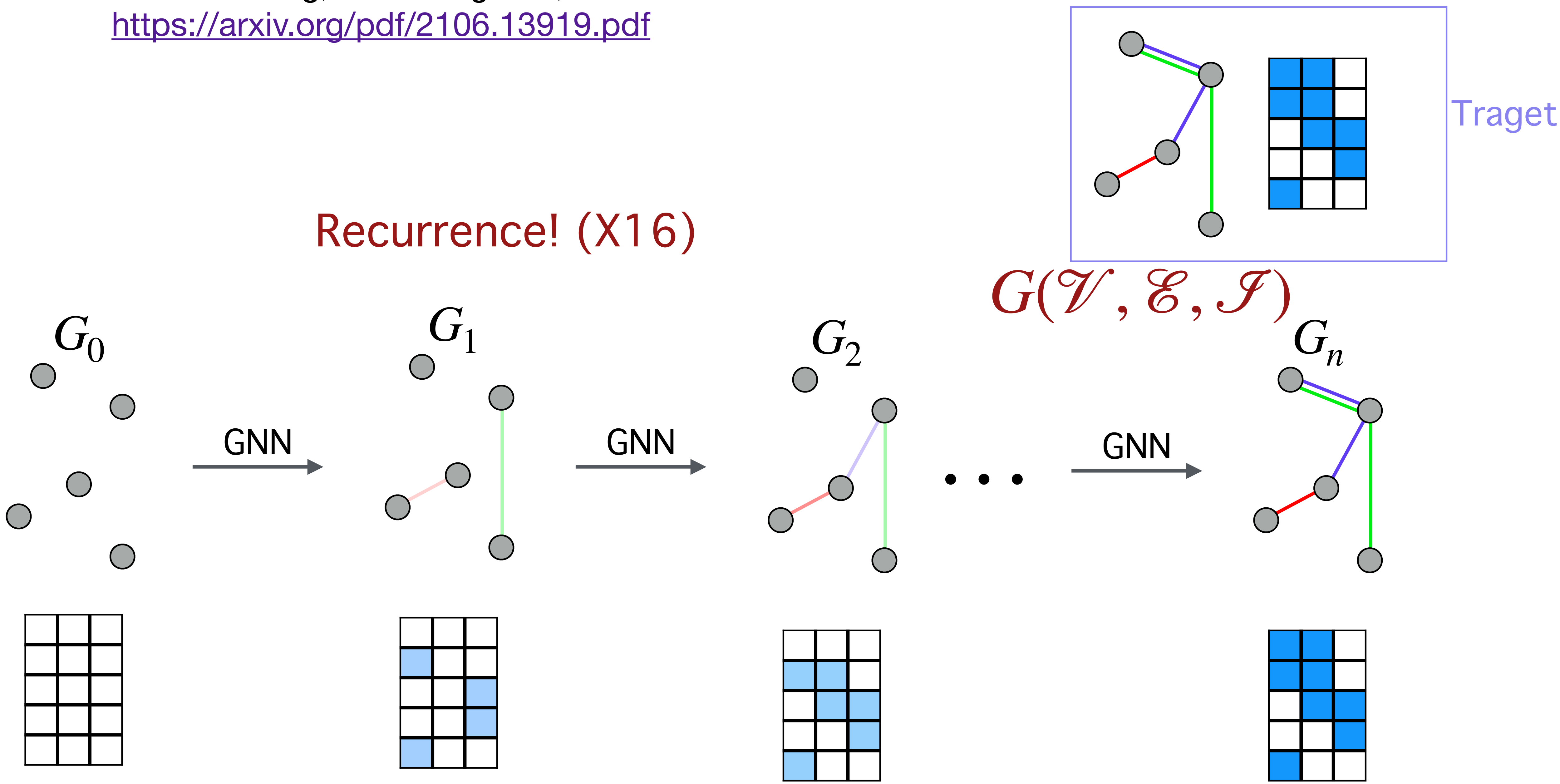
$$[I]_{ia} = \frac{E_{ia}}{\sum_{\text{particles } b} E_{ib}} = \frac{E_{ia}}{E_i}$$

KL Div $Loss_{inc} = \Sigma_a KL_i \left(I_{ia}^{targ}, Softmax_i(I_{ia}^{pred}) \right)$

Eia is the amount of energy that particle **a** contributes to the total energy **Ei** of node **i.**

Recurrently learning Hypergraph

Math based on D. Zhang, G. J. Burghout, C. G. M. Snuek
https://arxiv.org/pdf/2106.13919.pdf



Step 3

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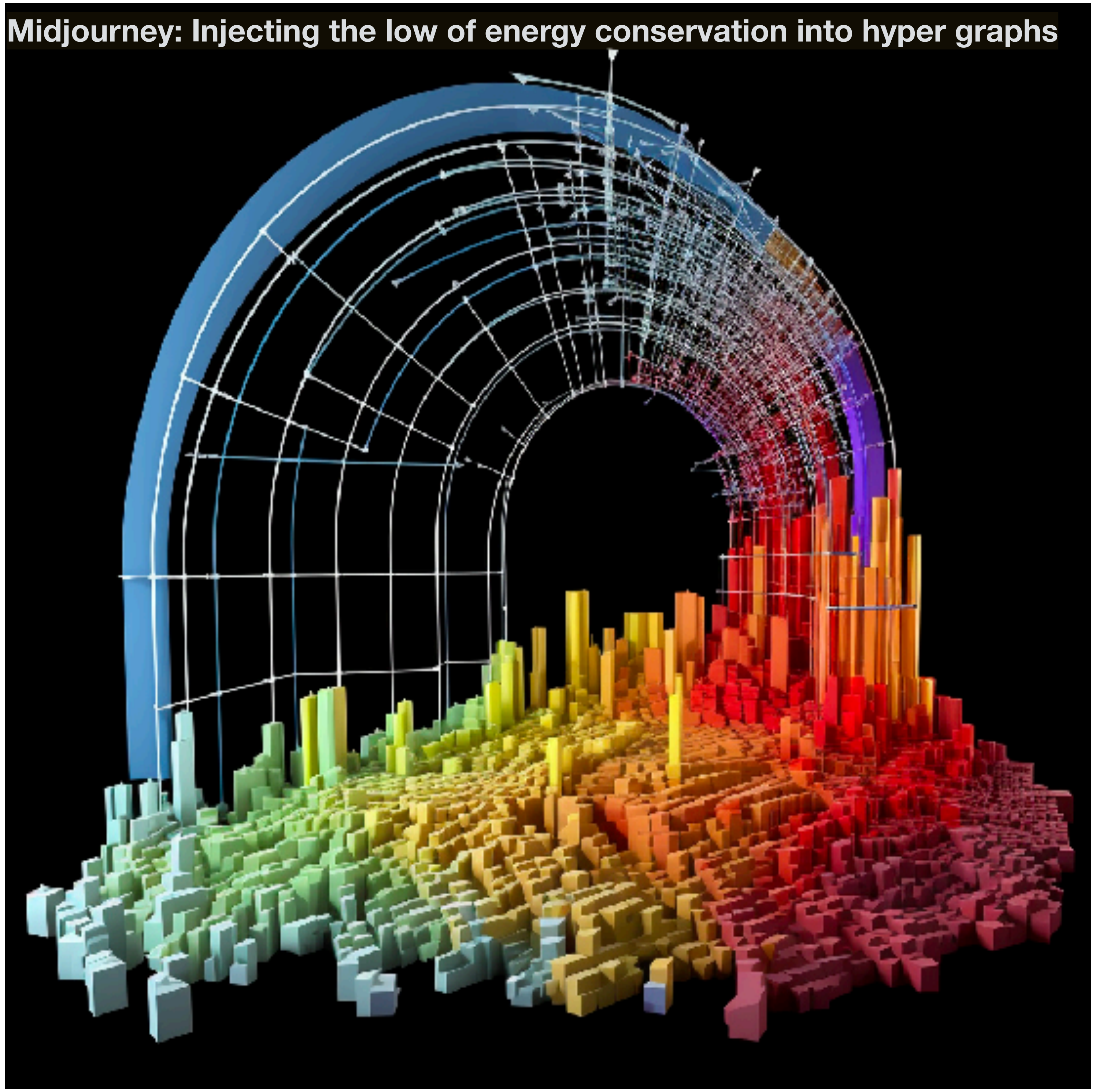
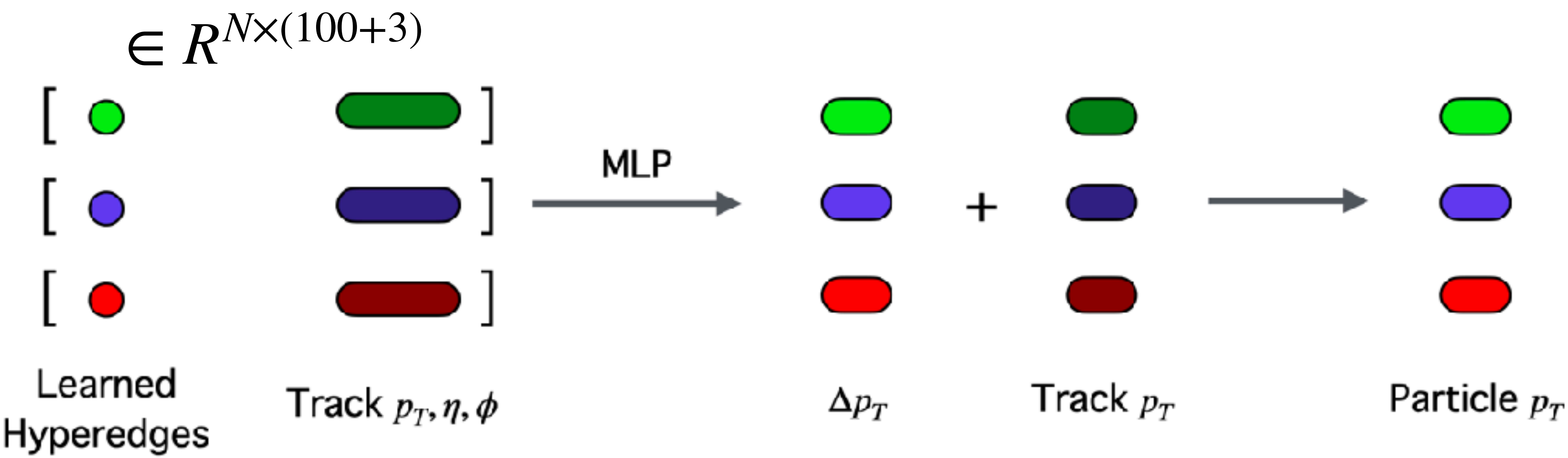
Interpretability



Charged Particles

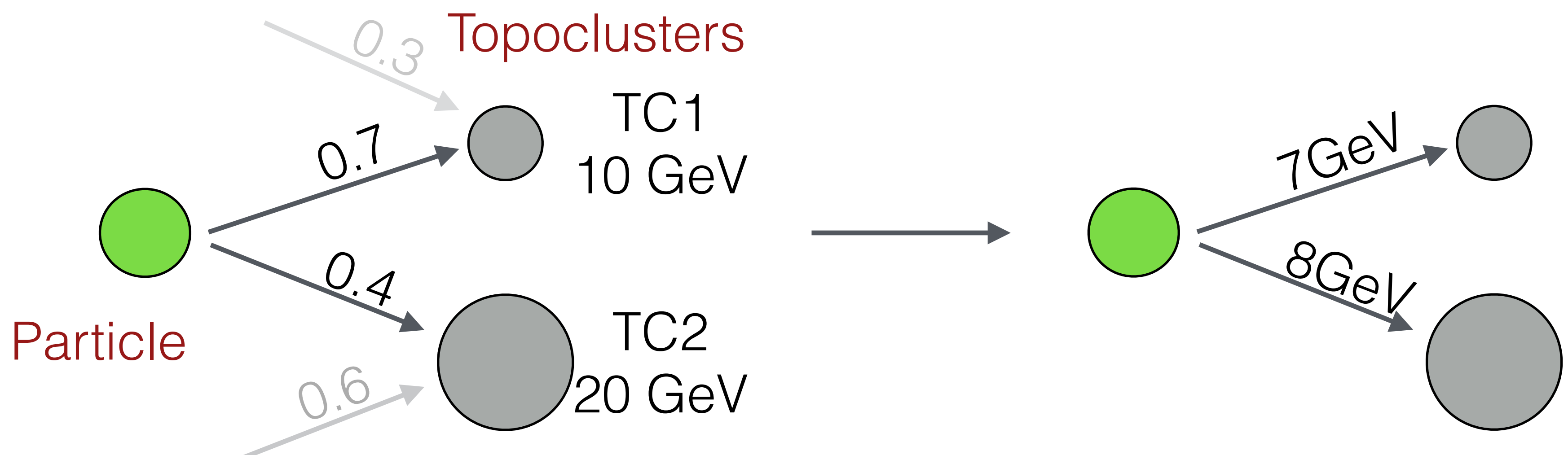
- Tracks are Good Proxies for Charged Particles pT & directions
- —> Separate the inference networks for Charged and Neutral particles
- **Take** η **and** ϕ **from the track**, and predict a **correction to track** p_T



Neutral Particles

Neutral particles

- Incidence matrix injects the Energy-Conservation into the learnt hyper-edges which by now can also serve as proxies for Neutral Particle



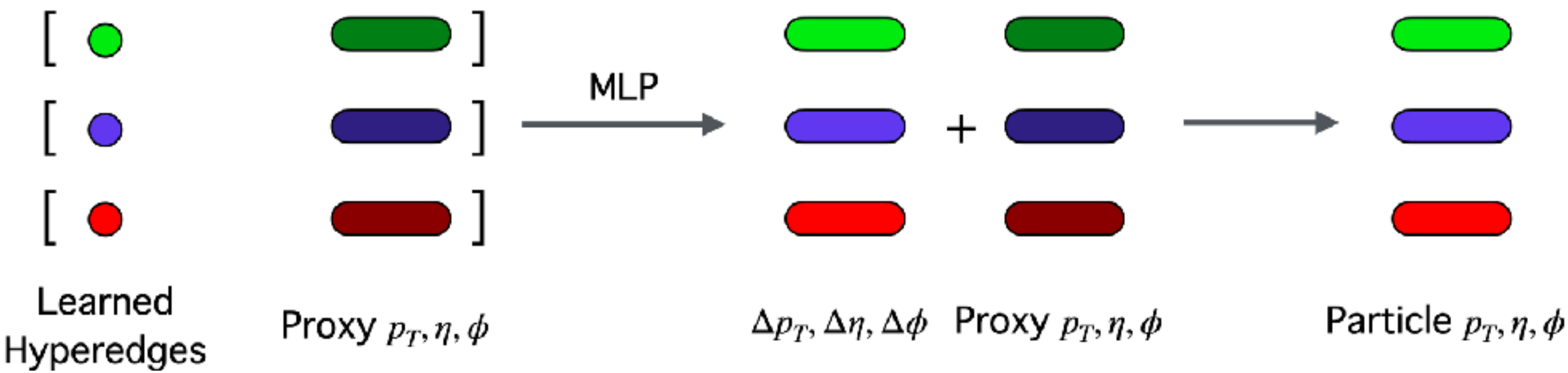
Proxy properties of

- E = E1 + E2 = 15GeV
- $\eta = \dfrac{7\eta_1 + 8\eta_2}{15}$
- $\phi = \dfrac{7\phi_1 + 8\phi_2}{15}$
- $p_T = \dfrac{E}{cosh(\eta)}$

$$Proxy^{Neutral} = (E, \eta, \phi) = \left(15, \frac{7\eta_1 + 8\eta_2}{15}, \frac{7\phi_1 + 8\phi_2}{15}\right)$$

