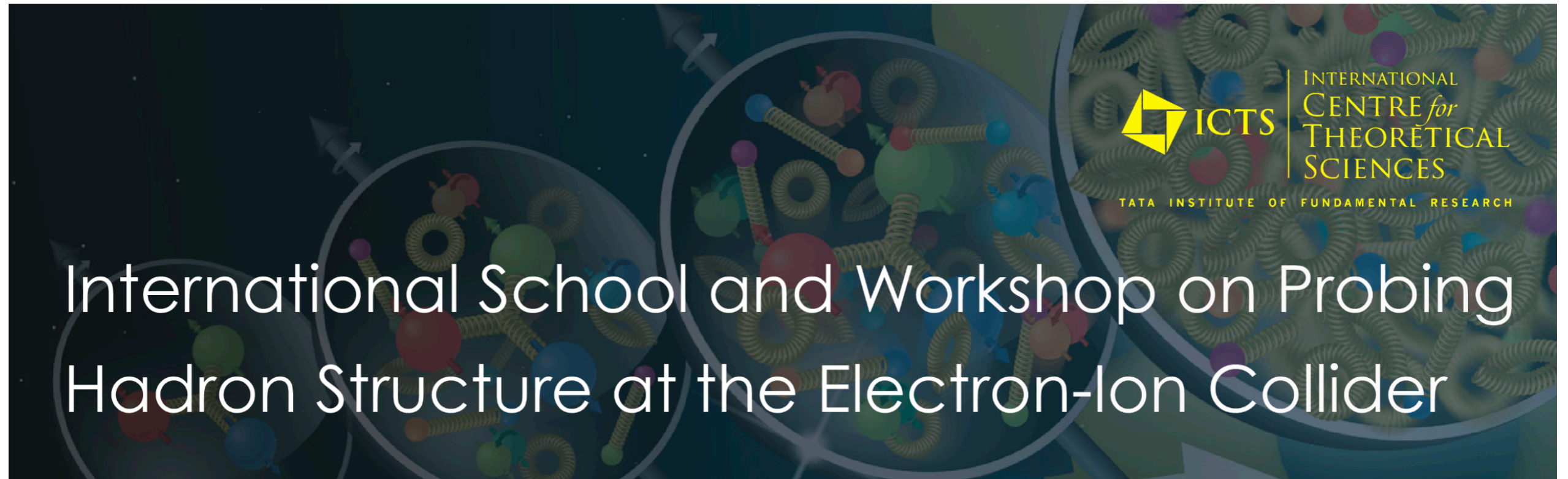


Machine Learning Knowledge exchange : from LHC to EIC



International School and Workshop on Probing
Hadron Structure at the Electron-Ion Collider



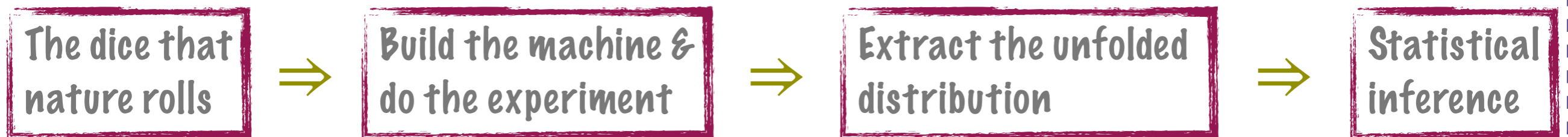
Sanmay Ganguly
IIT-Kanpur
sanmay@iitk.ac.in

The collider experimental program

Simulation based approach :

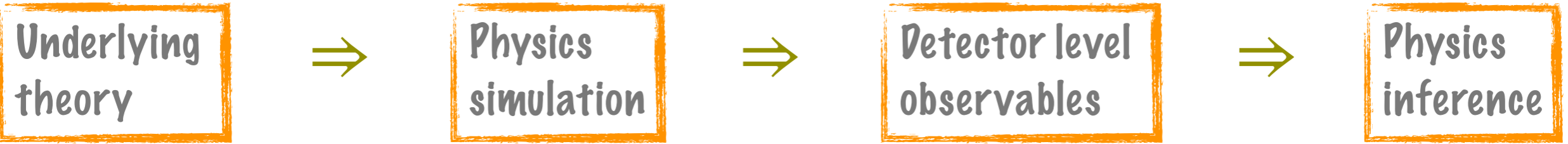


The real experiment :

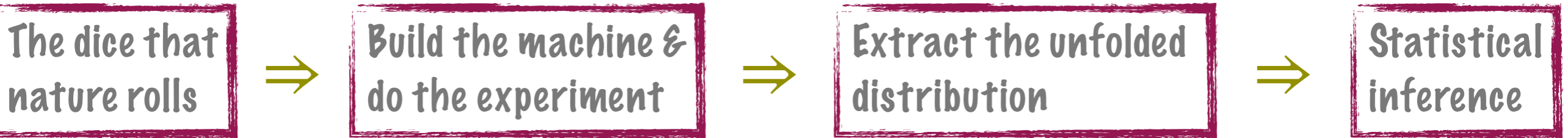


The collider experimental program

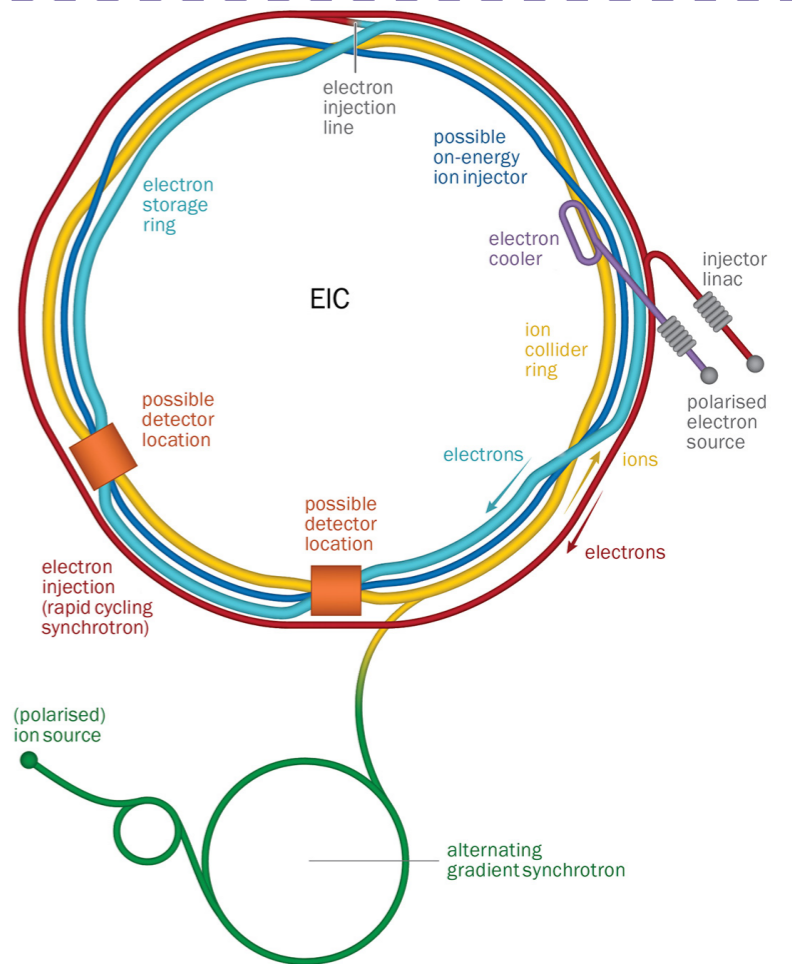
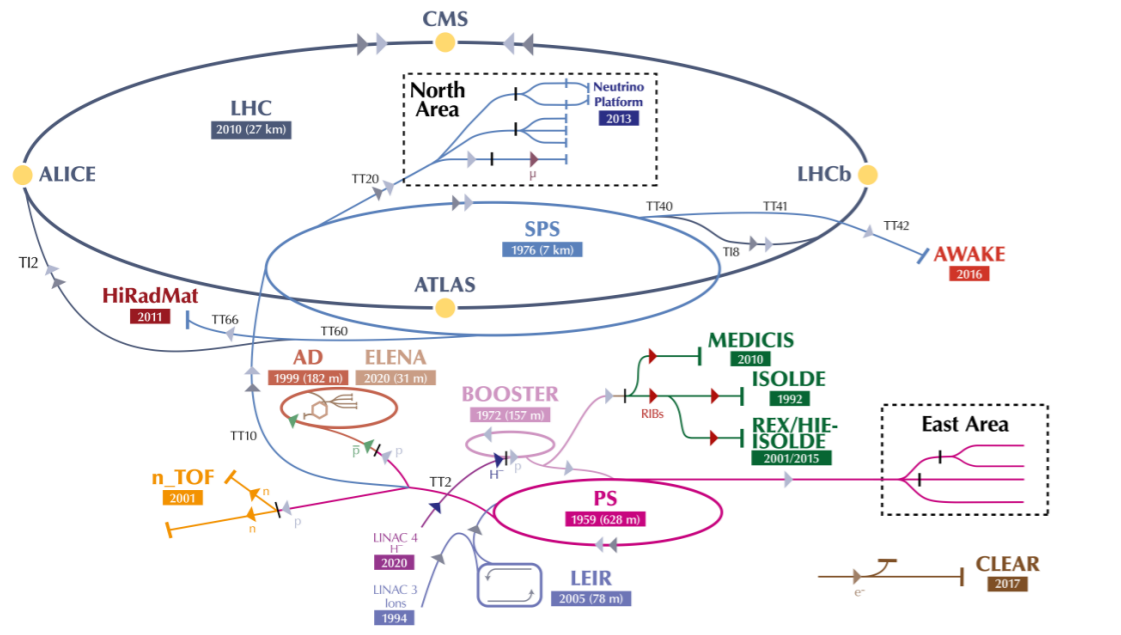
Simulation based approach :



The real experiment :



The CERN accelerator complex
Complexe des accélérateurs du CERN



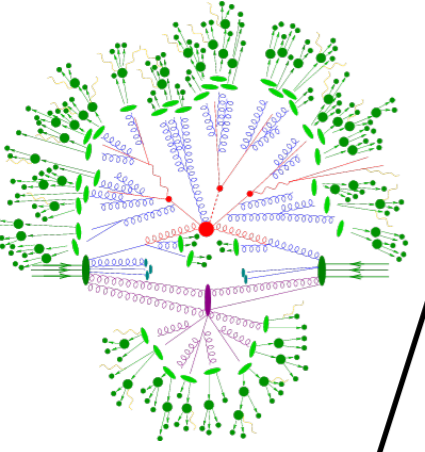
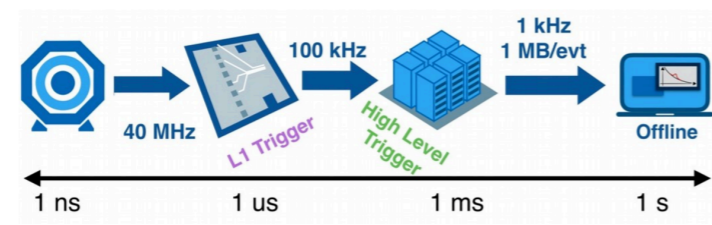
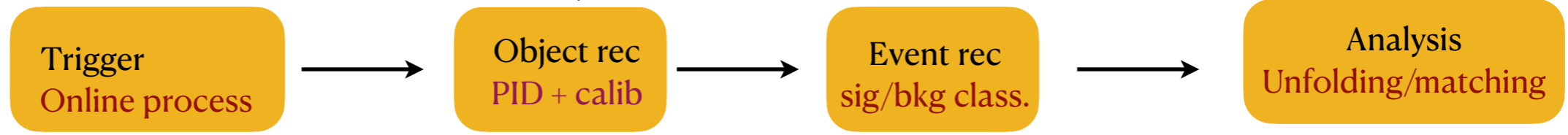
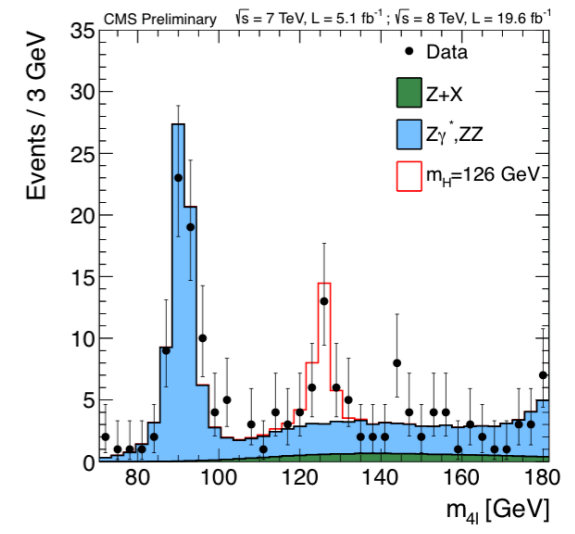
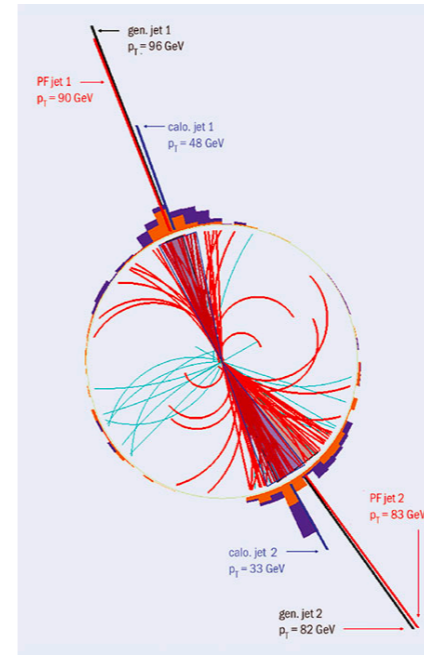
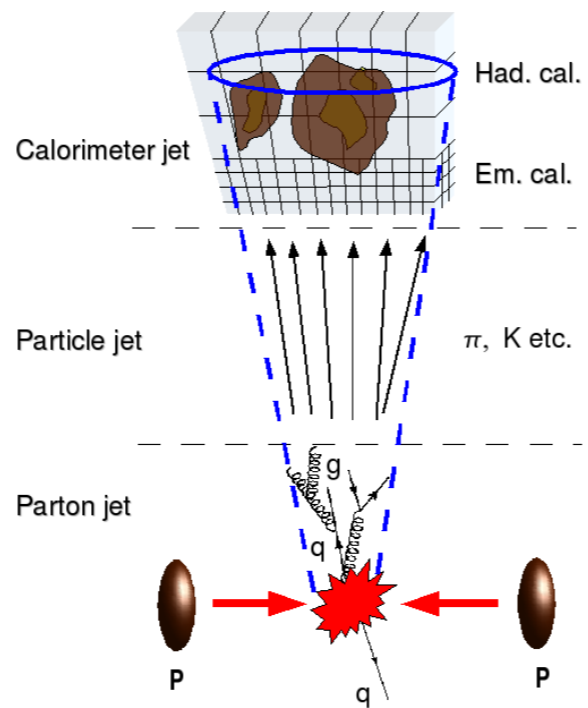
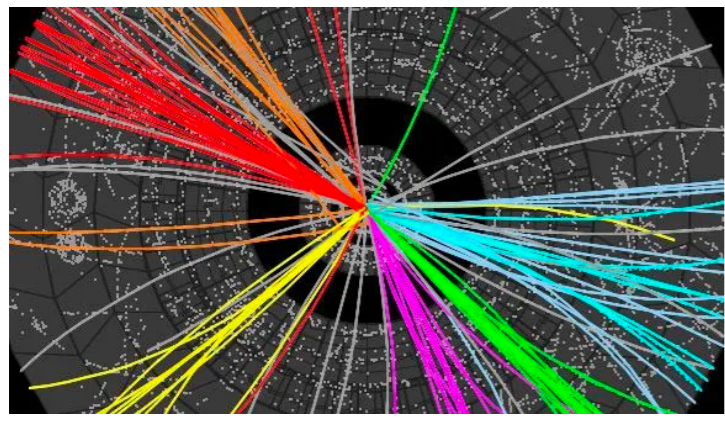
▶ H⁻ (hydrogen anions) ▶ p (protons) ▶ ions ▶ RIBs (Radioactive Ion Beams) ▶ n (neutrons) ▶ \bar{p} (antiprotons) ▶ e⁻ (electrons) ▶ μ (muons)

LHC - Large Hadron Collider // SPS - Super Proton Synchrotron // PS - Proton Synchrotron // AD - Antiproton Decelerator // CLEAR - CERN Linear Electron Accelerator for Research // AWAKE - Advanced WAKEfield Experiment // ISOLDE - Isotope Separator OnLine // REX/HIE-ISOLDE - Radioactive Experiment/High Intensity and Energy ISOLDE // MEDICIS // LEIR - Low Energy Ion Ring // LINAC - LINear ACcelerator //

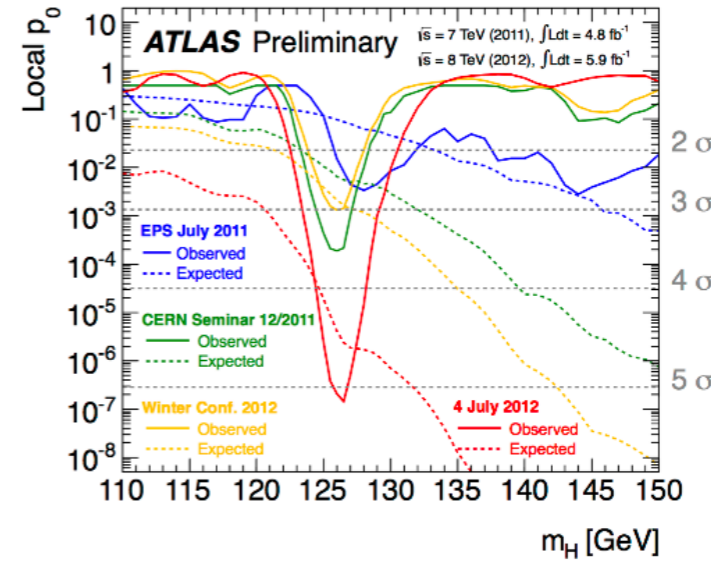
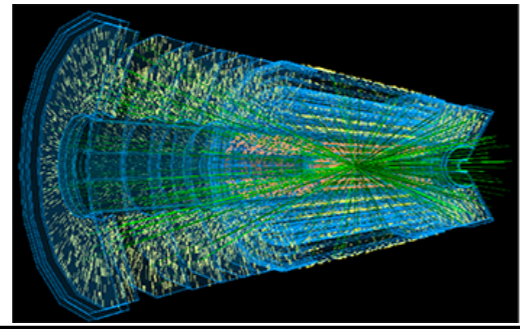
n_TOF - Neutrons Time Of Flight // HiRadMat - High-Radiation to Materials // Neutrino Platform
<https://cds.cern.ch/images/CERN-GRAPHICS-2022-001-1>

https://cerncourier.com/wp-content/uploads/2021/09/CCUSASupp21_EIC_fig1.jpg

The collider program flow-chain



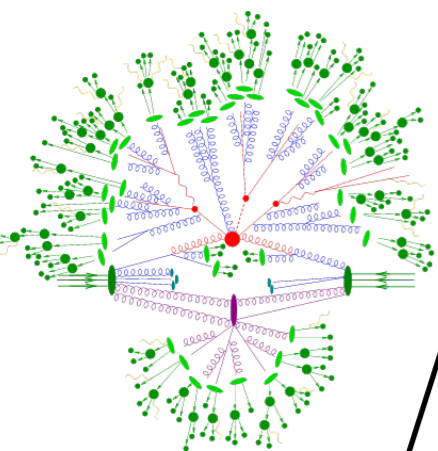
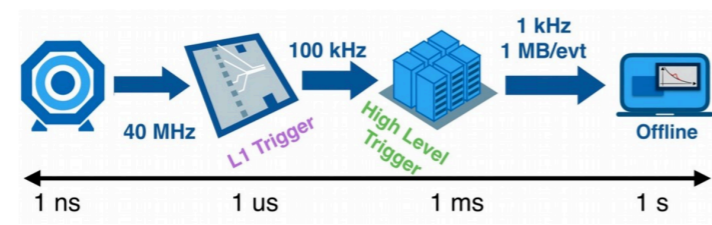
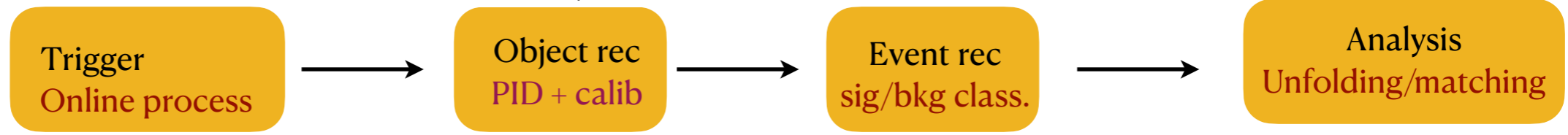
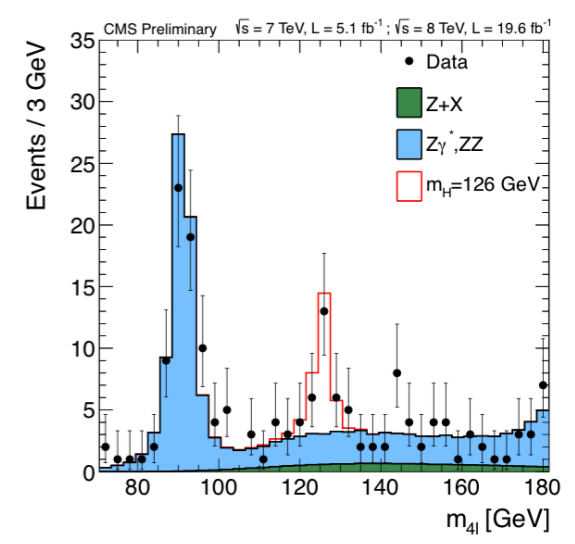
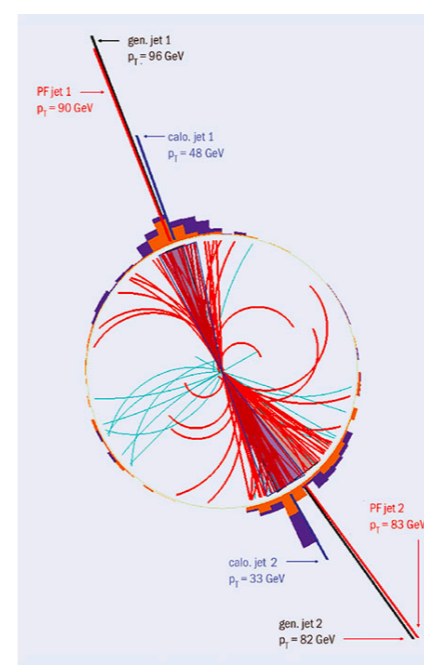
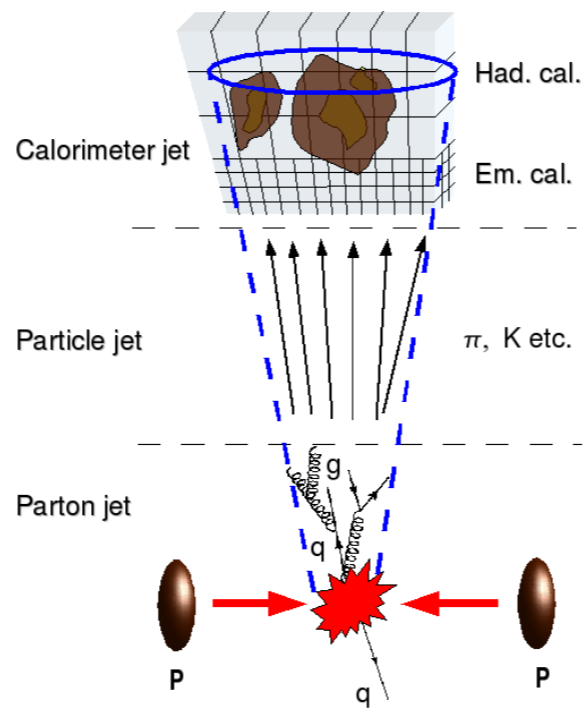
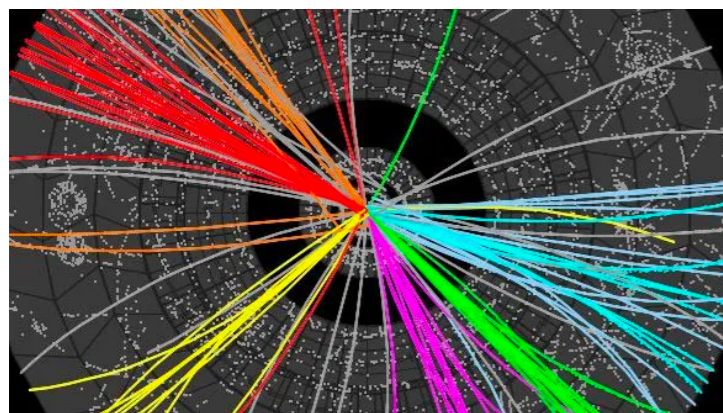
ME + PS generation
Detector Simulation



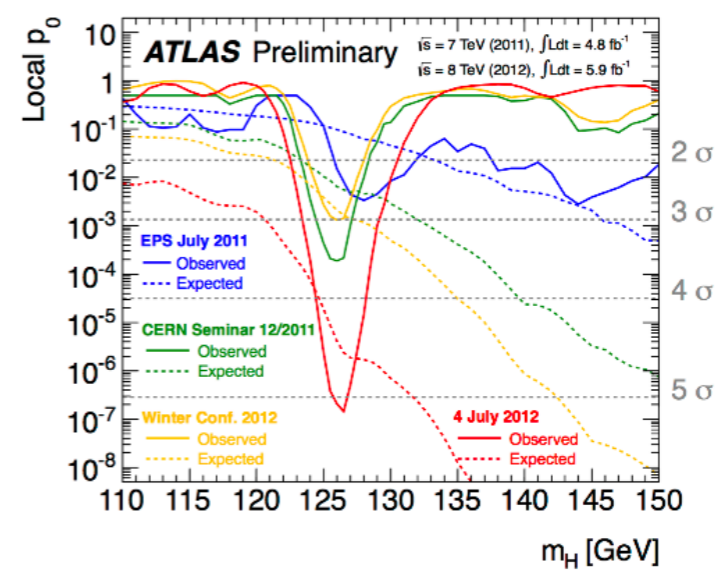
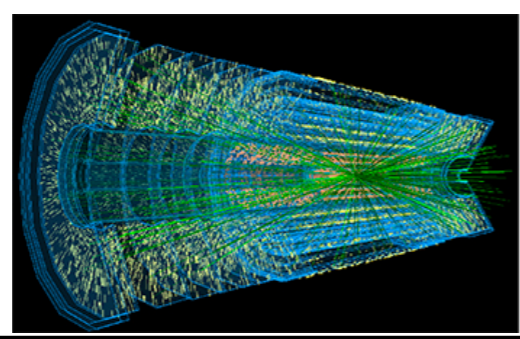
Inference

The collider program flow-chain

ML can (and will) play a role at every instance of this flow chain.

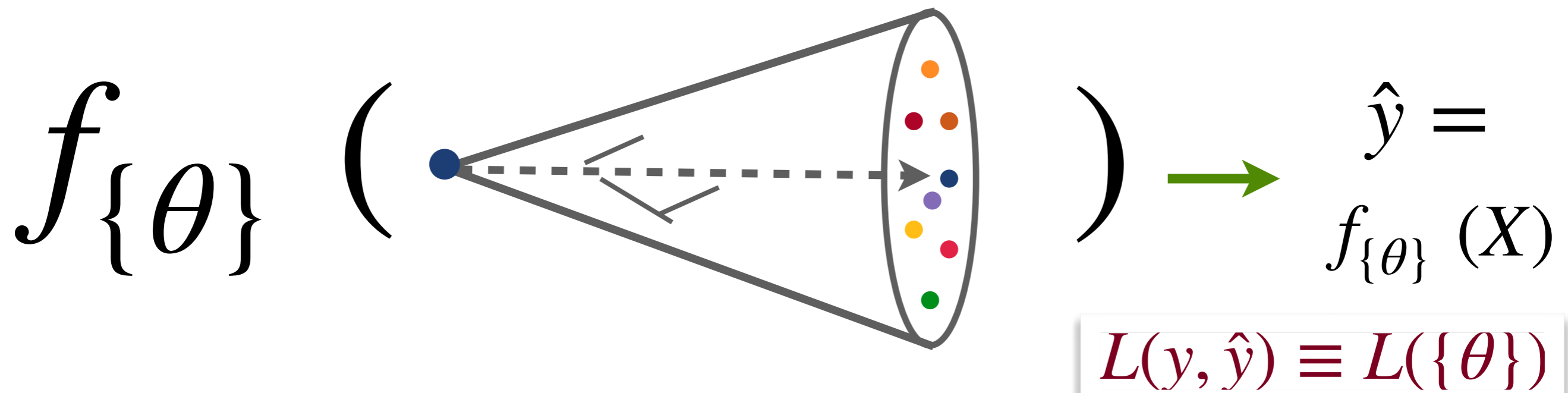


ME + PS generation
Detector Simulation



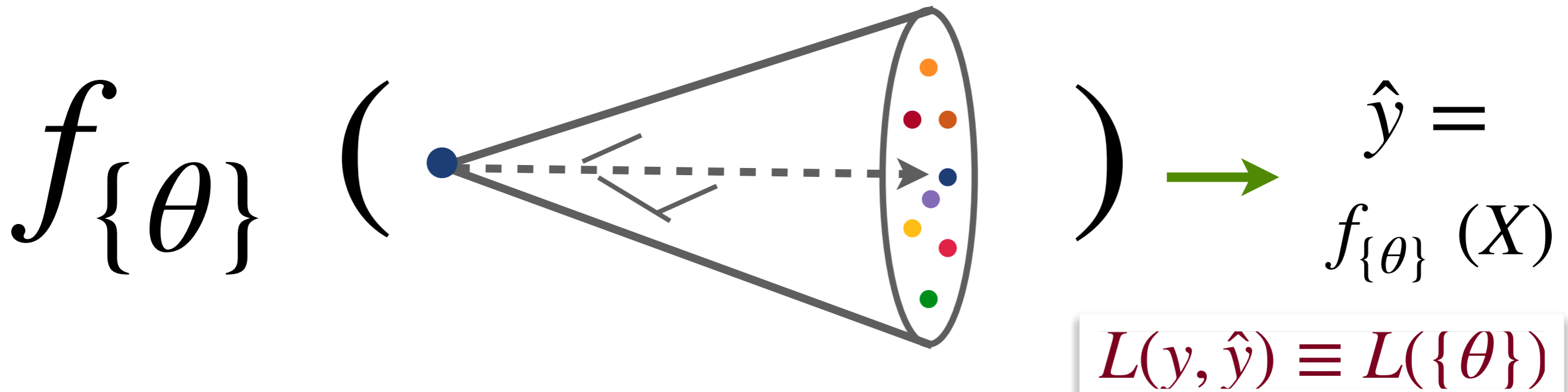
Inference

ML@Colliders : what's the broad task?



ML@Colliders : what's the broad task?

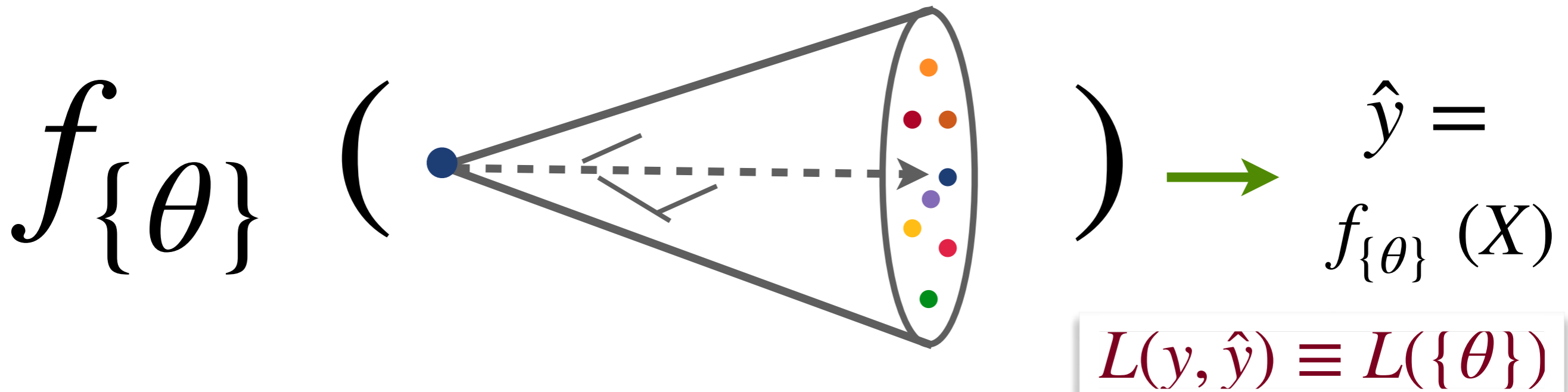
1. Decide the right representation of the data (images/graphs/trees..)



ML@Colliders : what's the broad task?

2. Choose a NN model
(CNN/GNN/)

1. Decide the right representation
of the data (images/graphs/trees..)

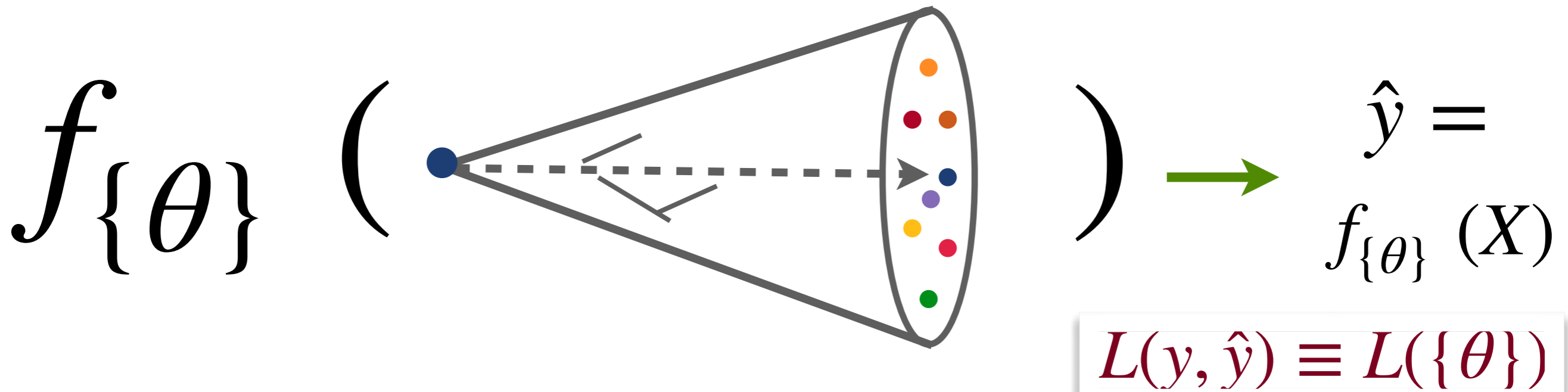


ML@Colliders : what's the broad task?

2. Choose a NN model
(CNN/GNN/)

1. Decide the right representation
of the data (images/graphs/trees..)

3. With a defined learning task,
compute the loss function.



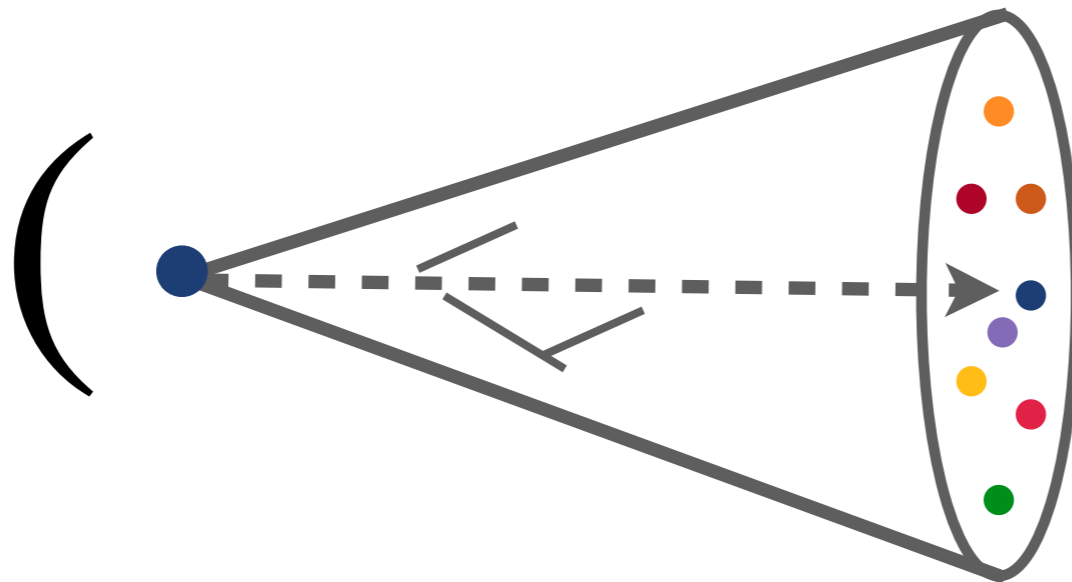
ML@Colliders : what's the broad task?

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of the data (images/graphs/trees..)

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compute the loss function.

$f_{\{\theta\}}$



Variation in data

$\hat{y} =$
 $f_{\{\theta\}}(X)$

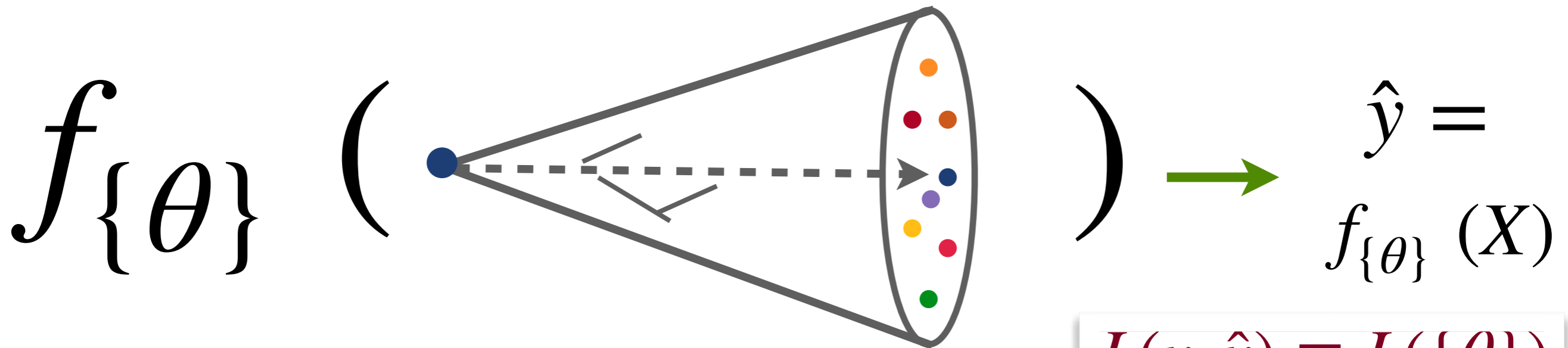
$$L(y, \hat{y}) \equiv L(\{\theta\})$$

ML@Colliders : what's the broad task?