Neutral Particles

$\in R^{N\times(100+3)}$



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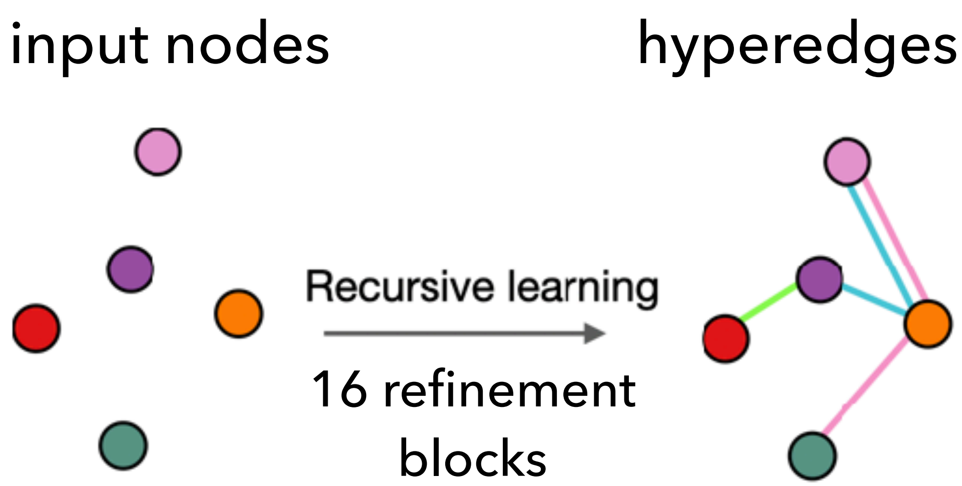
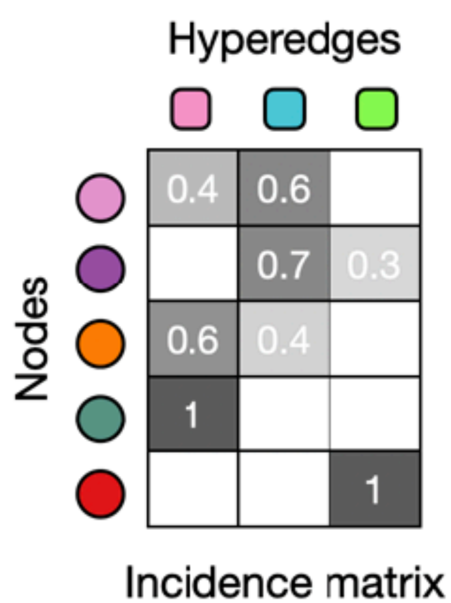
Overall **HGPflow** algorithm

1) predict incidence matrix



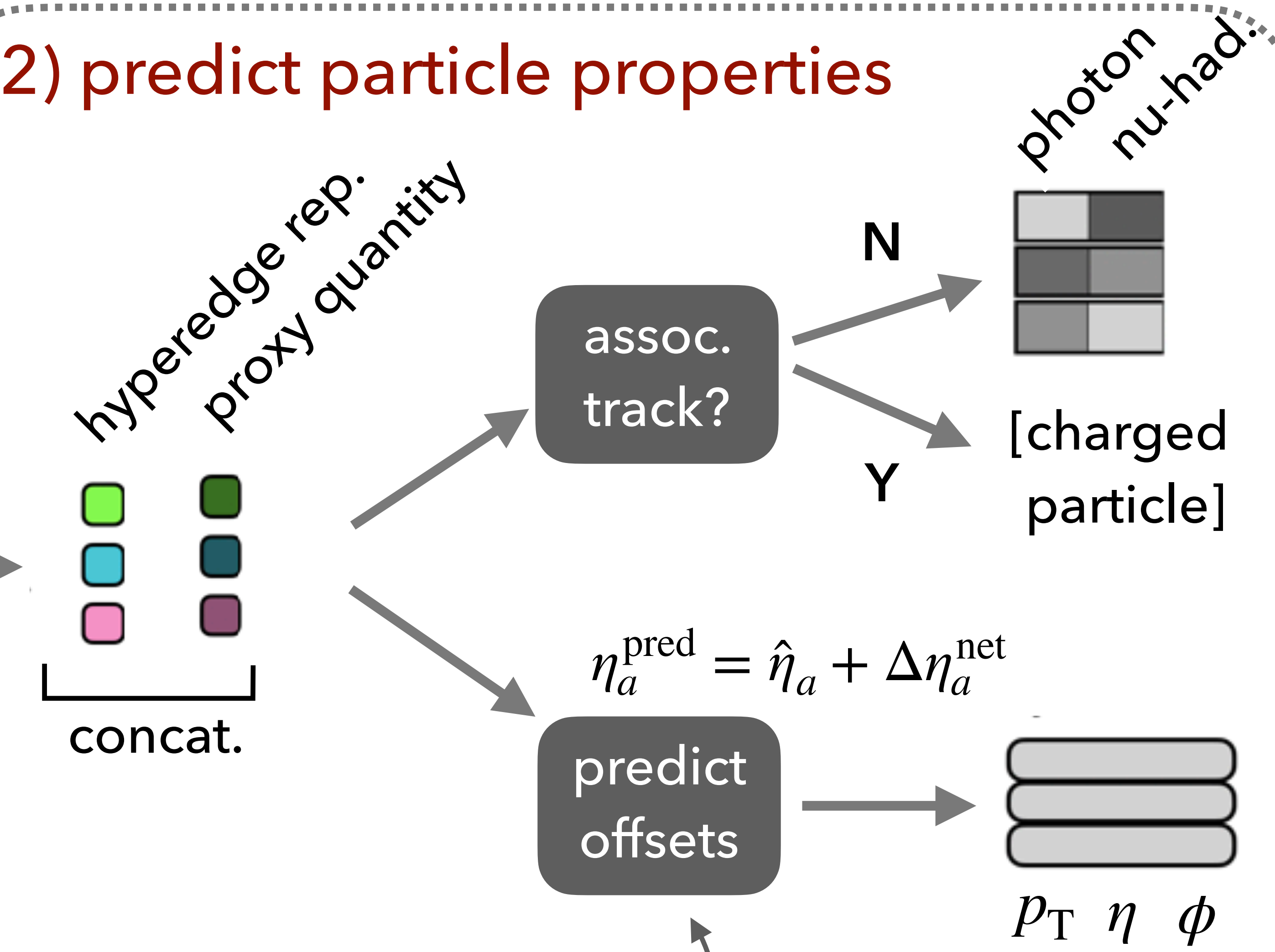
Energy-fraction incidence matrix

$$I_{ia} =$$



Recurrently predicting hypergraphs
arXiv:2106.13919

2) predict particle properties

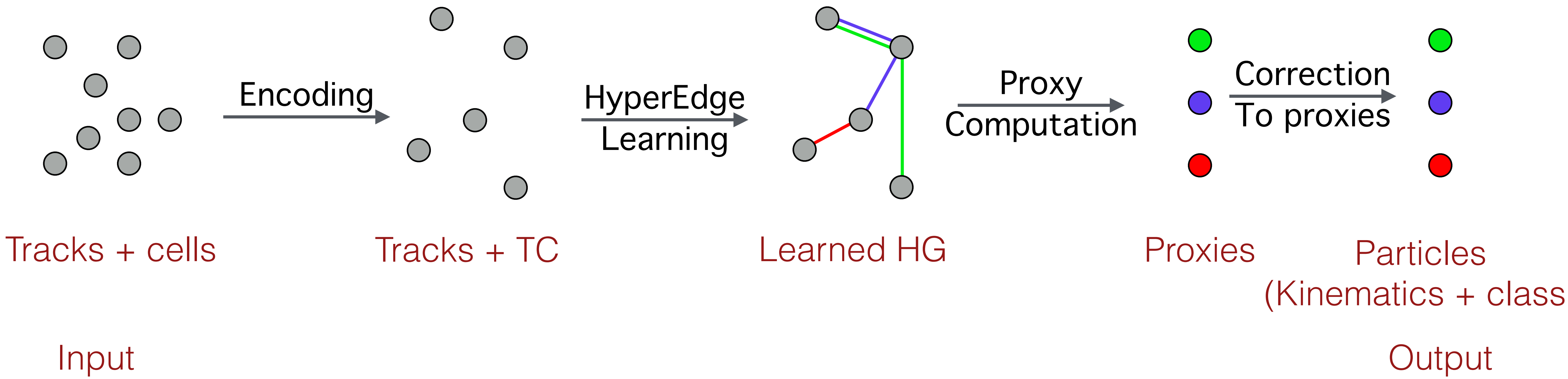


Energy-weighted proxy quantities:

$$E_{\blacksquare} = 0.60E_{\bullet} + 0.70E_{\bullet} + 0.40E_{\bullet}$$

$$\eta_{\blacksquare} = \eta_{\bullet}\frac{0.60E_{\bullet}}{E_{\blacksquare}} + \eta_{\bullet}\frac{0.70E_{\bullet}}{E_{\blacksquare}} + \eta_{\bullet}\frac{0.40E_{\bullet}}{E_{\blacksquare}}$$

Overall HGPflow algorithm



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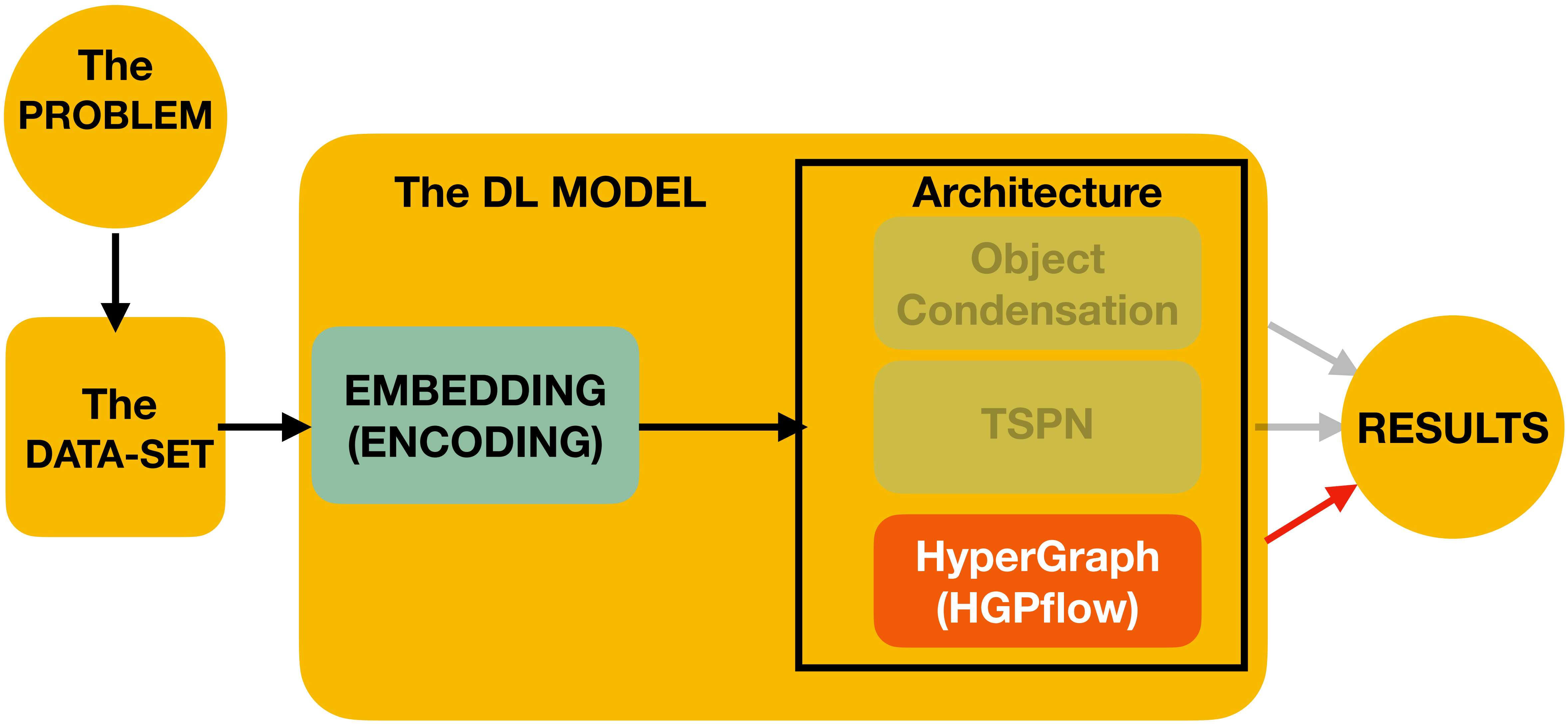
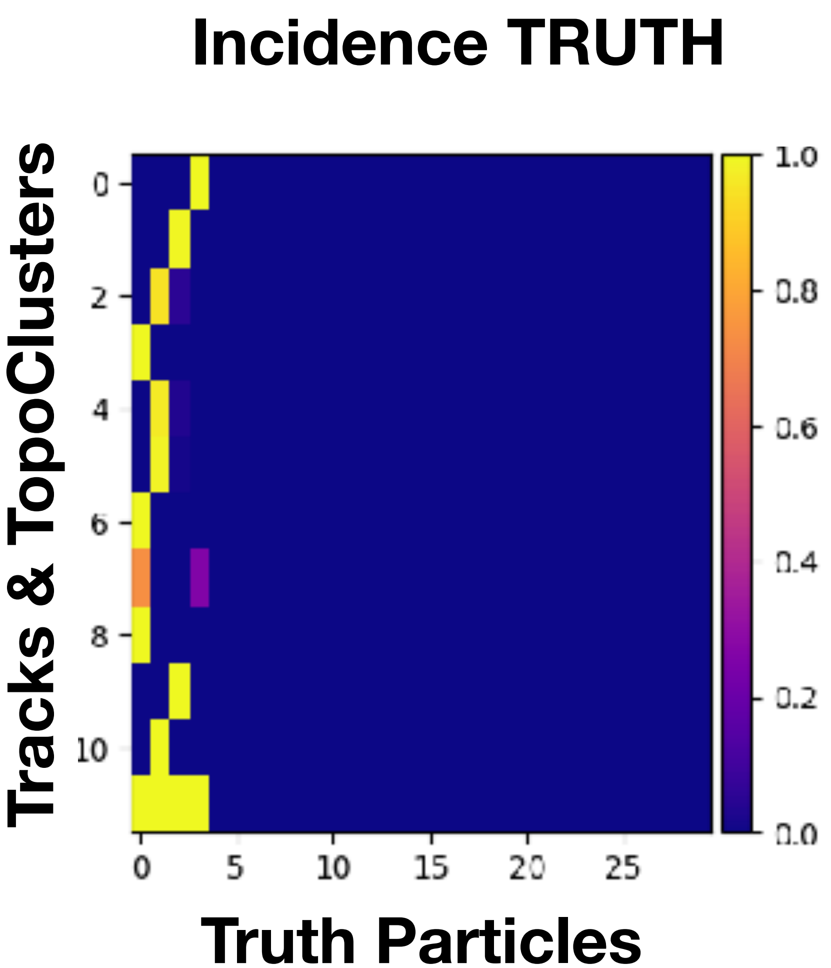
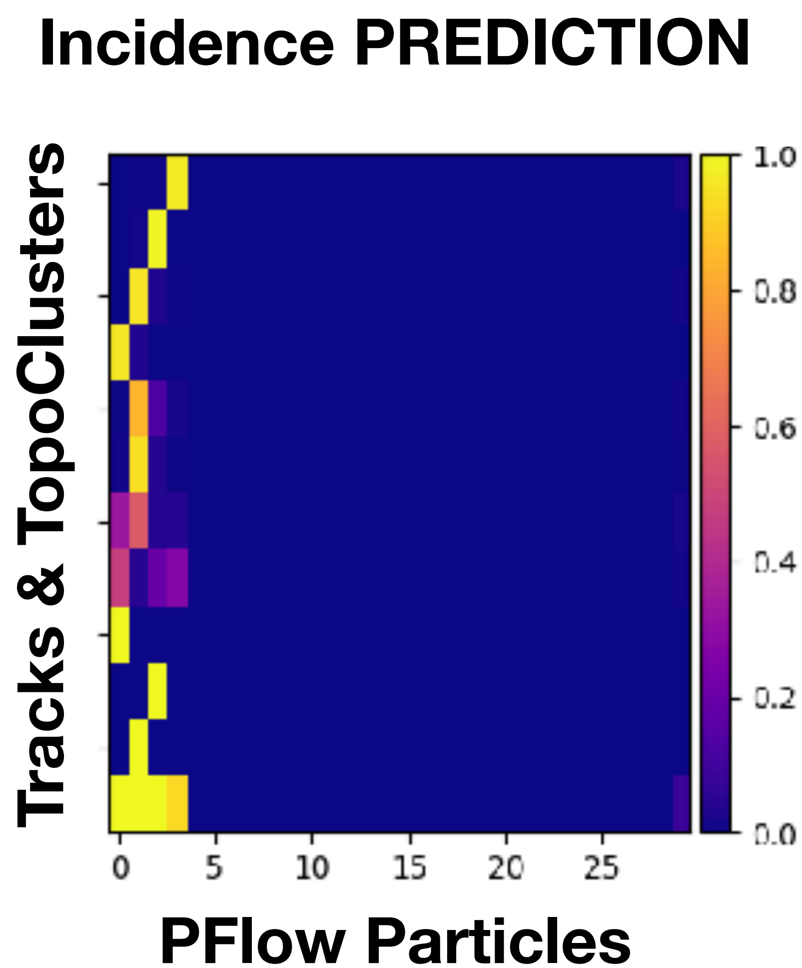
Diving into Deep Learning

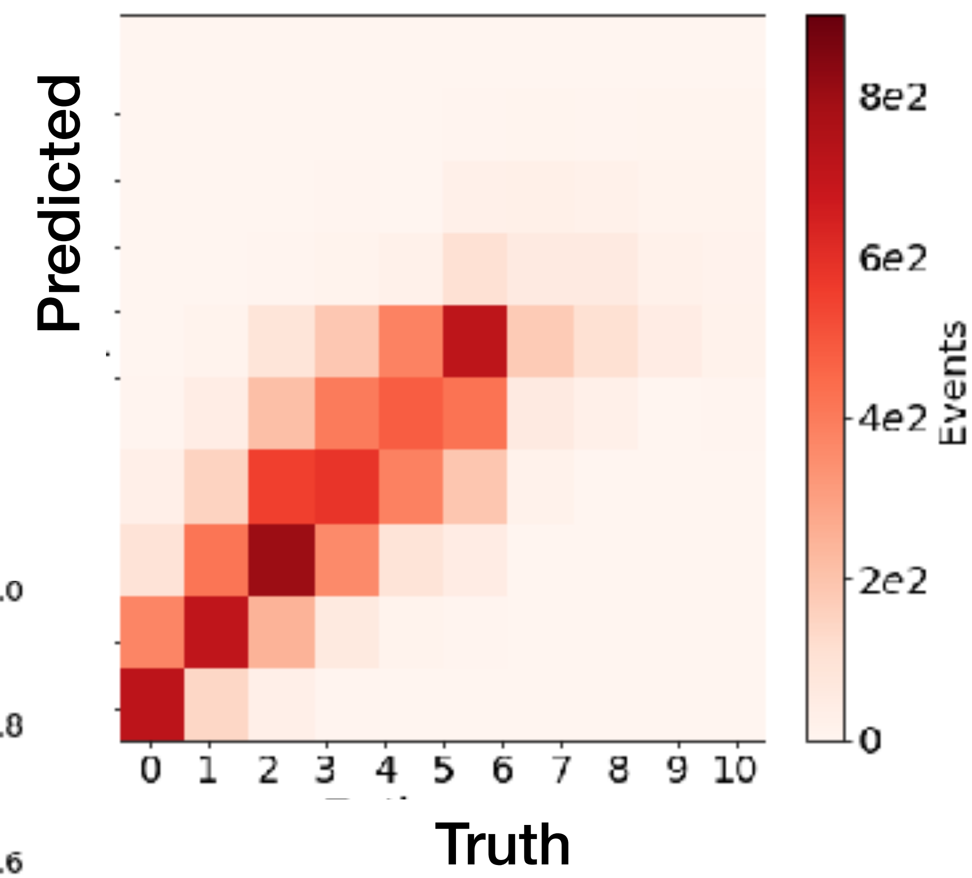


Cardinality of Neutral particles

- Fairly diagonal
- Cardinality prediction is much robust, by construction
- "local" reconstruction

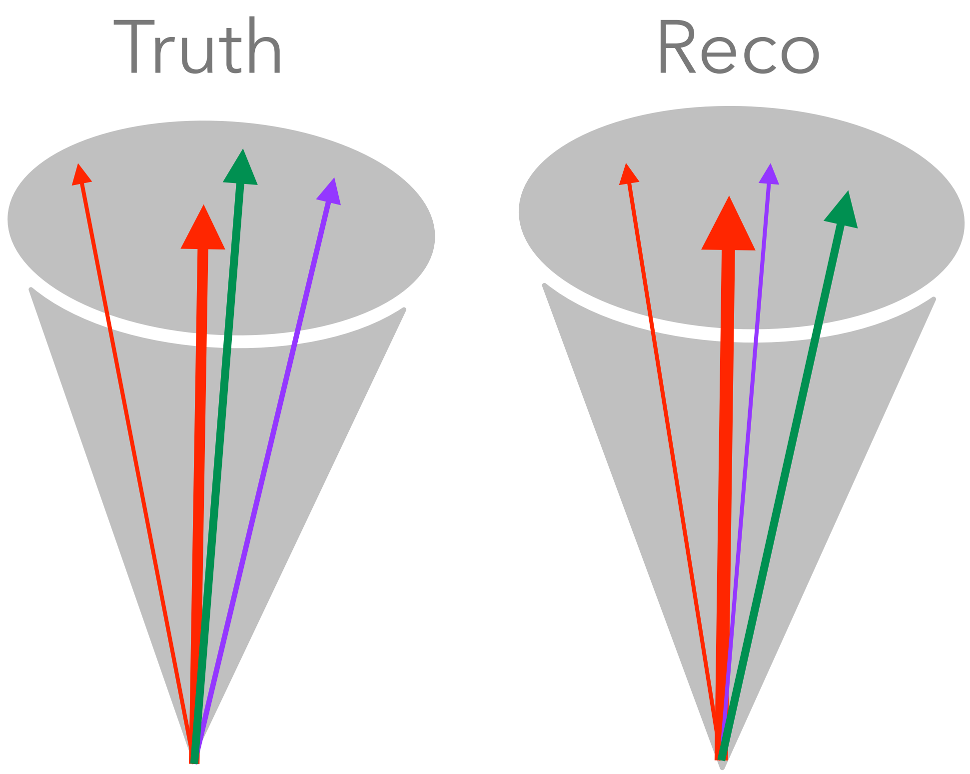






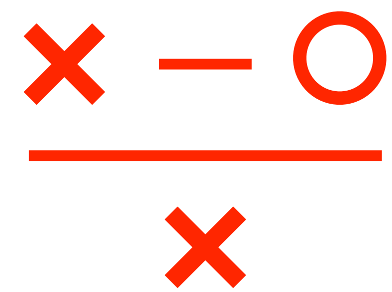
Comparing pred. vs target particles

- Jet-level quantities

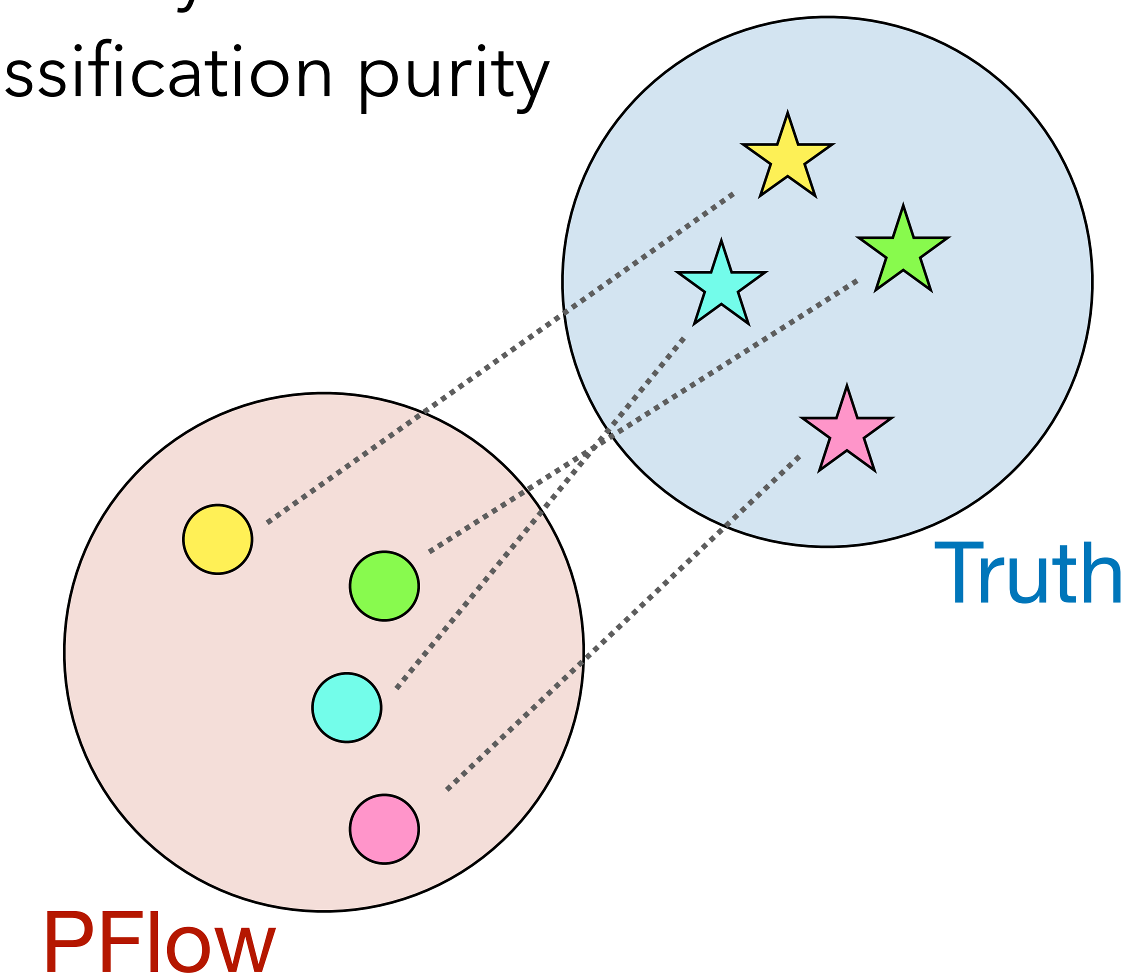


2) Performance metrics

- Particle angular, momentum residuals



- Efficiency and fake rate
- Classification purity



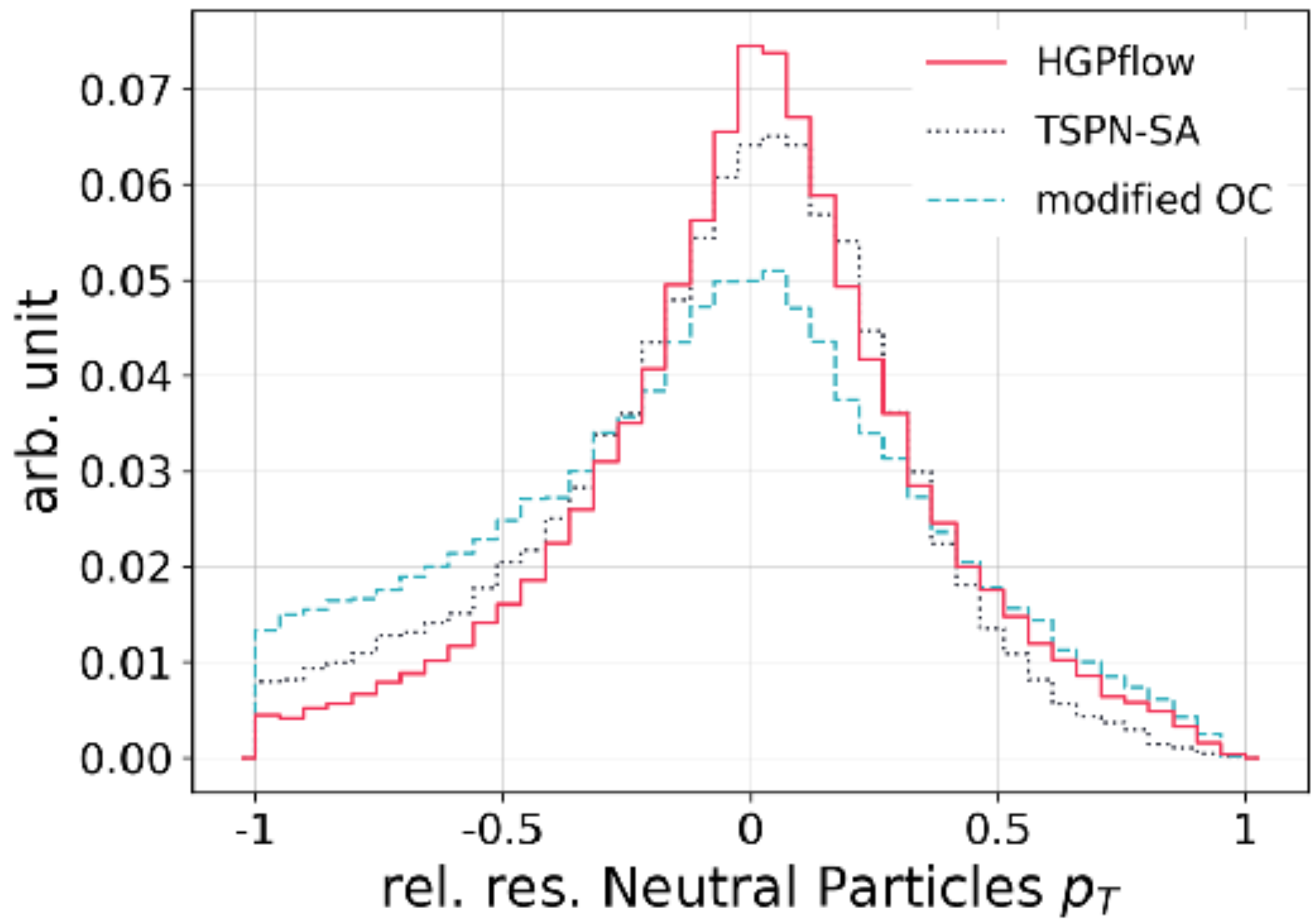
1) Hungarian matching:

$$d_{match} = \sqrt{\left(\frac{\Delta p_T}{p_T}\right)^2 + \Delta\eta^2 + \Delta\phi^2}$$

Neutral Particles (Photons & Hadrons)