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$$L(y, \hat{y}) \equiv L(\{\theta\})$$

Variation in data

Unsupervised

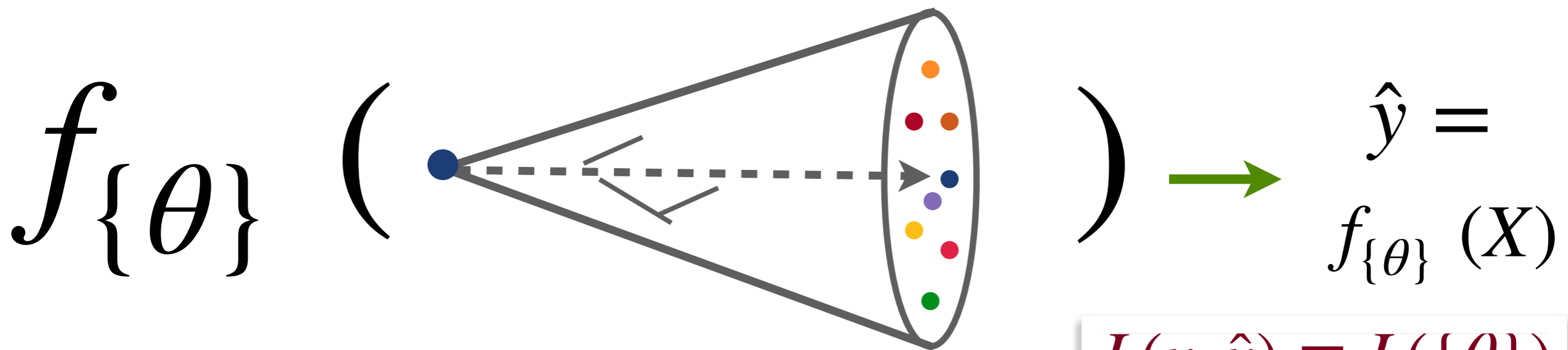
No-labels, the task is to
figure out $p(x)$ from which
the data is drawn. e.g. VAE

ML@Colliders : what's the broad task?

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$$L(y, \hat{y}) \equiv L(\{\theta\})$$

Variation in data

Unsupervised

Semi-supervised

No-labels, the task is to figure out $p(x)$ from which the data is drawn. e.g. VAE

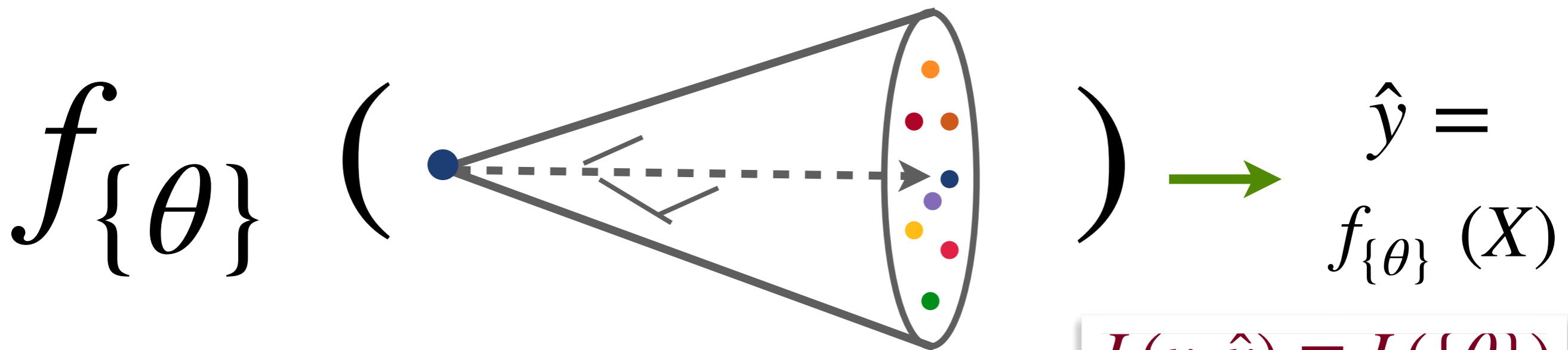
Noisy labels. estimate : $p(s\text{-enriched})/p(s\text{-depleted})$

ML@Colliders : what's the broad task?

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$$L(y, \hat{y}) \equiv L(\{\theta\})$$

Variation in data

Unsupervised

Semi-supervised

Weakly-supervised

No-labels, the task is to figure out $p(x)$ from which the data is drawn. e.g. VAE

Noisy labels. estimate : $p(s\text{-enriched})/p(s\text{-depleted})$

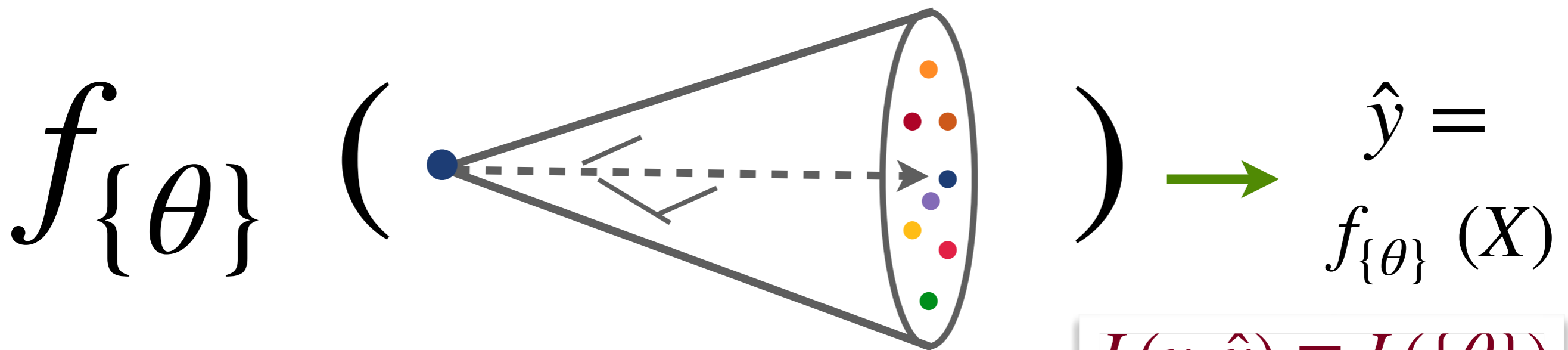
Partial labels. e.g. simulating : SM bkg vs many NP signals.

ML@Colliders : what's the broad task?

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$$L(y, \hat{y}) \equiv L(\{\theta\})$$

Variation in data

Unsupervised

Semi-supervised

Weakly-supervised

Supervised

No-labels, the task is to figure out $p(x)$ from which the data is drawn. e.g. VAE

Noisy labels. estimate : $p(s\text{-enriched})/p(s\text{-depleted})$

Partial labels. e.g. simulating : SM bkg vs many NP signals.

Learning on all the well labeled data.

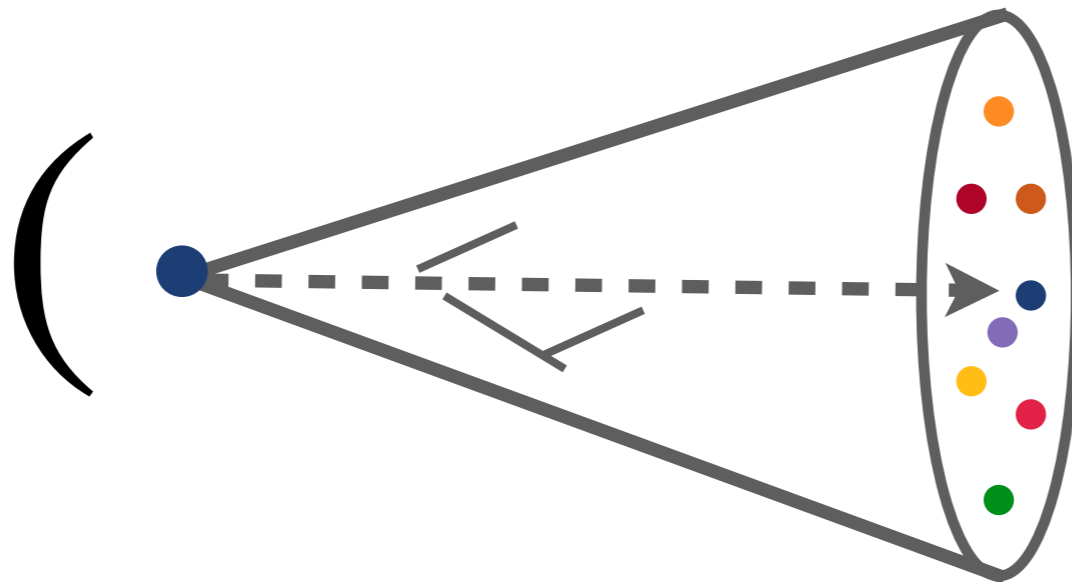
ML@Colliders : what's the broad task?

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$f_{\{\theta\}}$



$\hat{y} = f_{\{\theta\}}(X)$

$$L(y, \hat{y}) \equiv L(\{\theta\})$$

Self-supervised

Variation in data

Unsupervised

Semi-supervised

Weakly-supervised

Supervised

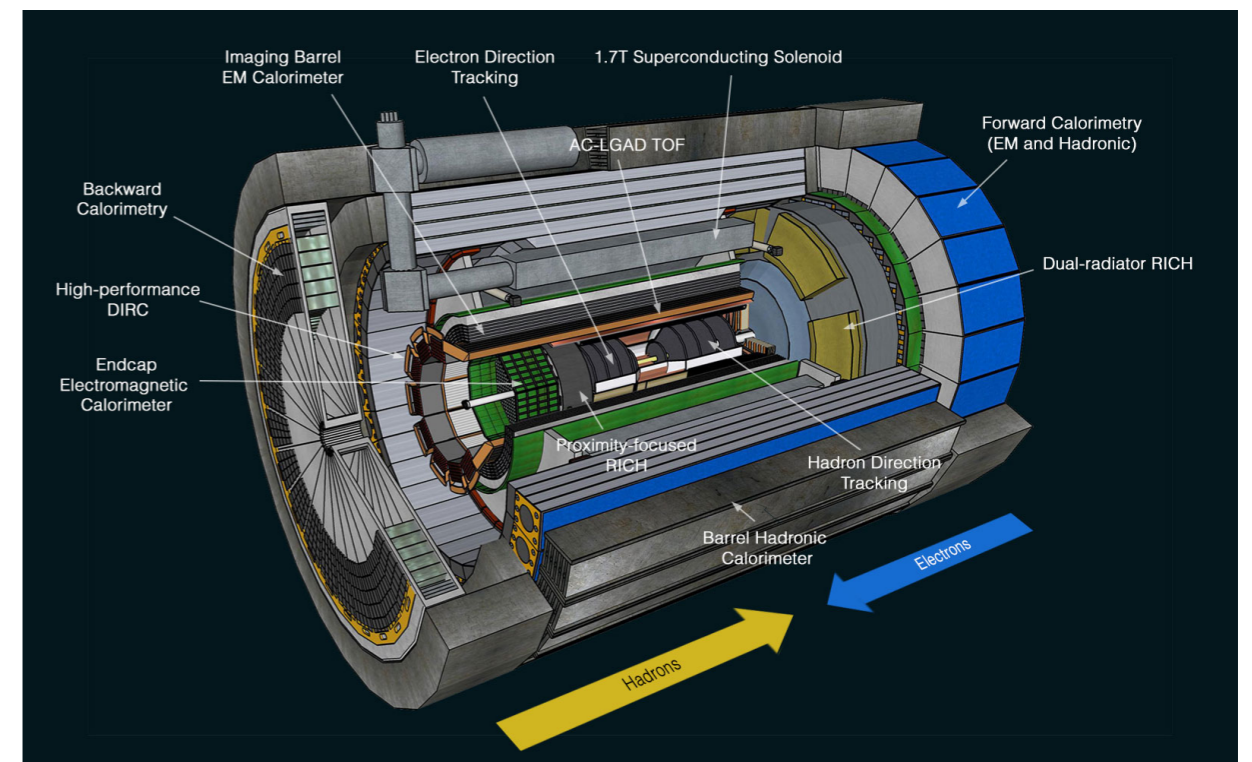
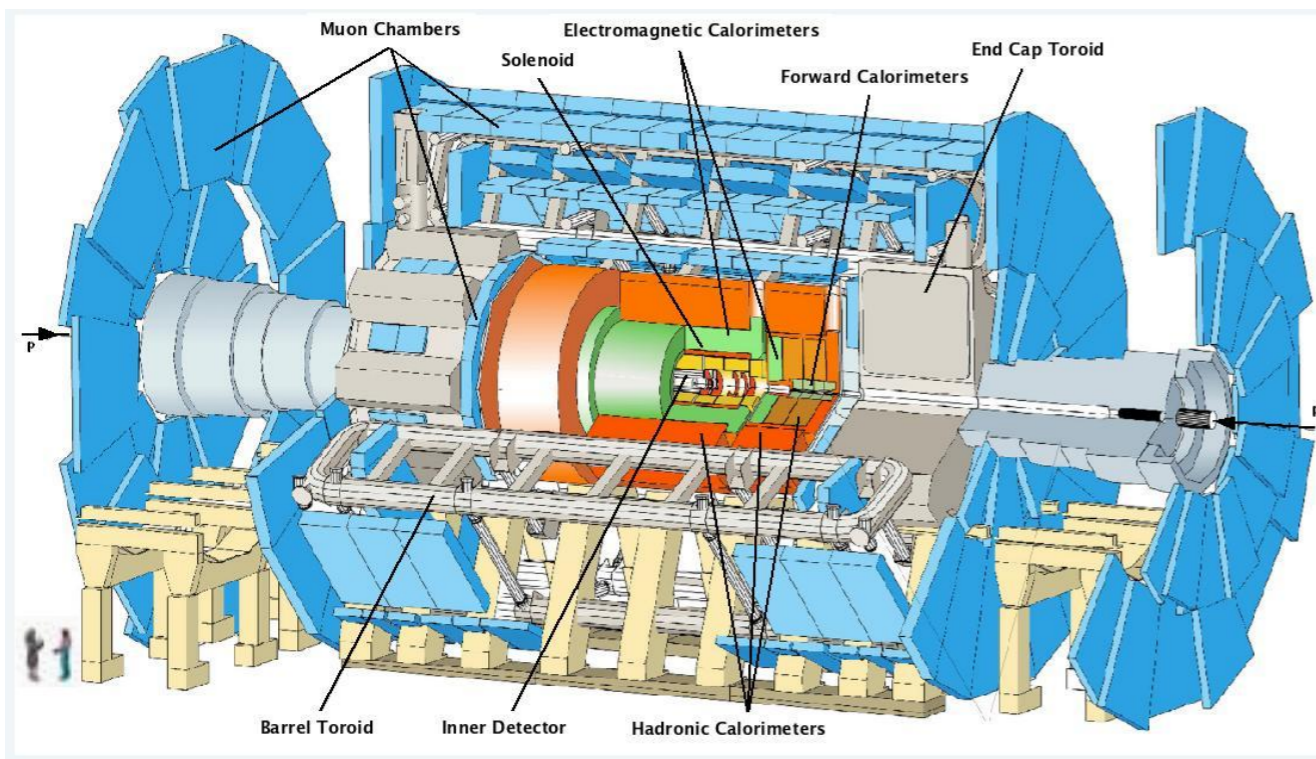
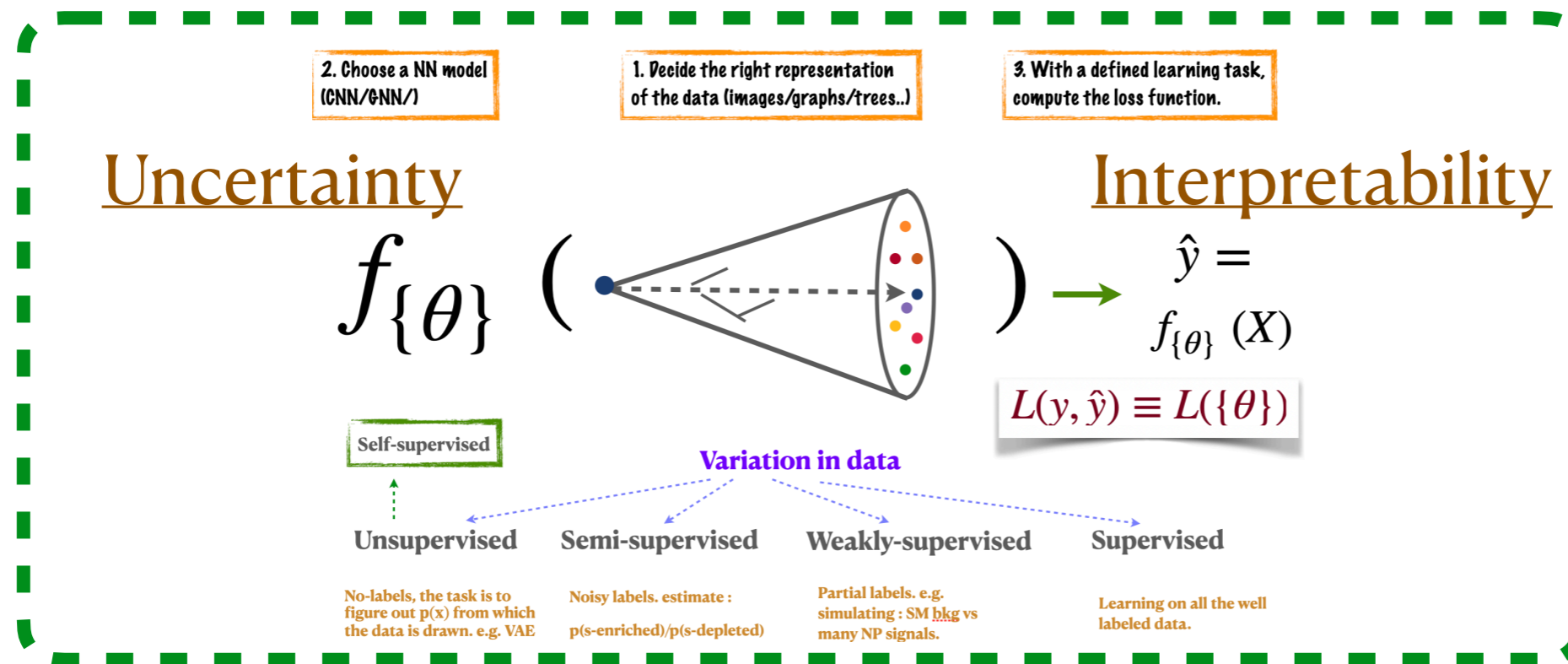
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Noisy labels. estimate : $p(s\text{-enriched})/p(s\text{-depleted})$

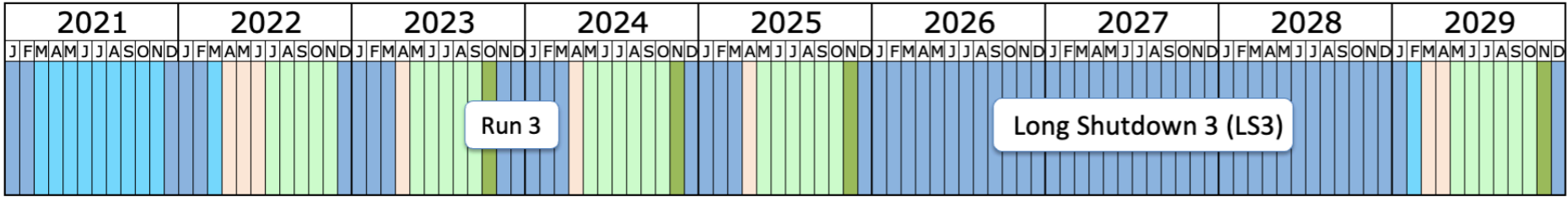
Partial labels. e.g. simulating : SM bkg vs many NP signals.

Learning on all the well labeled data.

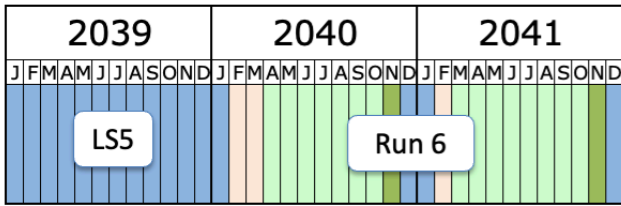
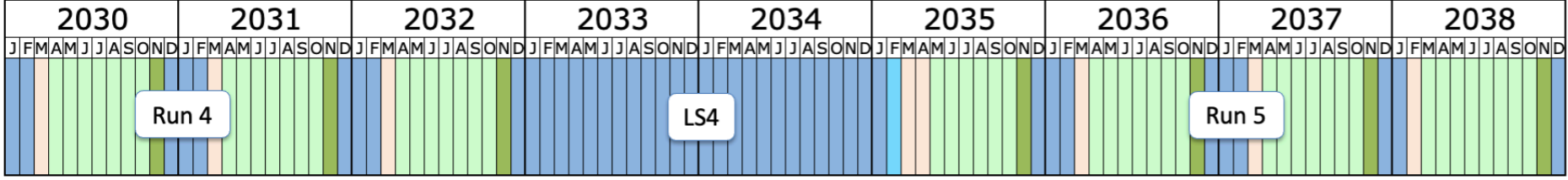
Looking the problem through ML lens



We have time for a coffee together

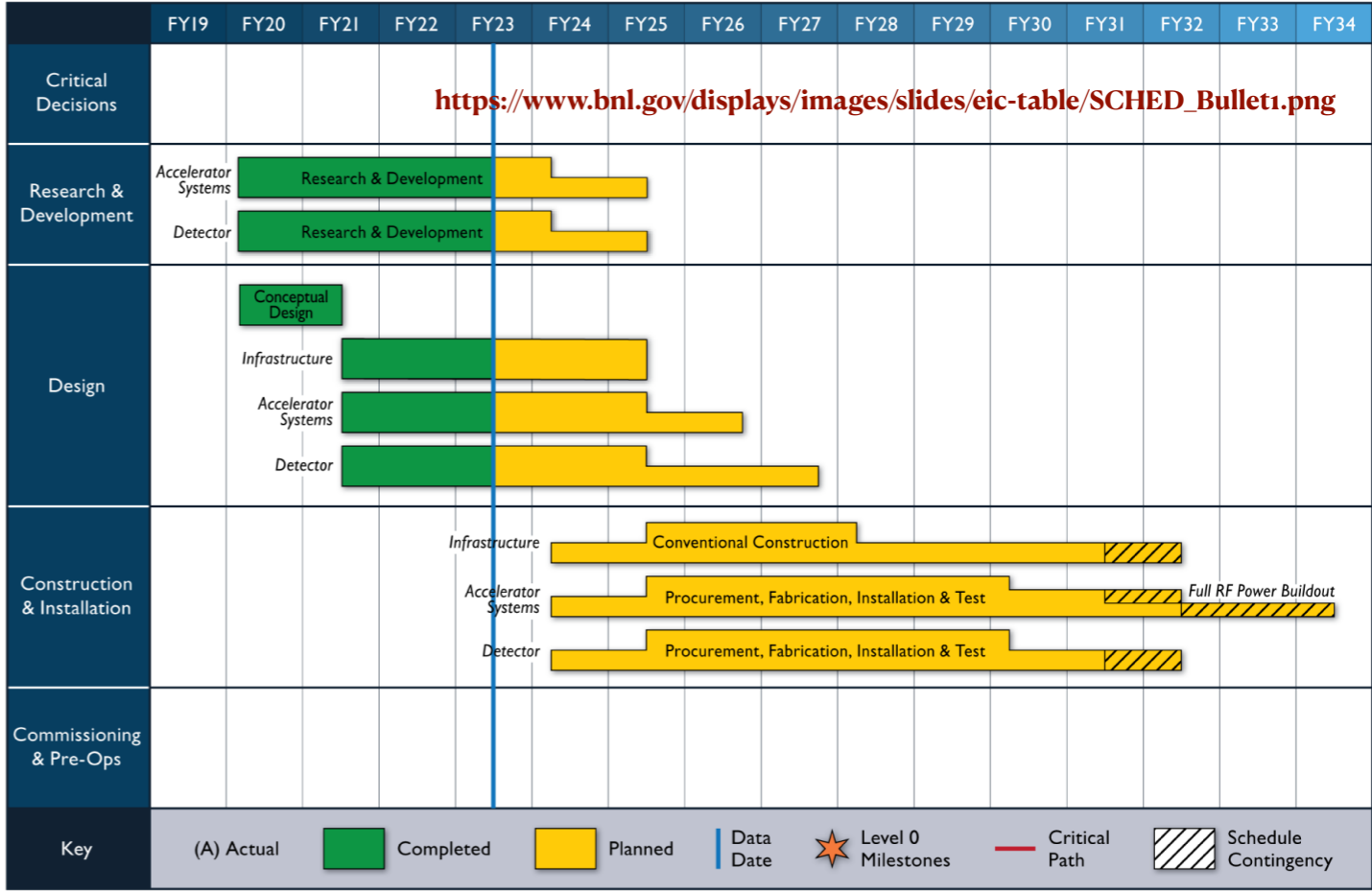


<http://lhc-commissioning.web.cern.ch/schedule/LHC-long-term.htm>

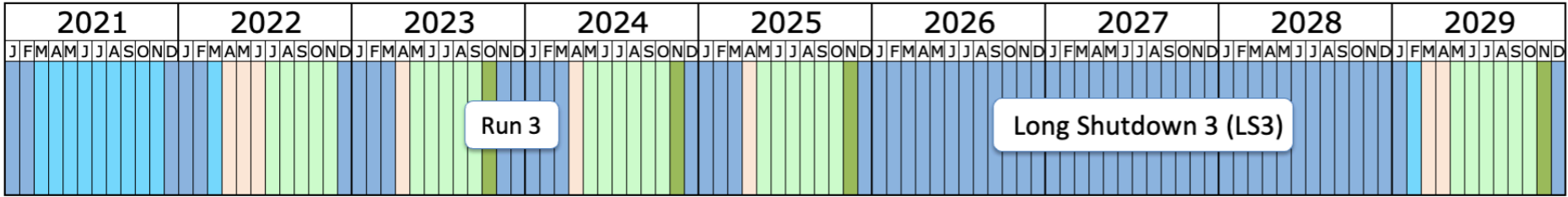


Last update: April 2023

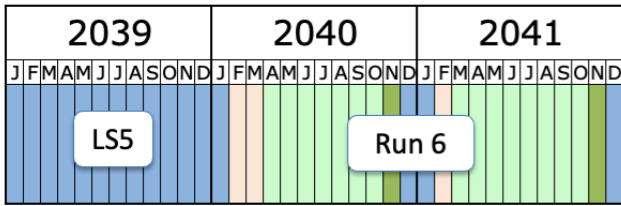
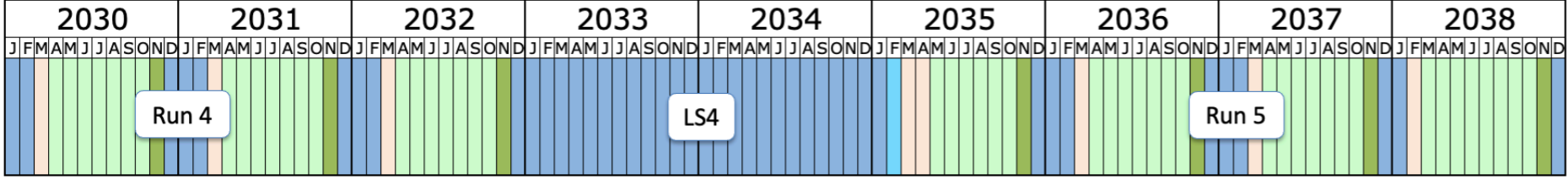
- Shutdown/Technical stop
- Protons physics
- Ions
- Commissioning with beam
- Hardware commissioning



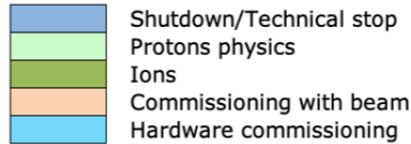
We have time for a coffee together



<http://lhc-commissioning.web.cern.ch/schedule/LHC-long-term.htm>



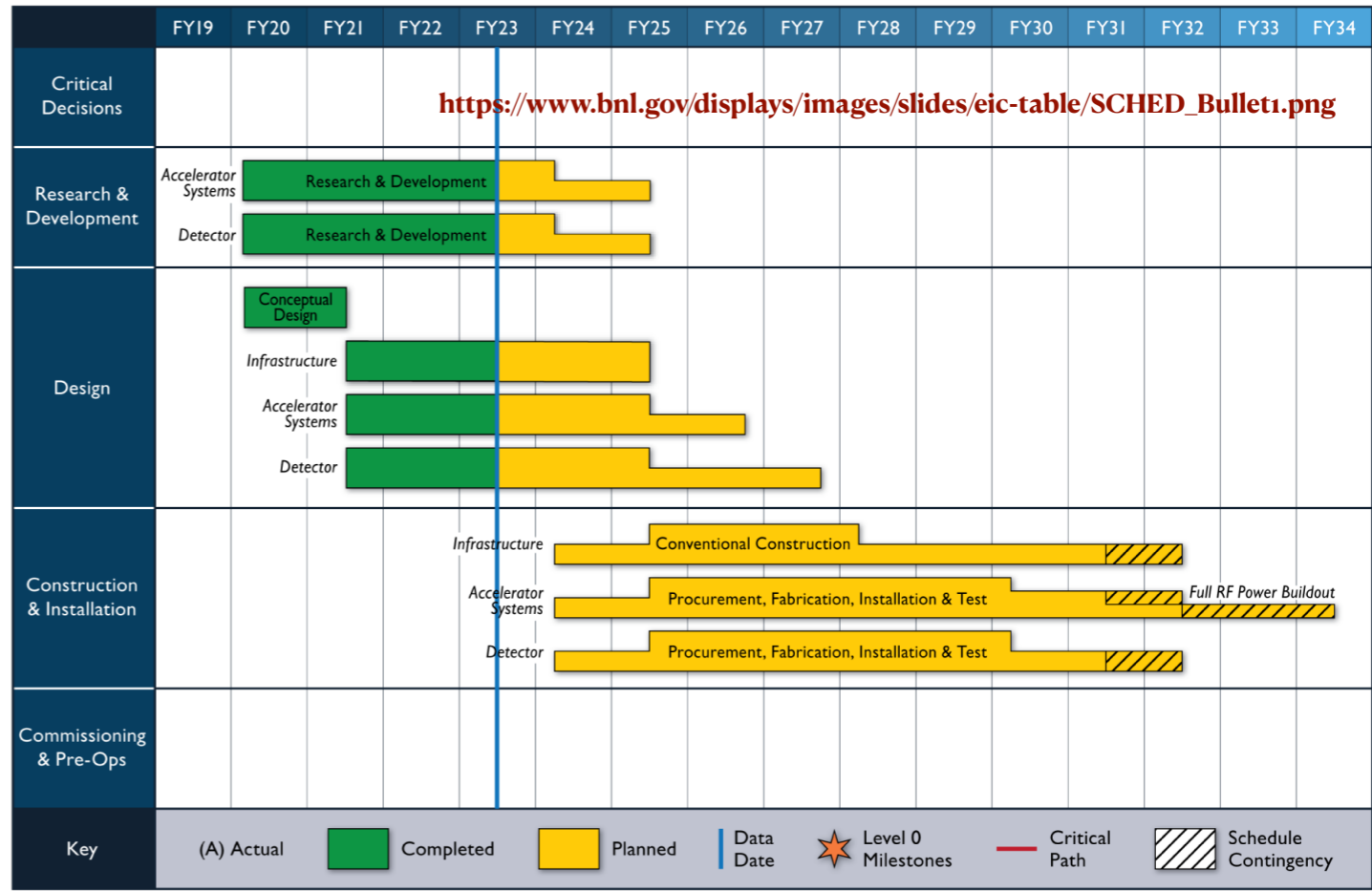
Last update: April 2023



There will be a decade of overlap between LHC and EIC.

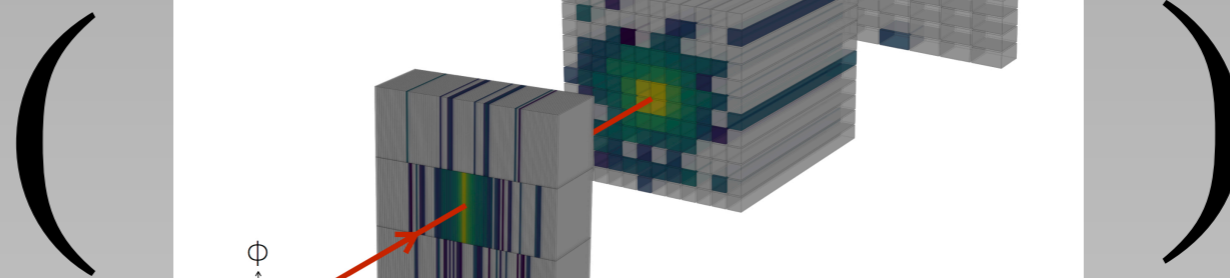
The probe of strong interaction program will have overlapping physics goals.

Through the ML lens the formulation of the problems will be closer.



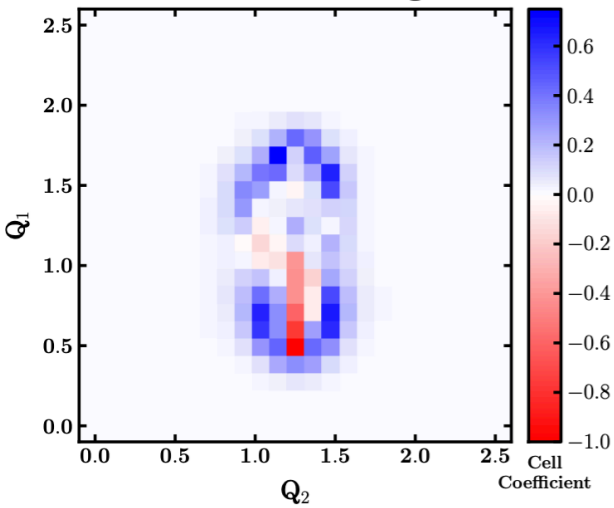
Calorimetry

Image from 1705.02355

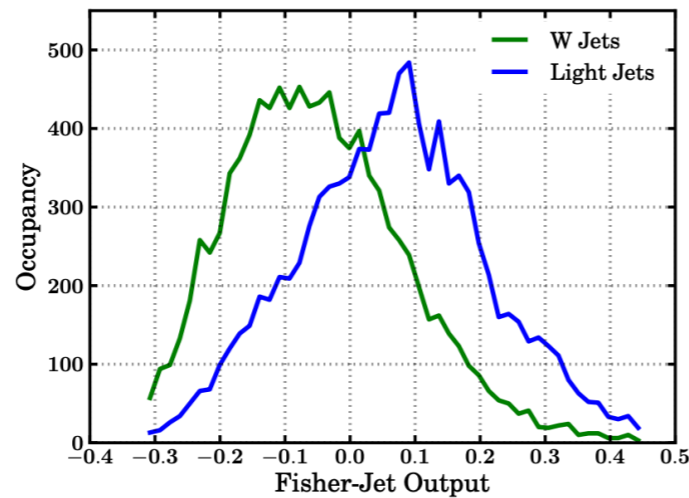
 $f_{\{\theta\}}$ 

Calorimetry + ML early works

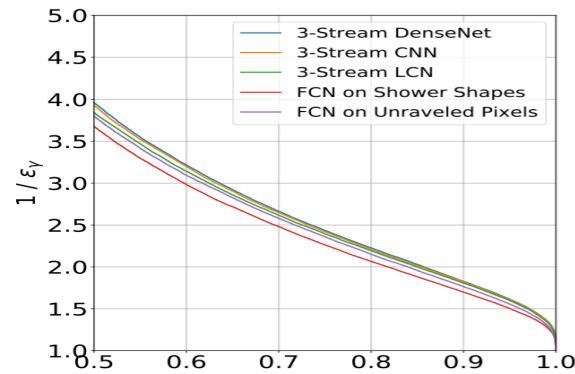
J. Cogan et-al JHEP 02 (2015) 118



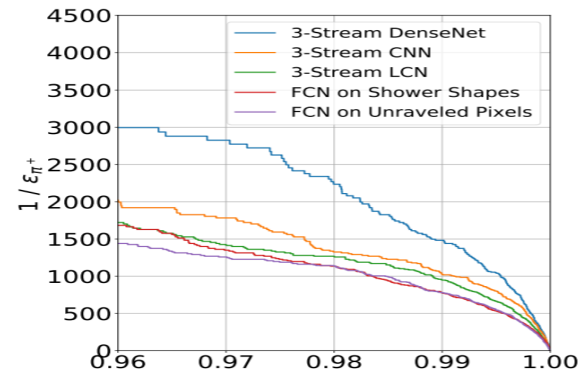
(a) Fisher-Jet



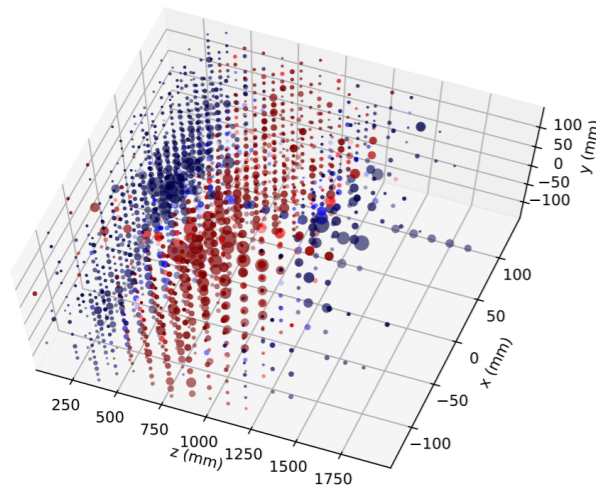
(b) Fisher-Jet Discriminant Output



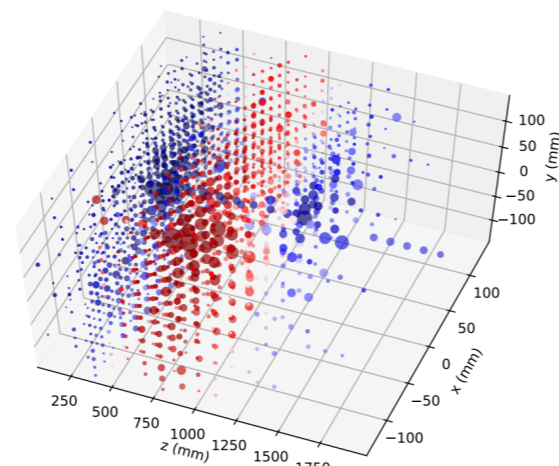
L. De Oliveira et-al NIM-A 951v162879
(a) ROC curves for $e^+ - \gamma$ classification