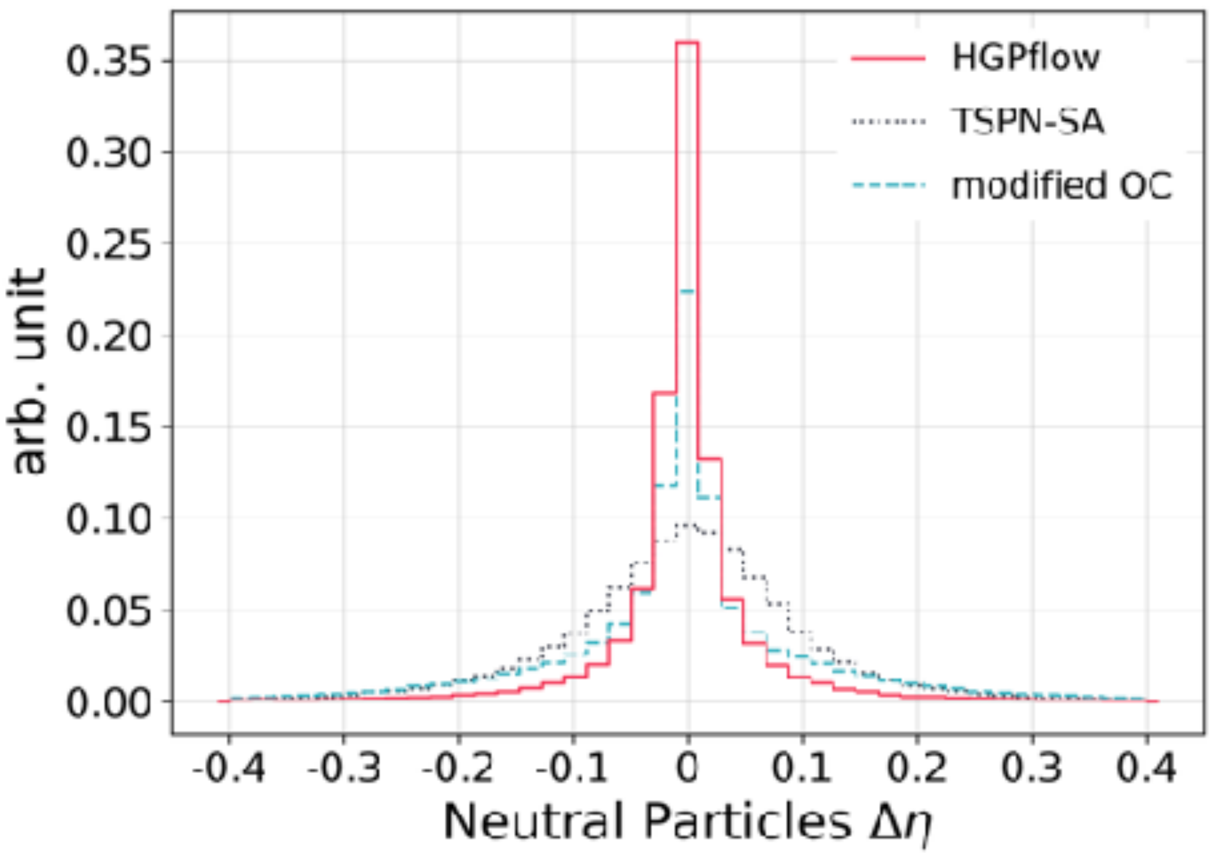
$$\frac{P_T^{truth} - P_T^{predicted}}{P_T^{truth}}$$

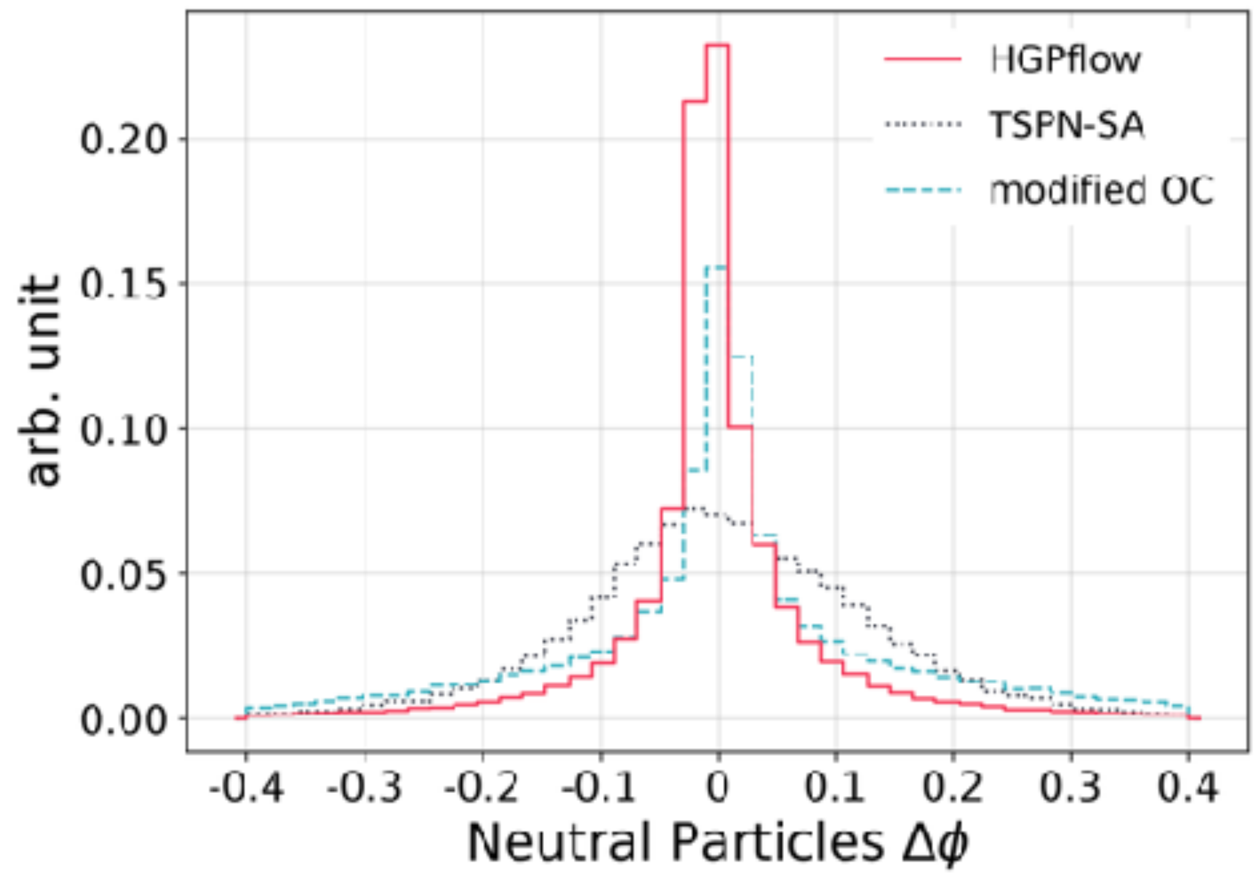
- HG can understand overlapping showers more precisely
- Helps in better reconstruction



F.A. Di Bello et. al. https://arxiv.org/abs/2212.01328

Neutral Particles (Photons & Hadrons)





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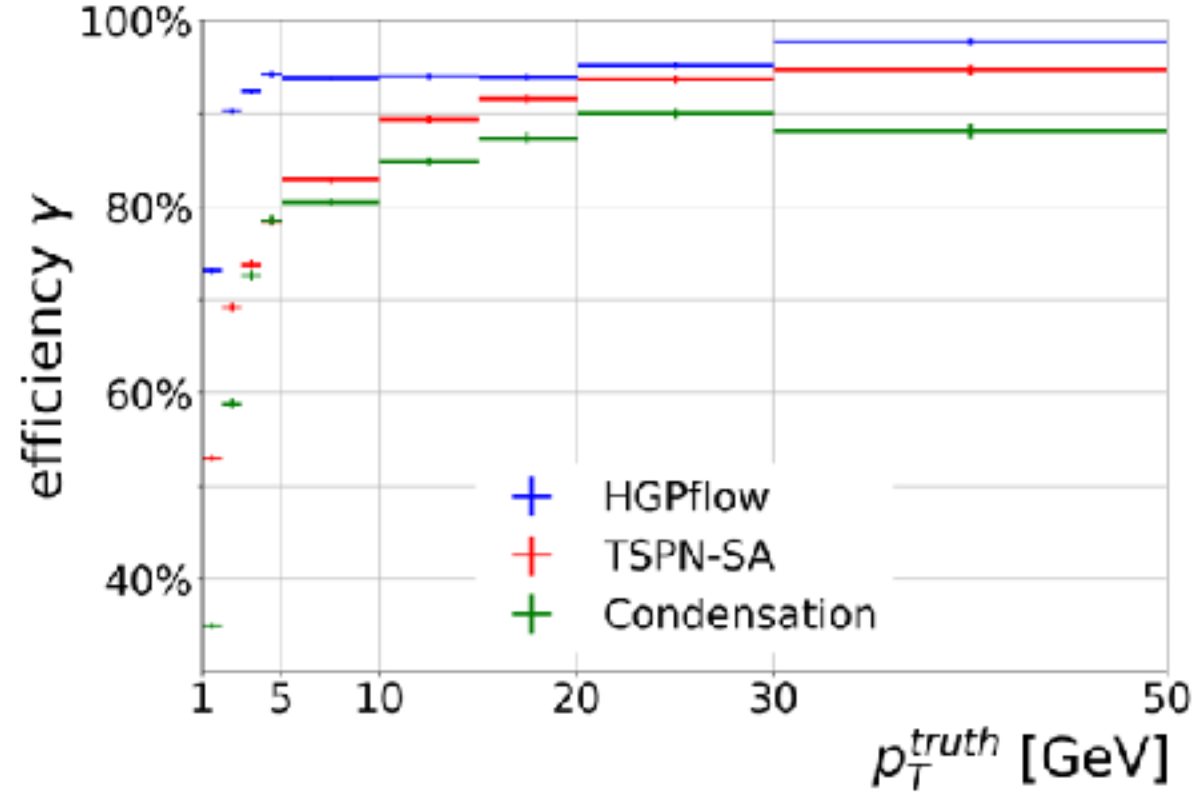
Photon efficiency:

- Supervised links b/w particle and input nodes assist in interpreting eff and fakes

$$\epsilon_{ff} = \frac{N_{match,pred}}{N_{target}}$$

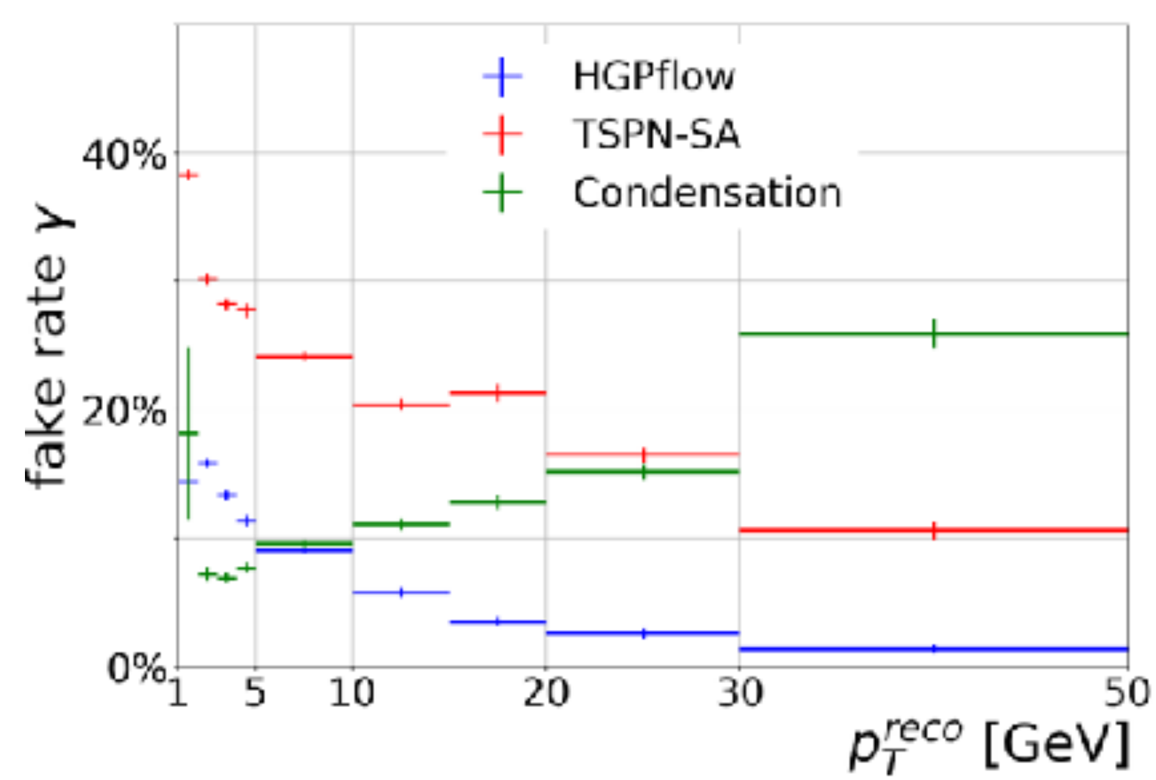
>90% above 2 GeV



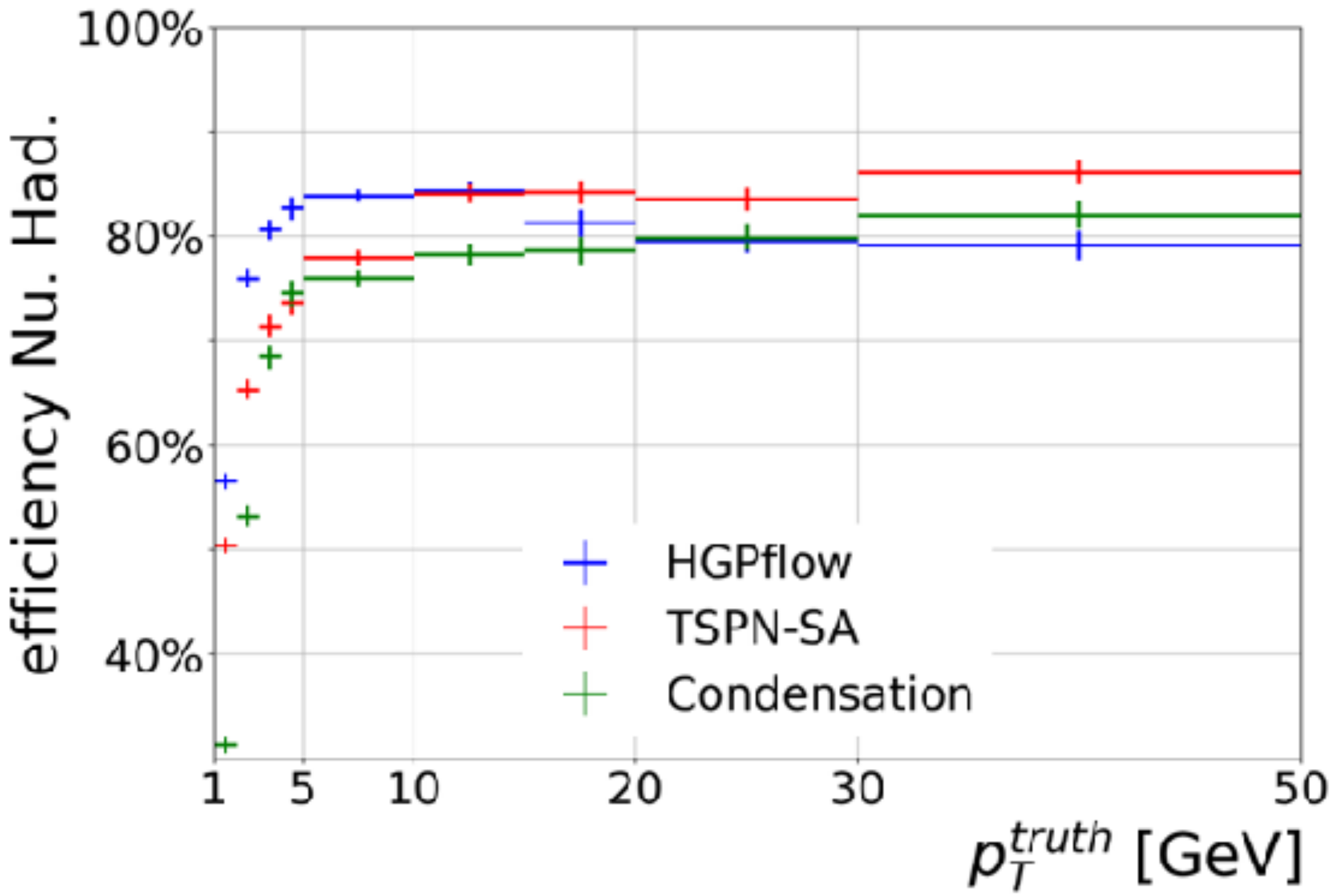
Photon fake rate:

$$fake = \frac{N_{unmatch,pred}}{N_{pred}}$$

<5% above 20 GeV



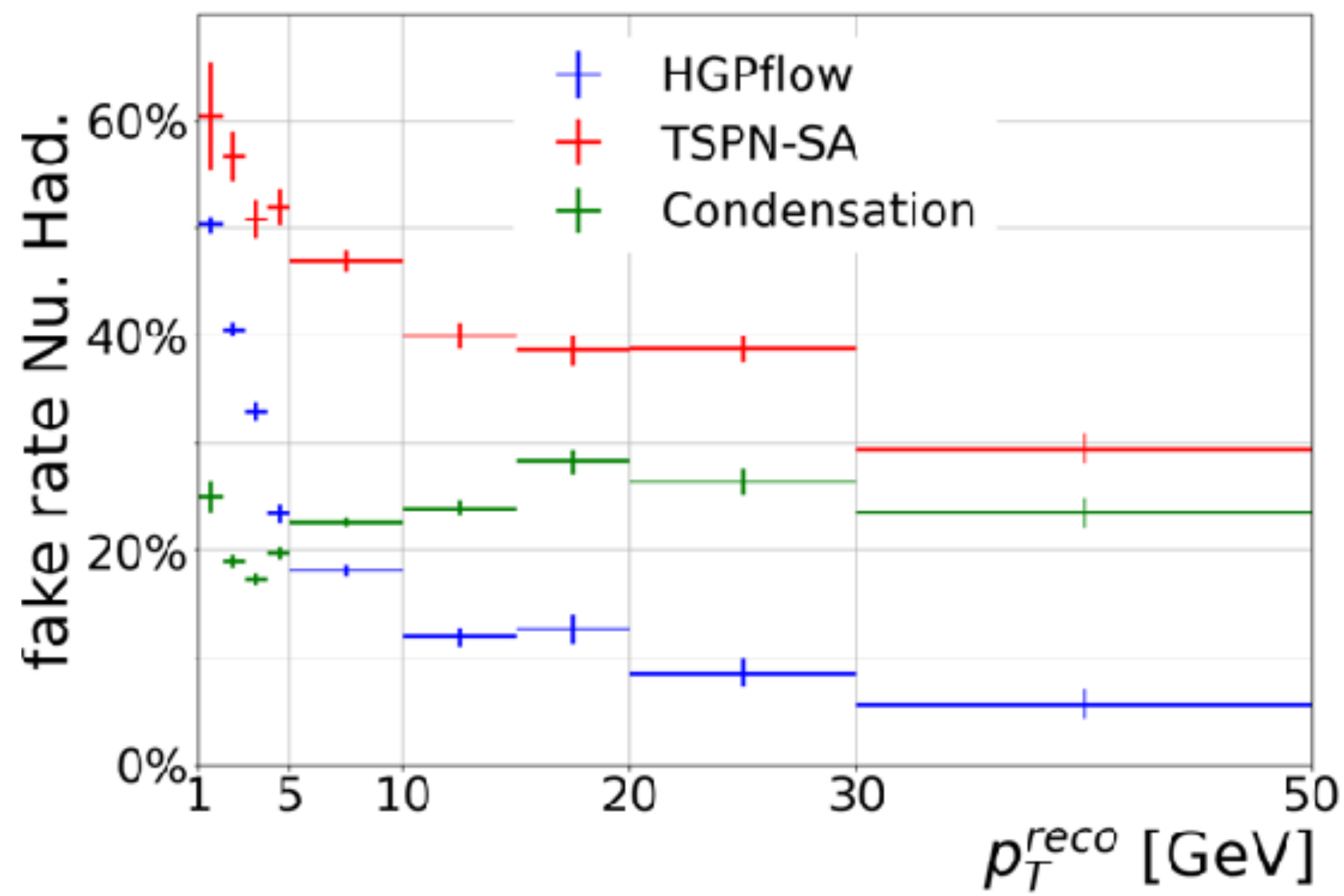
Nu. Had. efficiency:



$$\epsilon_{ff} = \frac{N_{match,pred}}{N_{target}}$$

≃ 80% above 3 GeV

Nu. Had. fake rate:



$$fake = \frac{N_{unmatch,pred}}{N_{pred}}$$

<10% above 20 GeV

Classification accuracy

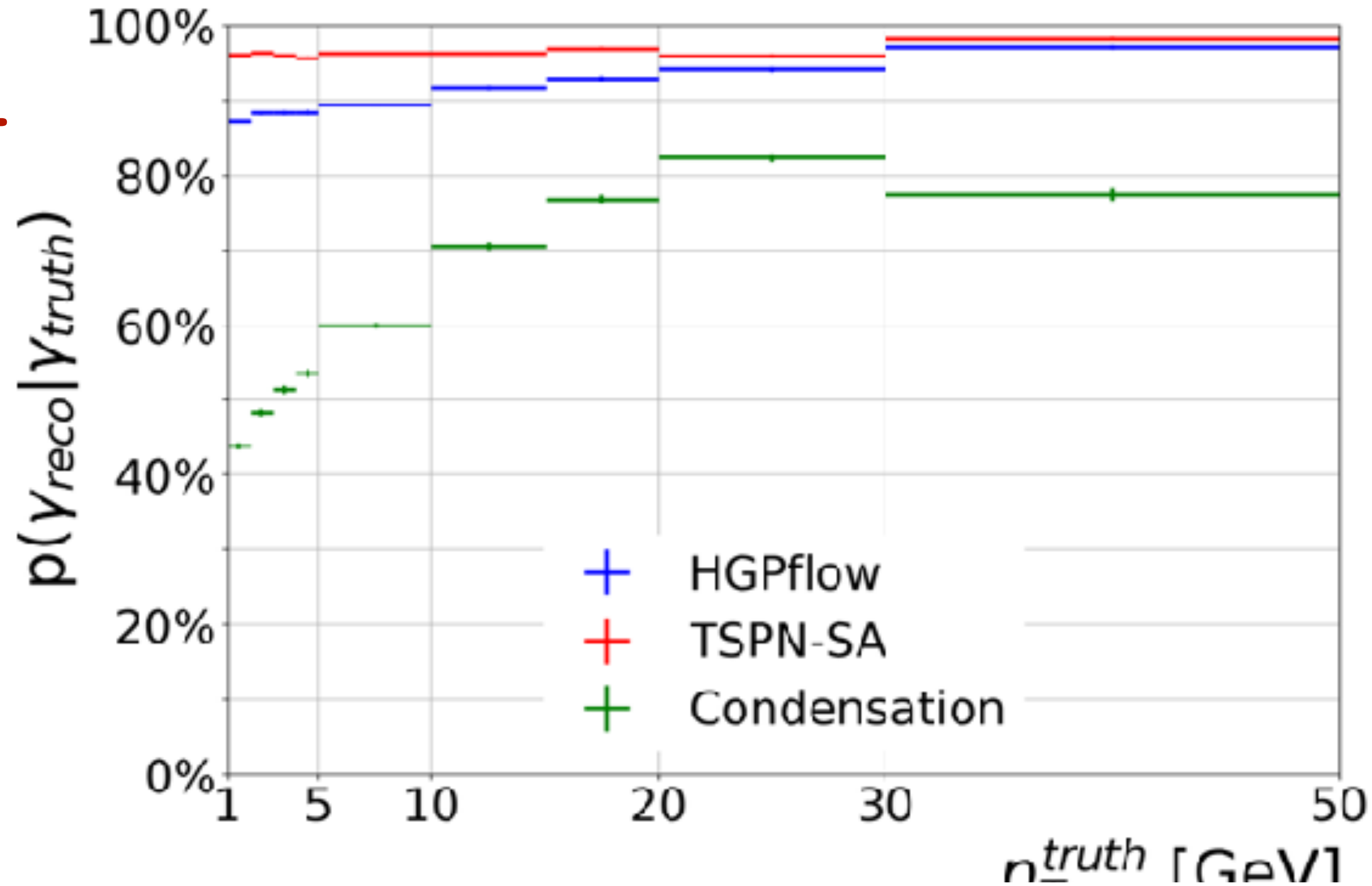
the probability that the predicted neutral particles which are matched to truth photons (neut hadrons) are assigned the correct class

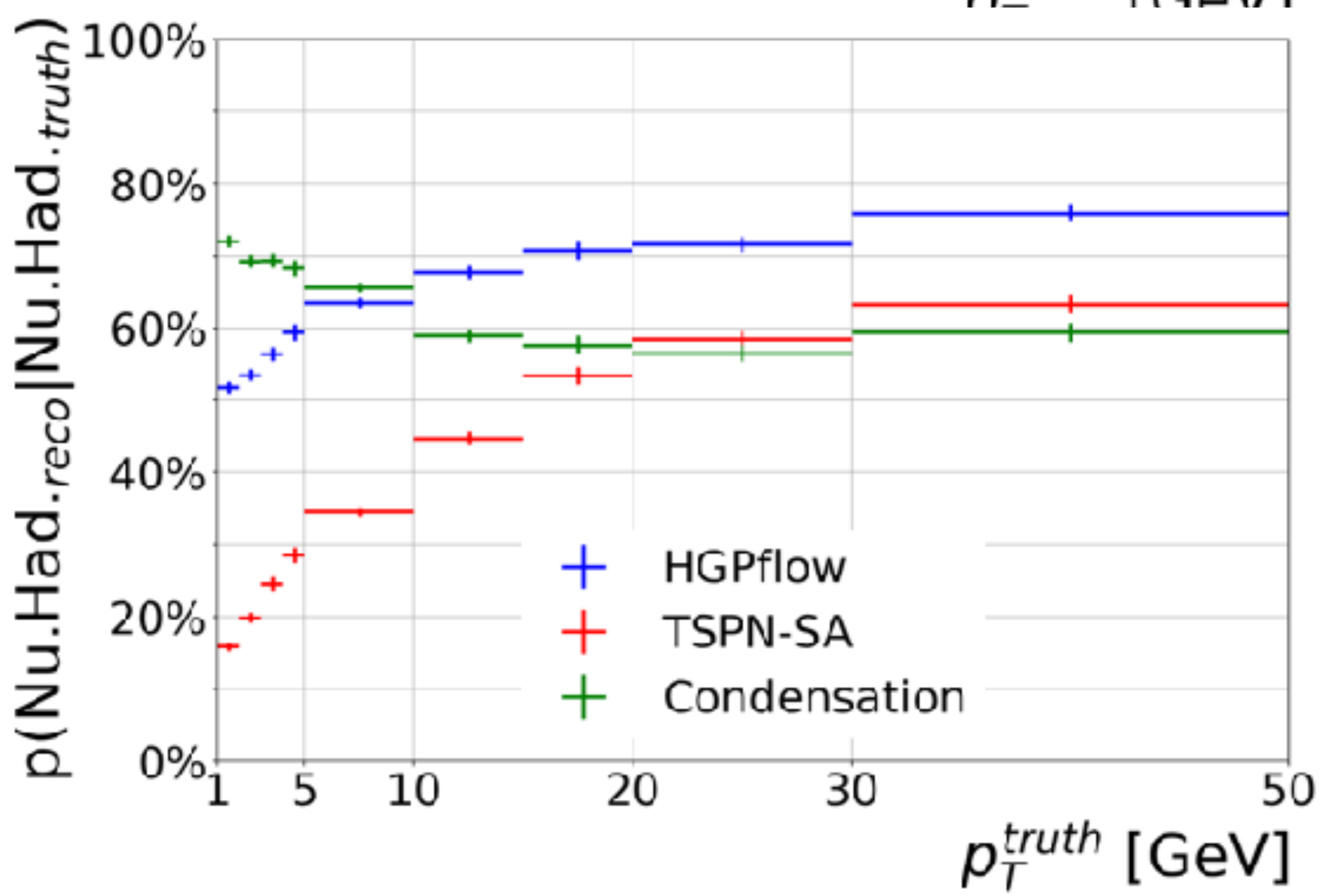
Photons

>90% above 5 GeV

Neutral Hadrons

>90% above 15 GeV

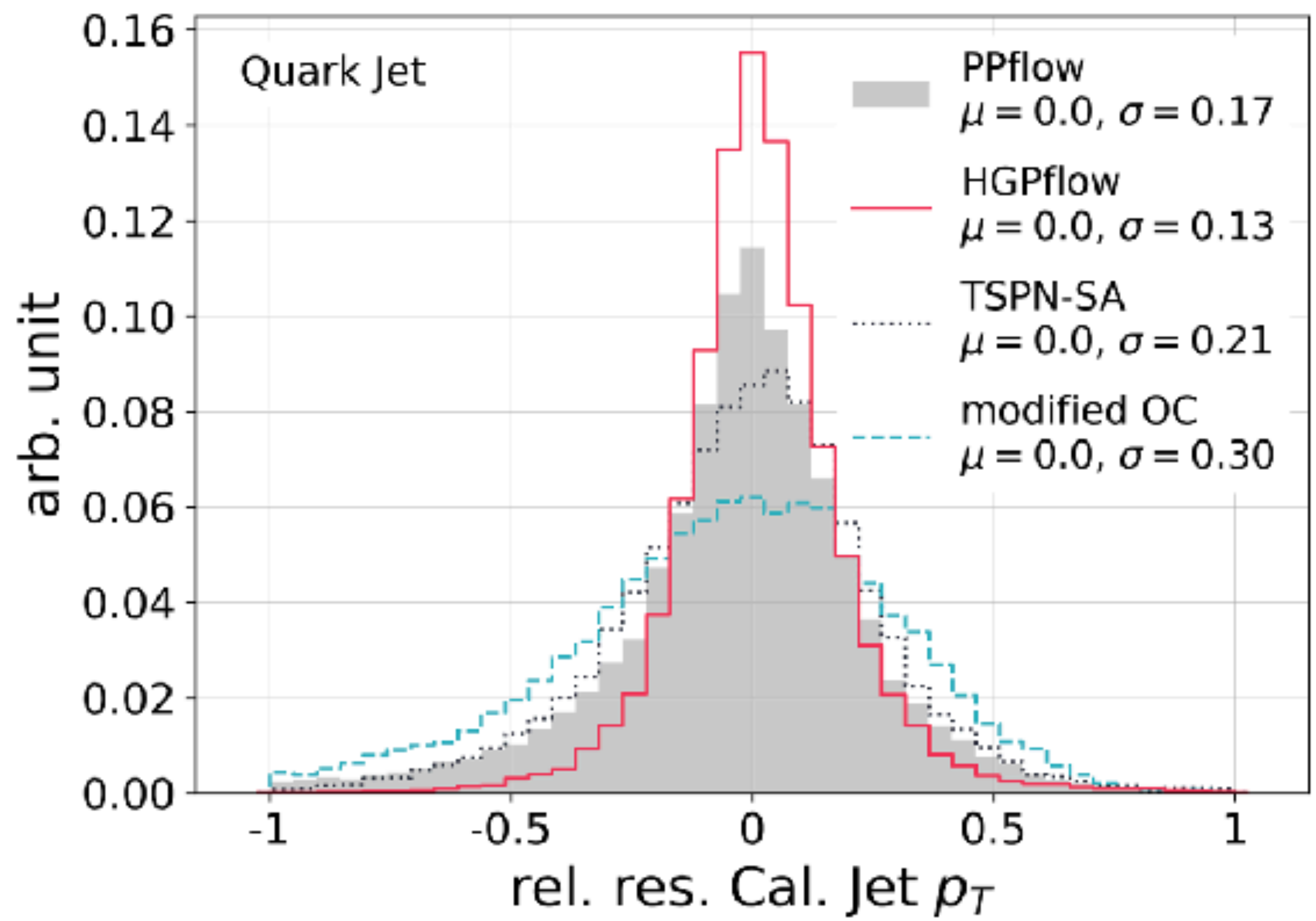




Improved Resolution!