(b) ROC curves for $e^+ - \pi^+$ classification



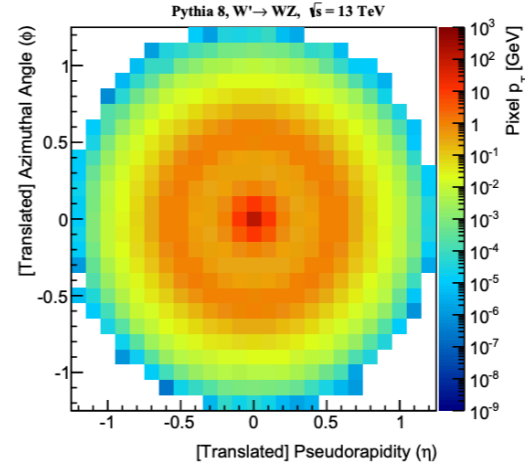
(a) Truth



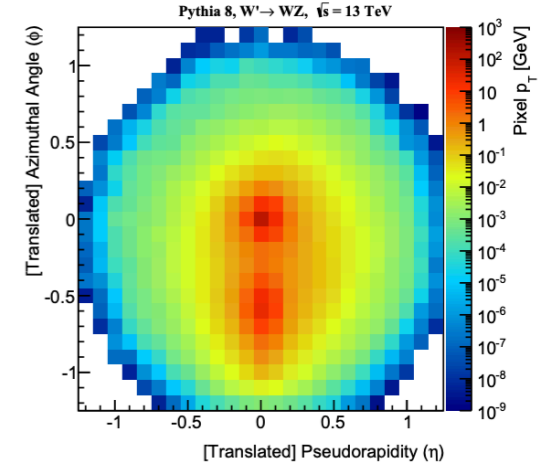
(b) Reconstructed

S. Qasim et-al EPJC 79 7 (2019) 608

$250 < p_T/\text{GeV} < 260 \text{ GeV}, 65 < \text{mass}/\text{GeV} < 95$

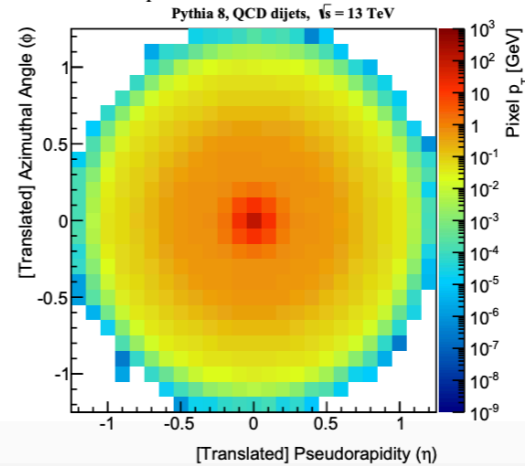


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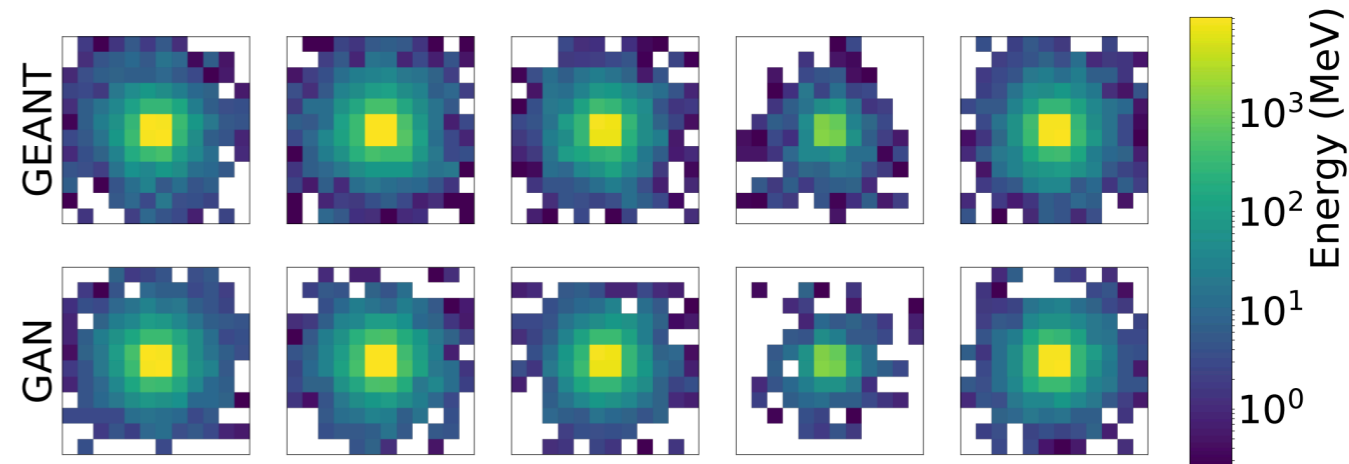
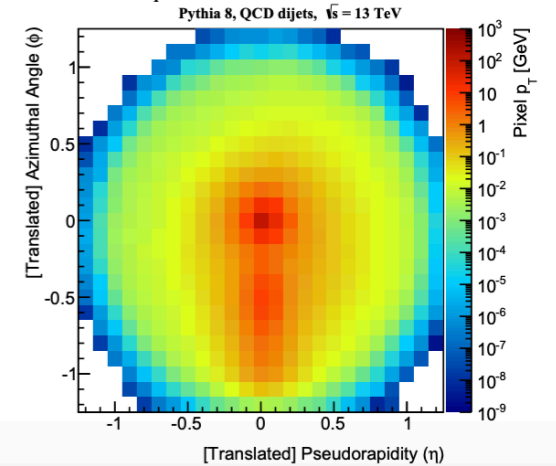


L. De Oliveira et-al JHEP 07 (2016) 069

$250 < p_T/\text{GeV} < 260 \text{ GeV}, 65 < \text{mass}/\text{GeV} < 95$



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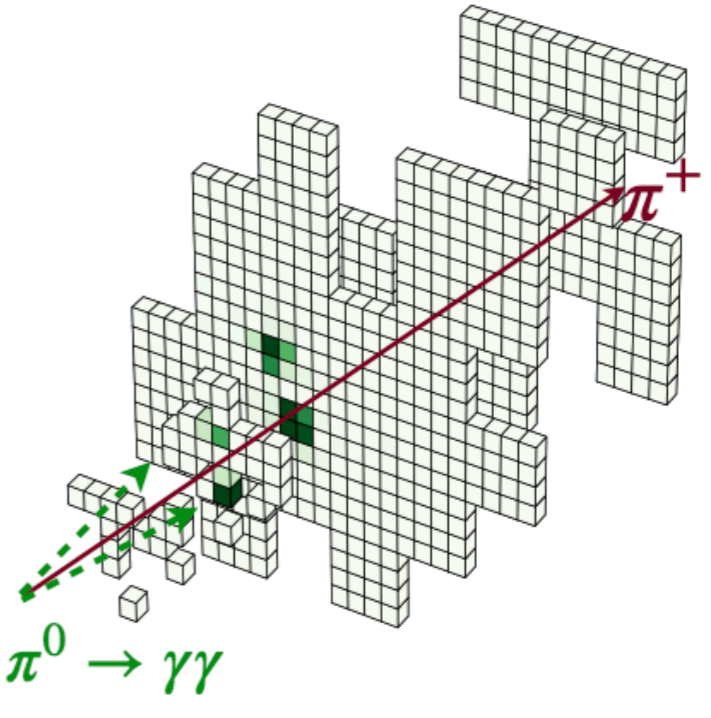
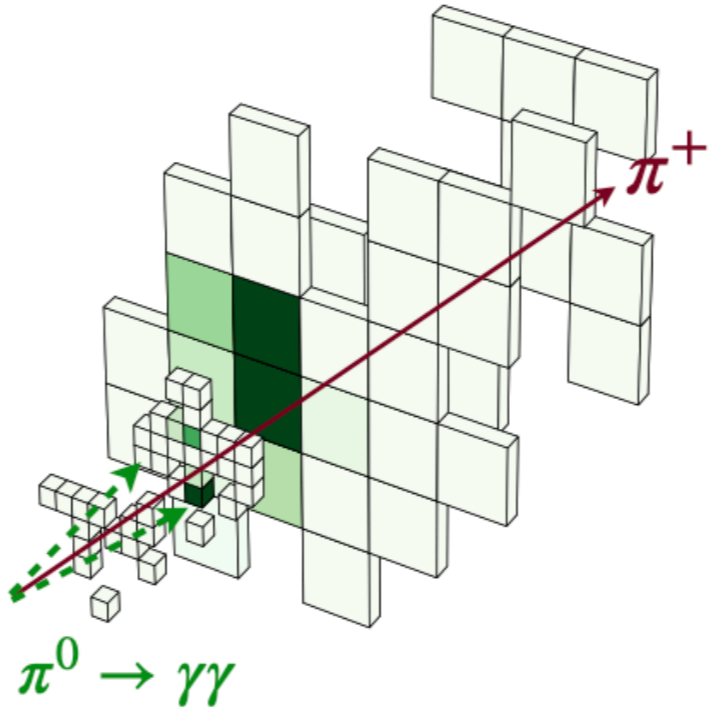
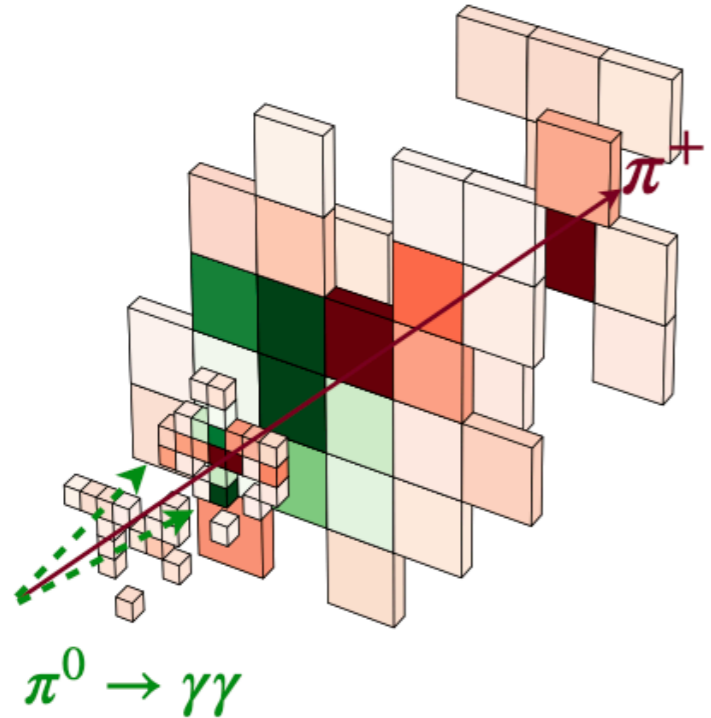


M. Paganini et-al PRD 97 (2018) 1, 014021

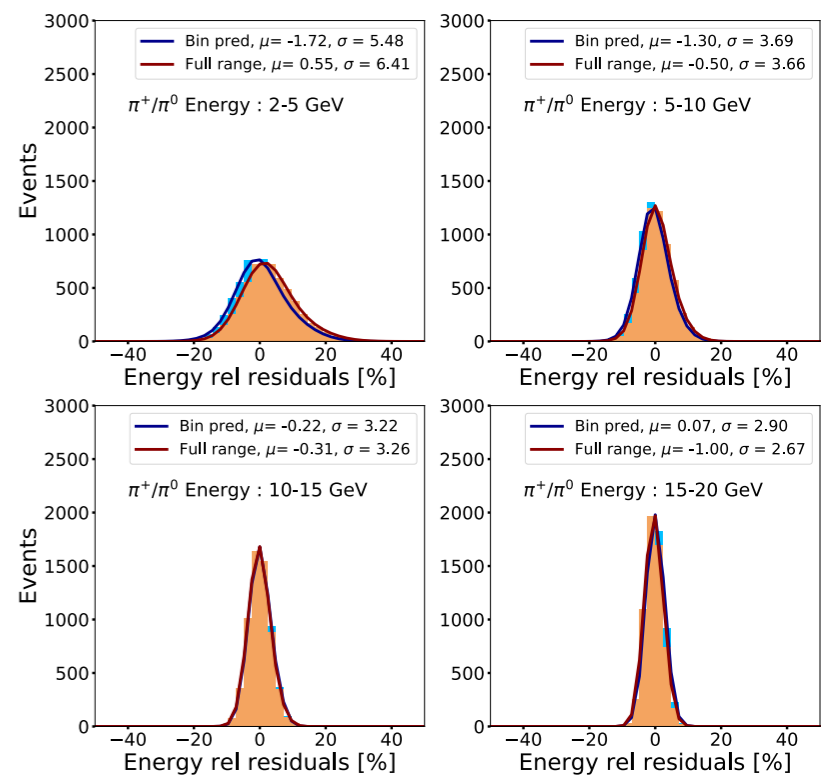
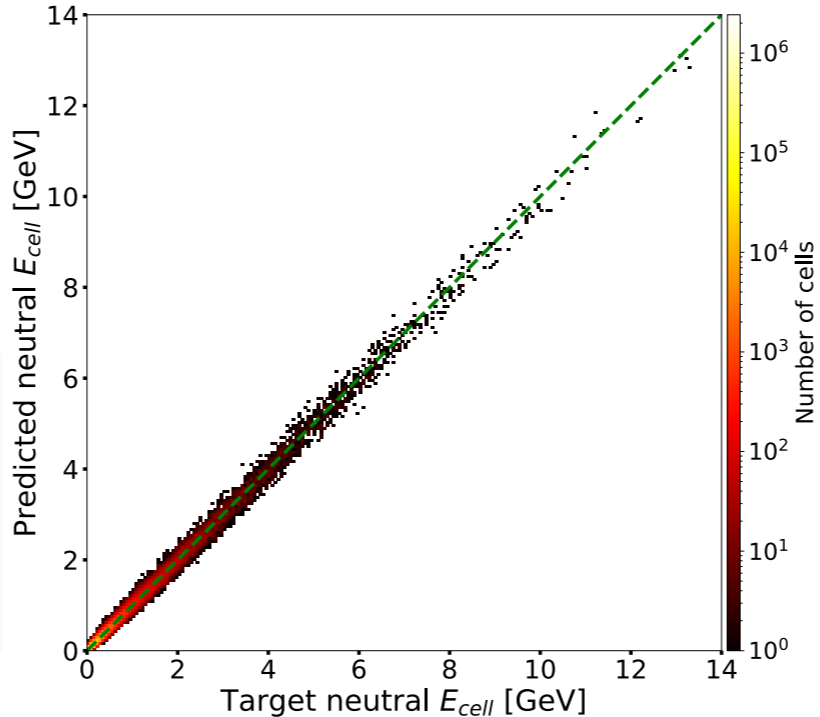
A 3-D view for topoclusters only

8 X 8 Low Res detector

32 X 32 High Res detector



The networks in general have good noise removal abilities.



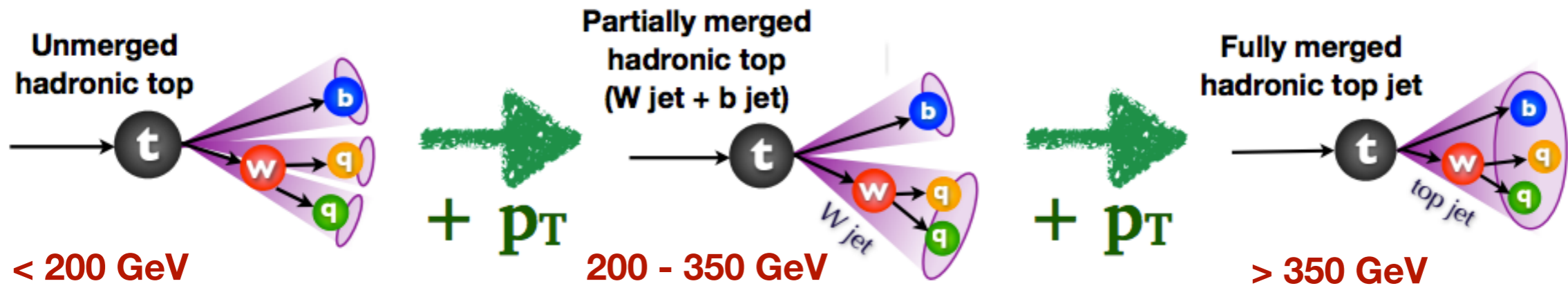
Towards a computer vision particle flow

Francesco Armando Di Bello, Sanmay Ganguly, Eilam Gross, Marumi Kado, Michael Pitt, Lorenzo Santi & Jonathan Shlomi

The European Physical Journal C 81, Article number: 107 (2021) | Cite this article

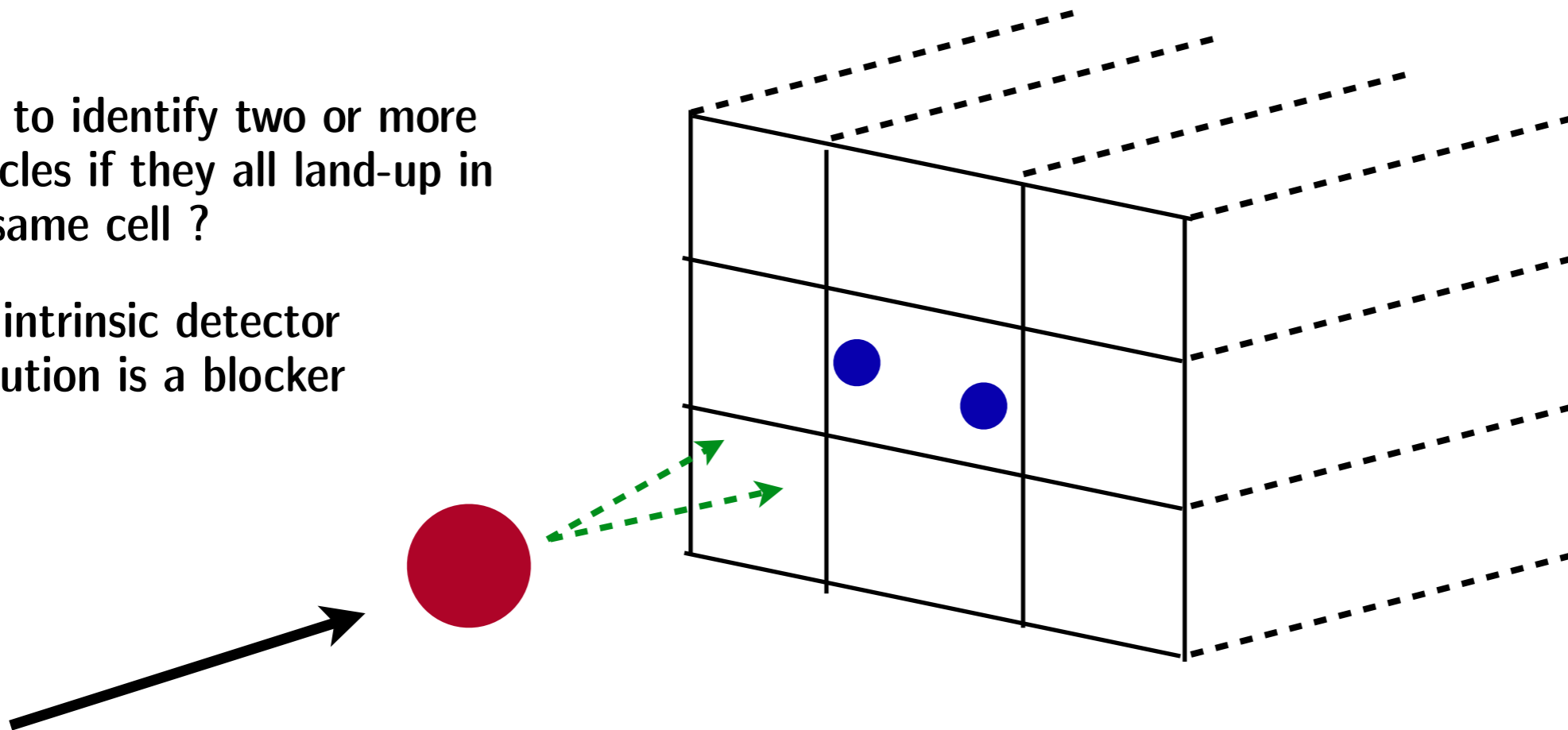
1341 Accesses | 13 Citations | 11 Altmetric | Metrics

When do intrinsic calorimeter sizes are limiting factors ?

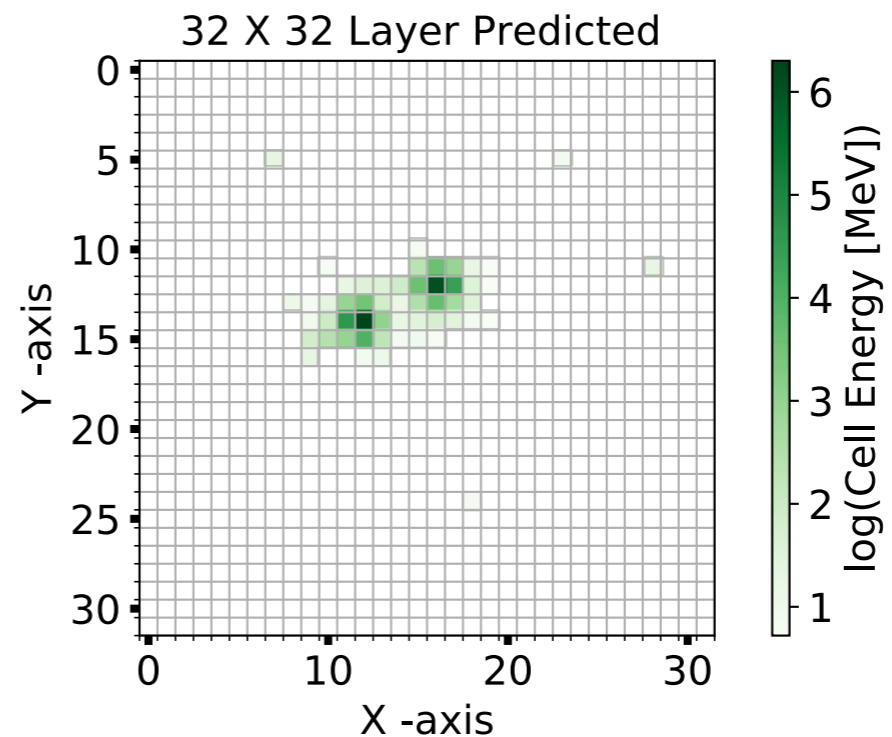
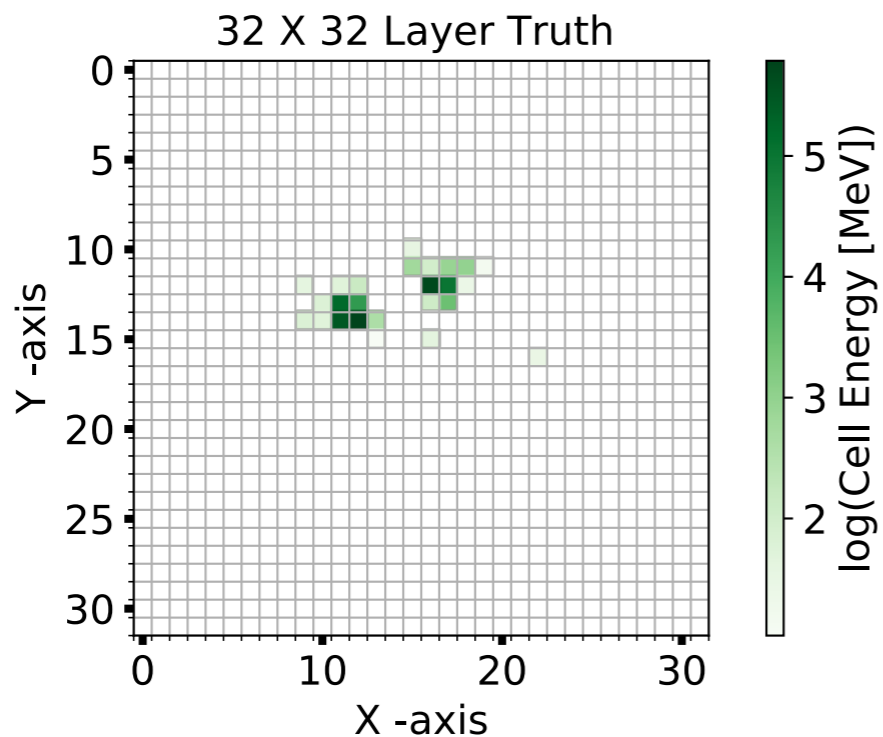
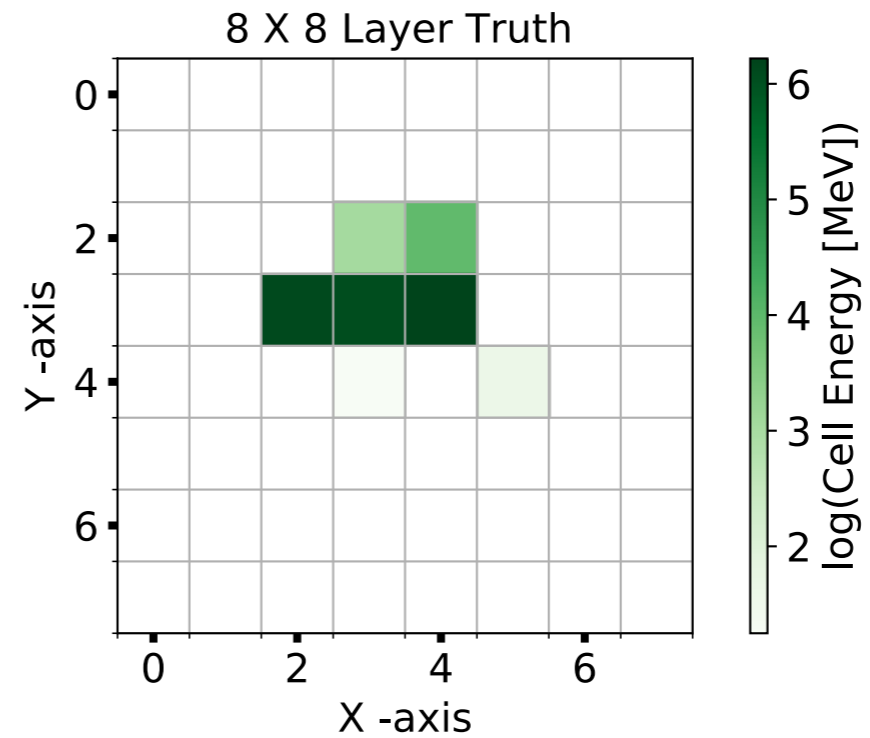
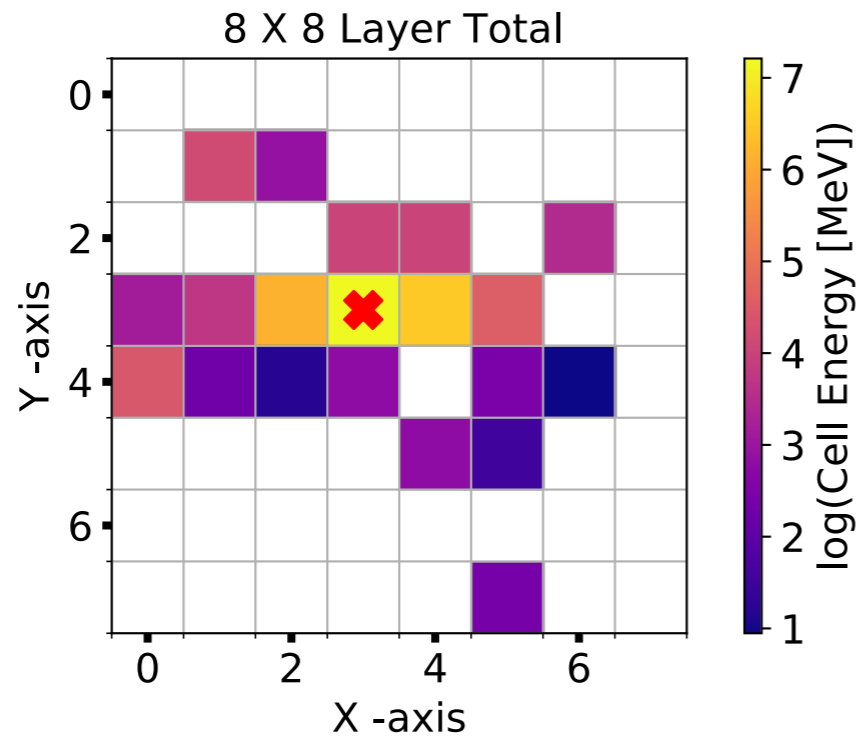


How to identify two or more particles if they all land-up in the same cell ?

The intrinsic detector resolution is a blocker

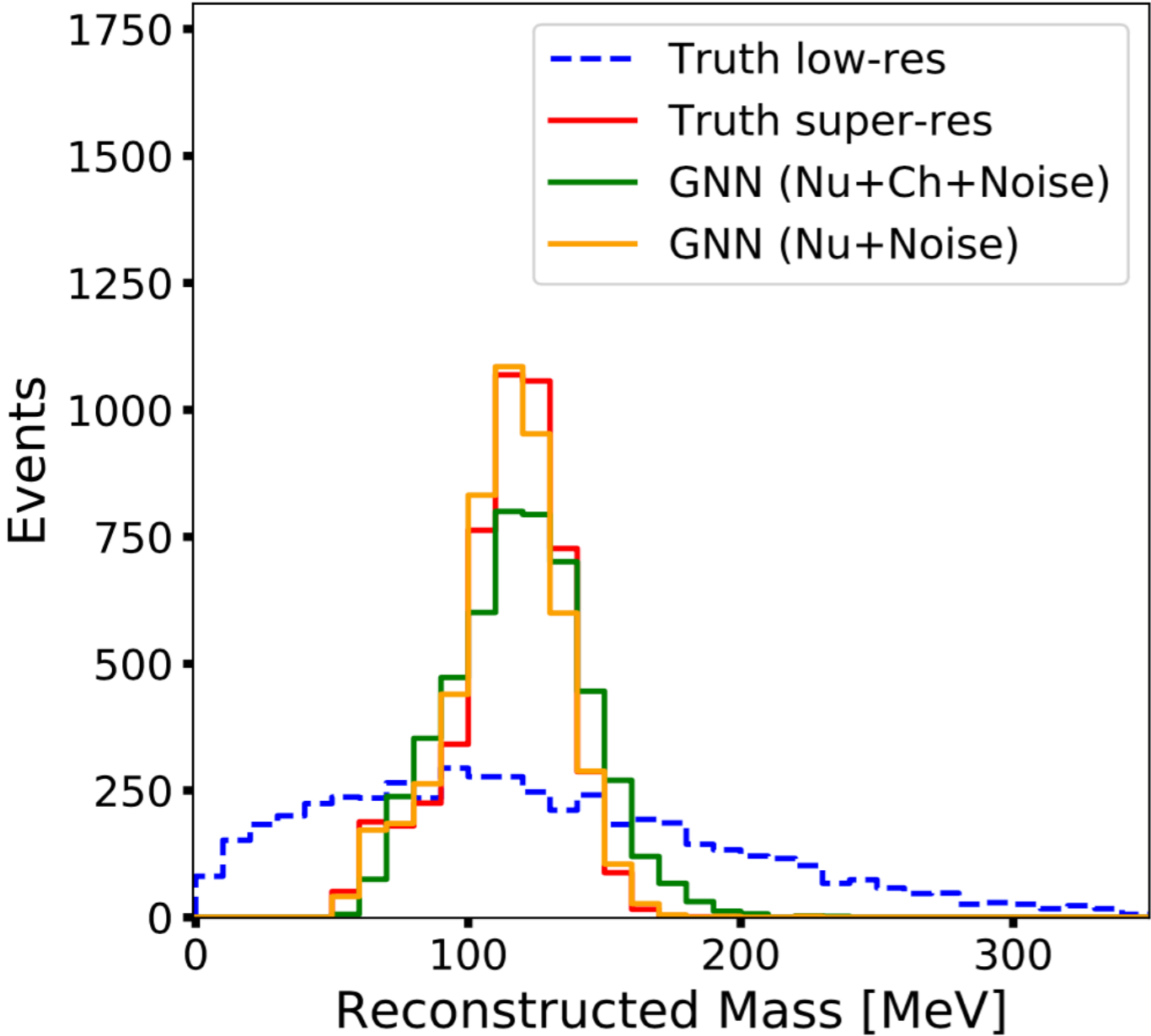
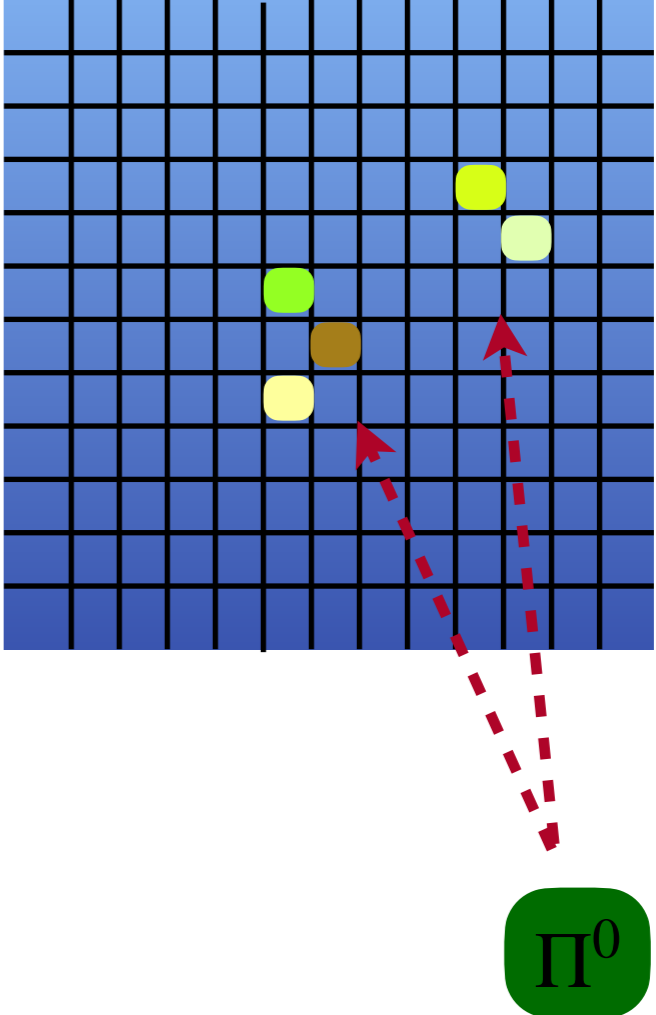


An event display for super-res prediction



The mass distribution

Invariant mass from reconstructed 4-vectors.



On the use of neural networks for energy reconstruction in high-granularity calorimeters **JINST 16 (2021) 12, P12036**
 N. Akchurin (Texas Tech.), C. Cowden (Texas Tech.), J. Damgov (Texas Tech.), A. Hussain (Texas Tech.), S. Kunori (Texas Tech.)

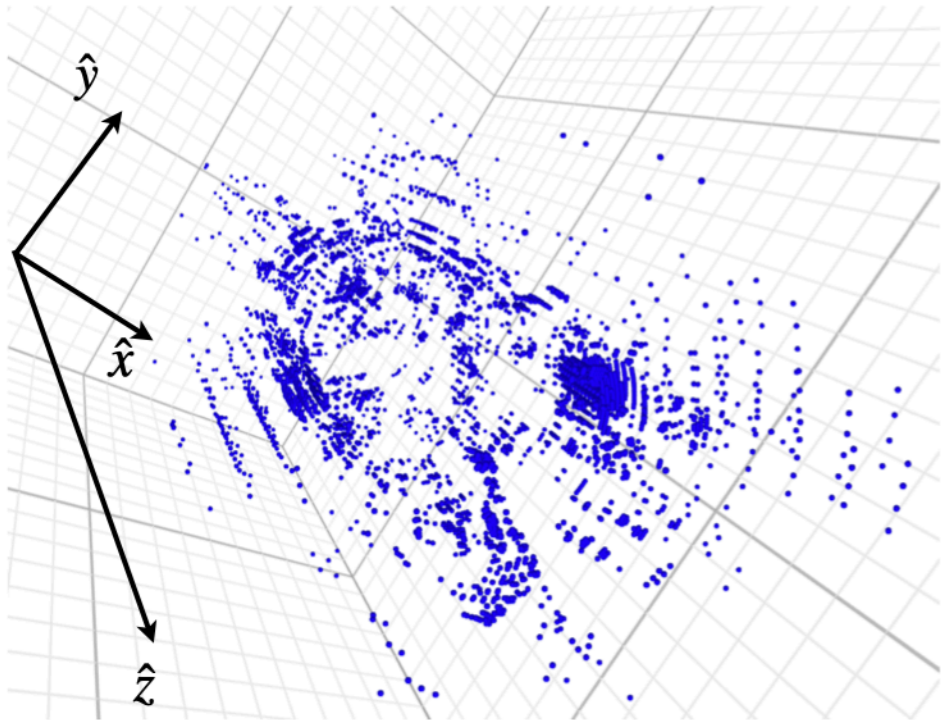
How to GAN Higher Jet Resolution
SciPost Phys. 13 (2022) 3, 064
 Pierre Baldi¹, Lukas Blecher², Anja Butter², Julian Collado¹, Jessica N. Howard³, Fabian Keilbach², Tilman Plehn², Gregor Kasieczka⁴, and Daniel Whiteson³

Higgs and top physics reconstruction challenges and opportunities at FCC-ee
Eur.Phys.J.Plus 137 (2022) 1, 39
 Patrizia Azzi (INFN, Padua and Padua U.), Loukas Gouskos (CERN), Michele Selvaggi (CERN), Frank Simon (Munich, Max Planck Inst.)

Test-beam and simulation studies towards RPWELL-based DHCAL #13
 Dan Shaked-Renous (Weizmann Inst.), Fernando Domingues Amaro (Coimbra U.), Purba Bhattacharya (Weizmann Inst.), Amos Breskin (Weizmann Inst.), Maximilien Chefdeville (Annecy, LAPP) et al. (Aug 26, 2022) **JINST 17 (2022) 12, P12008**

A high-granularity calorimeter insert based on SiPM-on-tile technology at the future Electron-Ion Collider **Nucl.Instrum.Meth.A 1047 (2023) 167866**
 Miguel Arratia (UC, Riverside), Kenneth Barish (UC, Riverside), Liam Blanchard (UC, Riverside), Huan Z. Huang (Southern California U.), Zhongling Ji (Southern California U.) et al. (Aug 10, 2022)

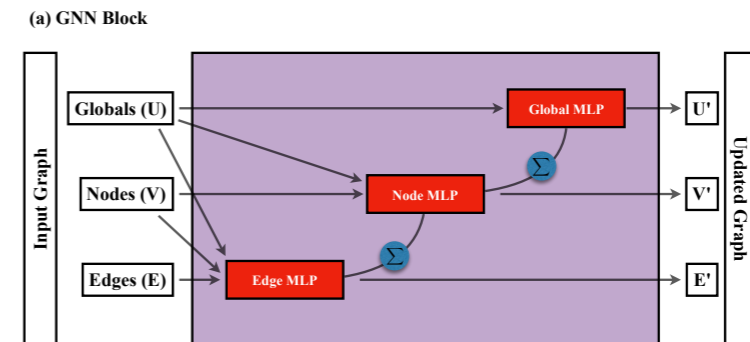
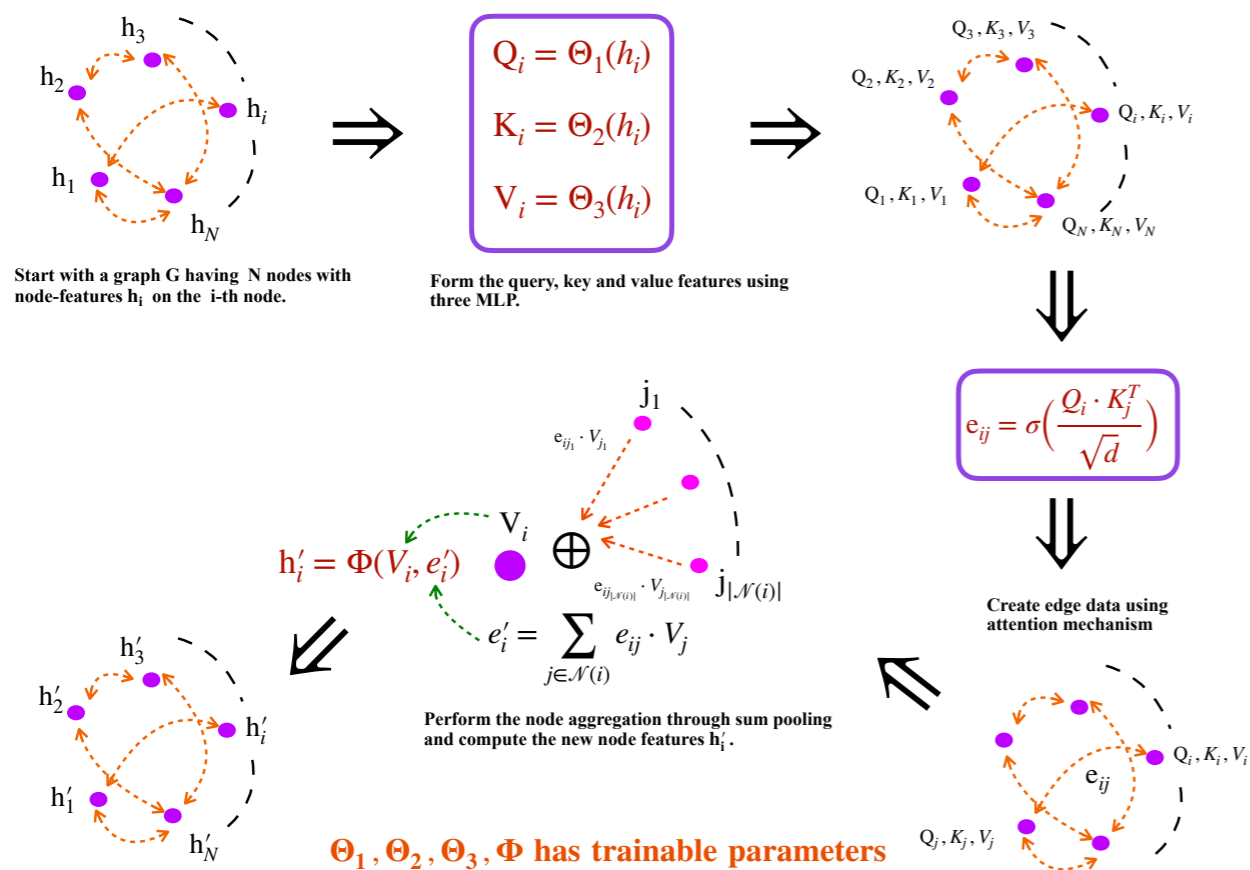
Pion identification within ATLAS



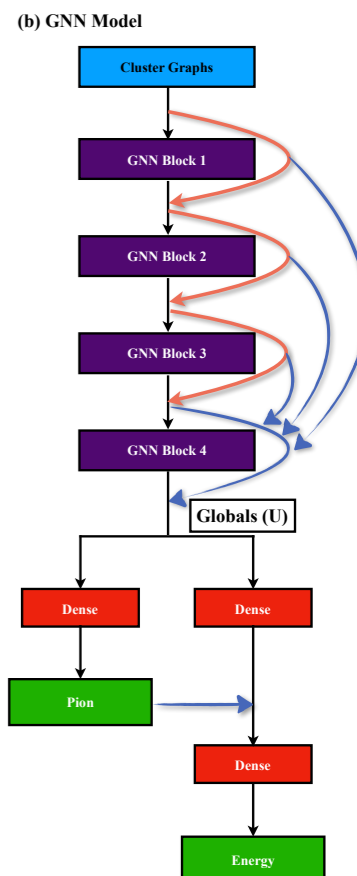
A classification & regression task is tested on ATLAS samples. The calibrated topocluster cells are used to form images & P.C.

ATL-PHYS-PUB-2020-040

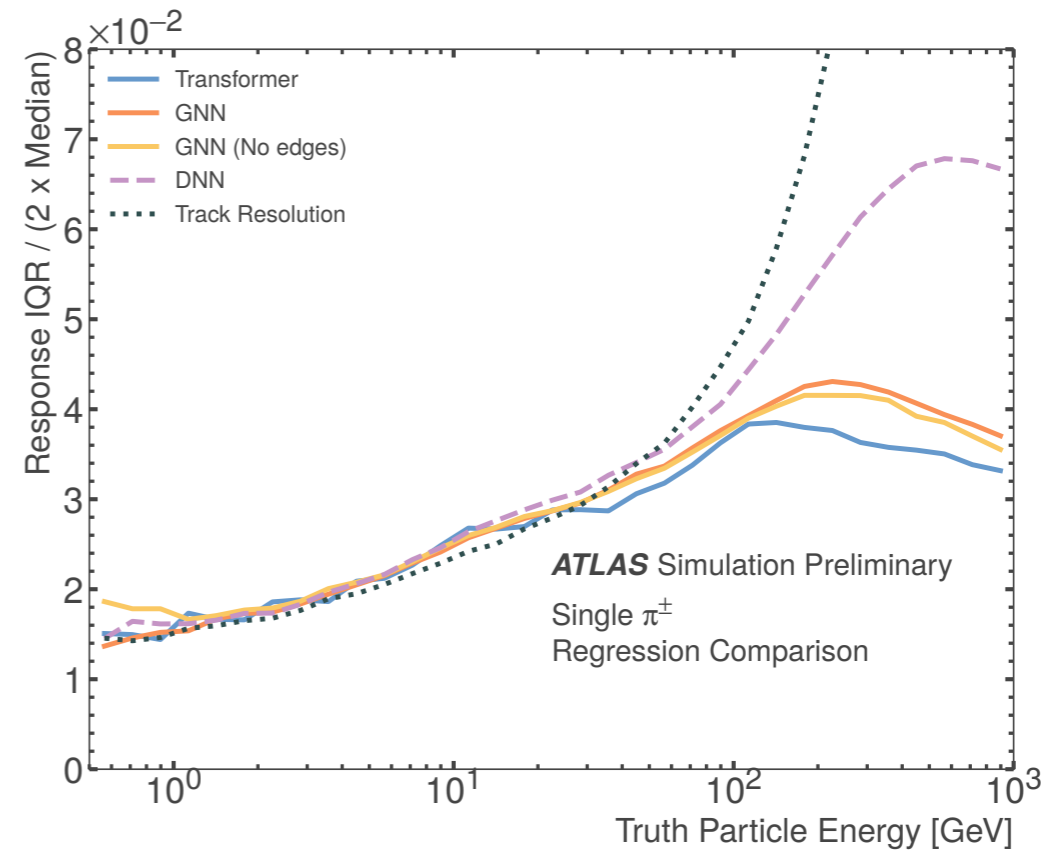
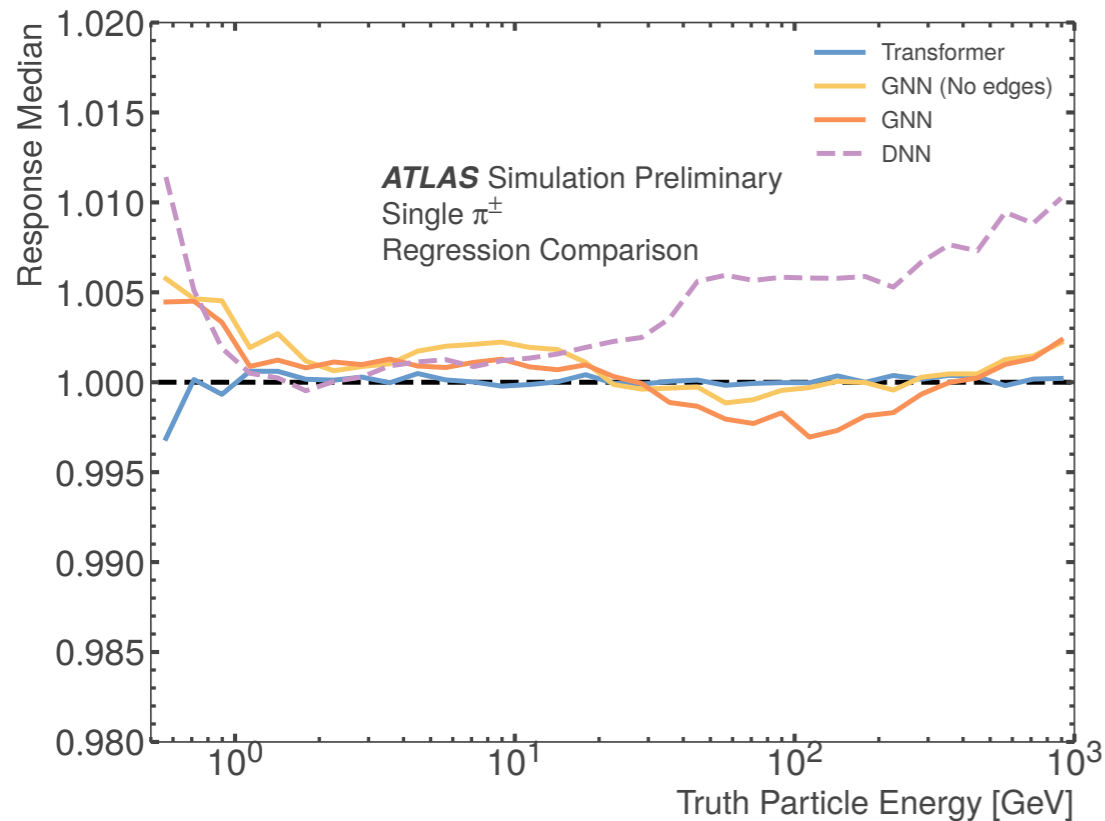
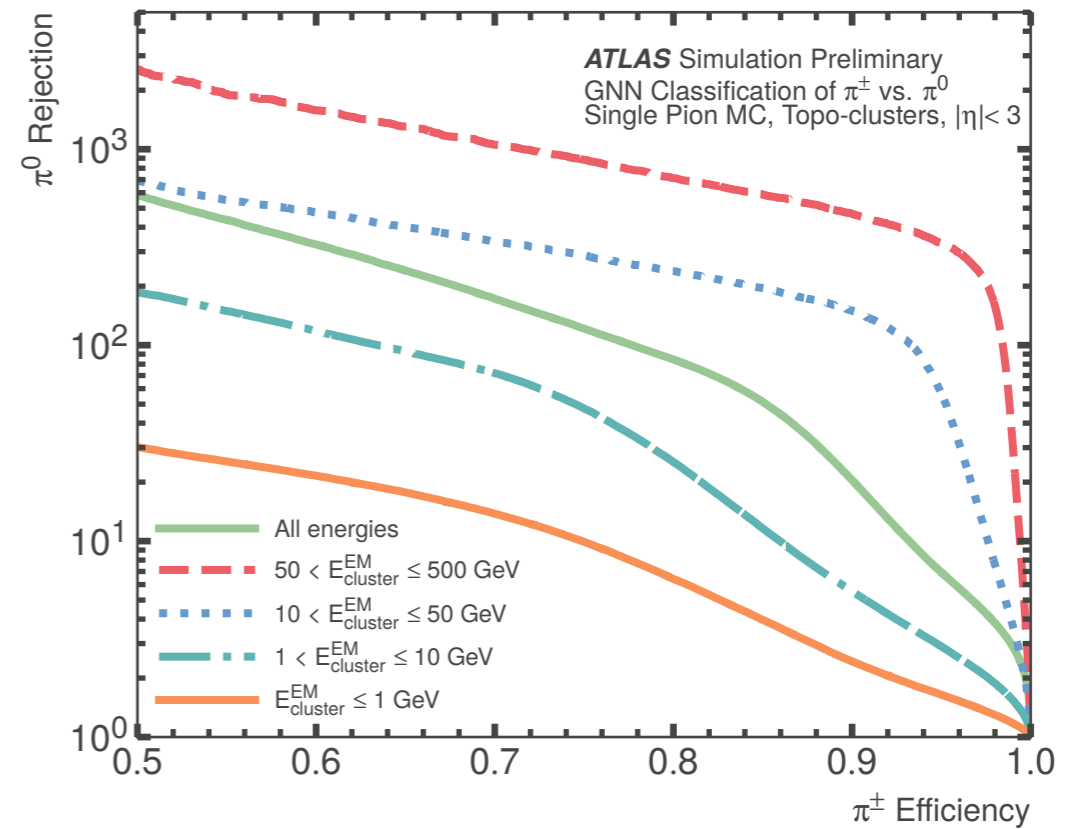
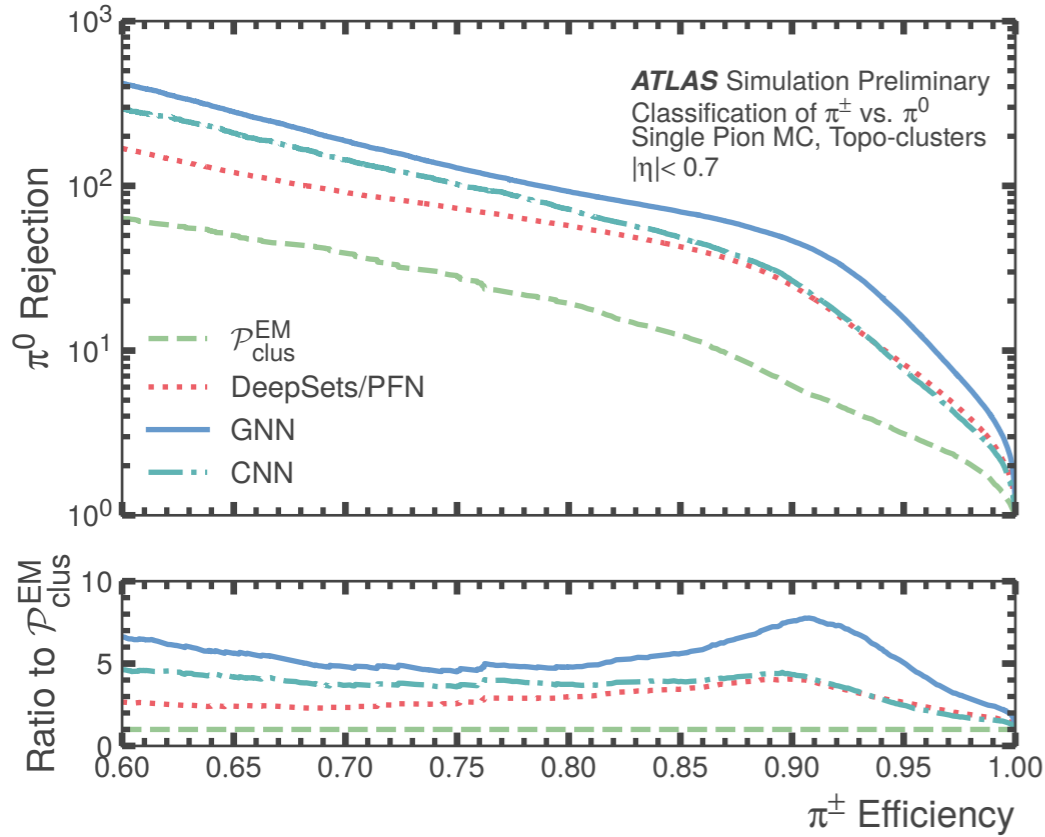
$$\mathcal{L} = (1 - \alpha) \mathcal{L}_{\text{classification}} + \alpha \mathcal{L}_{\text{Regression}}$$



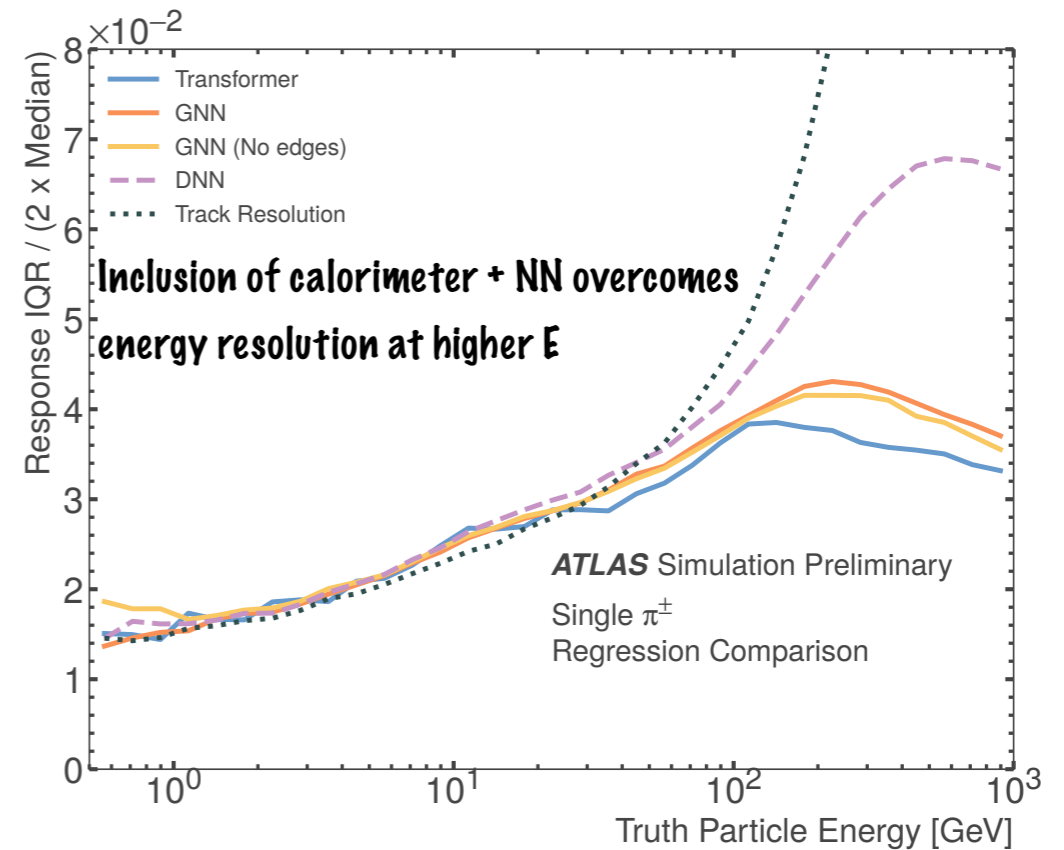
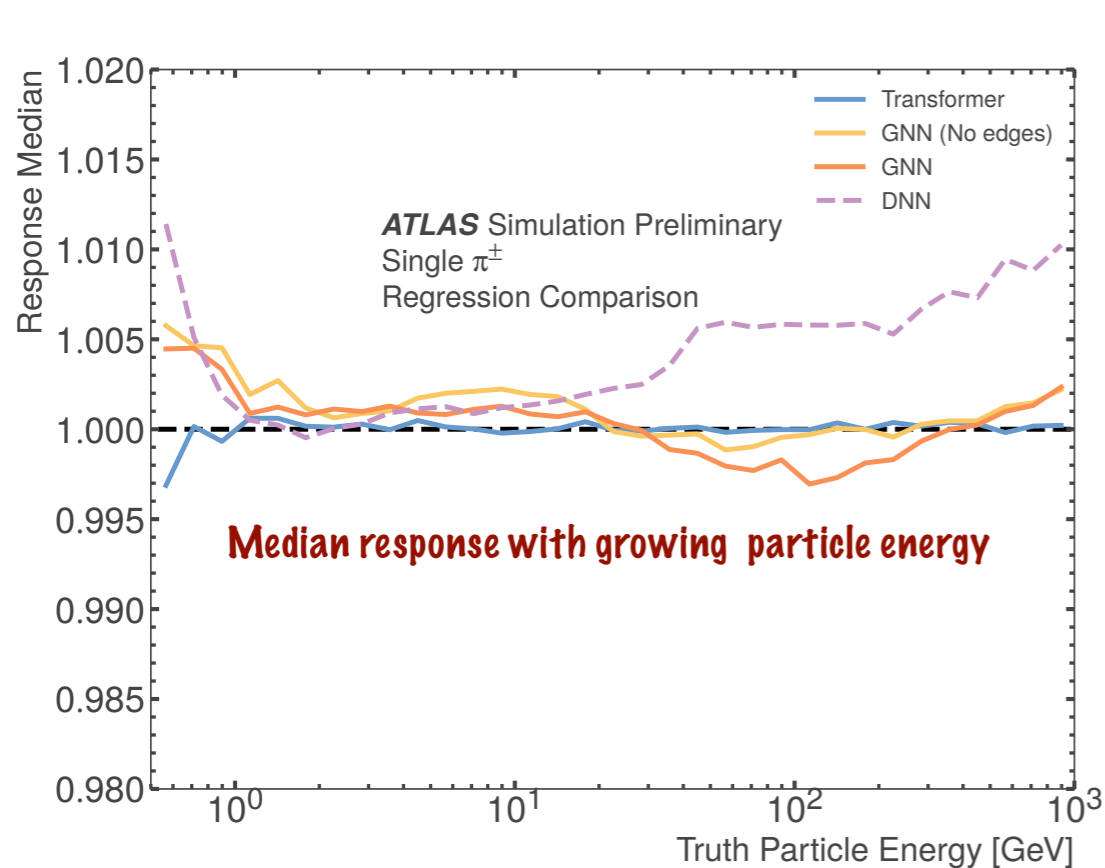
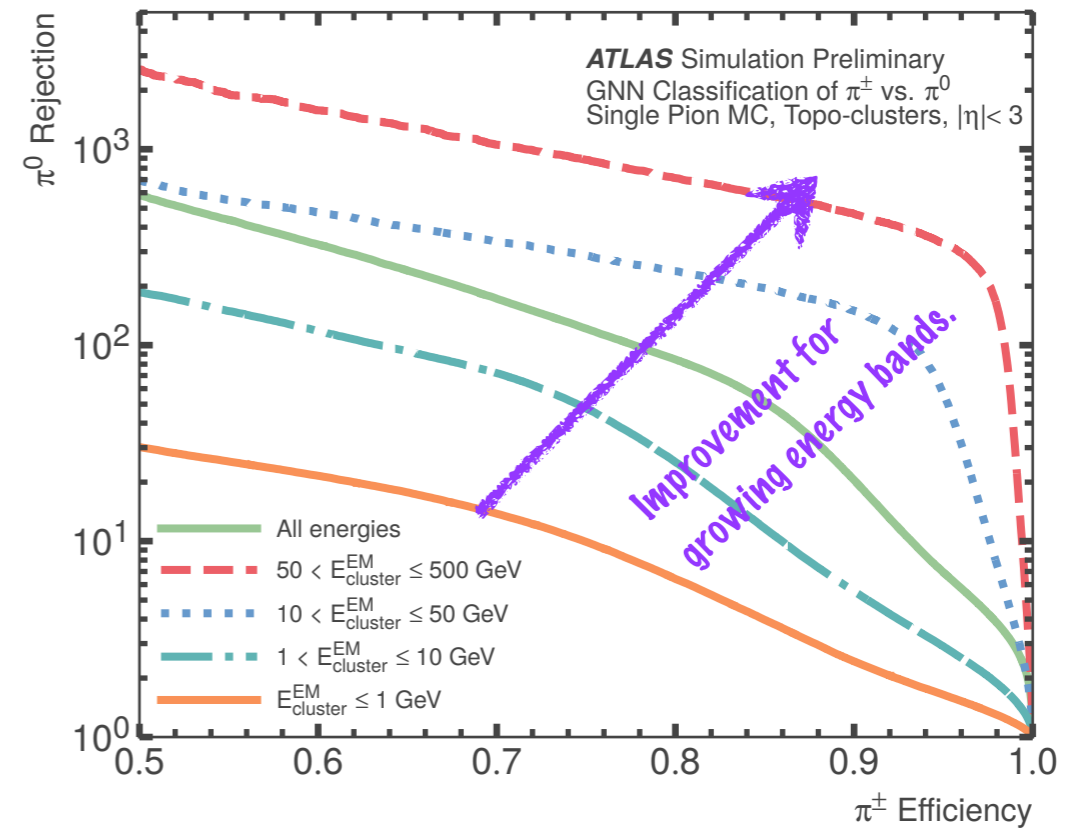
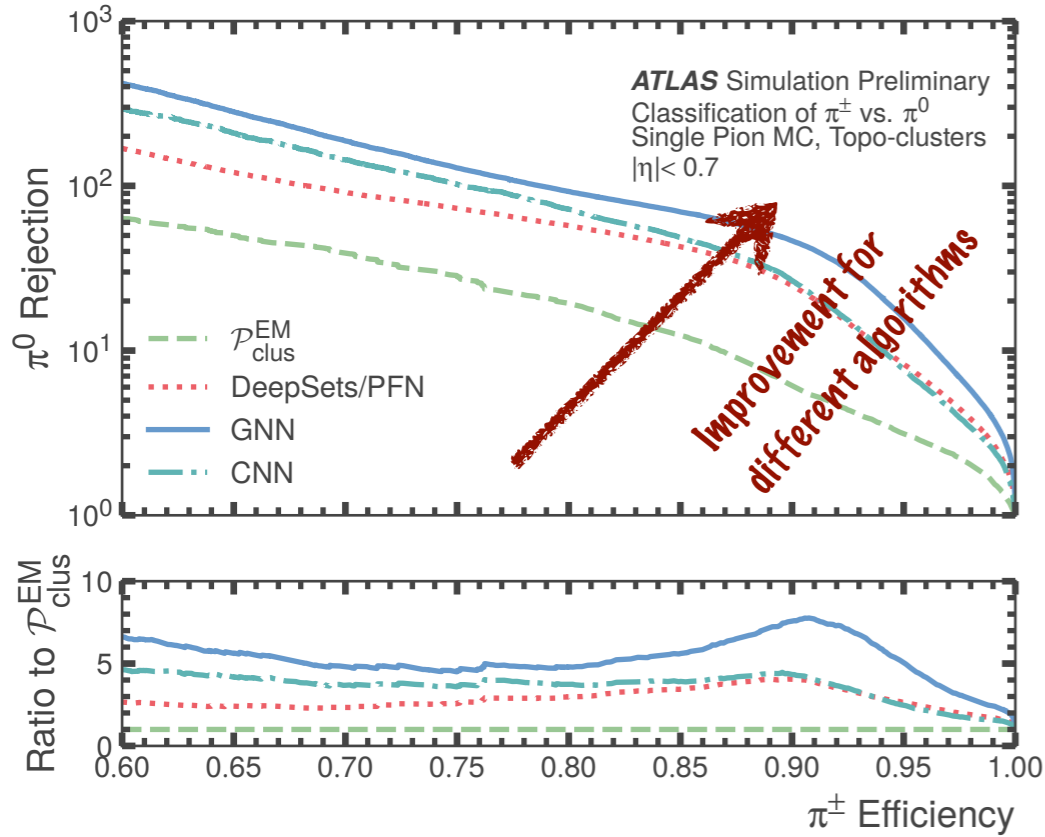
- MLP: 3 Dense Layers of 64 Neurons
- Dense: Dense Layer with 1 output Neuron
- Output Neuron
- Σ : Permutation-Invariant Aggregation
- \curvearrowright : Graph Concatenation
- \curvearrowleft : Globals Concatenation



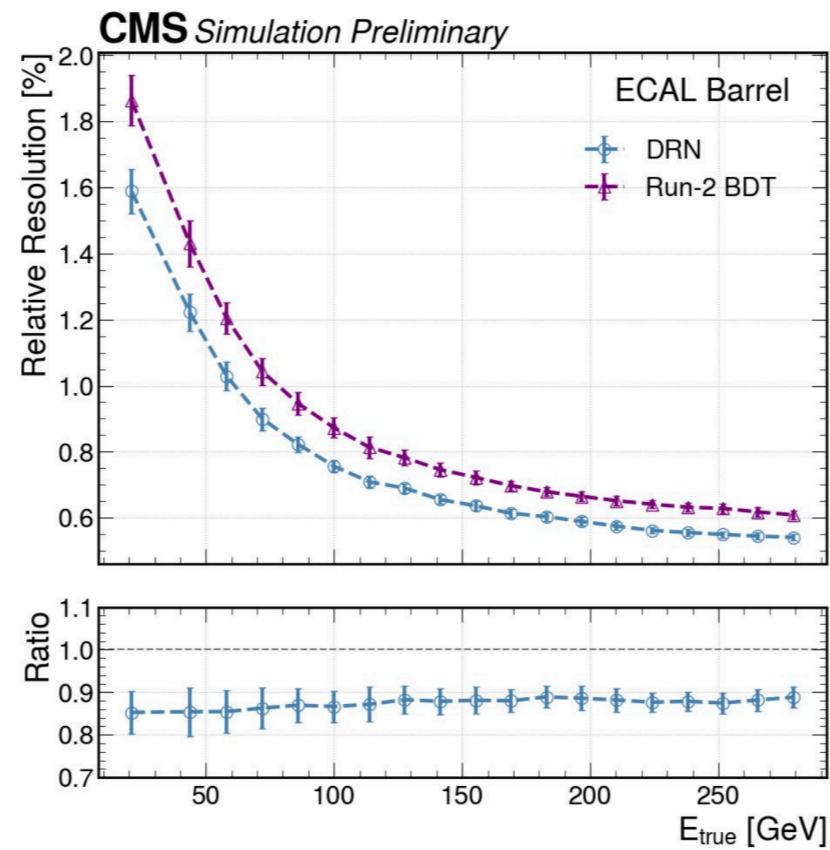
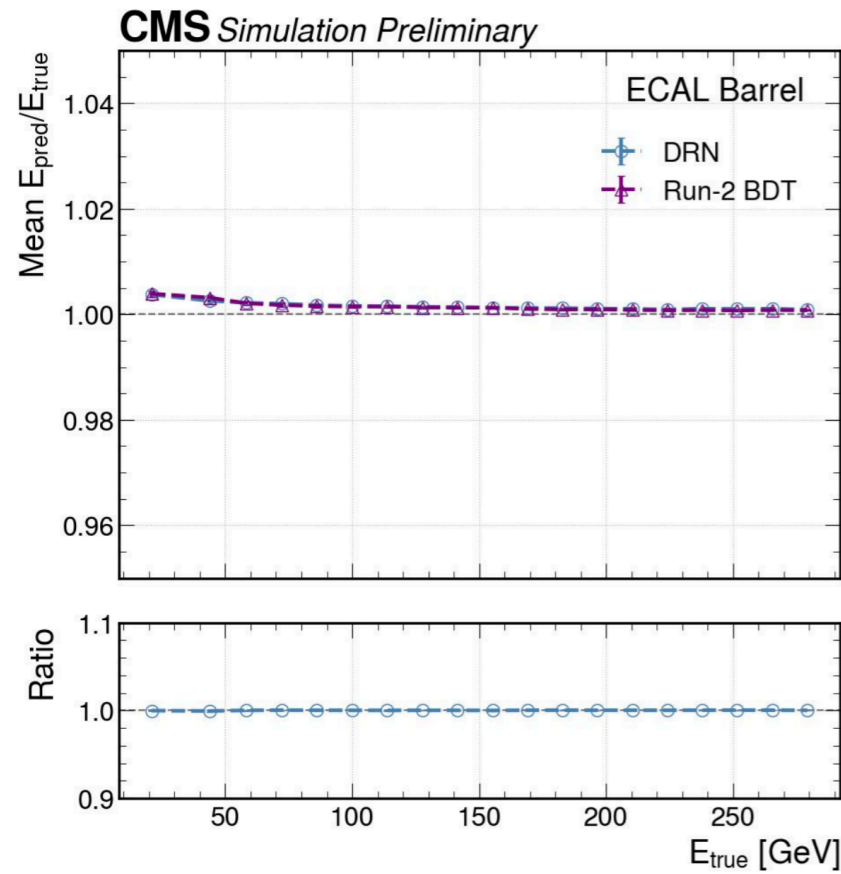
Pion identification within ATLAS



Pion identification within ATLAS

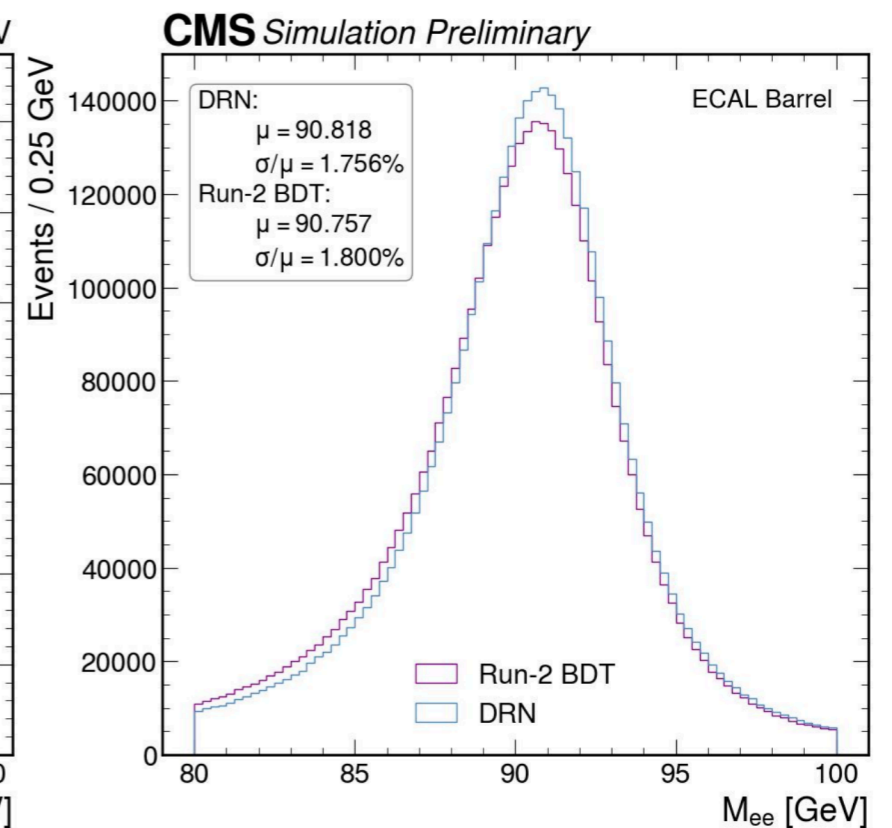
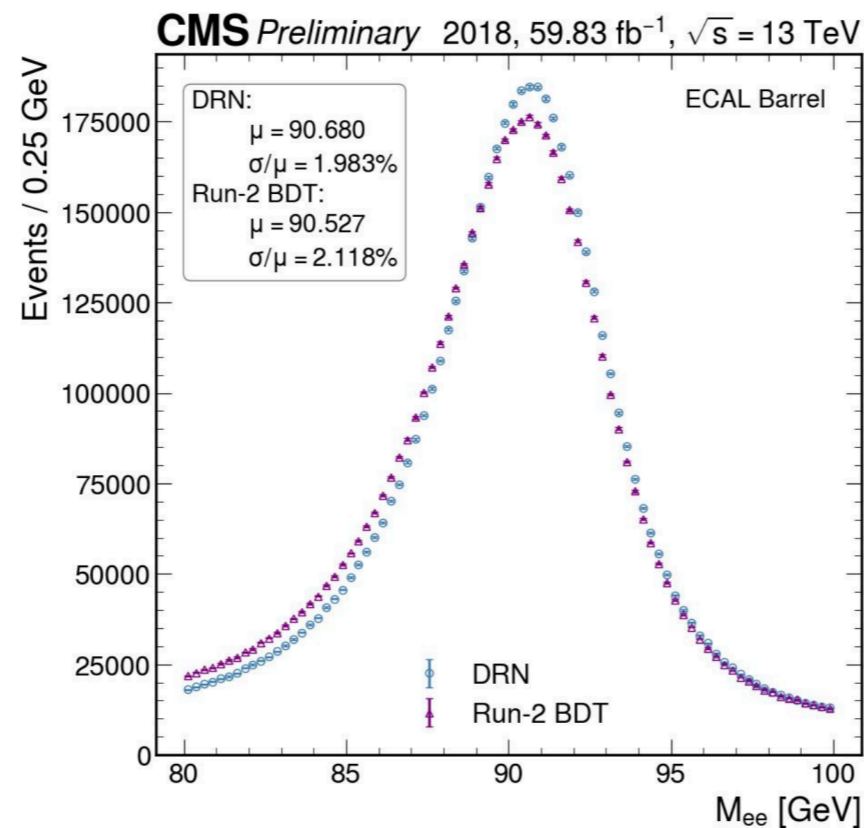


Electron identification within CMS

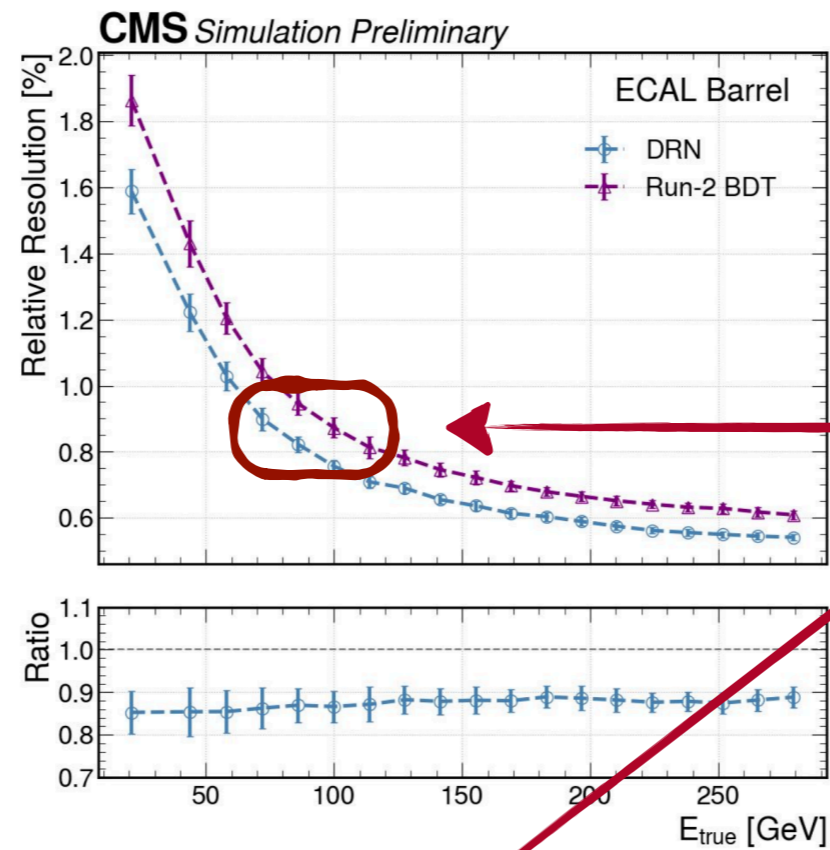
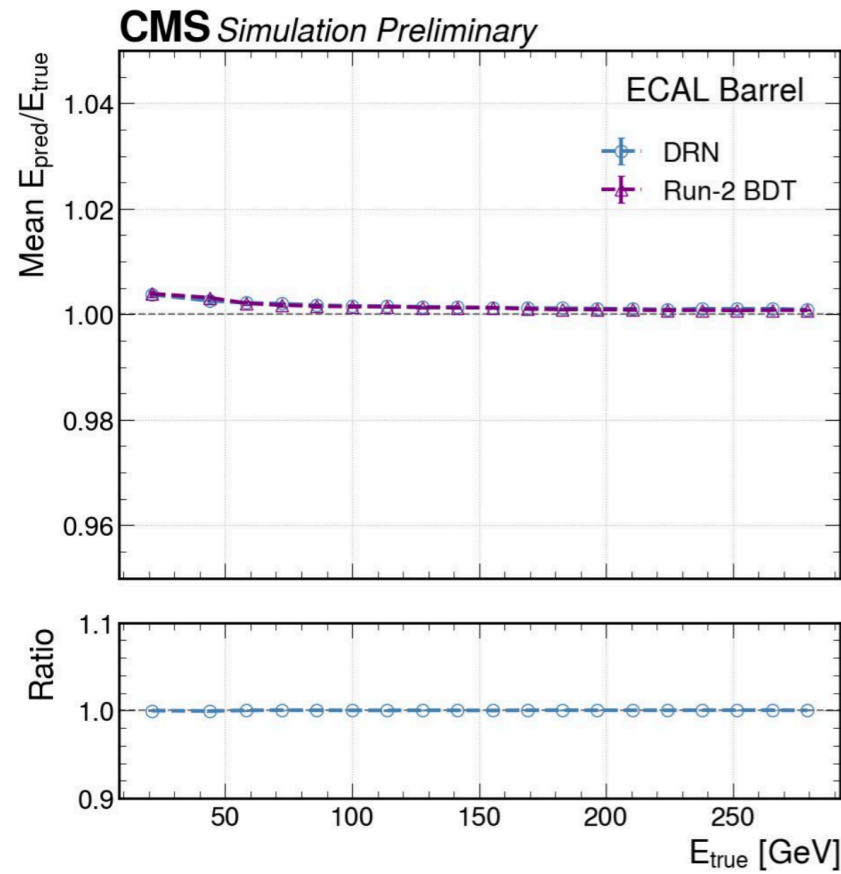