Jets (Quarks)

- The parametrization of PPflow is optimized for jet resolution
- ML algos were not trained on this objective



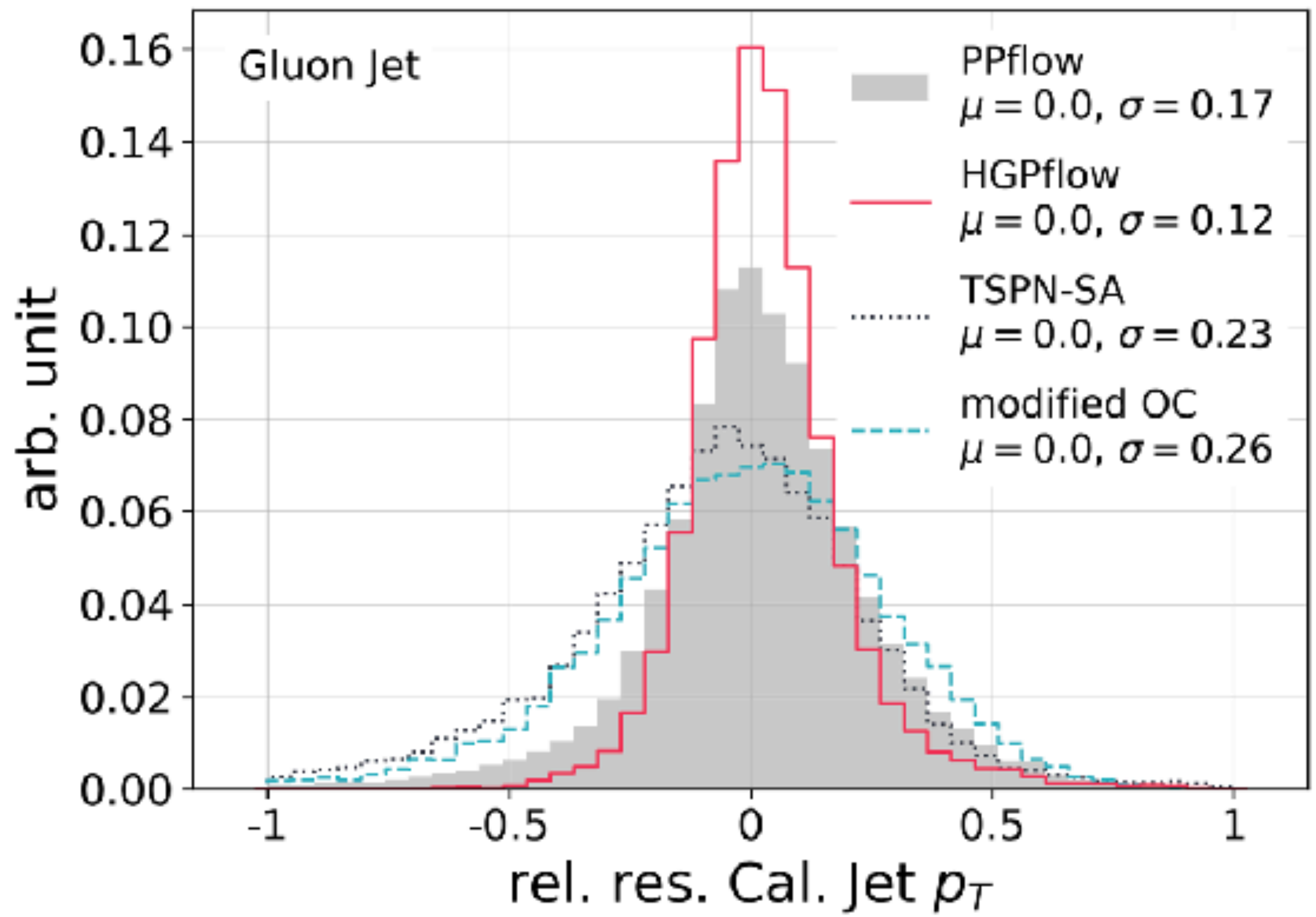
$$\frac{P_T^{truth} - P_T^{predicted}}{P_T^{truth}}$$

F.A. Di Bello et. al. https://arxiv.org/abs/2212.01328

Improved Resolution!

Jets (Gluons)

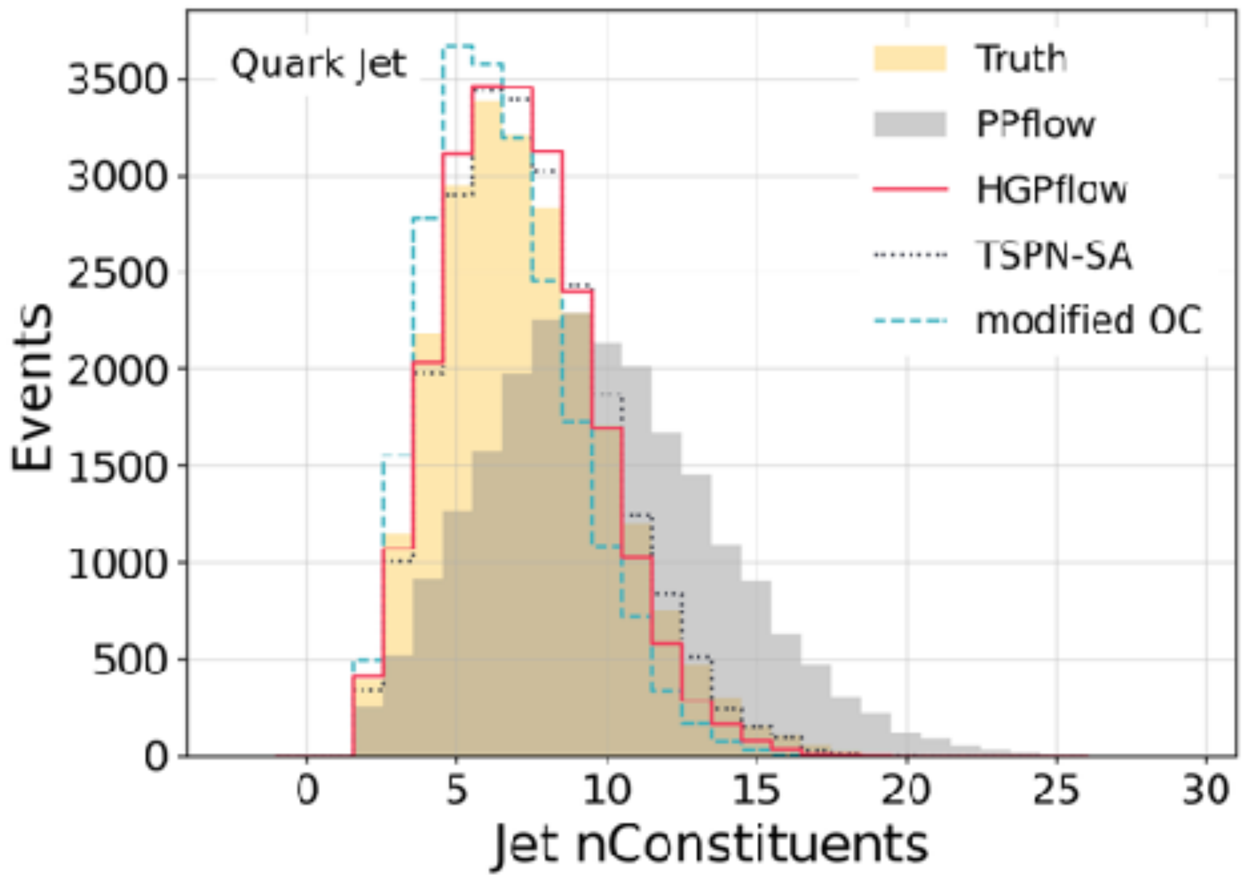
- HGPflow generalizes pretty well to gluon jets, though NOT TRAINED on Gluon Jets

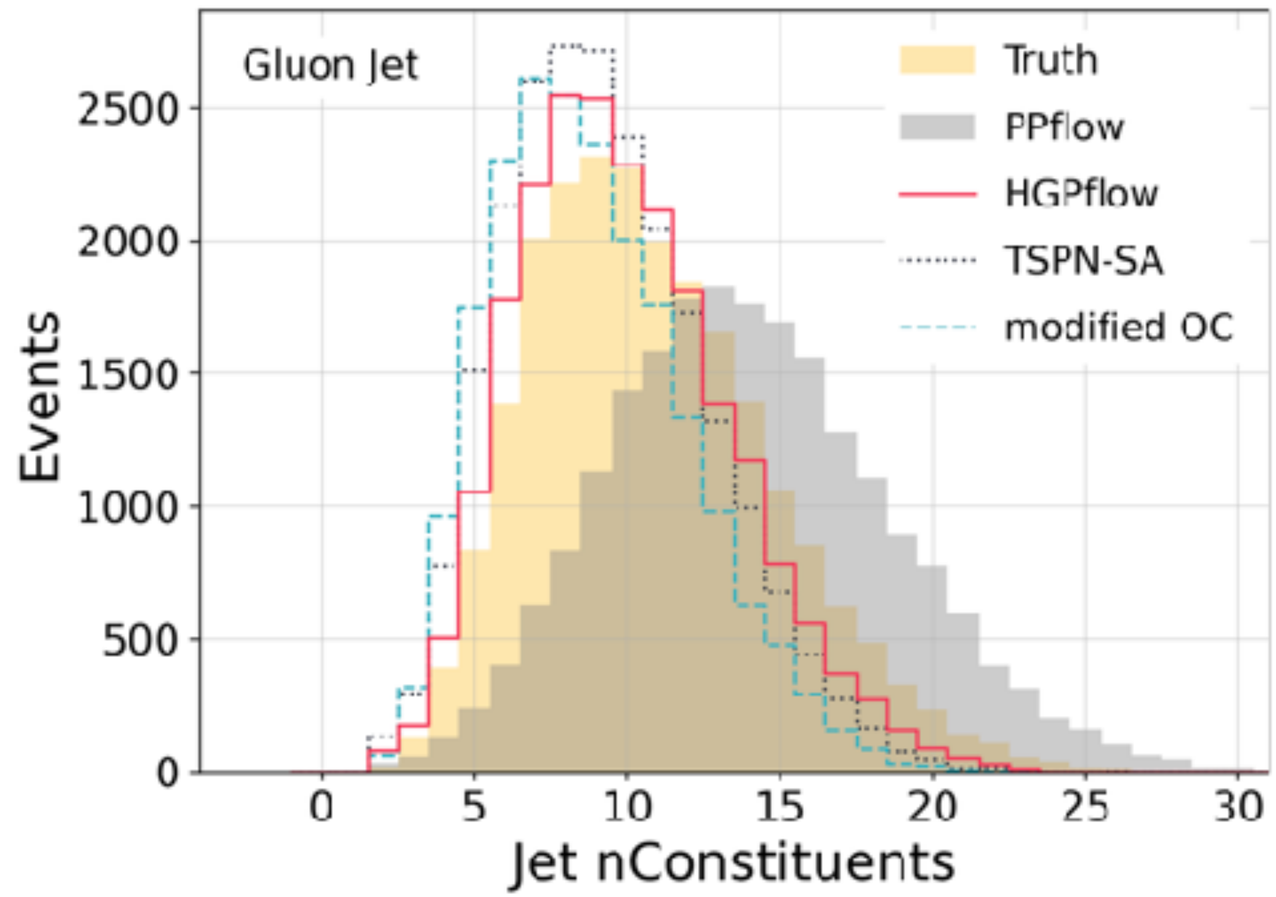


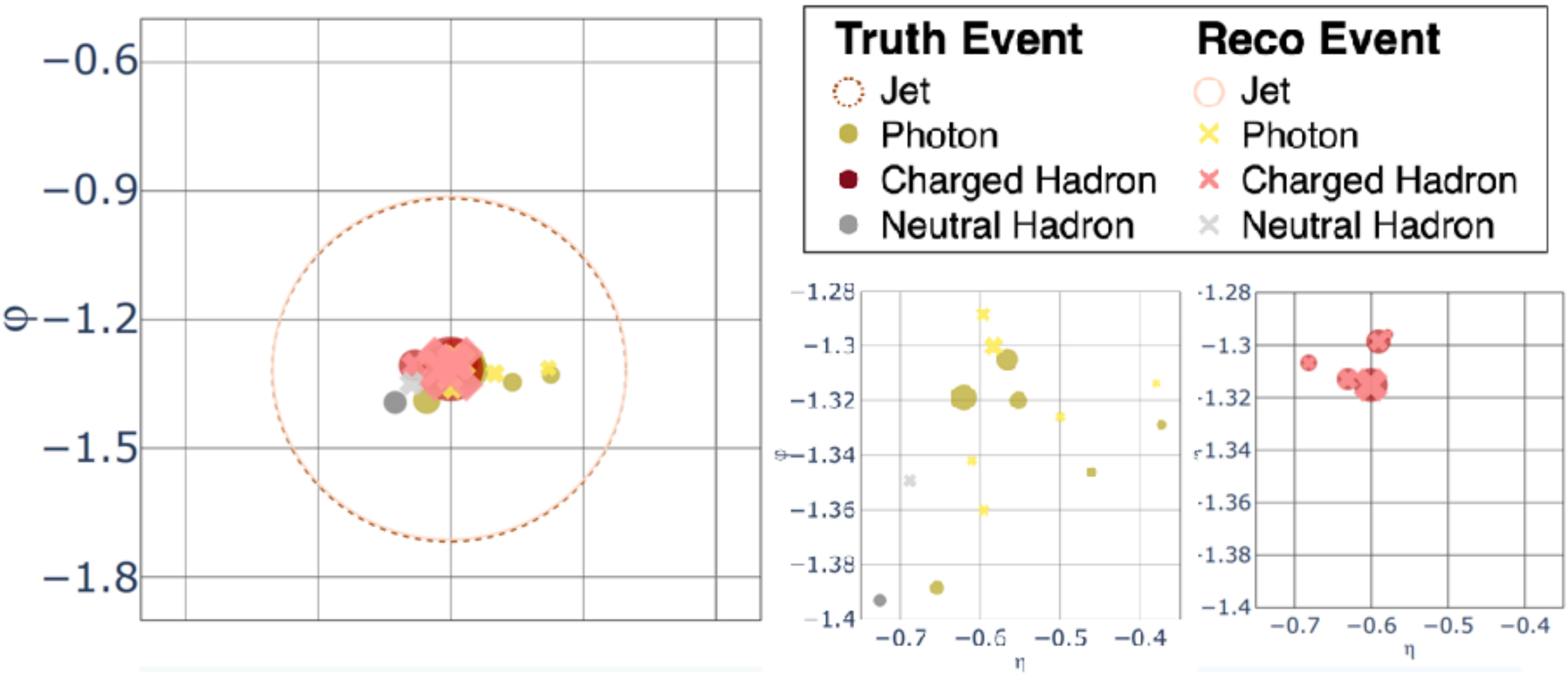
$$\frac{P_T^{truth} - P_T^{predicted}}{P_T^{truth}}$$