DRN is a dynamic GNN

CMS-DP2022_009



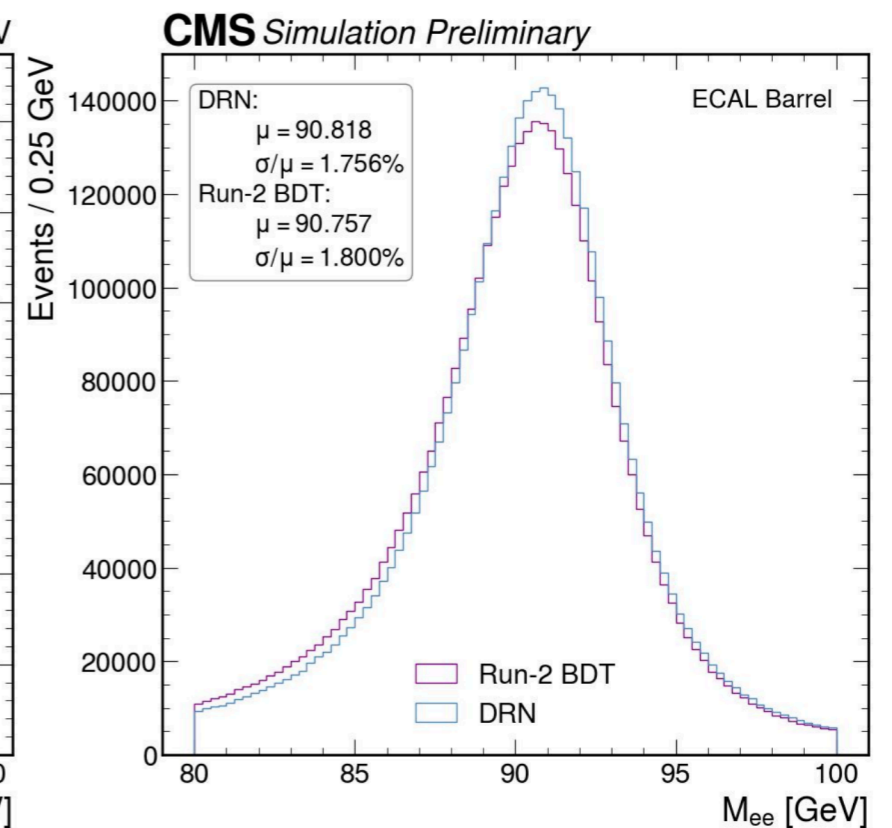
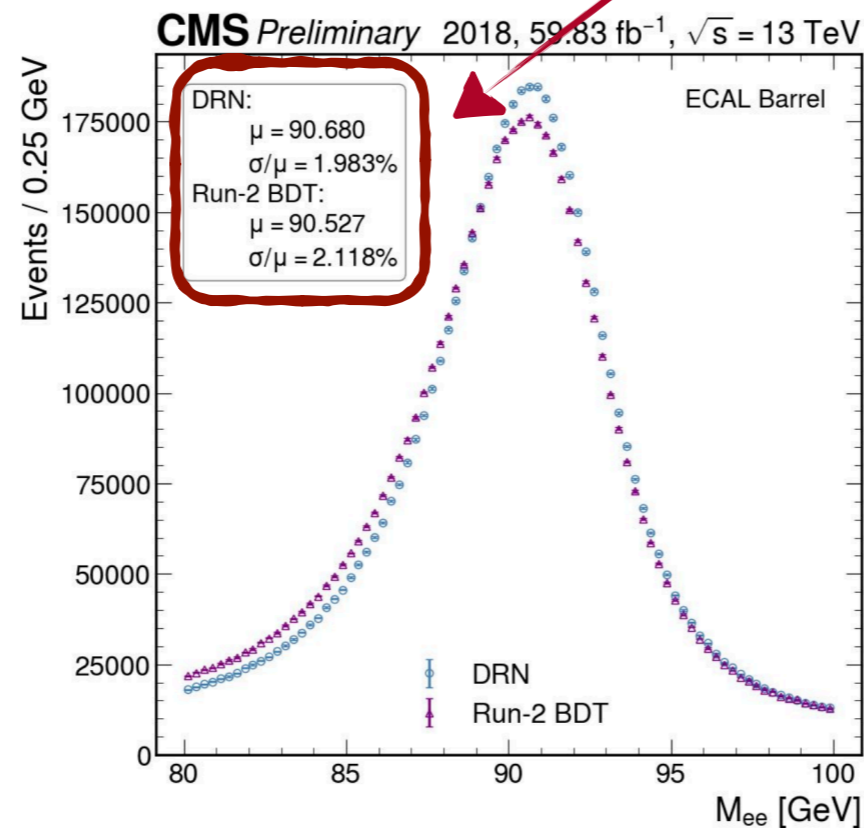
Electron identification within CMS



DRN is a dynamic GNN

Improvement from a modern ML algorithm

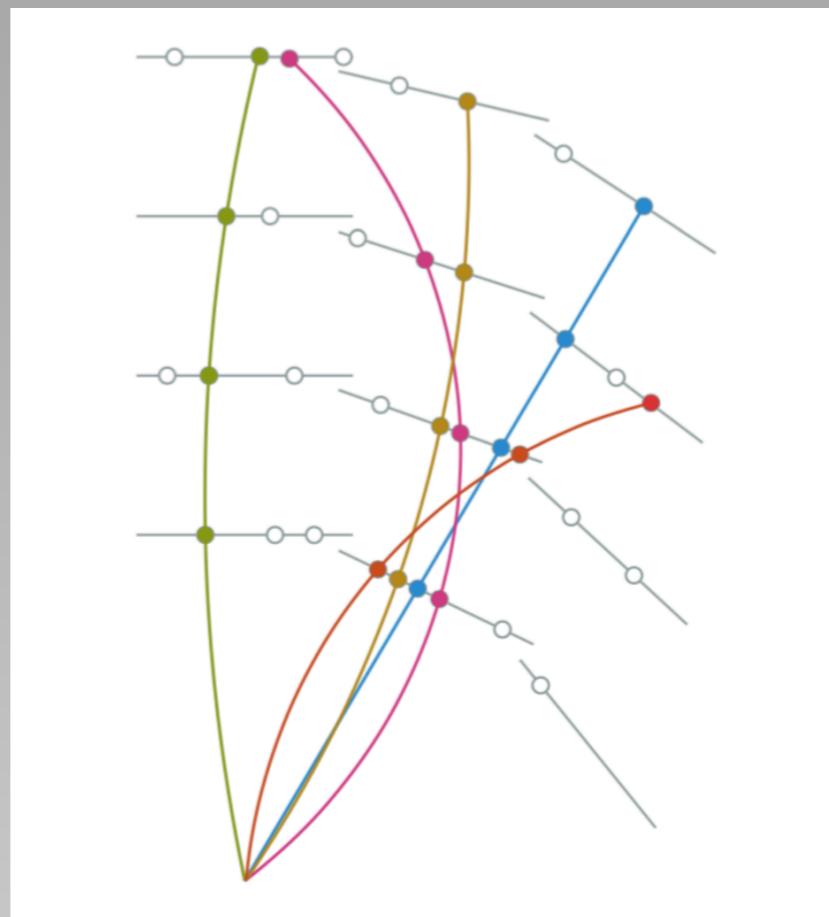
CMS-DP2022_009



Tracking

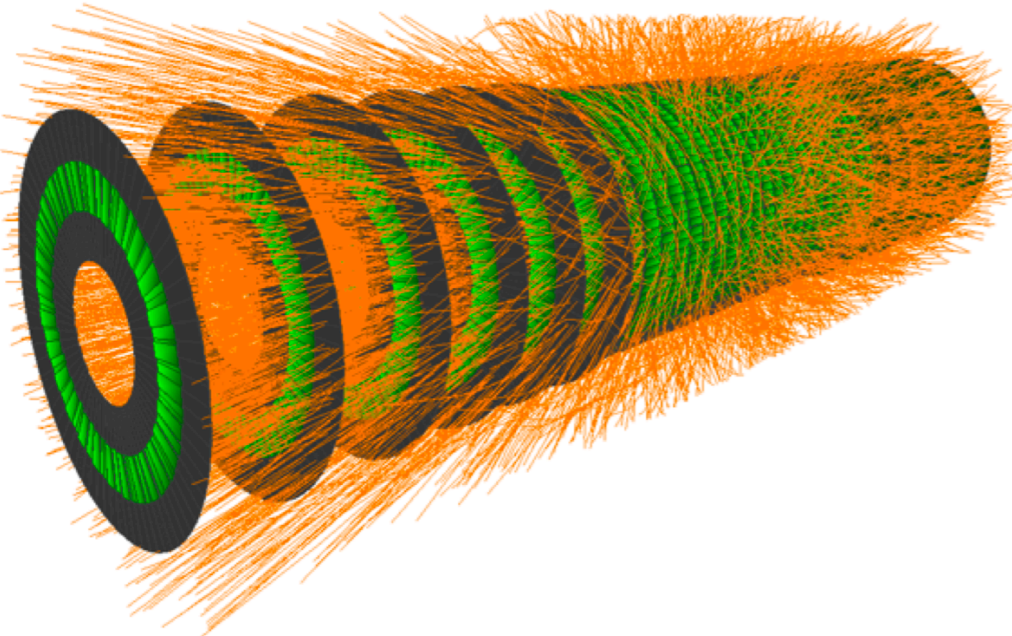
$f_{\{\theta\}}$

(

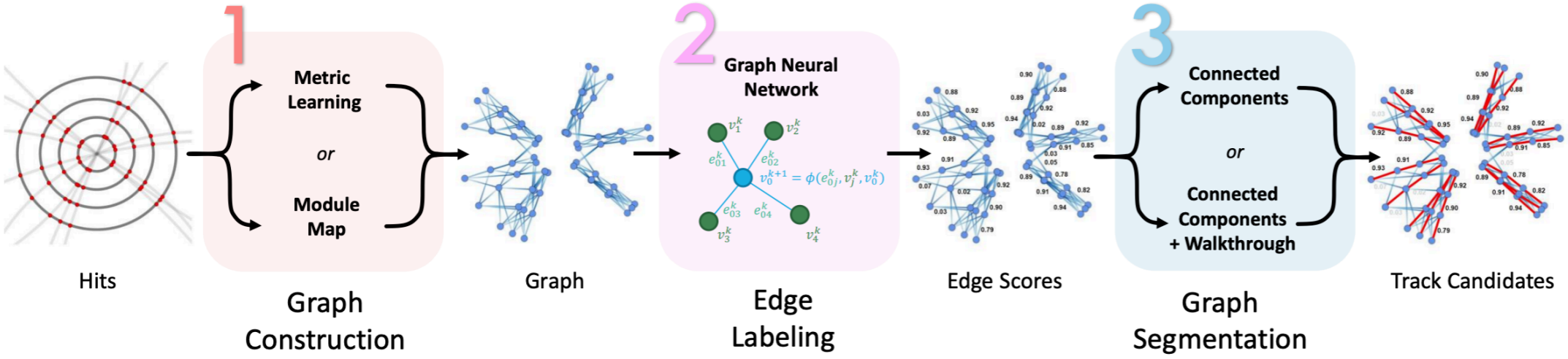
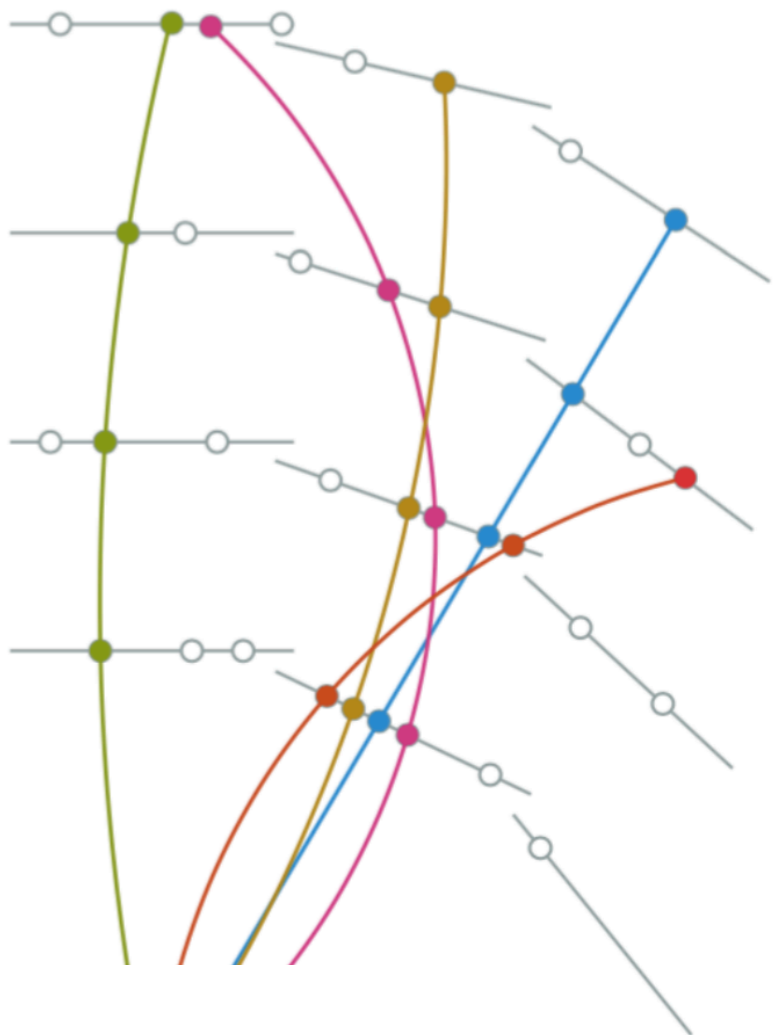


)

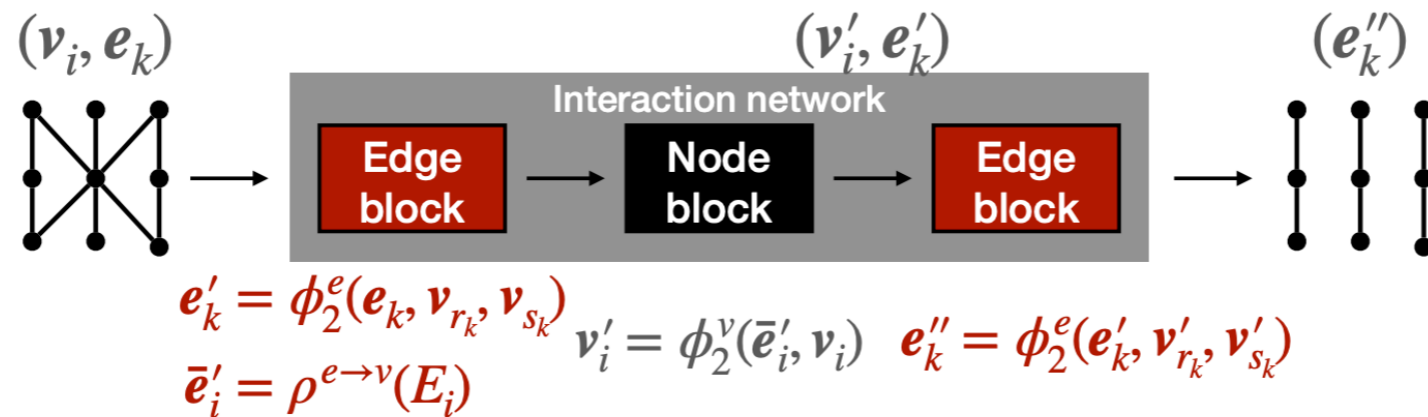
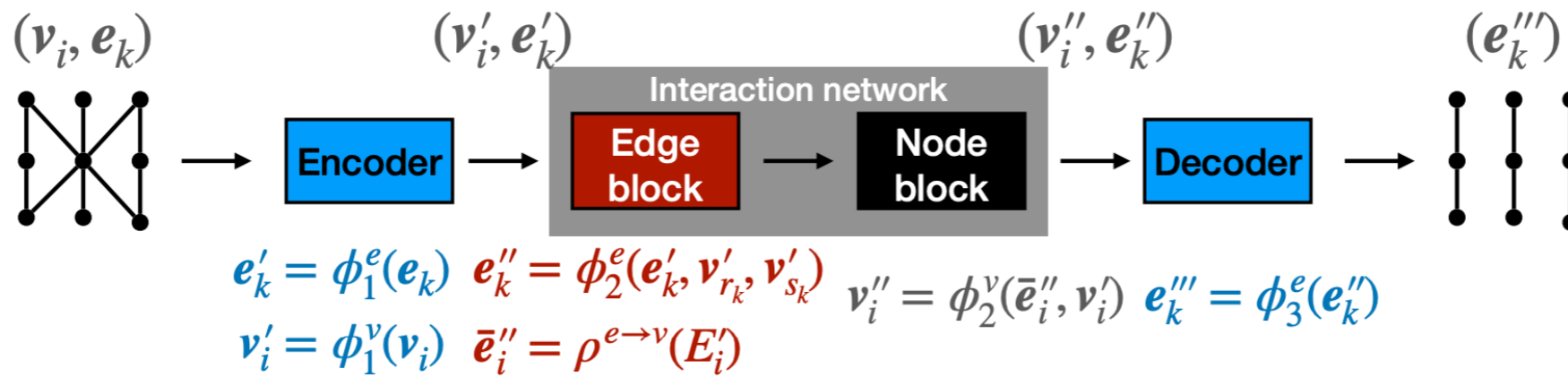
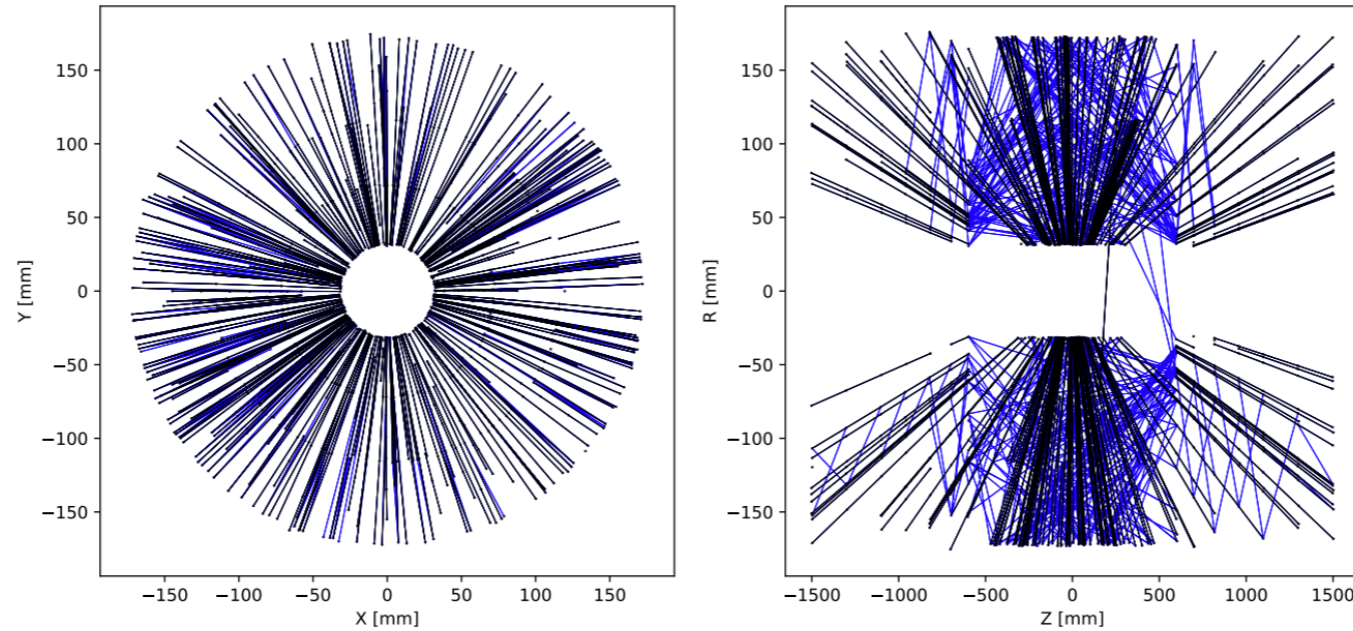
Tracking & ML



An exponentially large edge finding problem

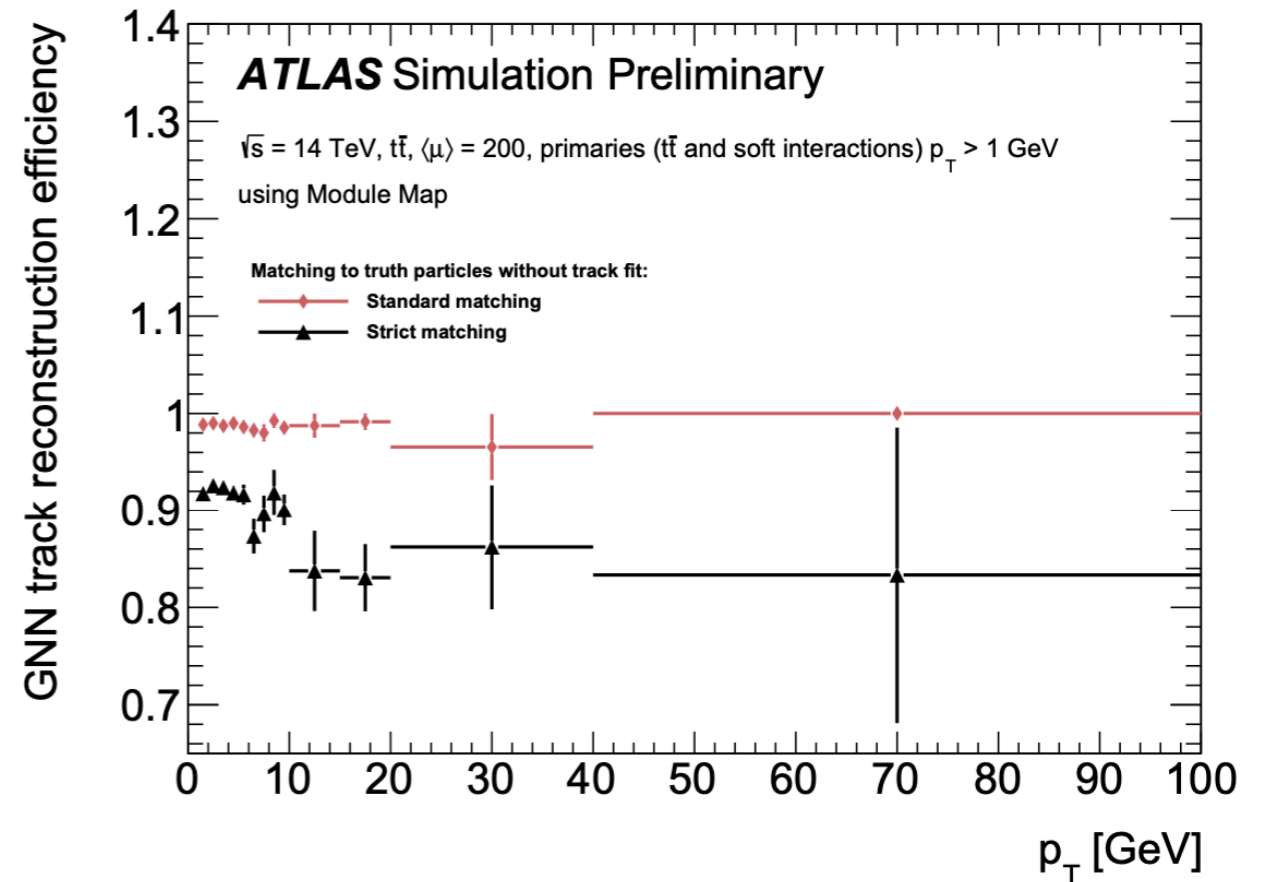
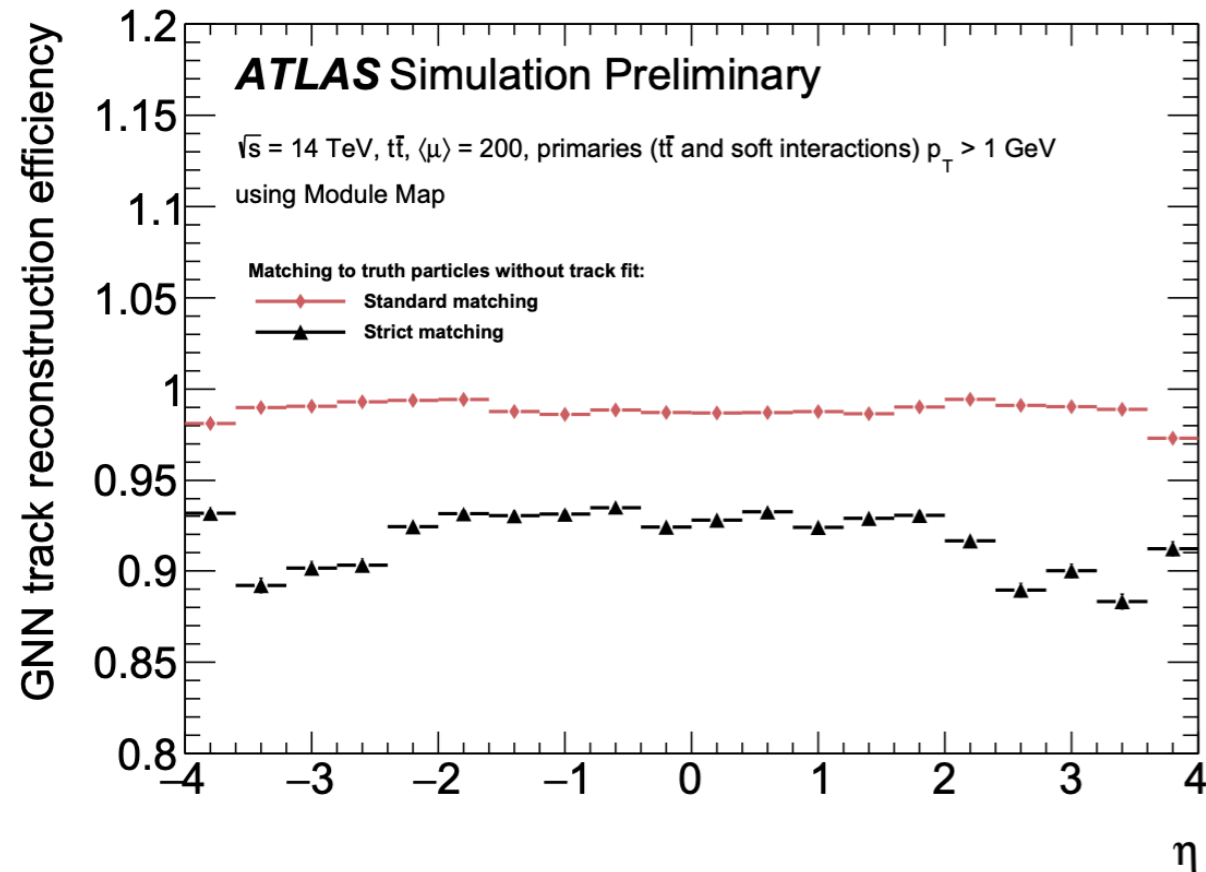
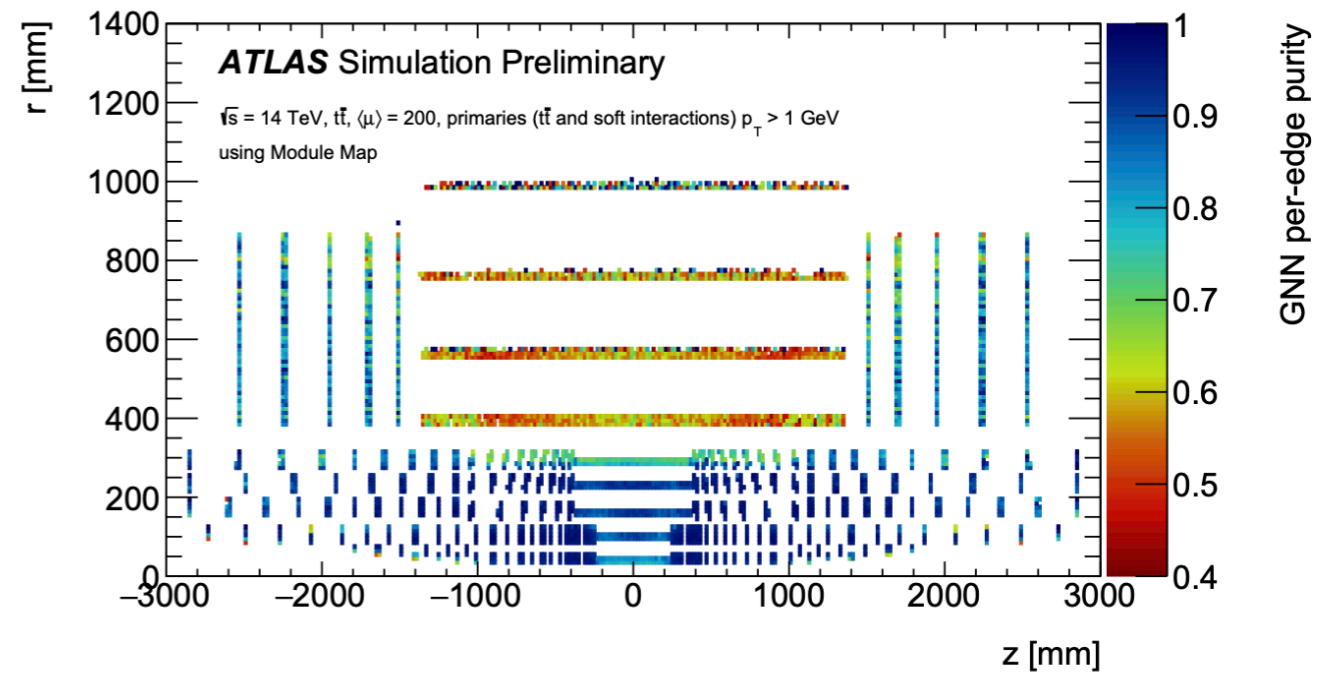
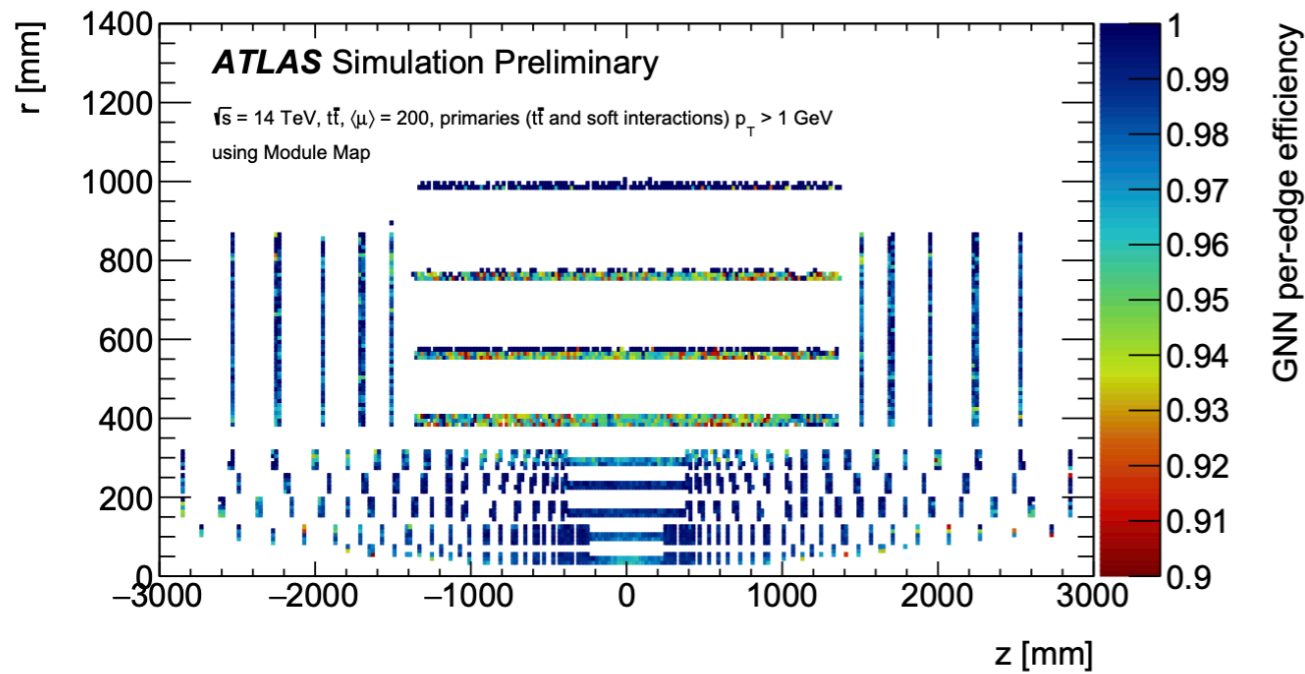


Tracking & ML

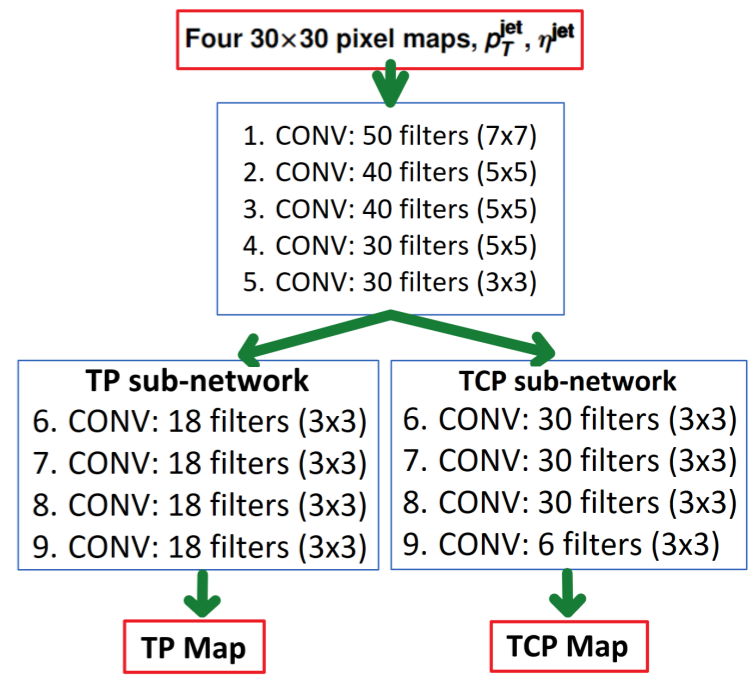
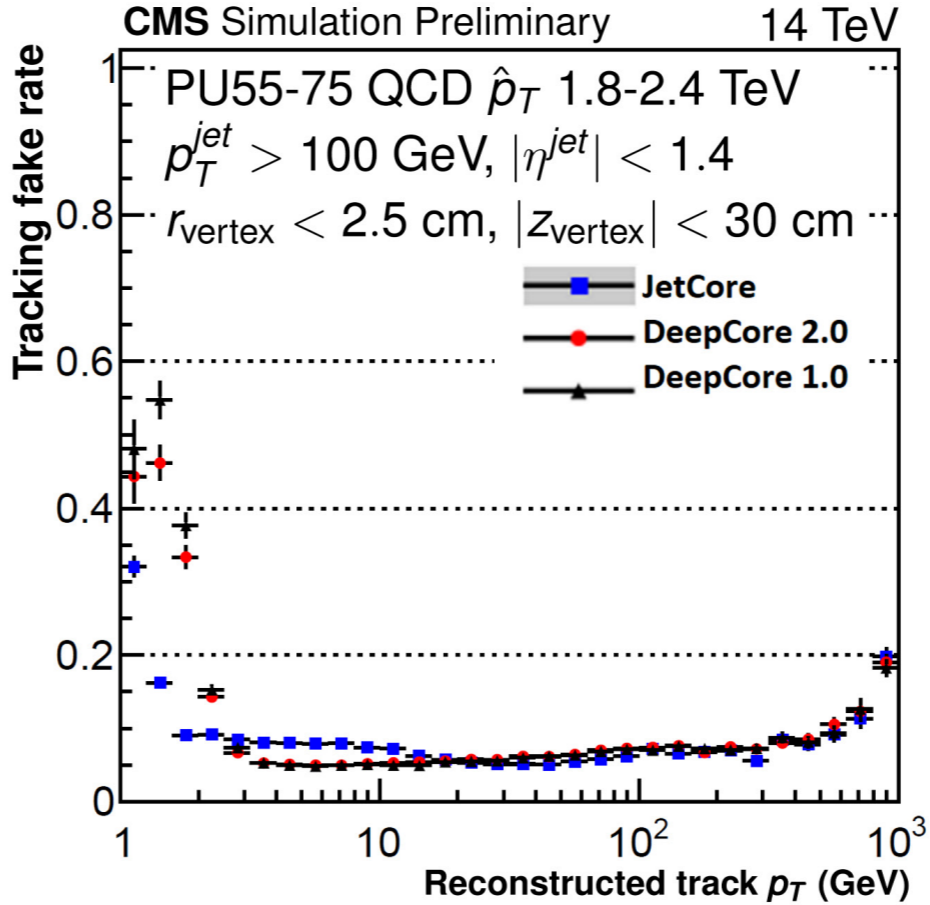
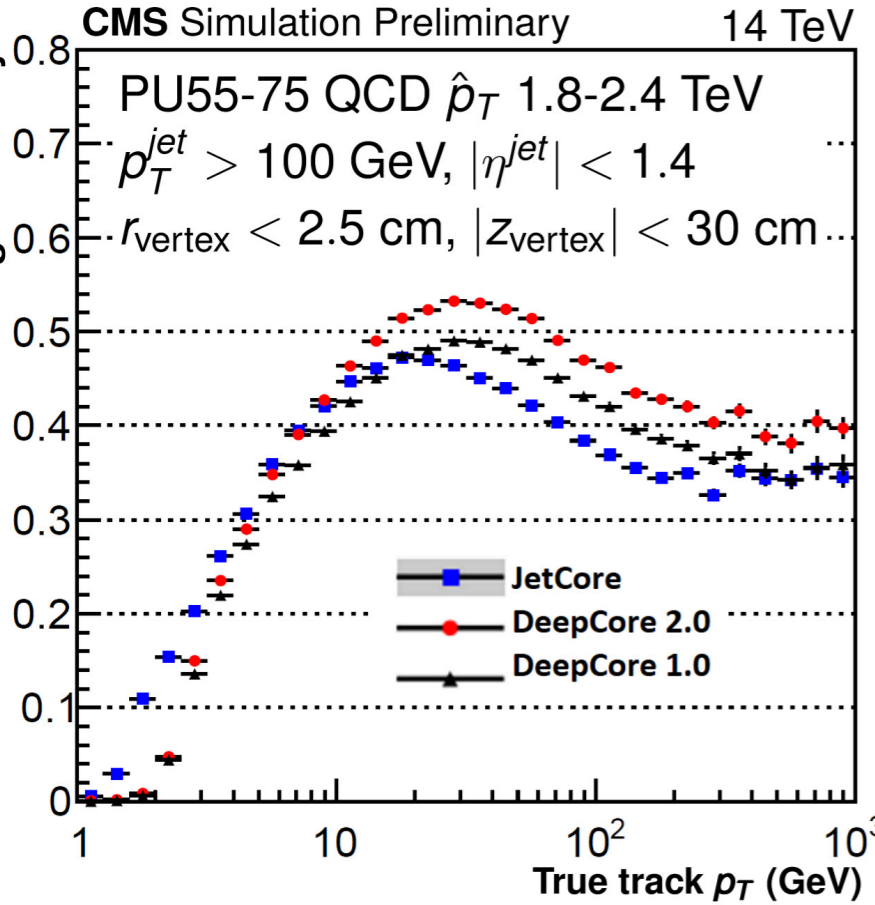
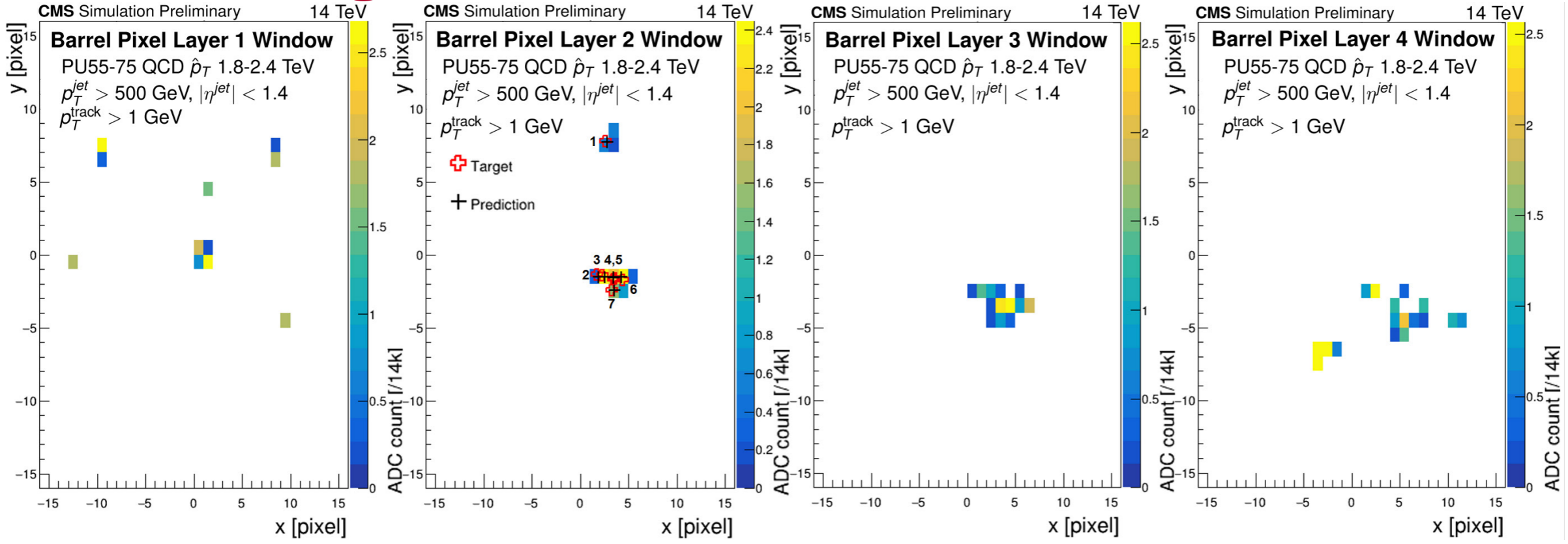