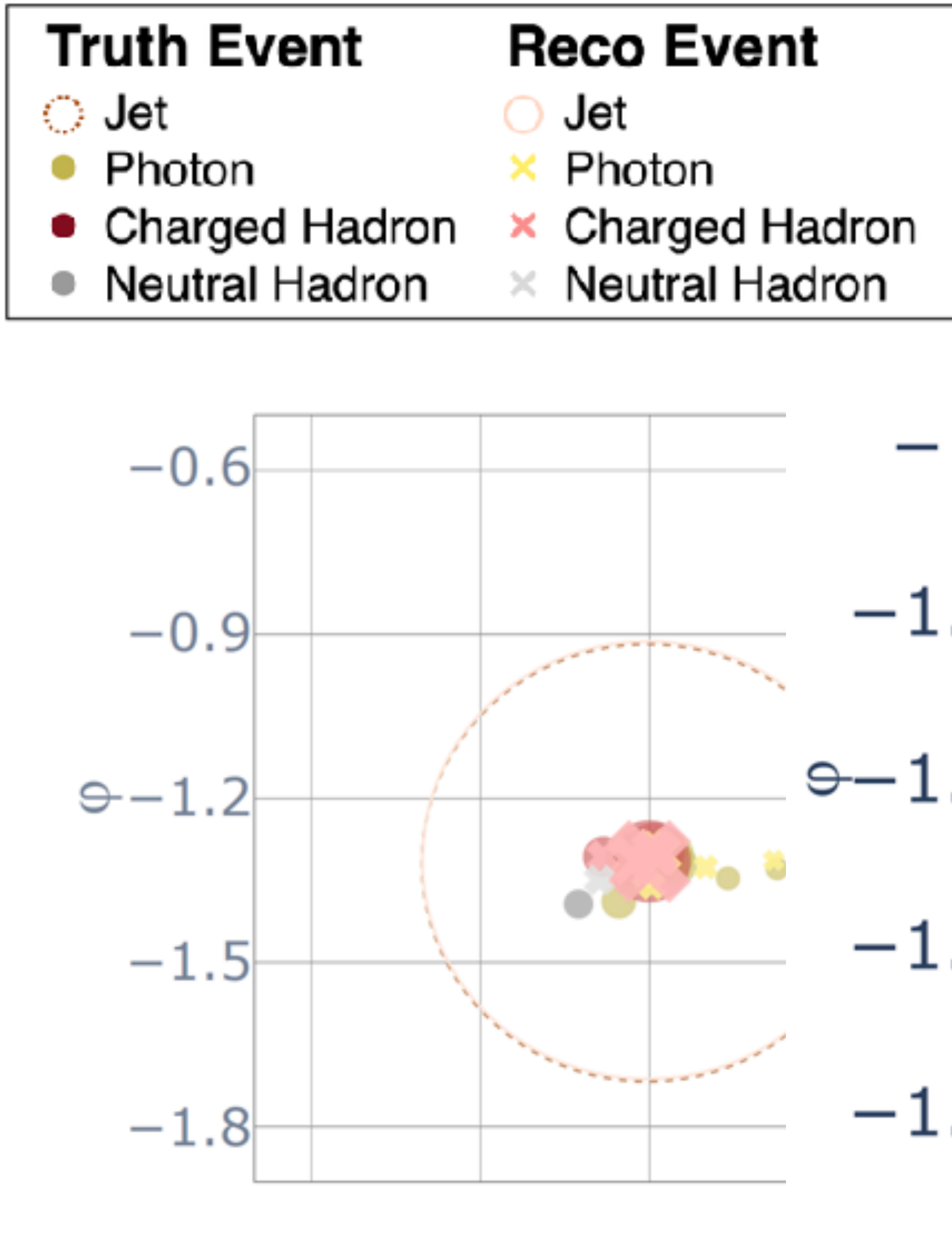
F.A. Di Bello et. al. https://arxiv.org/abs/2212.01328

Jet constituent

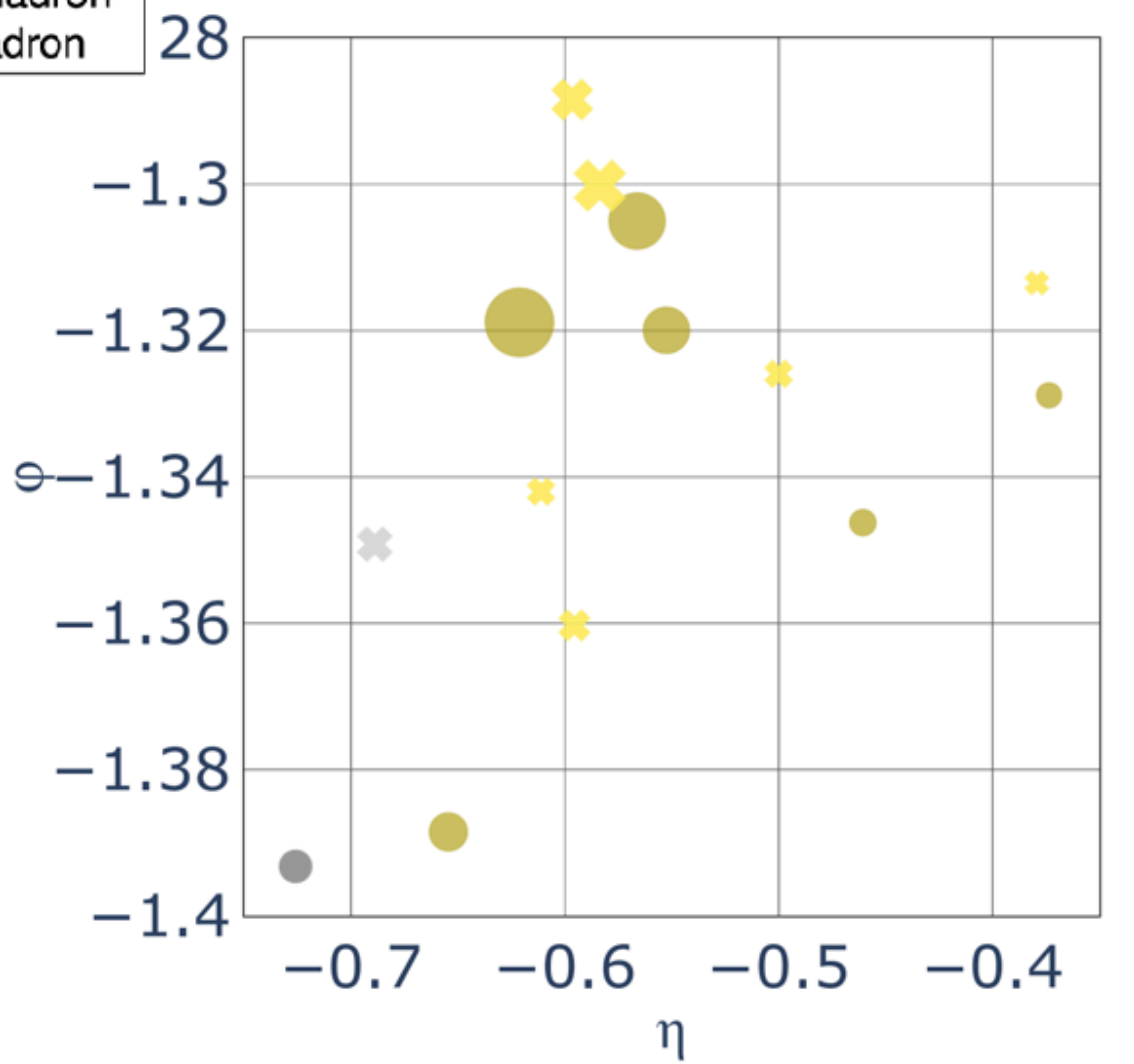


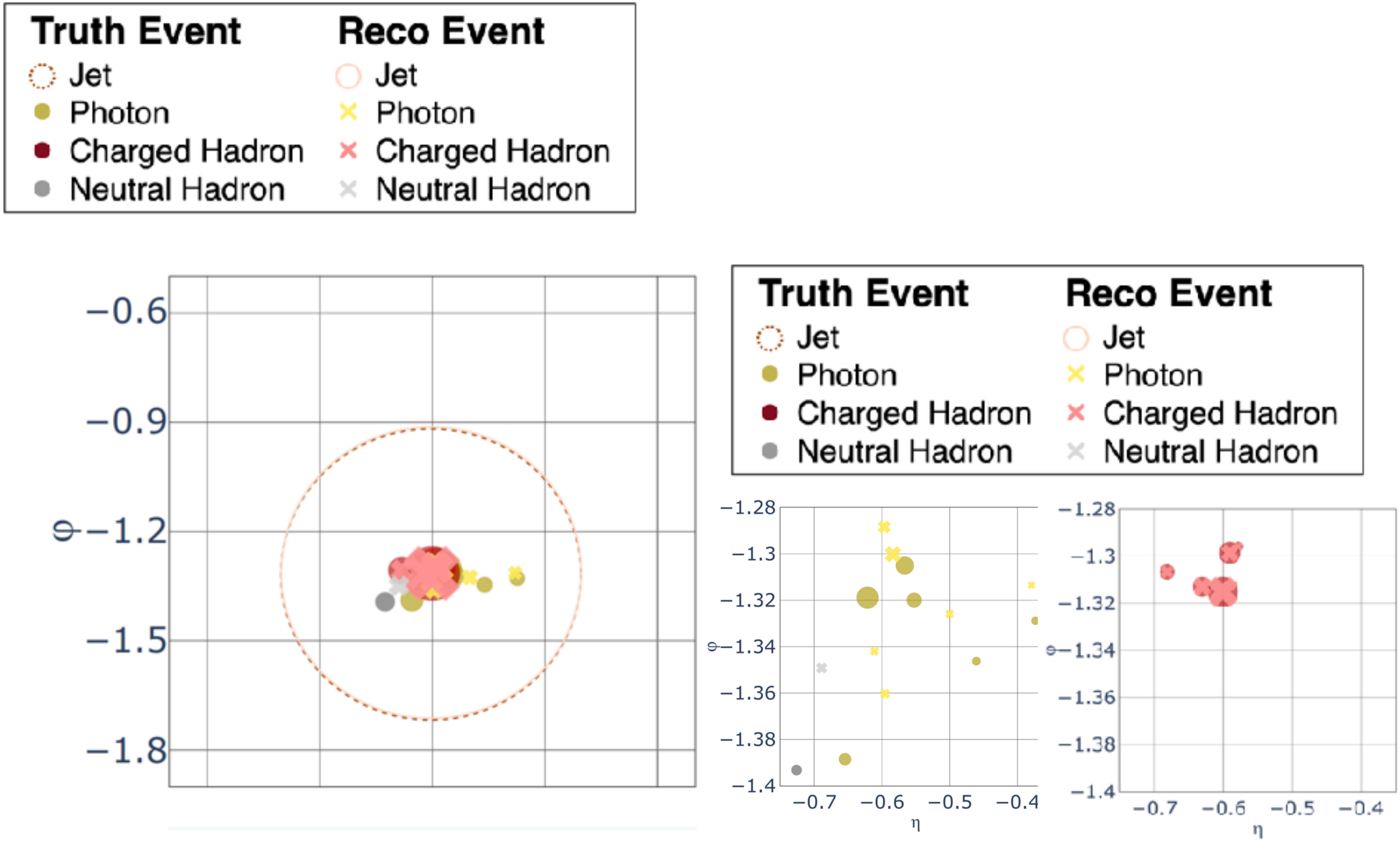



Truth Event
Jet
Photon
Charged Hadron
Neutral Hadron
Reco Event
Jet
Photon
Charged Hadron
Neutral Hadron
φ
−0.6
−0.9
−1.2
−1.5
−1.8
−1.28
−1.3
−1.32
−1.34
−1.36
−1.38
−1.4
−0.7
−0.6
−0.5
−0.4
η