Tracking & ML : ATLAS

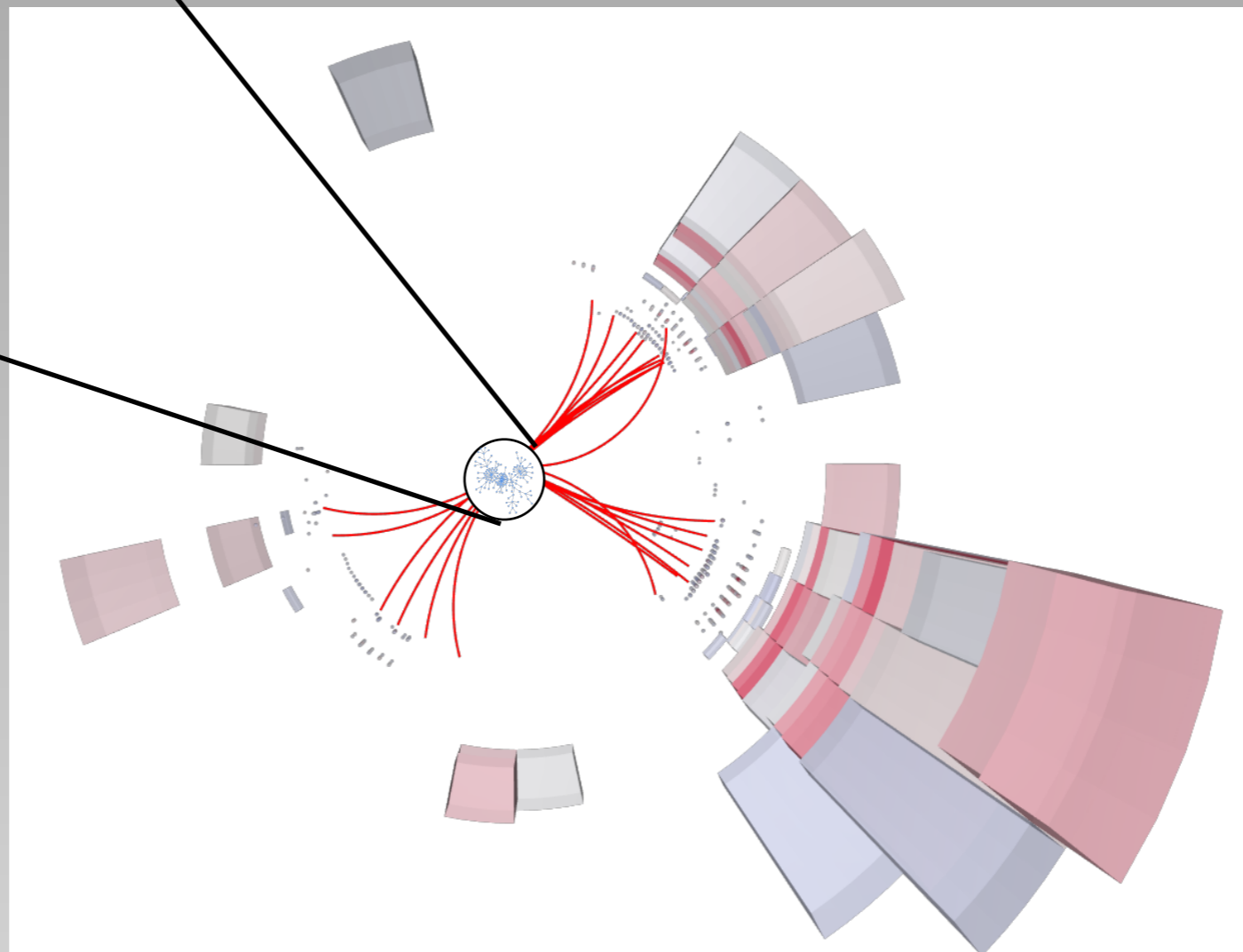
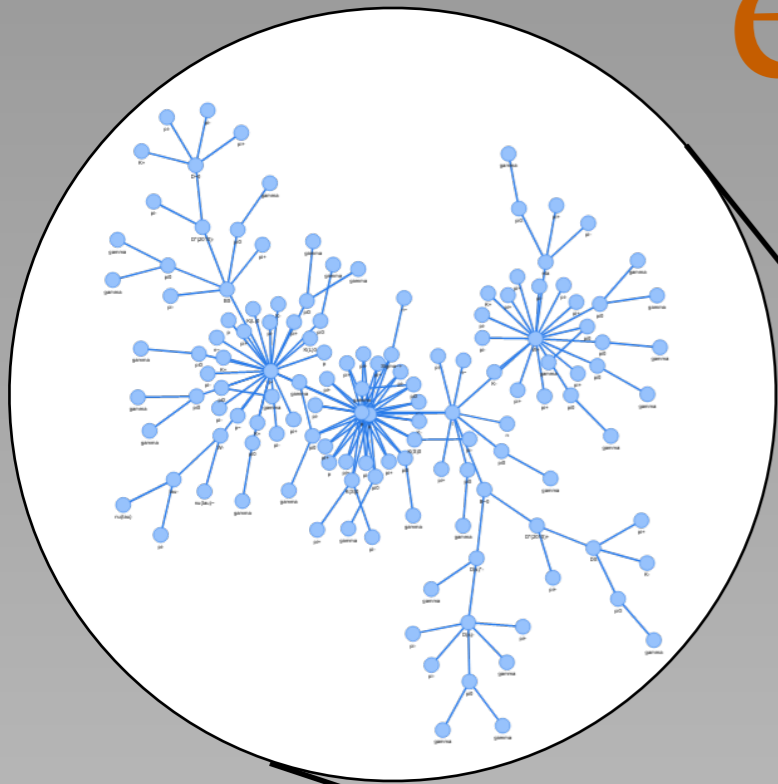
ATL-ITK-PROC-2022-006



Tracking & ML : CMS



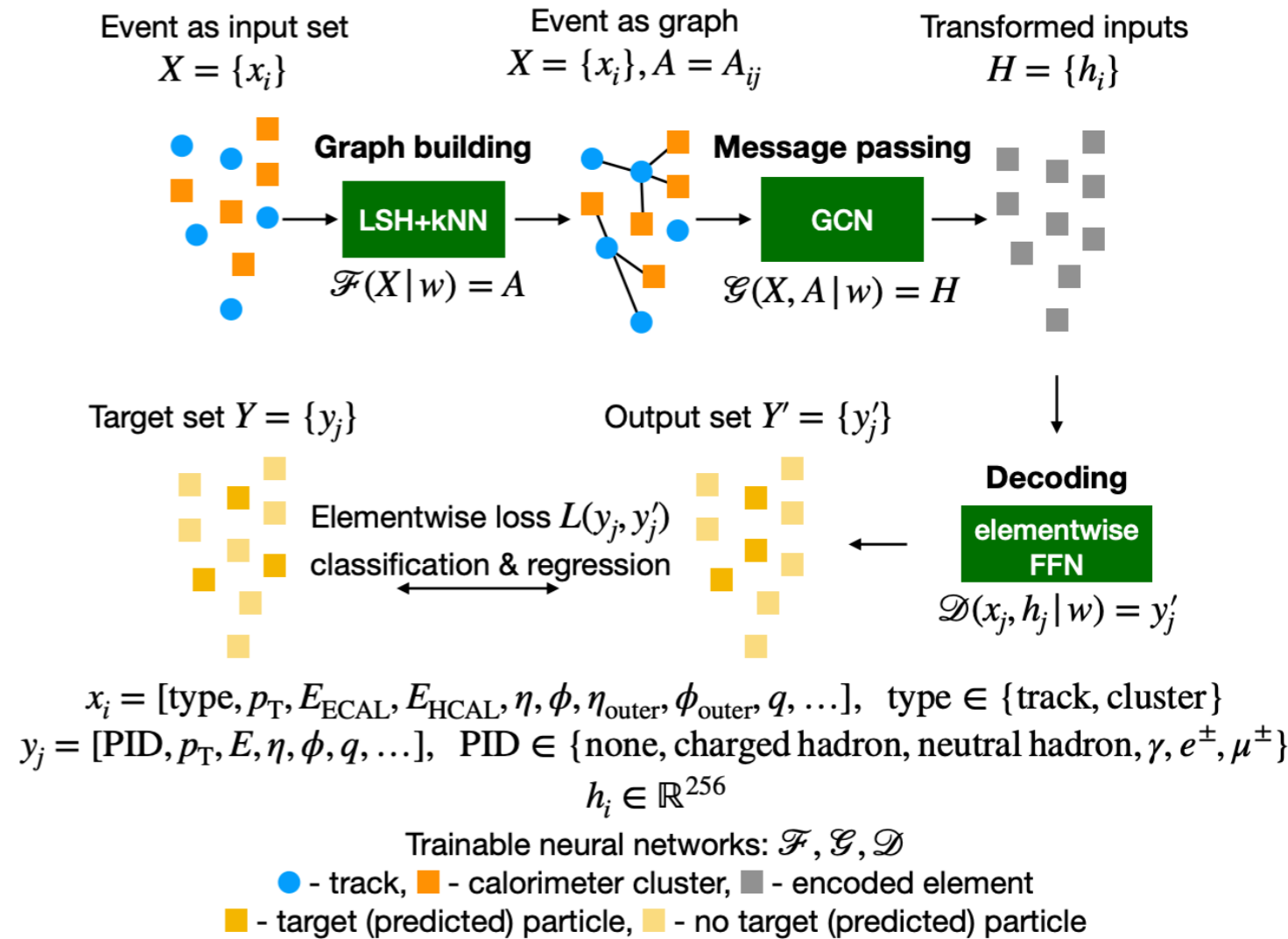
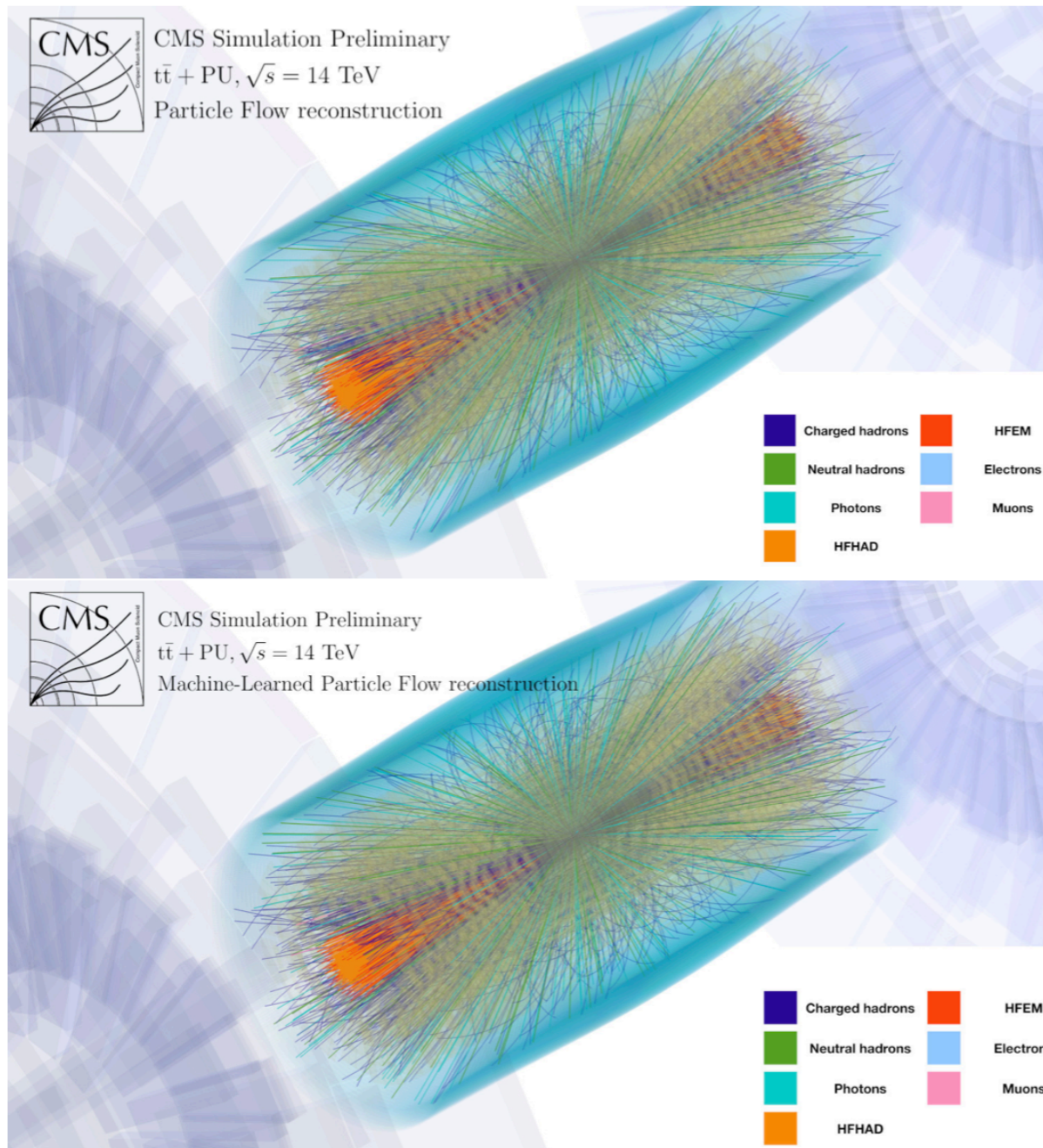
Particle-Flow event reconstruction



$f_{\{\theta\}}$ (

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Full ML driven PFlow : MLPF

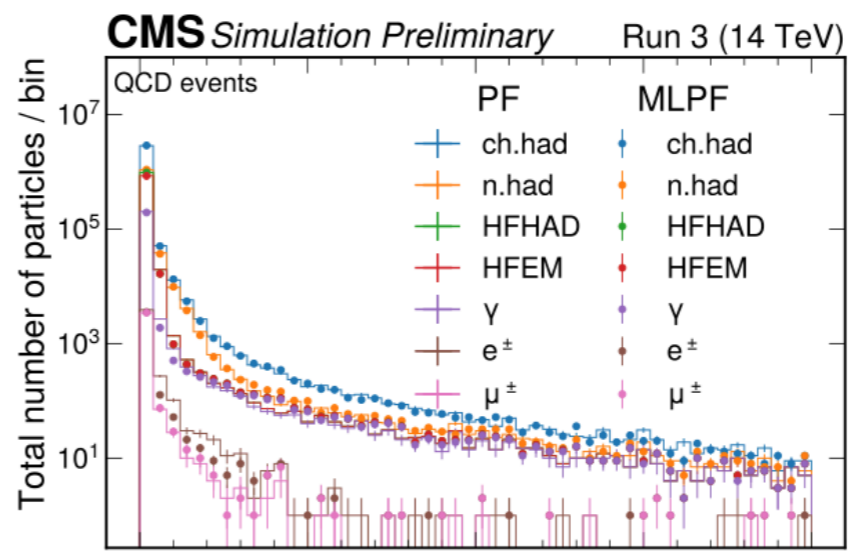
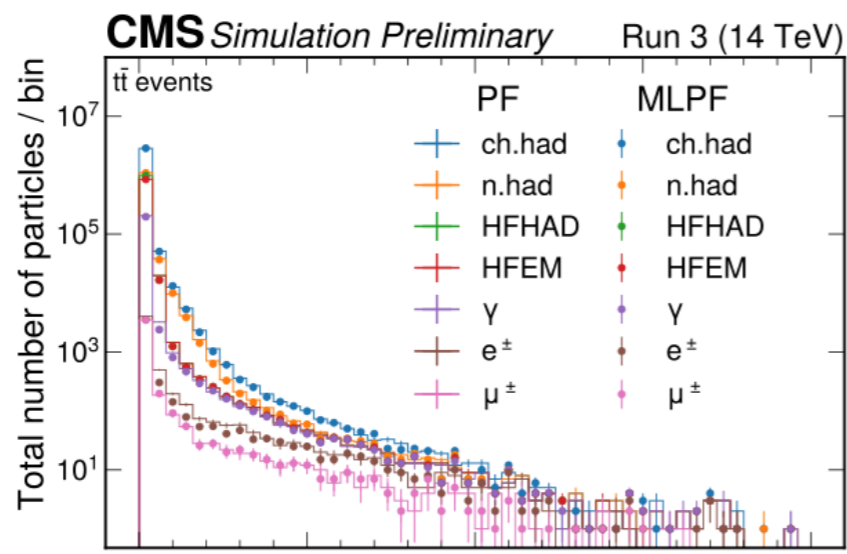


MLPF

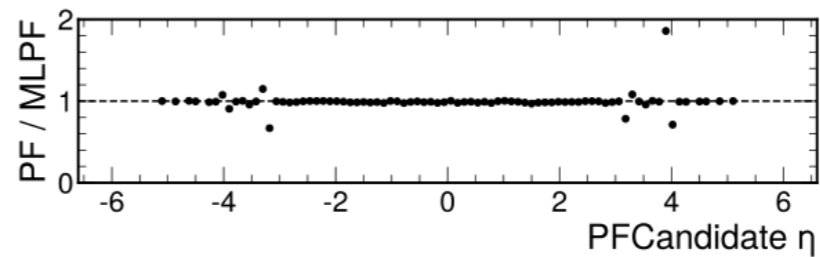
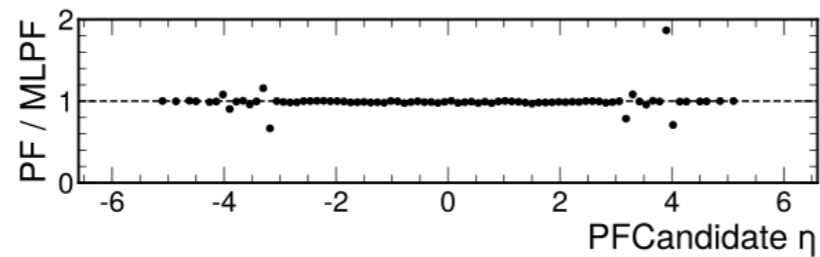
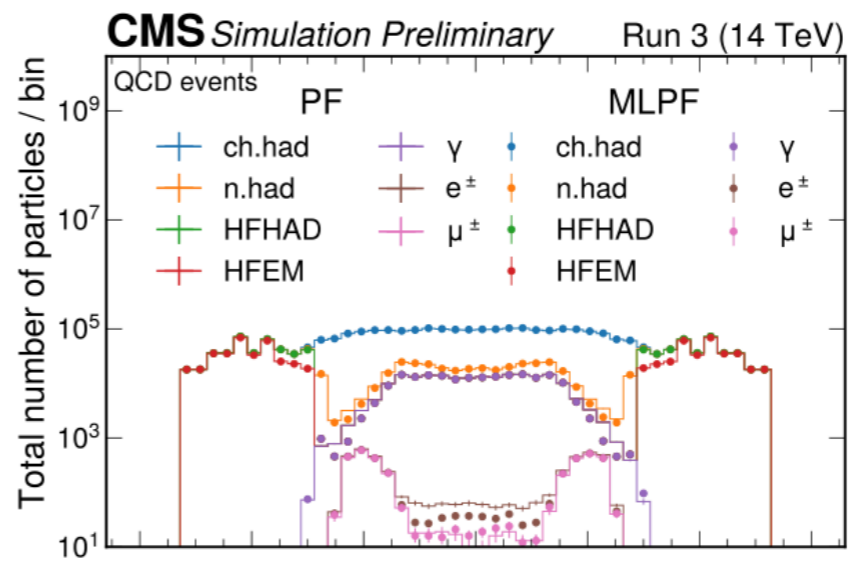
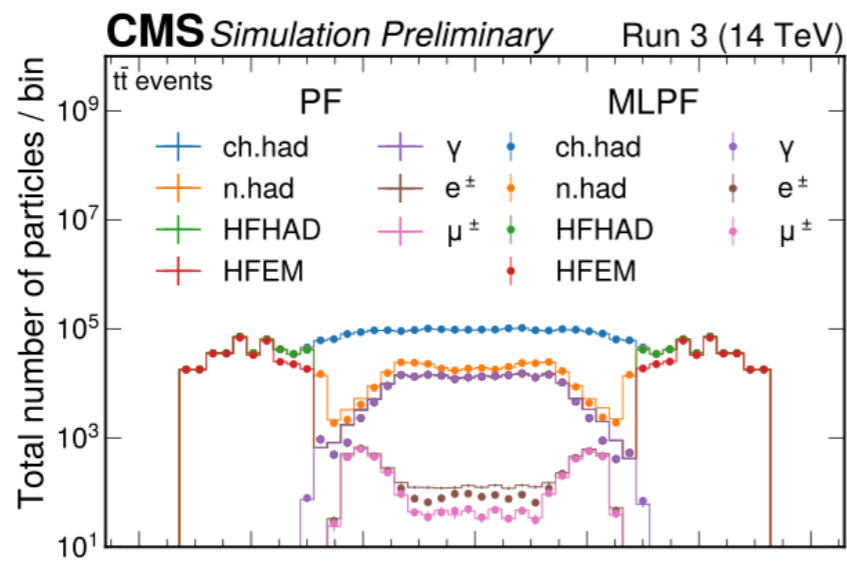
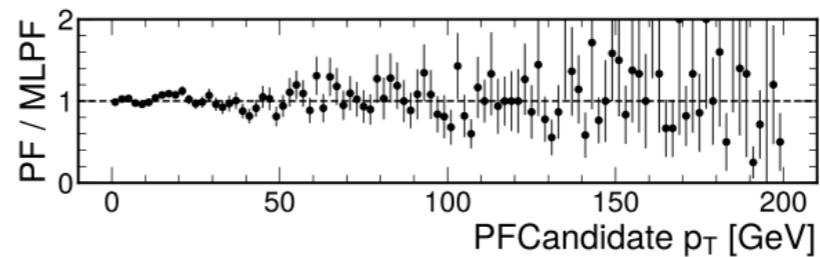
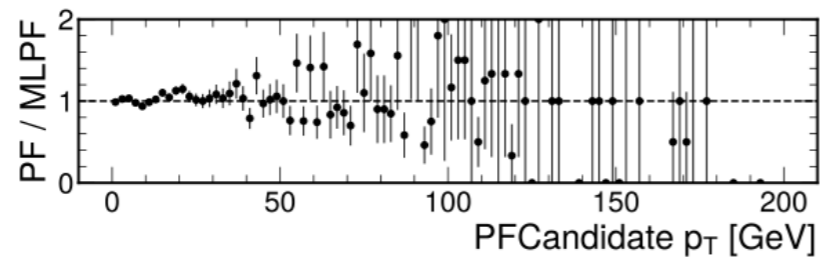
Eur. Phys. J. C (2021) 81: 381
 J. Pata et. al.

PF lepton, hadron, photon = F_{PF} (track hits + calo cells)

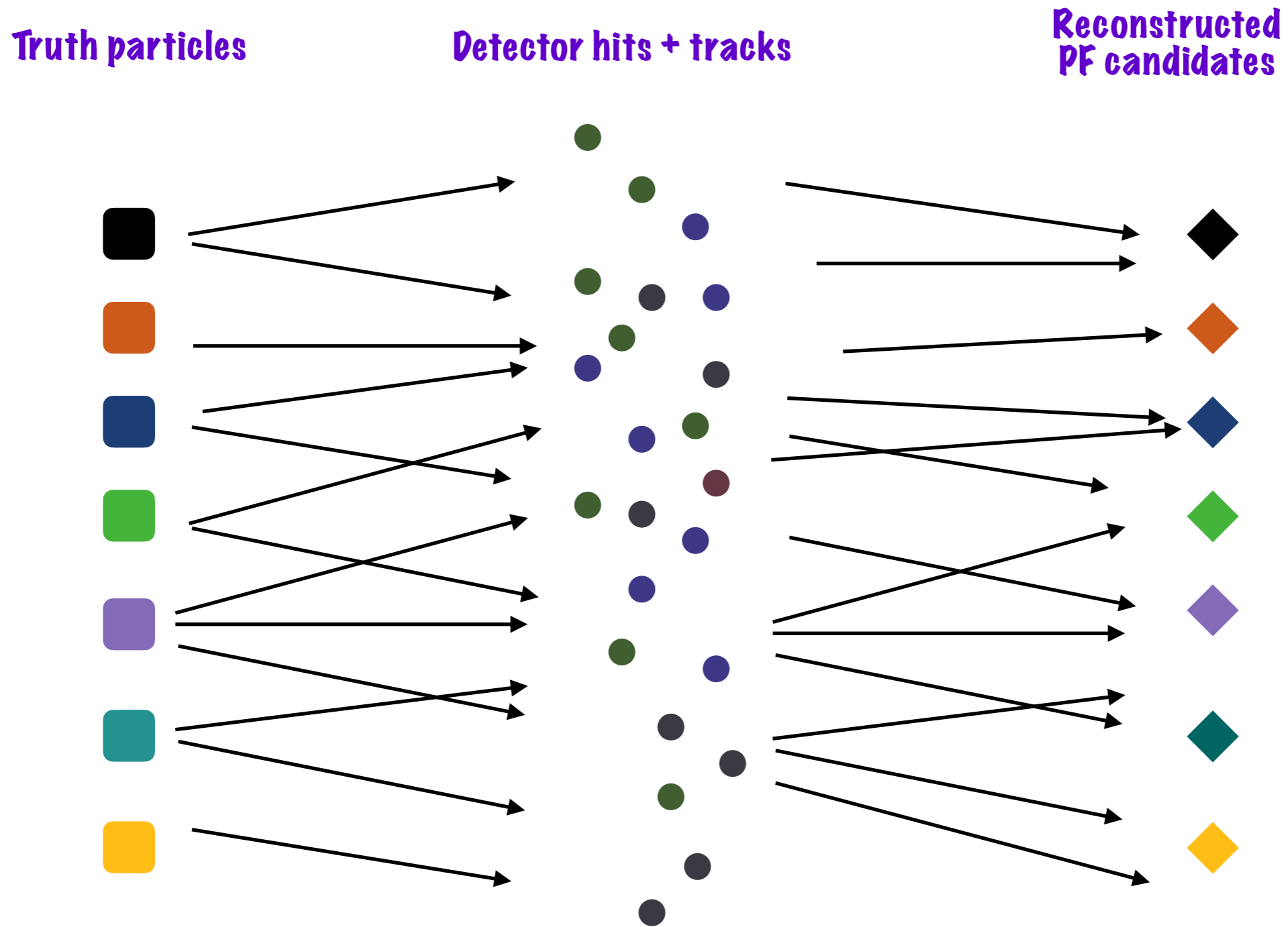
Combining track + calo for PFlow



MLPF
arXiv : 2203.00330
J. Pata et. al.



What's the core data structure?

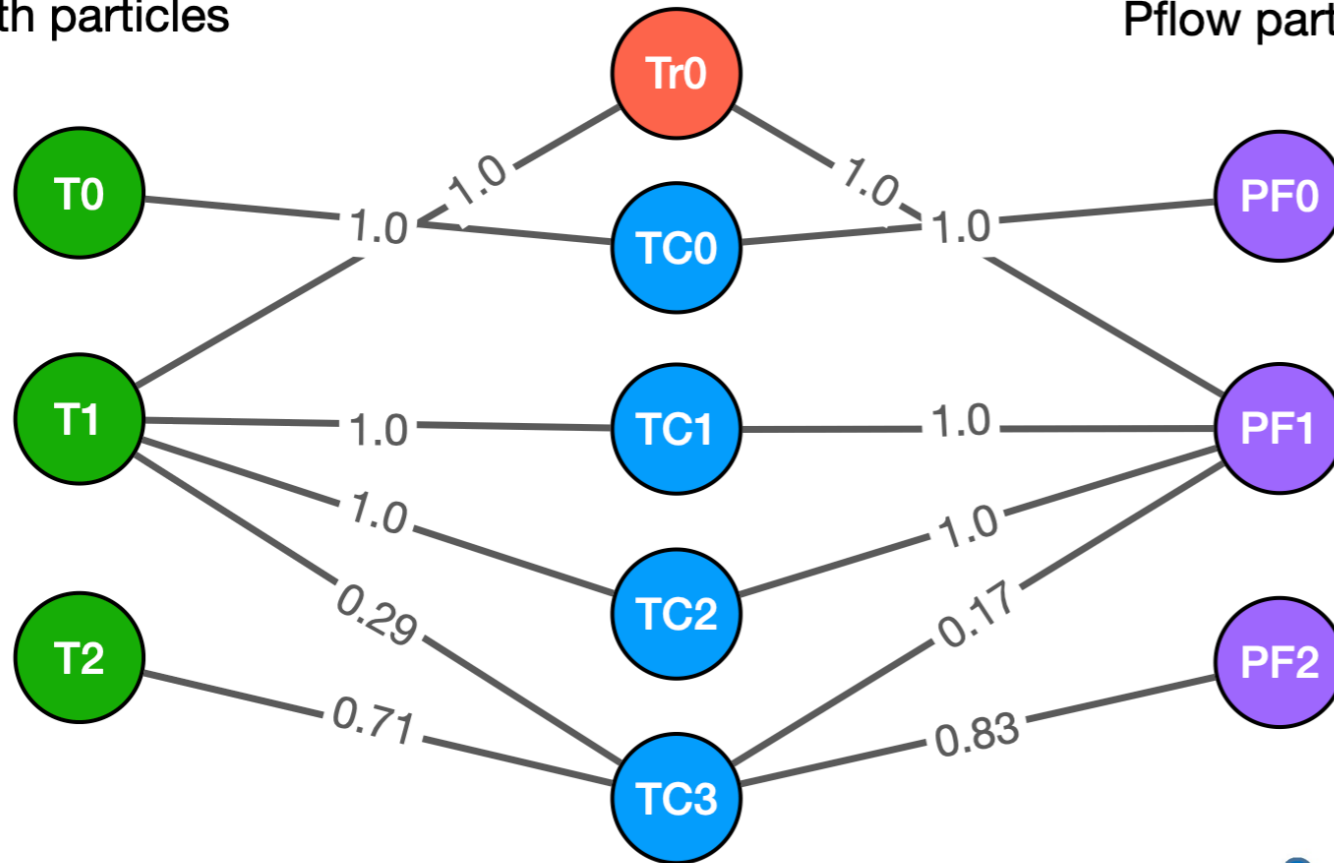


What's the core data structure?

Nodes
(Tracks, topoclusters)

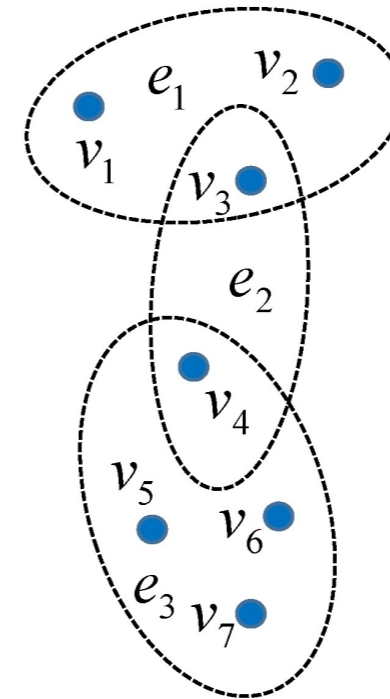
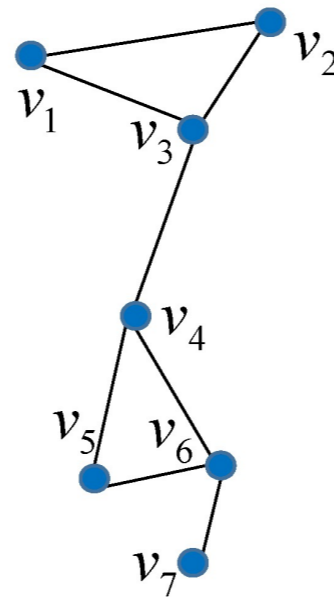
Truth particles

Pflow particles



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

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



	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

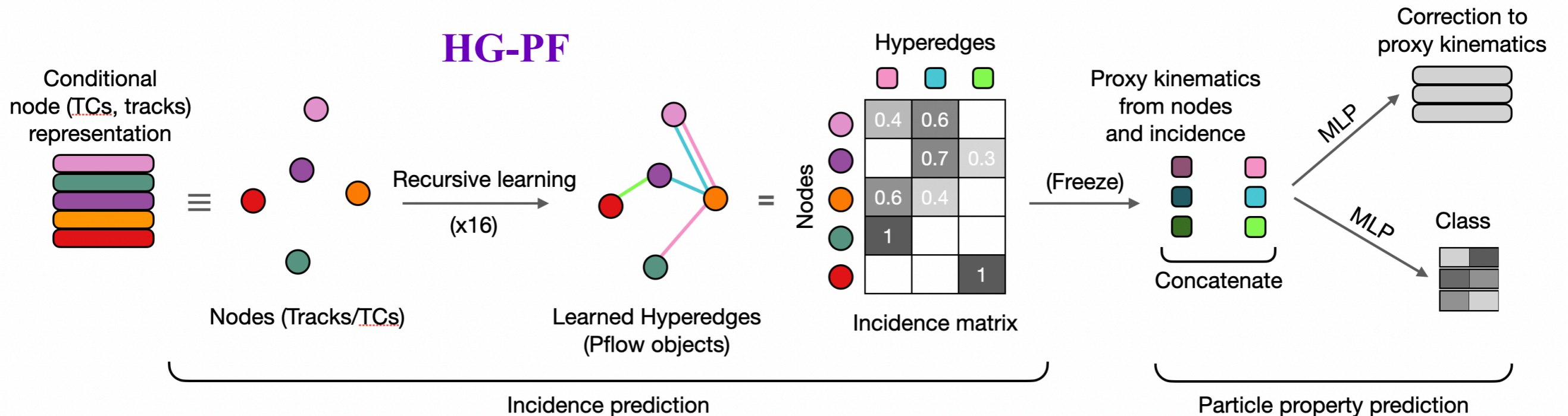
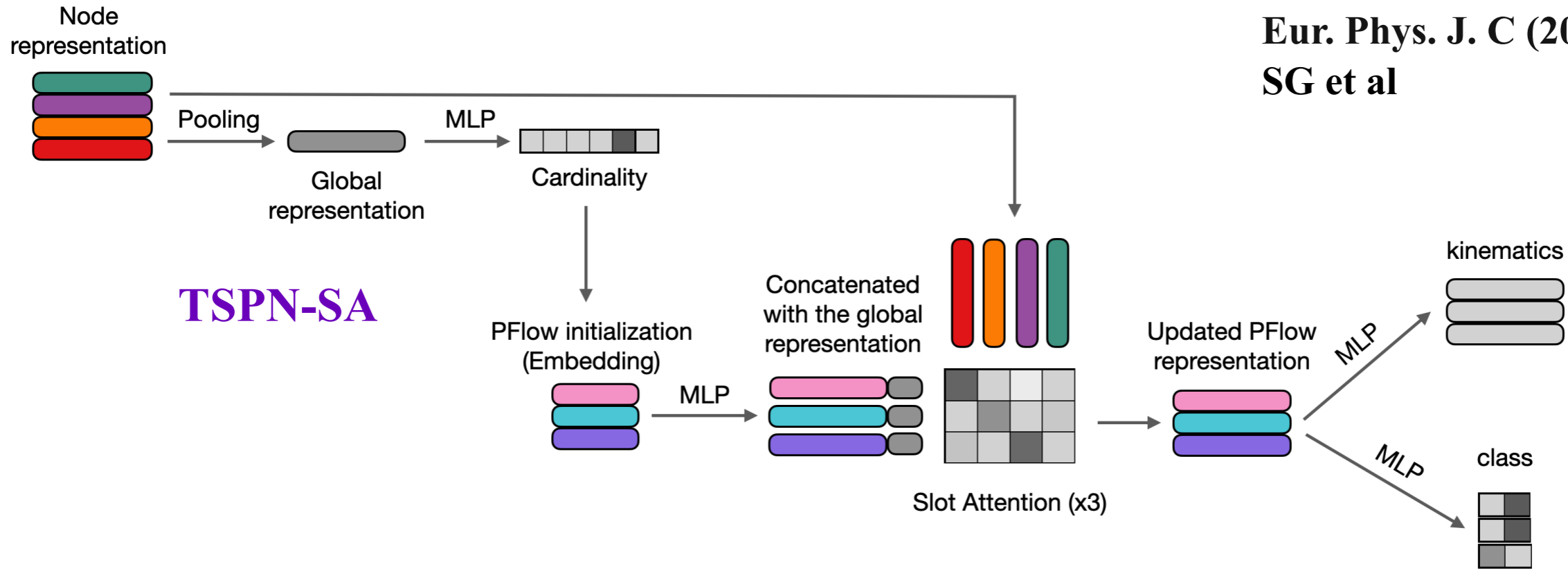
(a) Simple graph

(b) Hypergraph \mathbf{G}

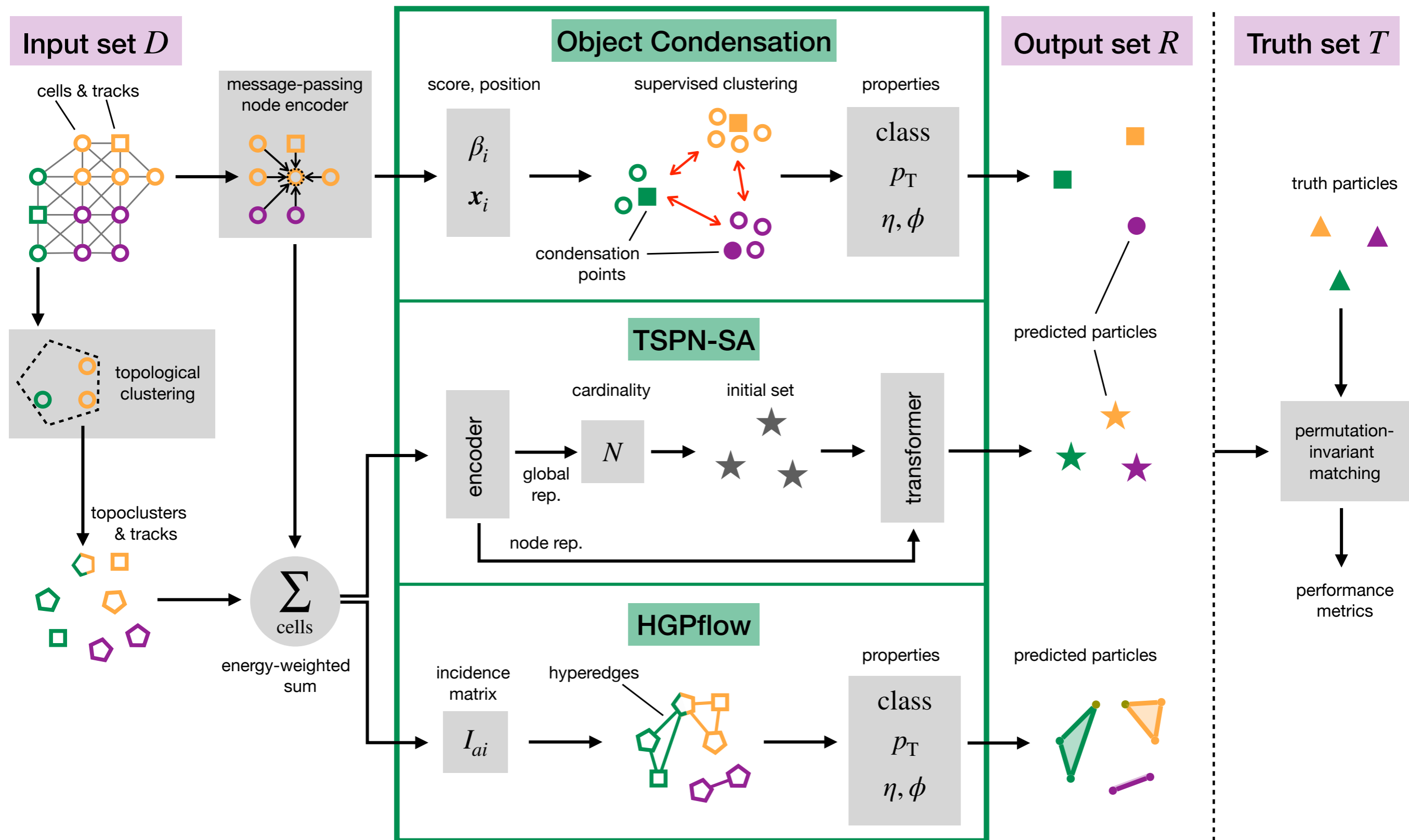
(c) Incidence matrix \mathbf{H}

The new networks we tried

Eur. Phys. J. C (2023) 83:596
SG et al



The network flow comparisons



Design of the performance metrics

- Efficiency and fake rate
- Classification purity
- Particle angular and momentum resolution
- Jet-level quantities

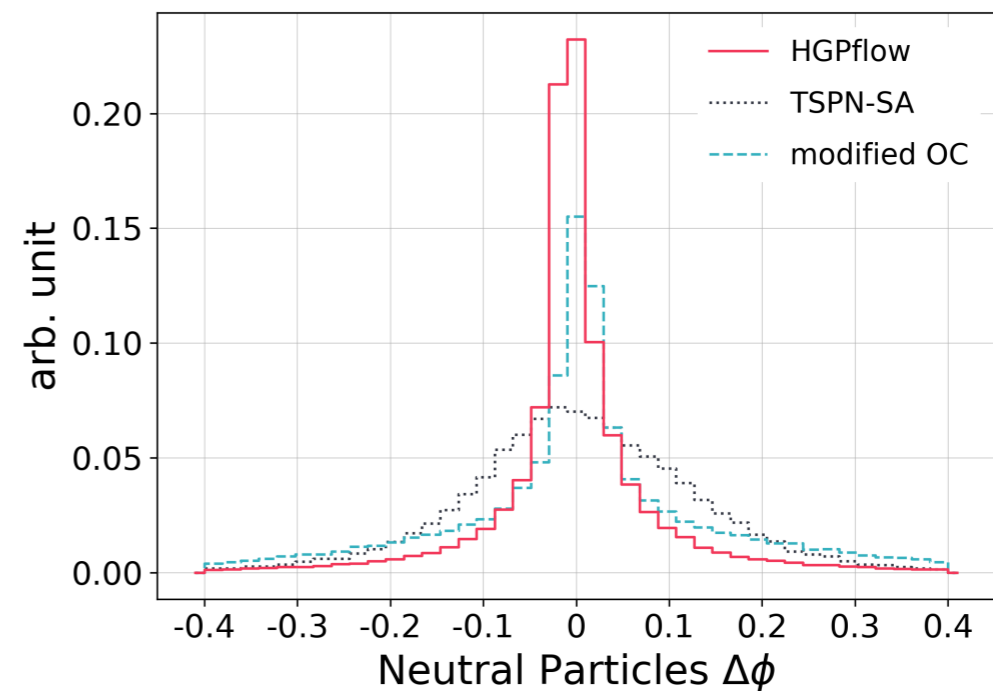
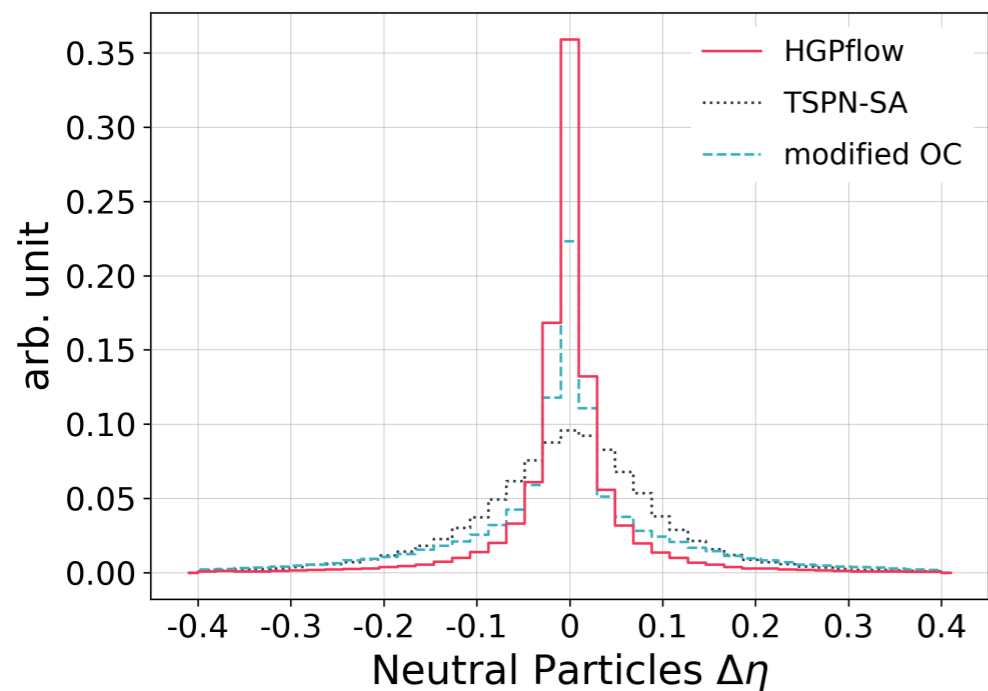
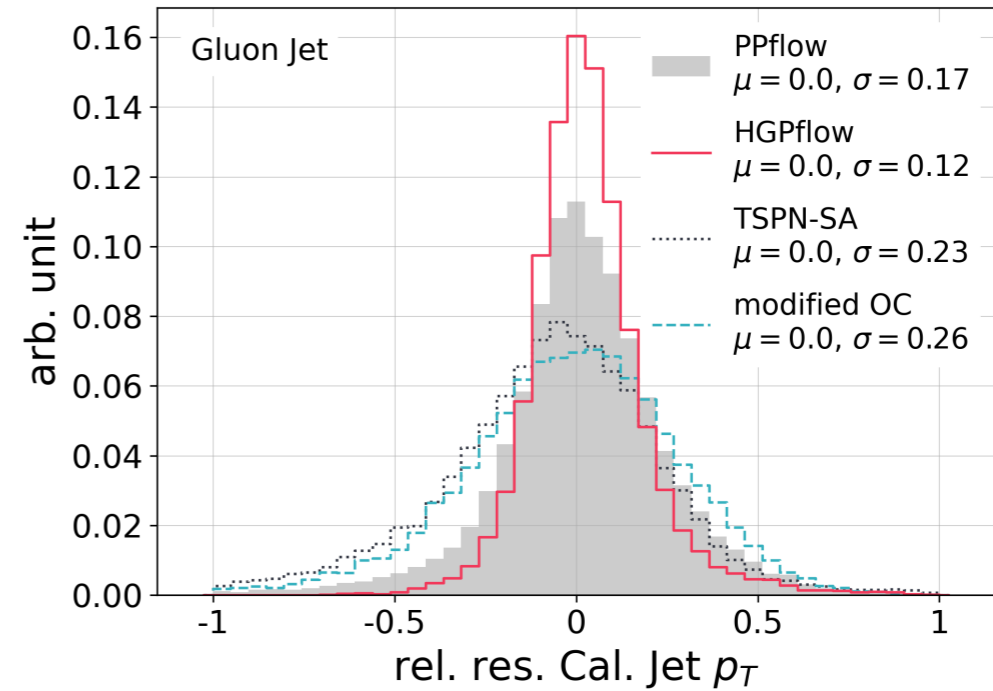
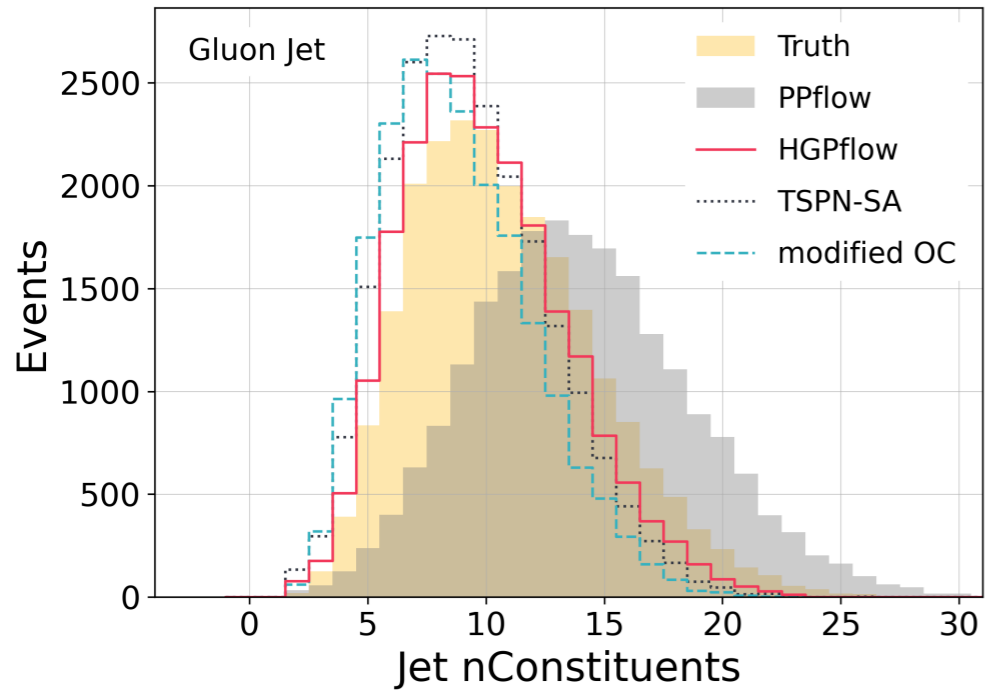
The efficiency and fake rate are defined as follows:

$$\varepsilon \equiv \frac{N(\text{matched pred})}{N(\text{targ})}, \quad f \equiv \frac{N(\text{unmatched pred})}{N(\text{pred})}$$

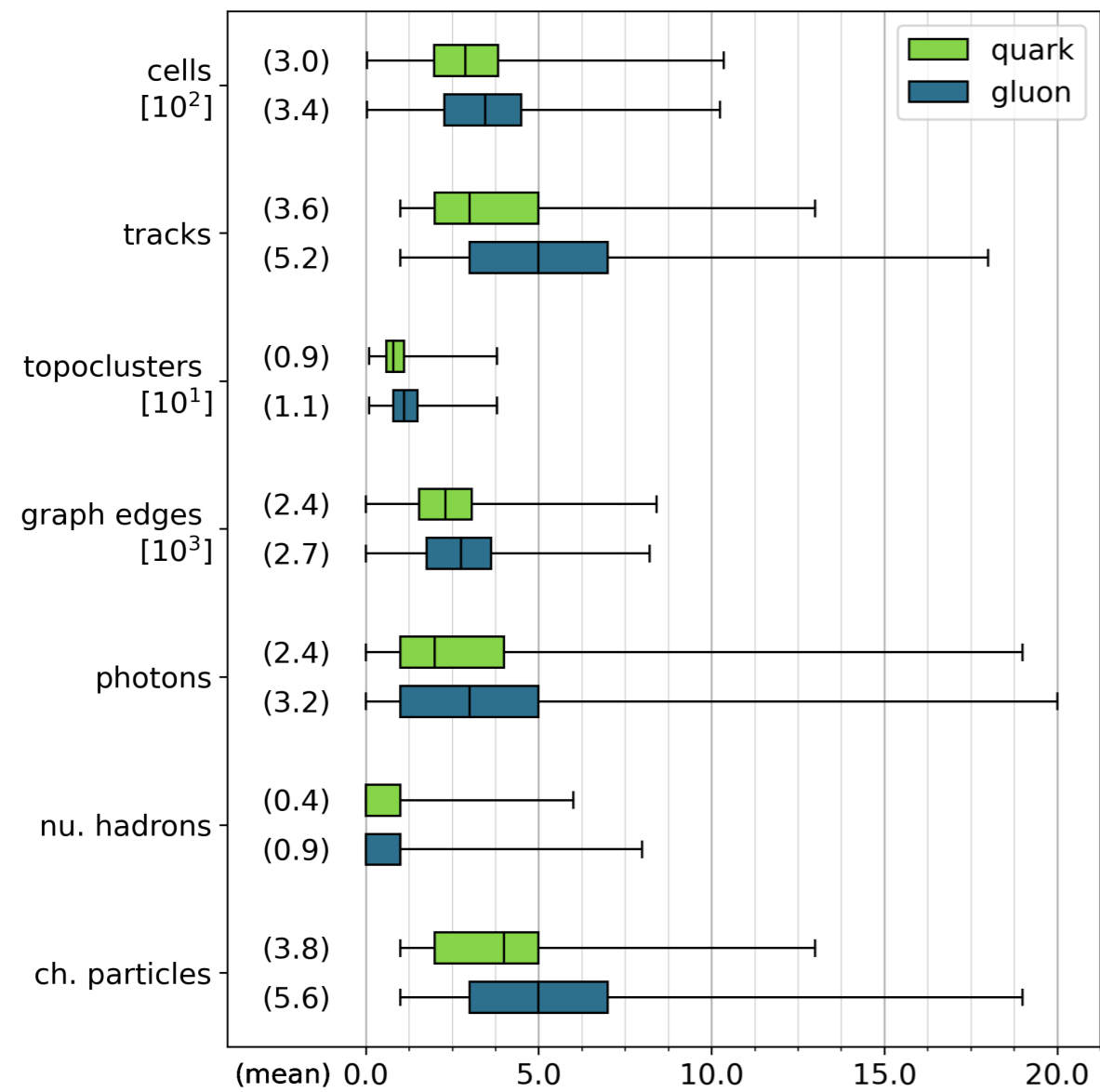
Set-to-set matching is done using the Hungarian distance :

$$\sqrt{c_{p_T}(\Delta p_T/p_T^{\text{truth}})^2 + C_{\Delta R}(\Delta R)^2}$$

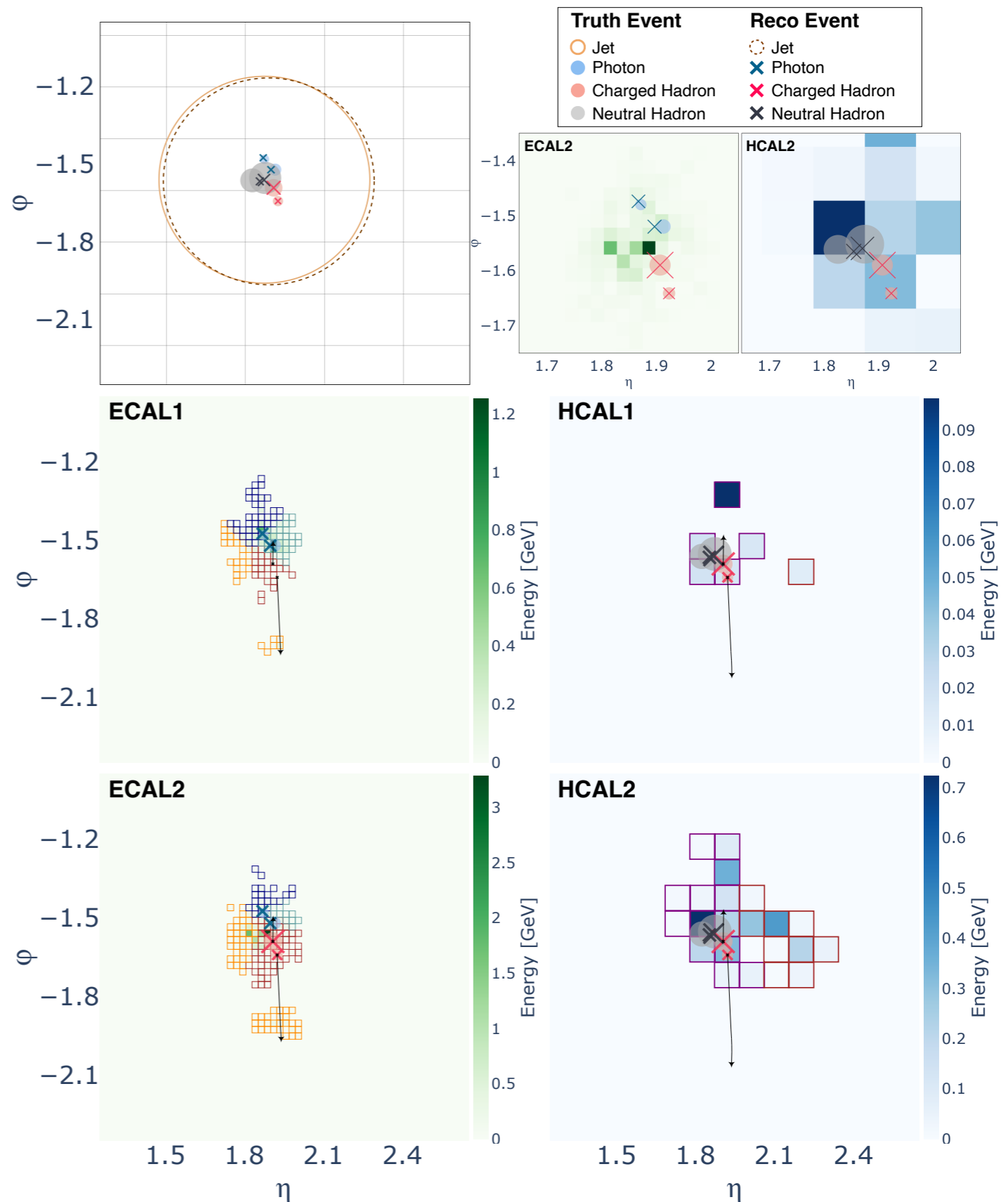
$$\mathcal{L}_{\text{hung}}(A, B) = \min_{\pi \in P} \sum_{a_i \in A} d(a_i, b_{\pi(i)})$$



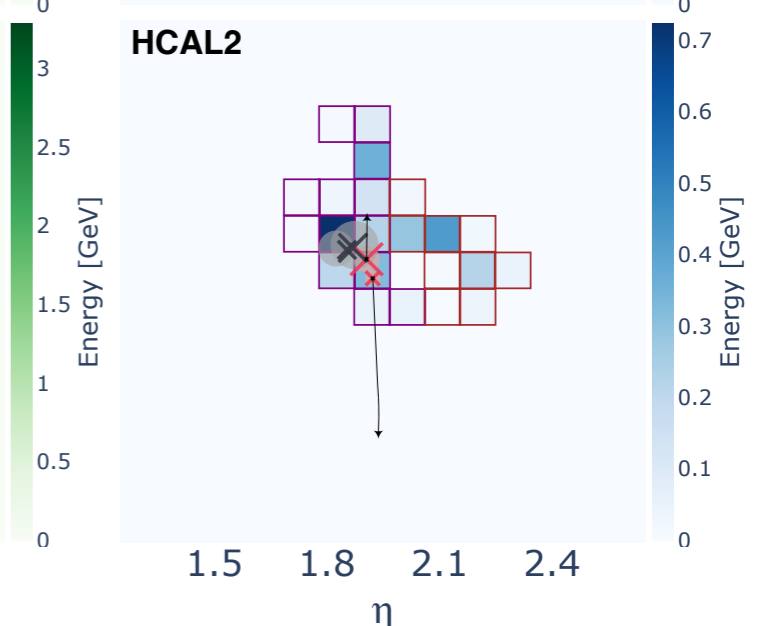
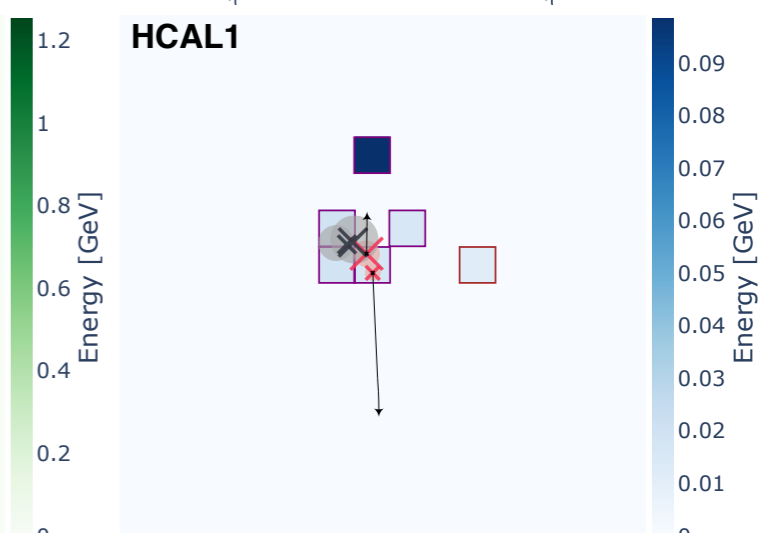
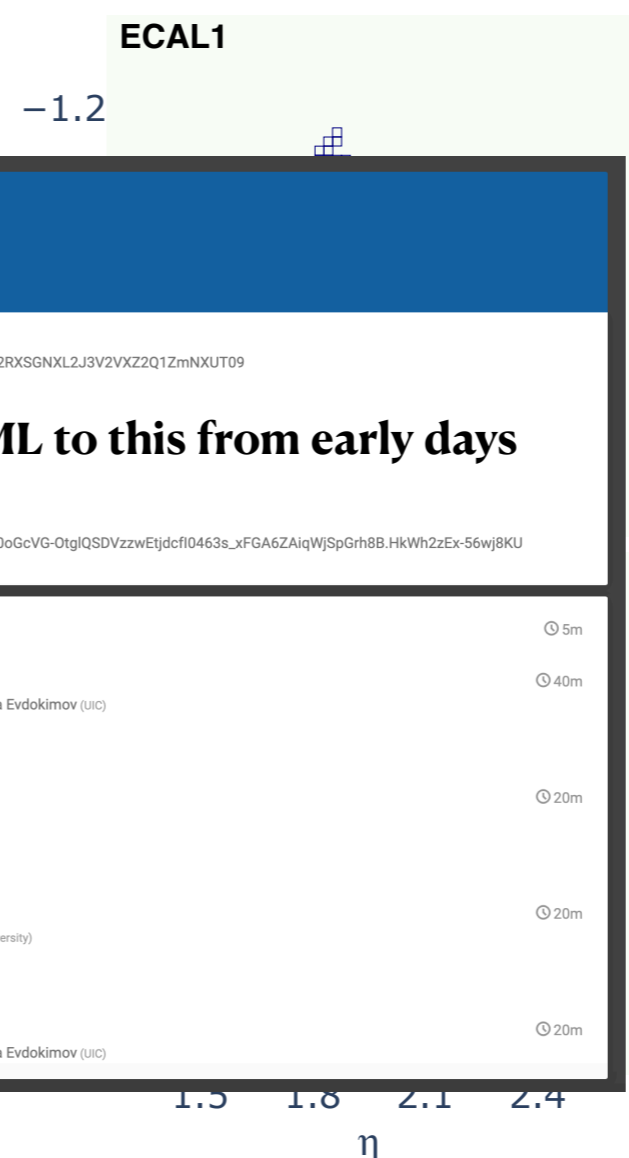
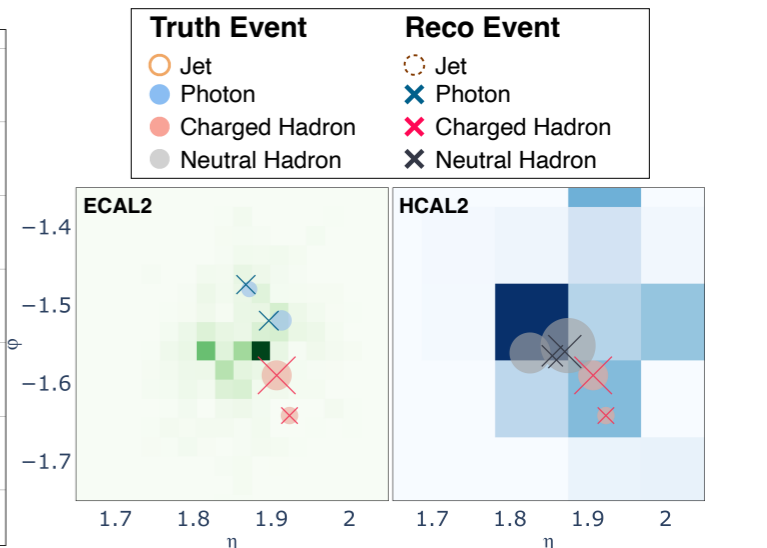
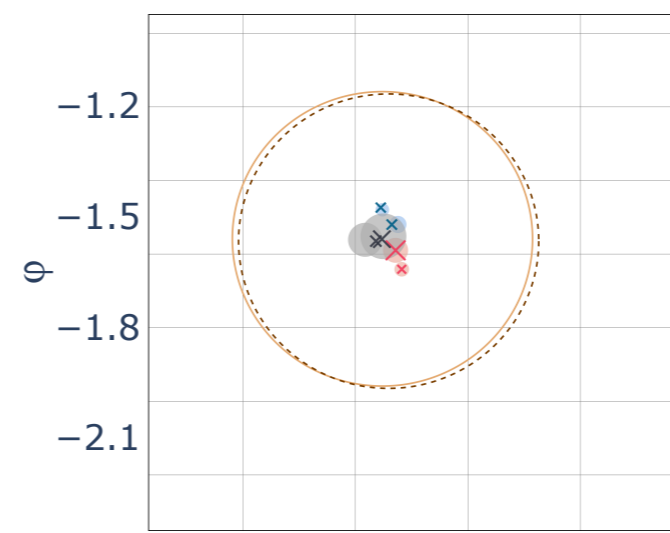
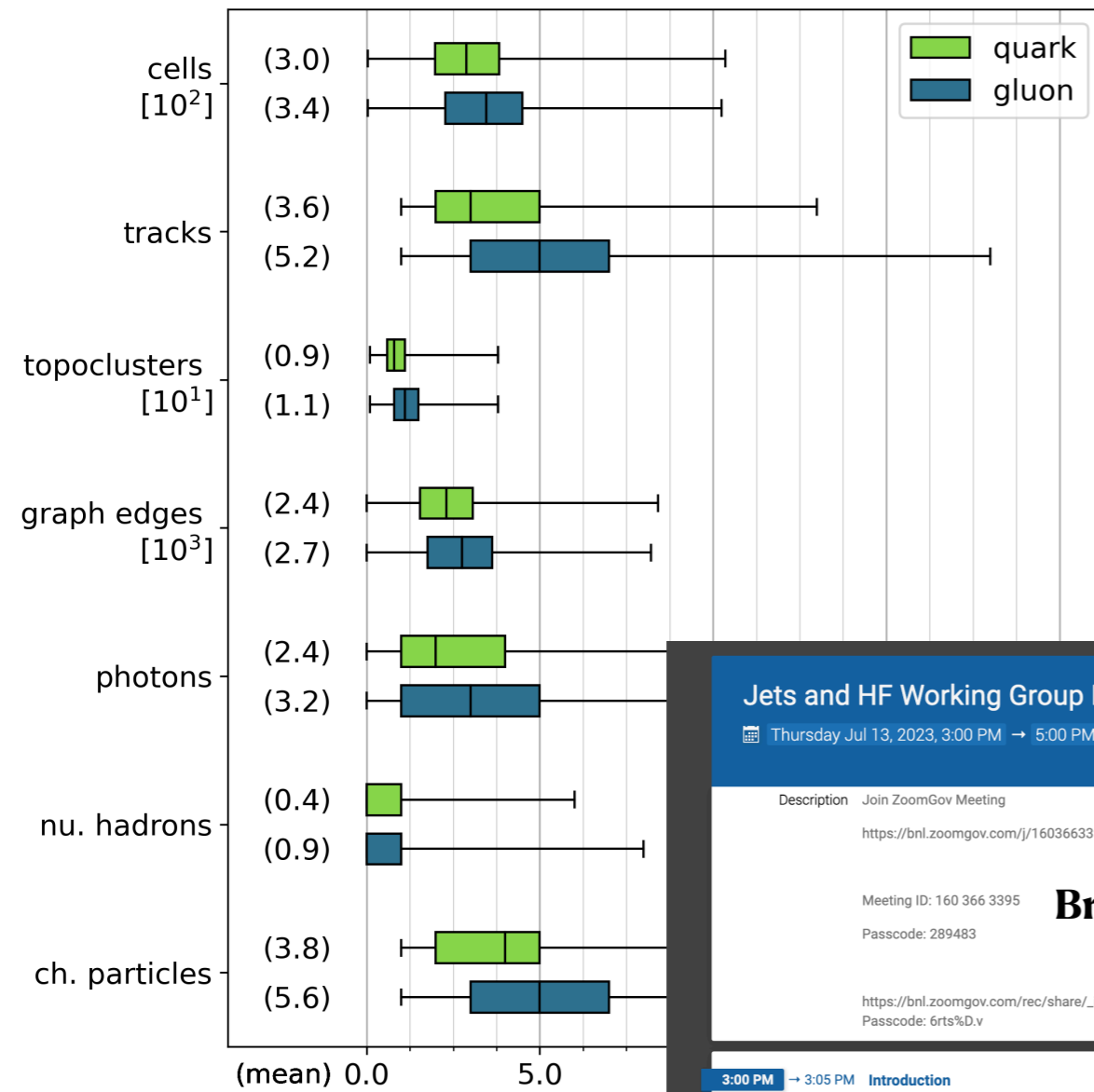
Data complexity & sample output



HG-PFlow seems to be doing a better job among the compared methods



Data complexity & sample output



Jets and HF Working Group Meeting

Thursday Jul 13, 2023, 3:00 PM → 5:00 PM US/Eastern

Description: Join ZoomGov Meeting
<https://bnl.zoomgov.com/j/1603663395?pwd=RHpSY2RXSGNXL2J3V2VXZ2Q1ZmNXUT09>

Meeting ID: 160 366 3395
 Passcode: 289483

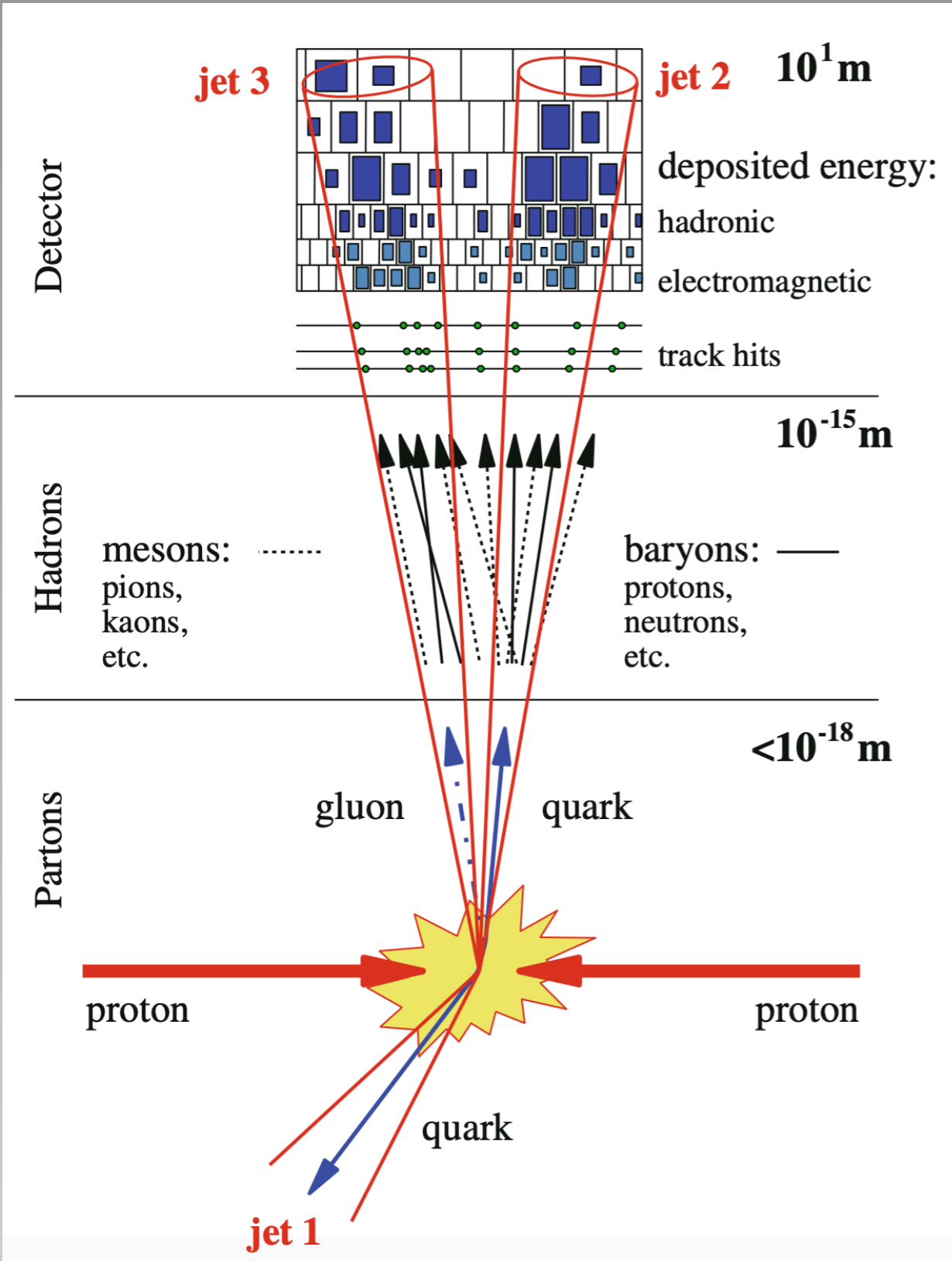
Bring ML to this from early days

https://bnl.zoomgov.com/rec/share/_ipKV0vIU6ryhT30oGcVG-OtglQSDVzzwEtjdcf10463s_xFGA6ZaiqWjSpGrh8B.HkWh2zEx-56wj8KU
 Passcode: 6rts%D.v

3:00 PM → 3:05 PM	Introduction	🕒 5m
3:05 PM → 3:45 PM	Particle Flow in CMS Speakers: Brian Page (Brookhaven National Laboratory), Olga Evdokimov (IUC)	🕒 40m
3:45 PM → 4:05 PM	PF implementation survey Speaker: Derek Anderson (Iowa State University)	🕒 20m
4:05 PM → 4:25 PM	PF experience @ sPHENIX Speaker: Antonio Carlos Oliveira da Silva (Iowa State University)	🕒 20m
4:25 PM → 4:45 PM	Benchmark Discussion Speakers: Brian Page (Brookhaven National Laboratory), Olga Evdokimov (IUC)	🕒 20m

HG-PFlow seems to a better job among methods

Jet tagging



$$\{p_1, p_2, \dots, p_n\}$$

Jet Algorithm (for CA, kT, anti-kT)

$$\{j_1, j_2, \dots, j_k\}$$

$$\{p_1, p_2, \dots, p_n\} = F(q)$$

The forward problem is not computable from first principle

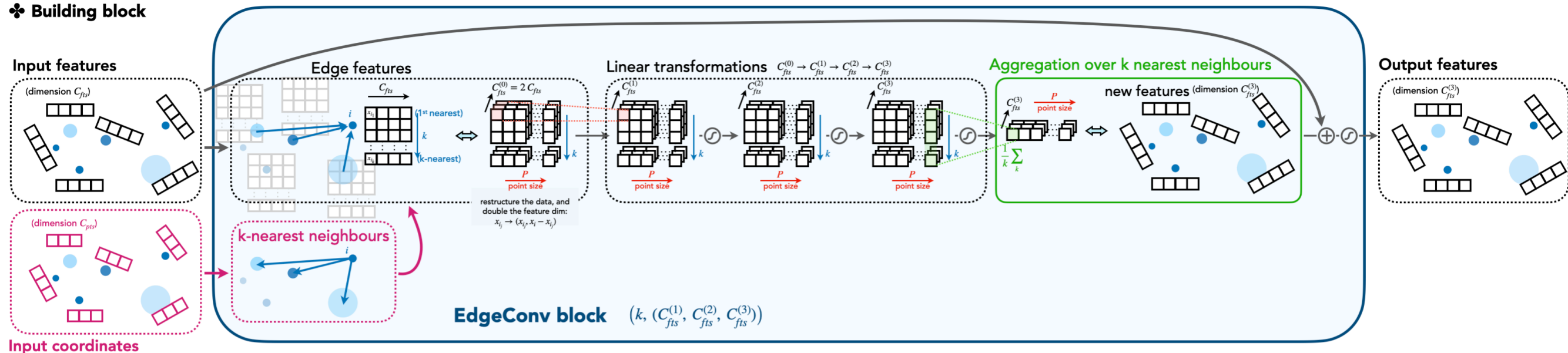
The question of jet tagging is how do we define the inverse problem?