6 photons + 1 neutral had

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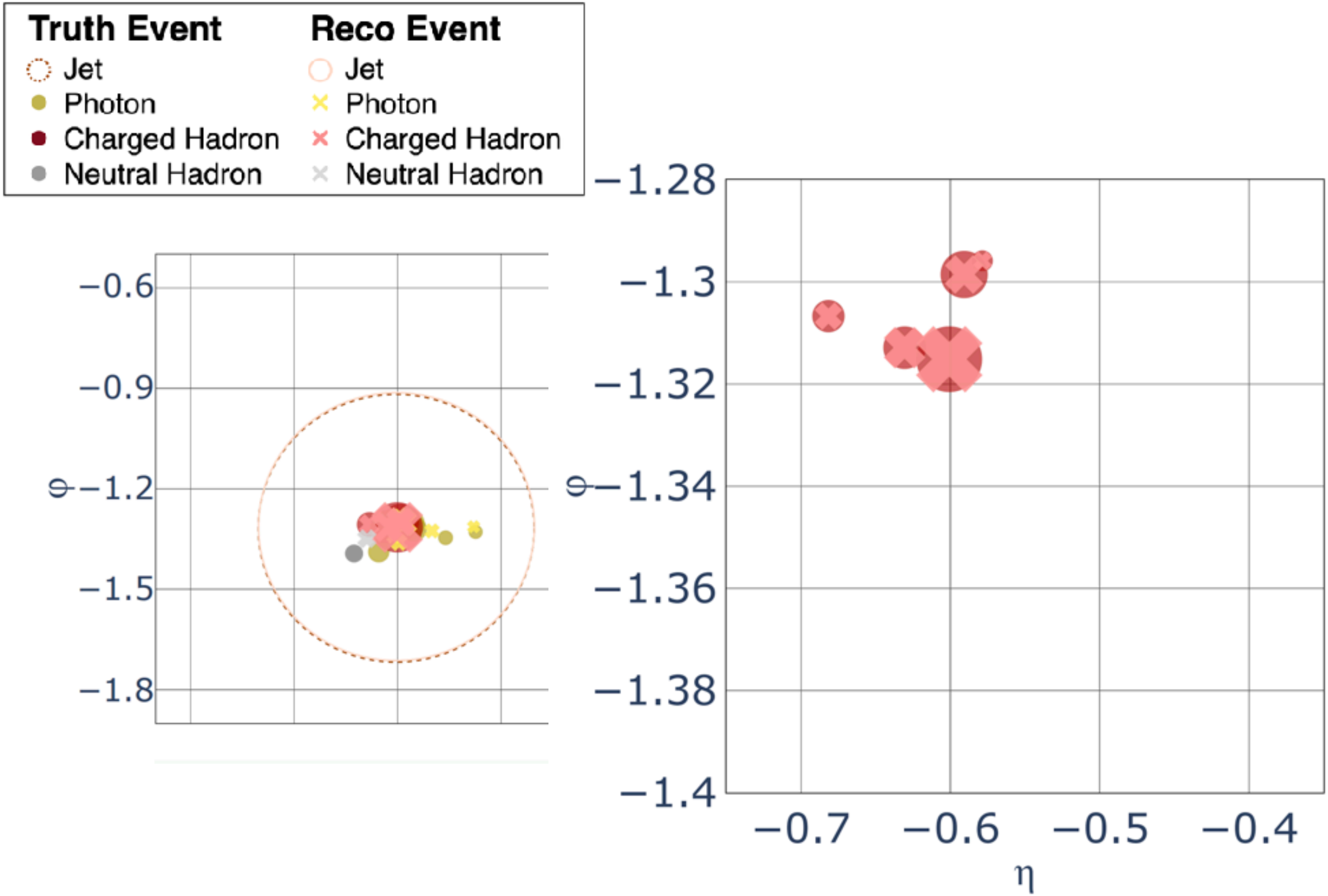
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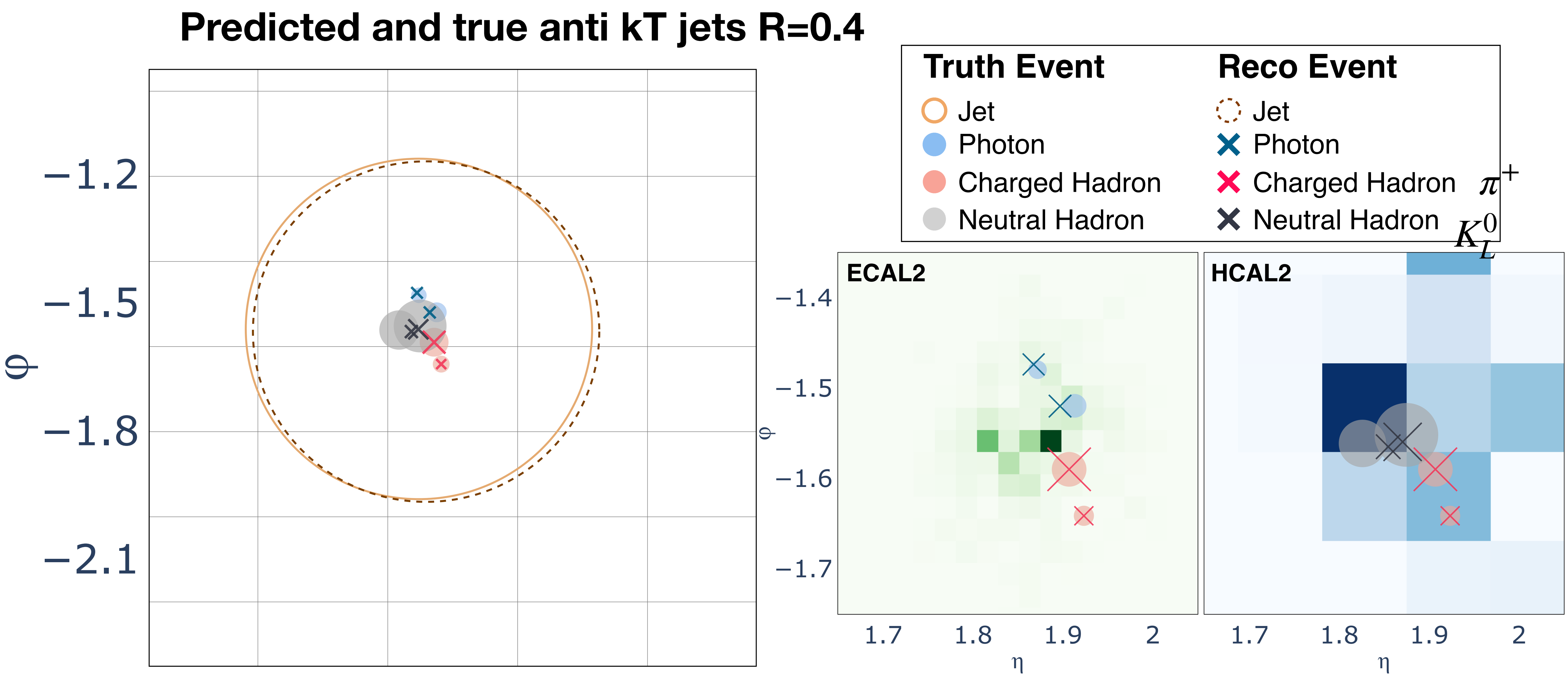
η

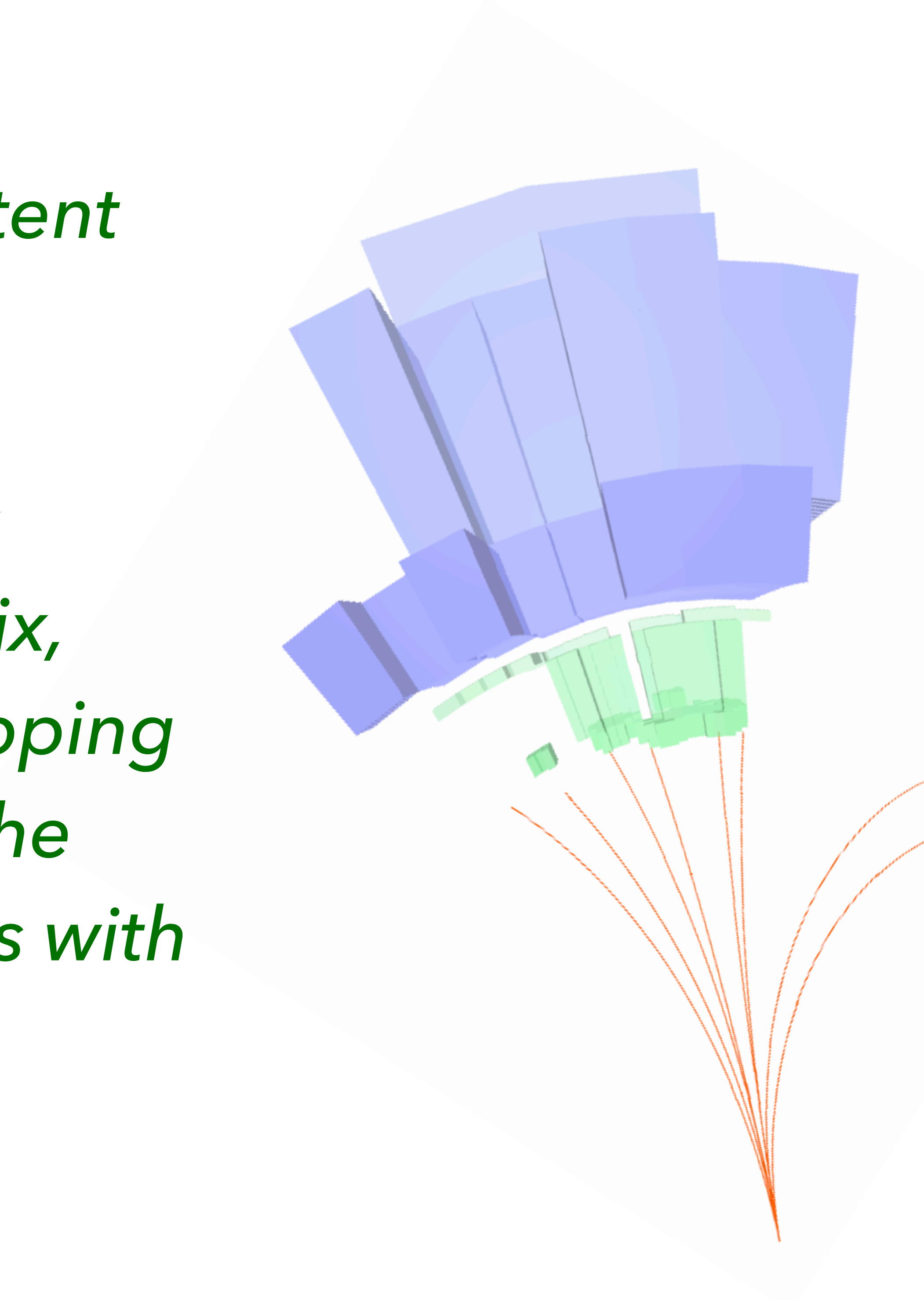
Event Display
Reconstruction with HGPflow



A Comment

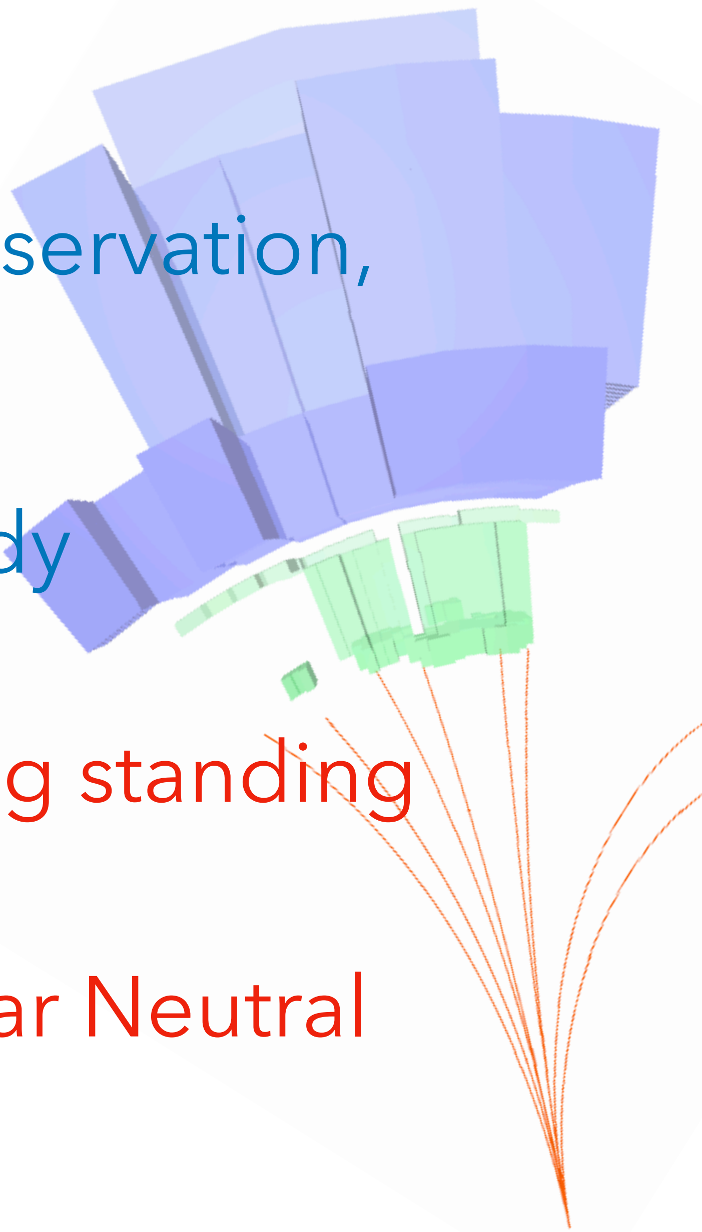
- Why HG{flow is Superior to SA

  - The attention weights in SA have a latent rather than physical meaning and are learned in an unsupervised way.
    On the other hand, HGPflow not only explicitly predicts the incidence matrix, which is the key to unraveling overlapping particle showers, but expresses it in the physical basis of energy contributions with a built in physics induction bias



Conclusion

- *HGPflow (HyperGrpahs PFlow)*:
  hyperedges proxies for particles
  - ✓ Enables physically-interpretable results
  - ✓ Introduces inductive bias towards energy conservation,
  - ✓ Predictions interpretable from physics pov
  - ✓ Shows excellent performance, best in our study



- HGPFlow seems to provide a solution to the long standing Particle Flow problem;
  Allowing to reconstruct particles and in particular Neutral constituents inside a Jet.

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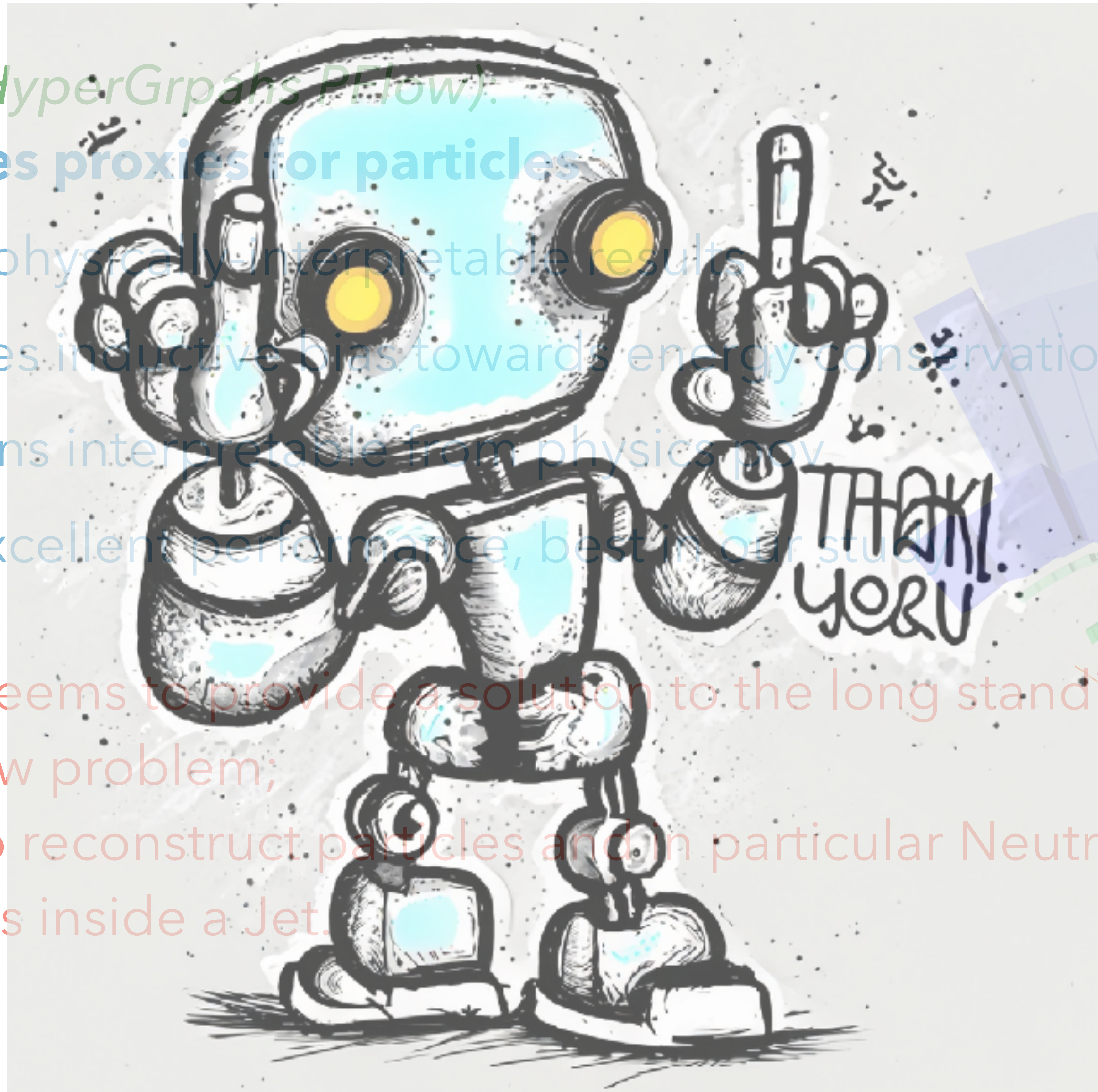

backup