$$q = F^{-1}(\{p_1, p_2, \dots, p_n\}) ?$$

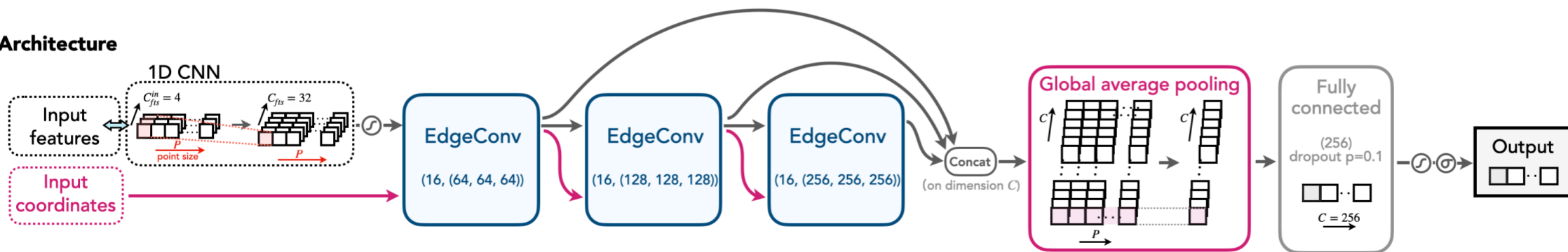
Object tagging

Particle Net : 1902.08570
 Huilin Qu, Loukas Goukos

Building block



Architecture



arXiv > cs > arXiv:1801.07829

Computer Science > Computer Vision and Pattern Recognition

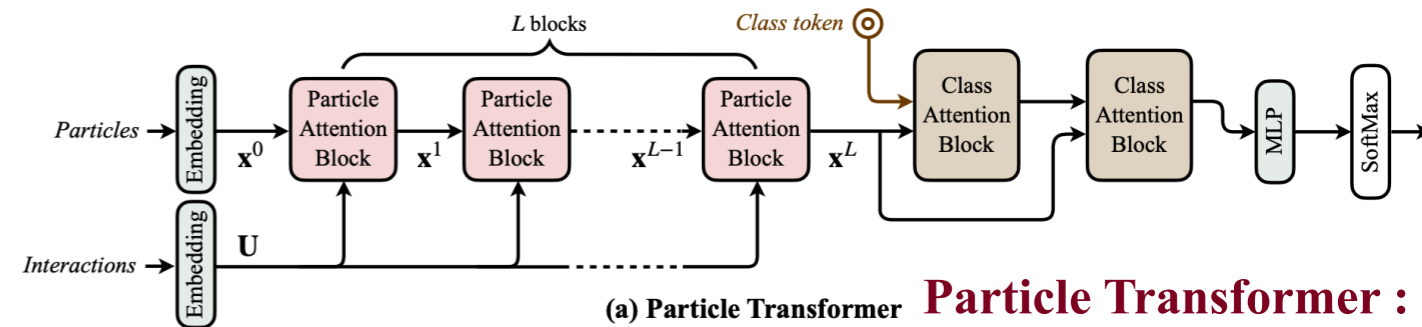
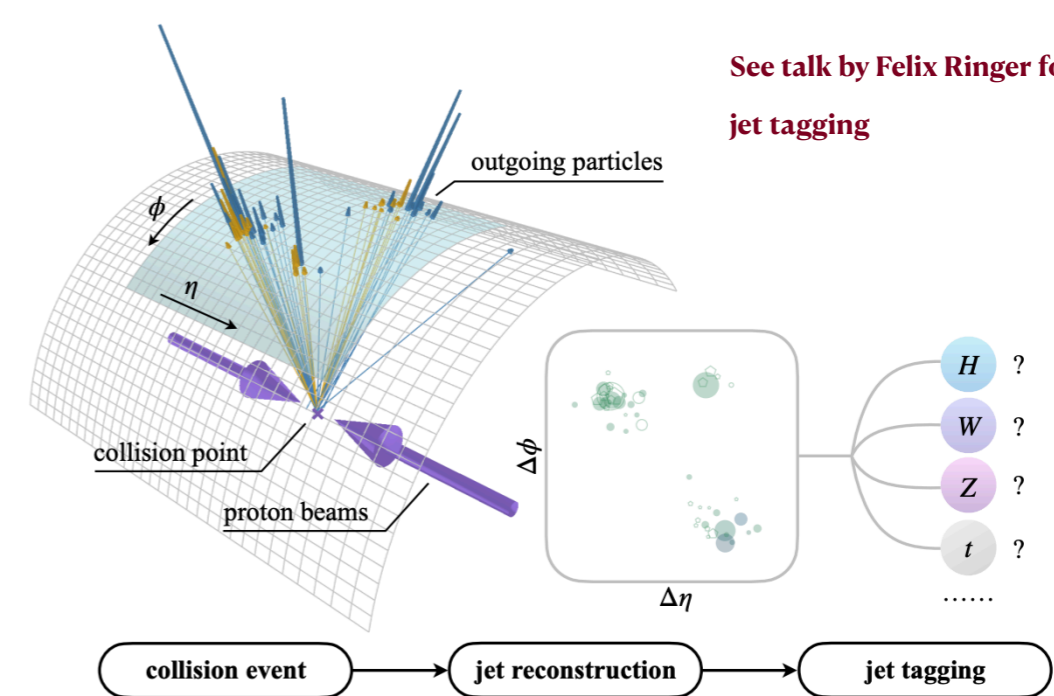
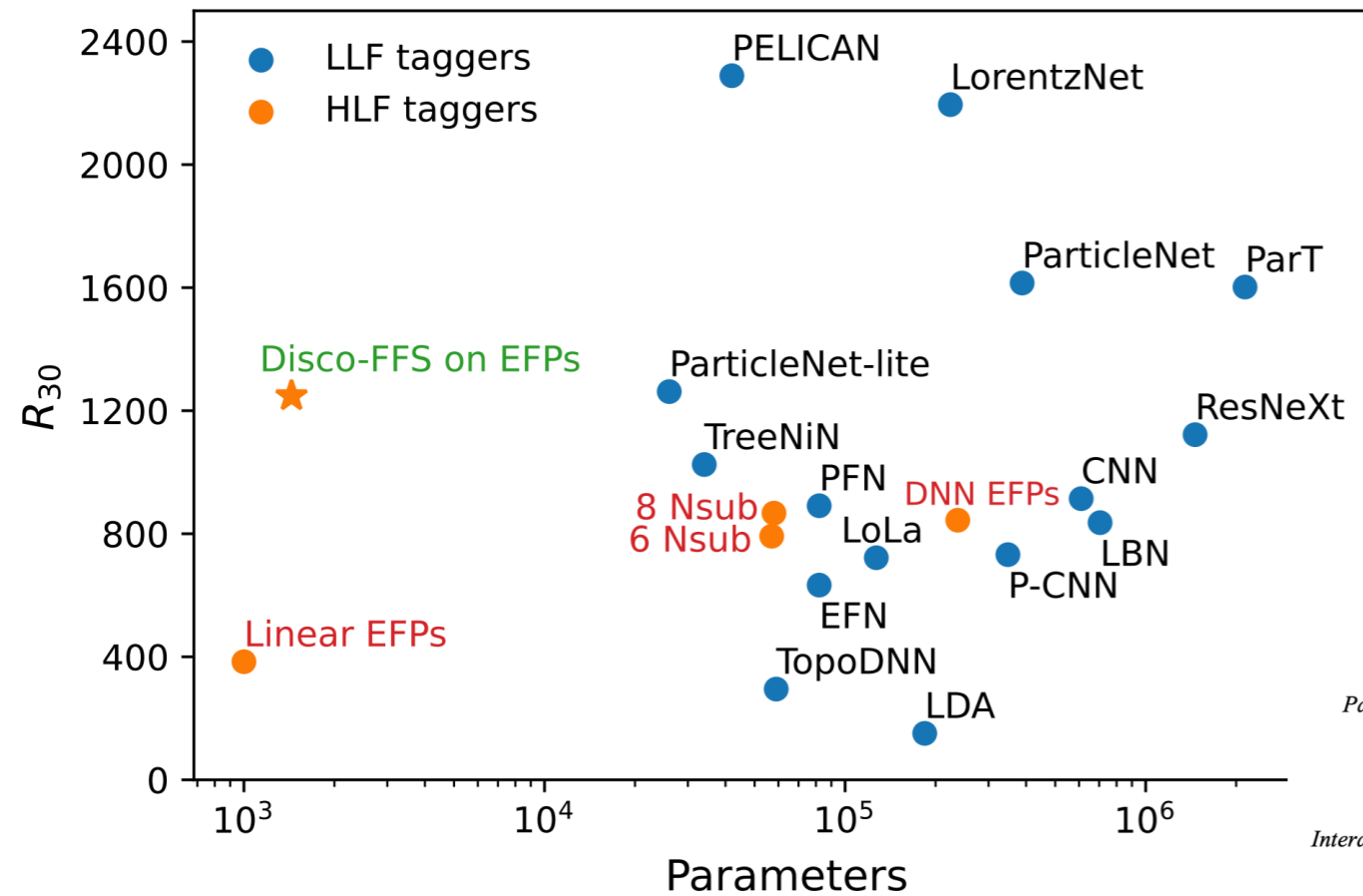
[Submitted on 24 Jan 2018 (v1), last revised 11 Jun 2019 (this version, v2)]

Dynamic Graph CNN for Learning on Point Clouds

Yue Wang, Yongbin Sun, Ziwei Liu, Sanjay E. Sarma, Michael M. Bronstein, Justin M. Solomon

Object tagging

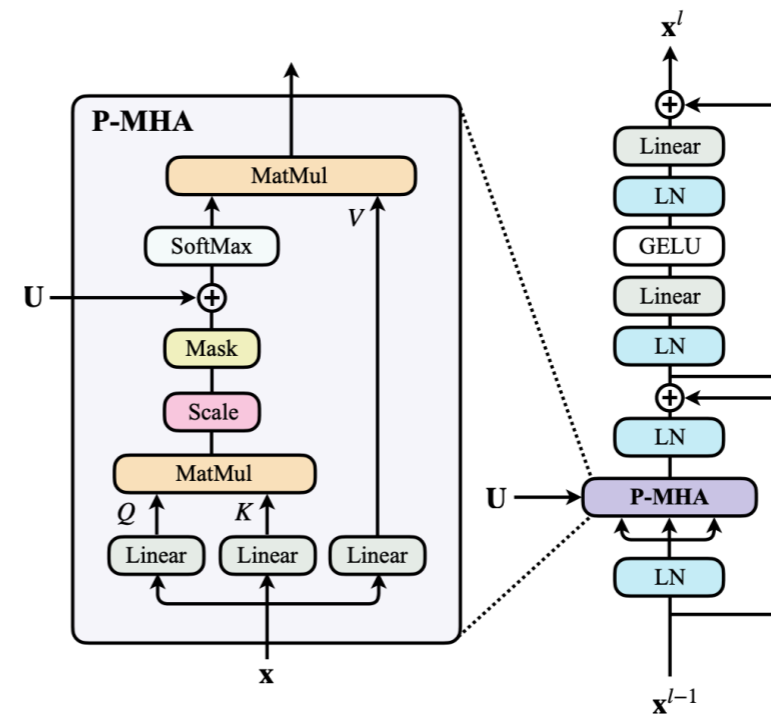
See talk by Felix Ringer for ML based EIC jet tagging



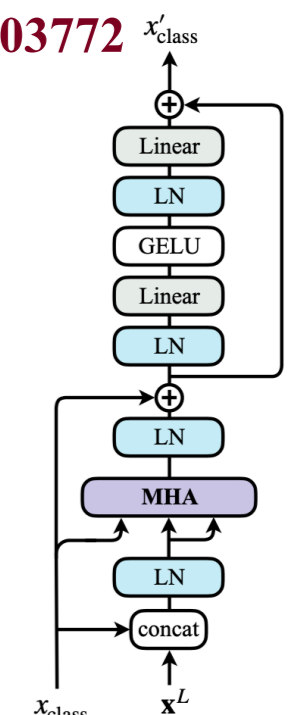
(a) Particle Transformer

Particle Transformer :
2202.03772

	Accuracy	AUC	Rej _{50%}	Rej _{30%}
P-CNN	0.930	0.9803	201 ± 4	759 ± 24
PFN	—	0.9819	247 ± 3	888 ± 17
ParticleNet	0.940	0.9858	397 ± 7	1615 ± 93
JEDI-net (w/ $\sum O$)	0.930	0.9807	—	774.6
PCT	0.940	0.9855	392 ± 7	1533 ± 101
LGN	0.929	0.964	—	435 ± 95
rPCN	—	0.9845	364 ± 9	1642 ± 93
LorentzNet	0.942	0.9868	498 ± 18	2195 ± 173
ParT	0.940	0.9858	413 ± 16	1602 ± 81
ParticleNet-f.t.	0.942	0.9866	487 ± 9	1771 ± 80
ParT-f.t.	0.944	0.9877	691 ± 15	2766 ± 130

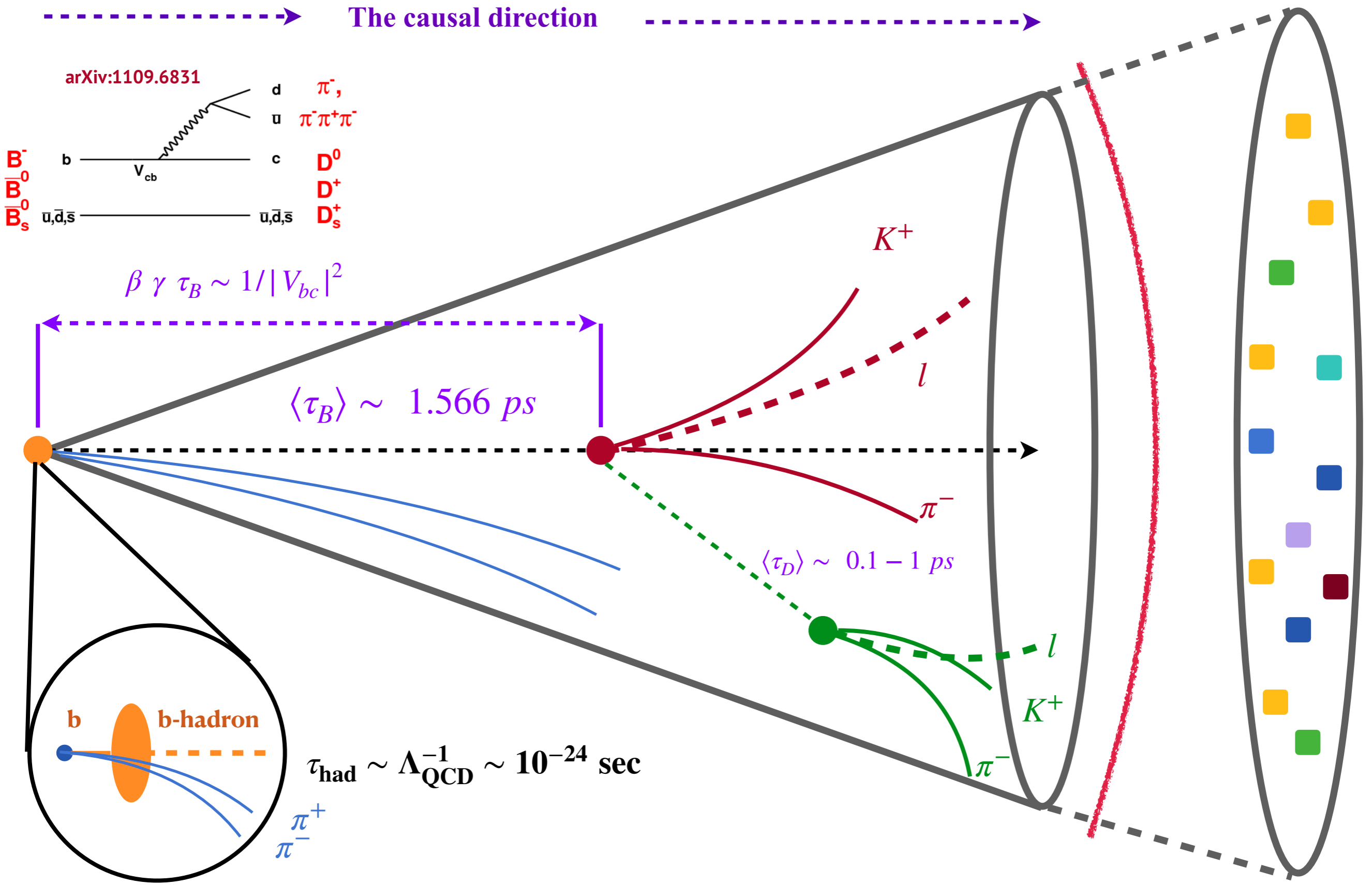


(b) Particle Attention Block

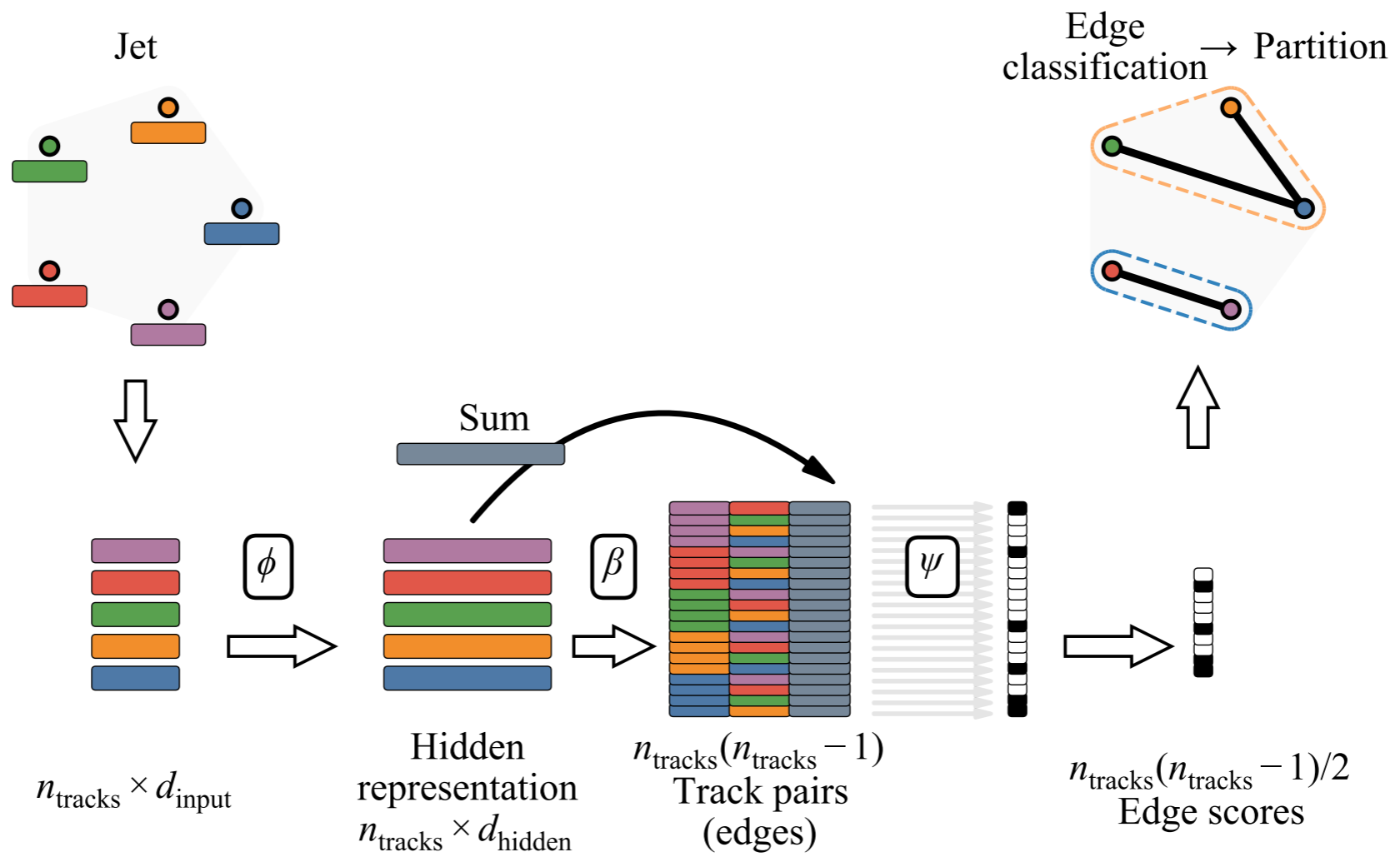
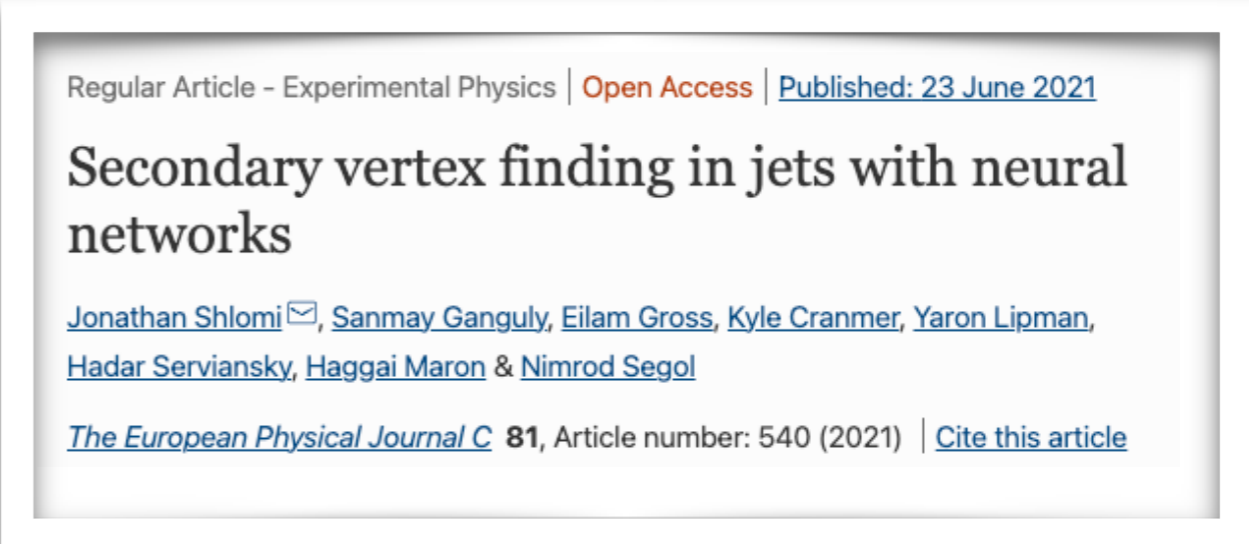
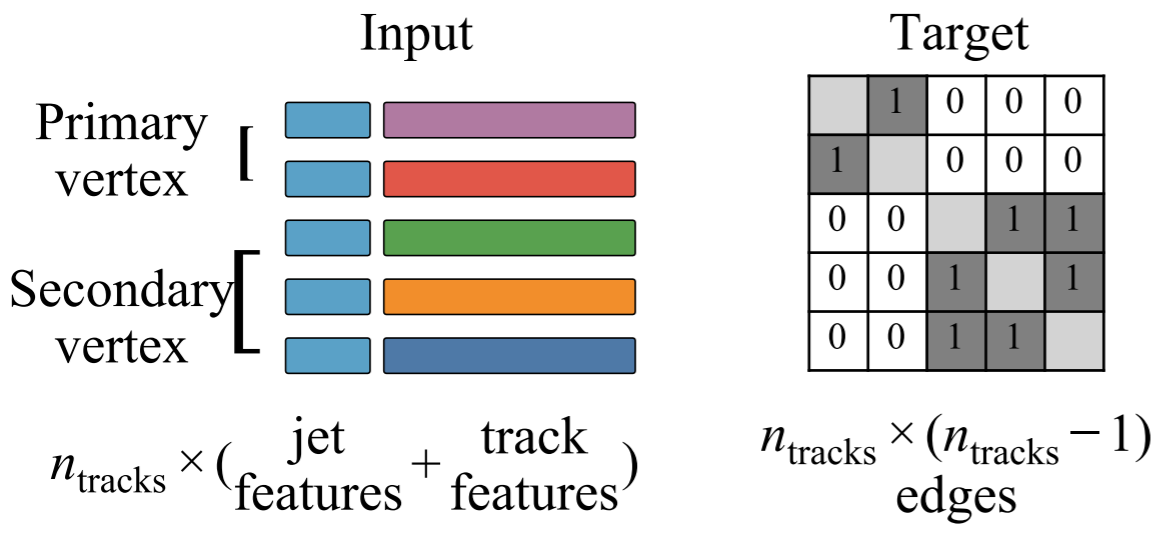


(c) Class Attention Block

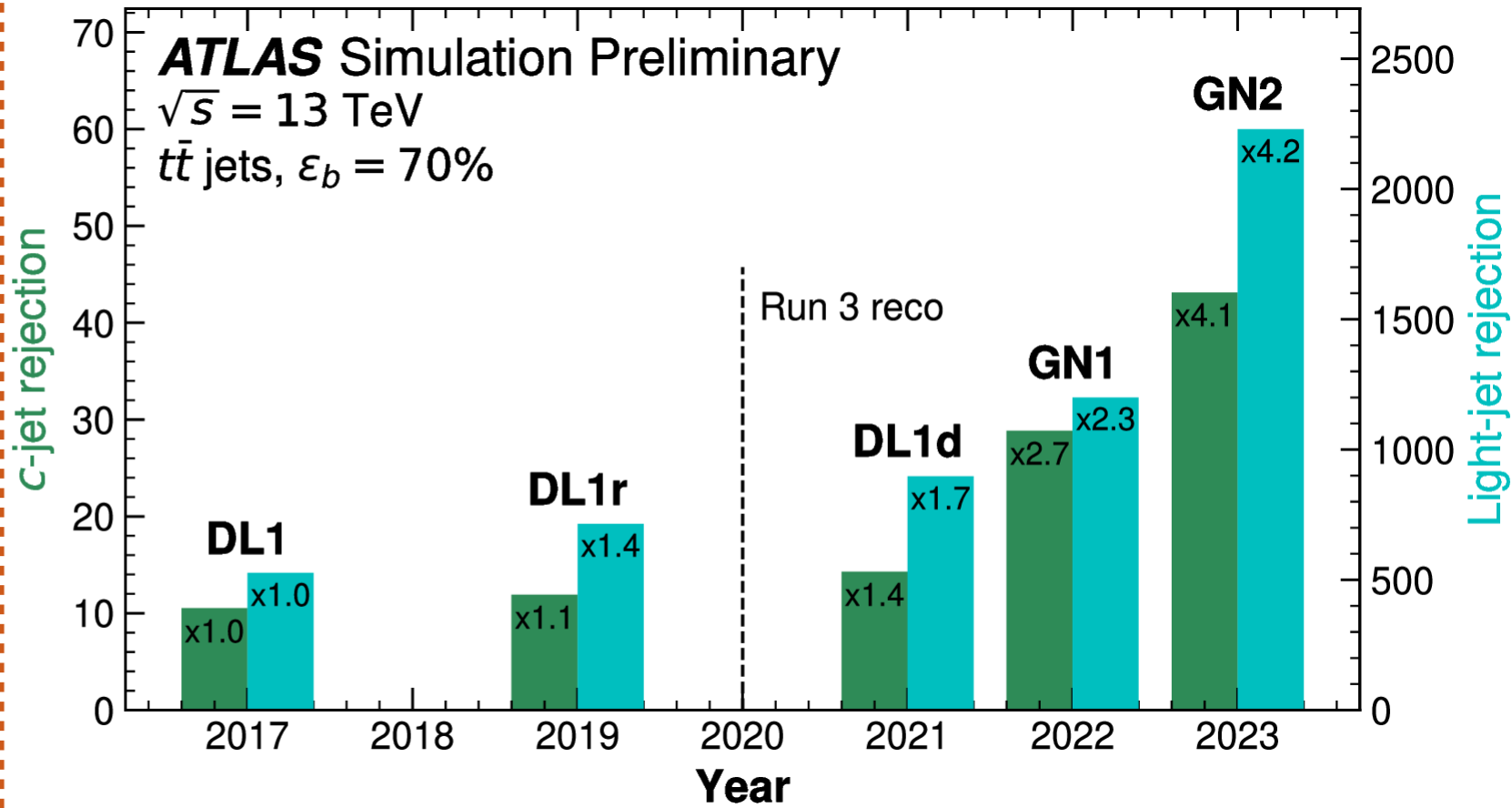
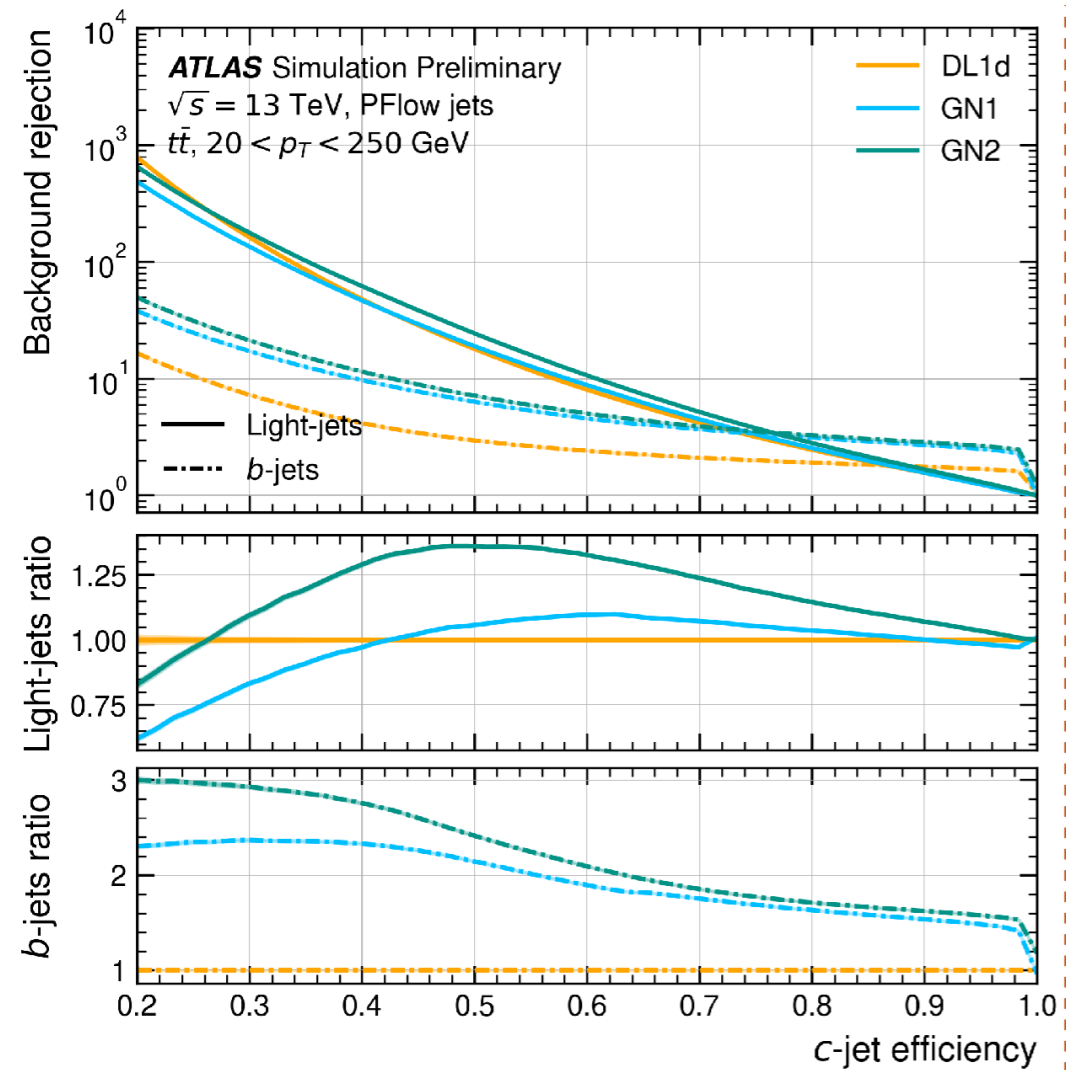
Anatomy of heavy-quark hadronization



Set2Graph proposal for flavor-tagging



Set2Graph model within ATLAS



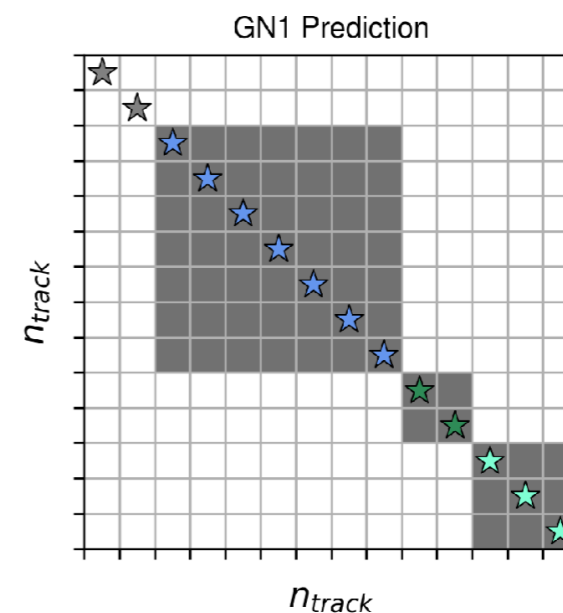
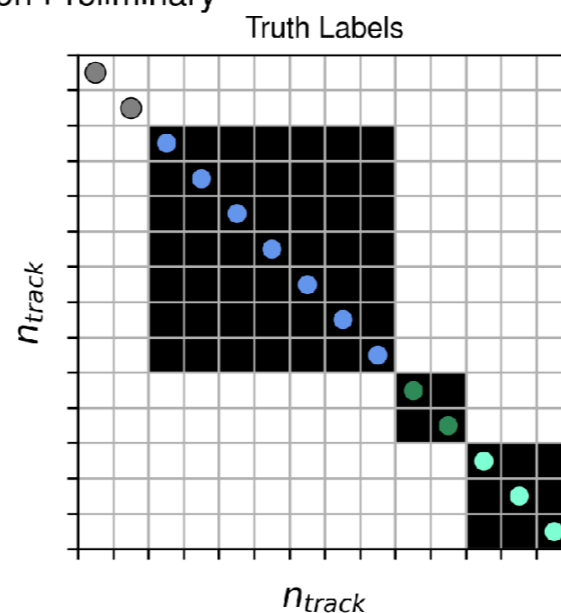
Sizable improvement over the current DL1r algorithm.

For a c-tagging working point ~ 30%, a significant gain in Rejection rate is obtained.

ATLAS Simulation Preliminary
 $\sqrt{s} = 13$ TeV
 $t\bar{t}$ jets

Truth b -jet
 $p_T = 134.1$ GeV

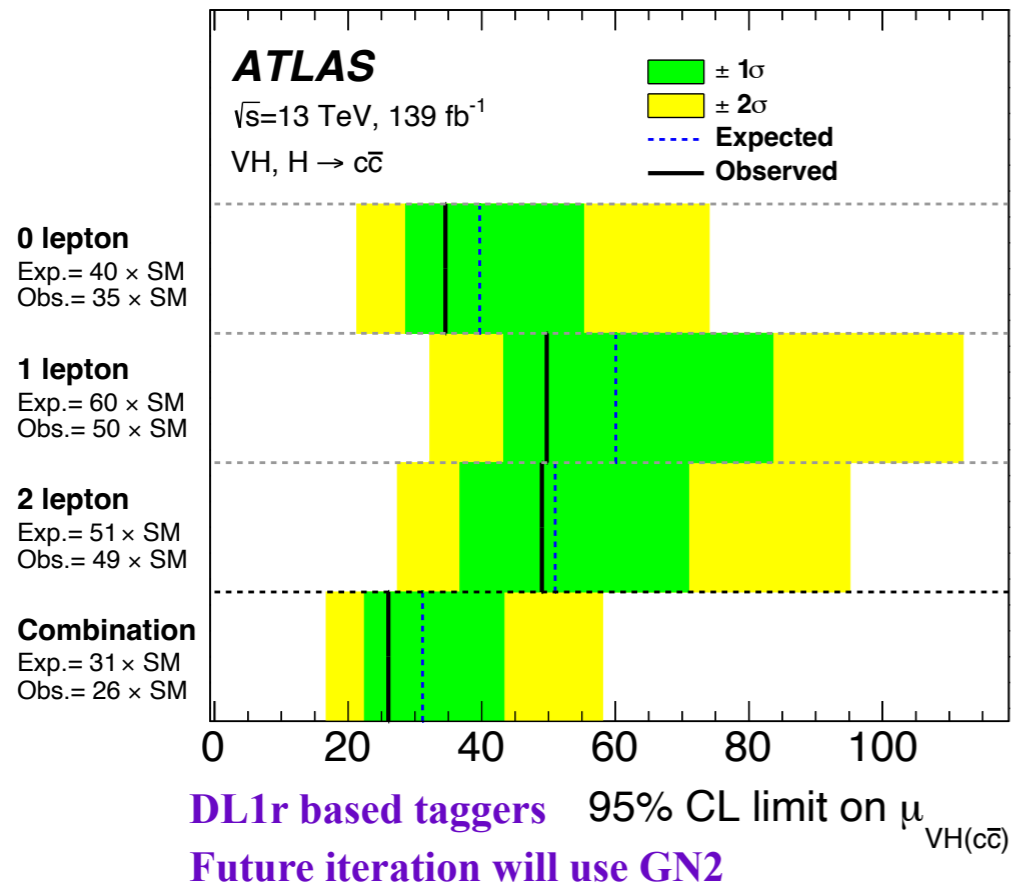
$\rho_b = 0.995$
 $\rho_c = 0.005$
 $\rho_u = 0.000$



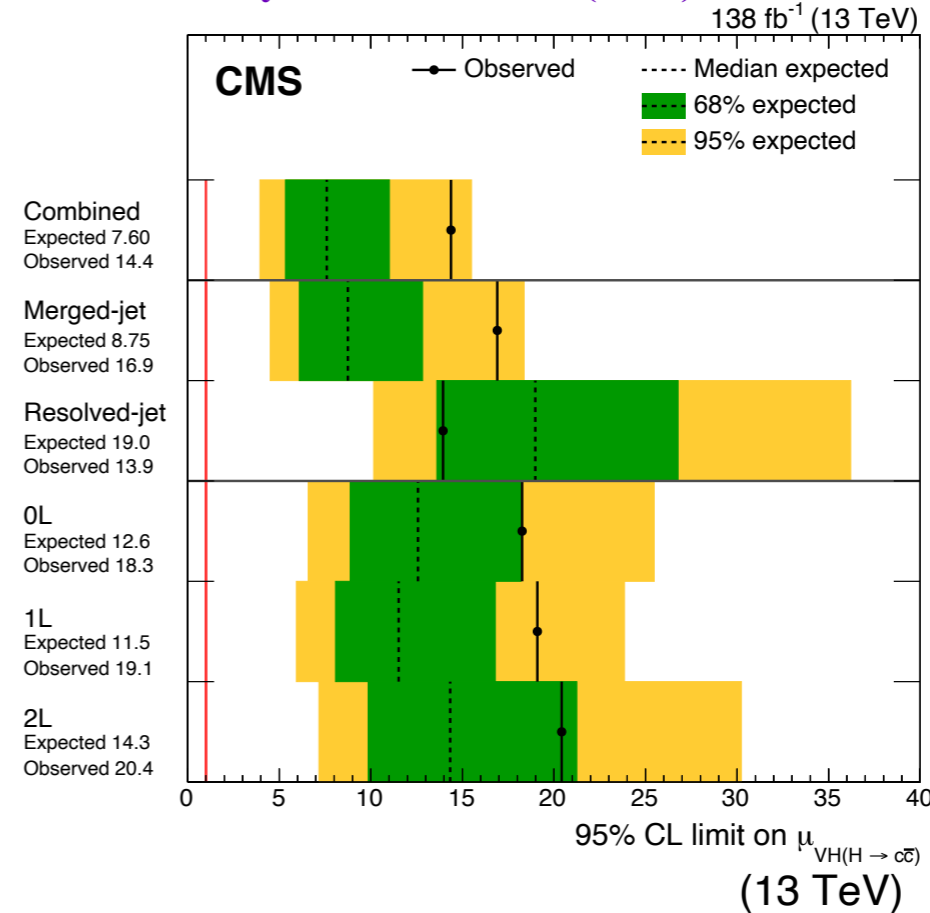
- Truth
- ★ Predicted
- Pileup
- Fake
- Primary
- FromB
- FromBC
- FromC
- FromTau
- OtherSecondary

Direct physics application of the taggers

Eur. Phys. J. C (2022) 82:717

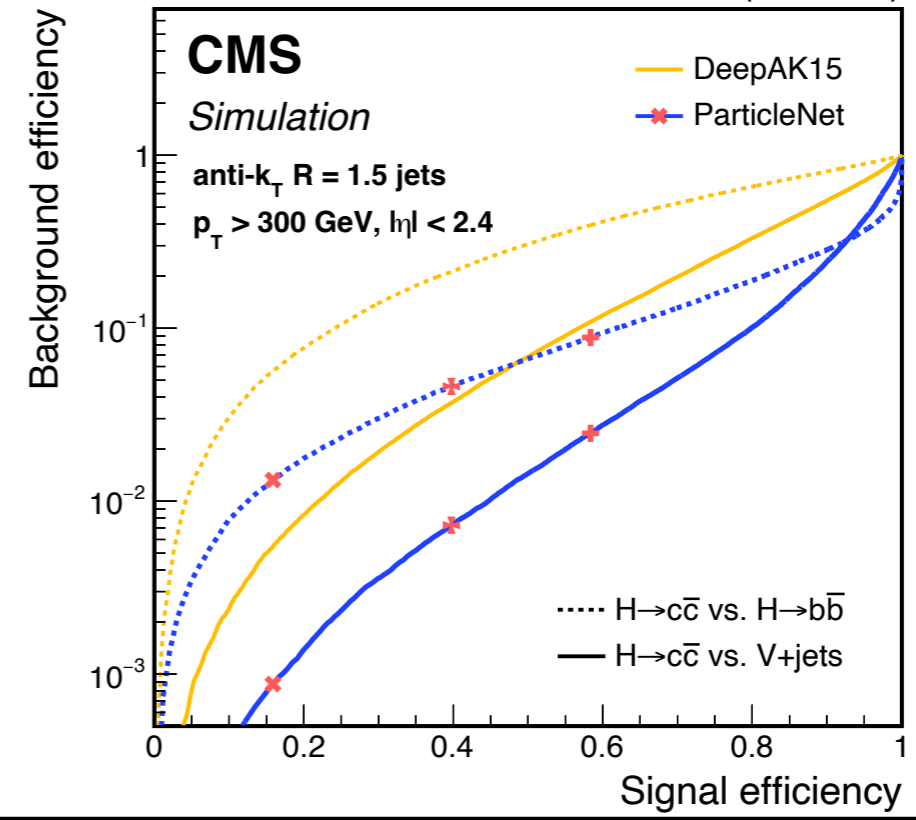


Phys. Rev. Lett. 131 (2023) 061801

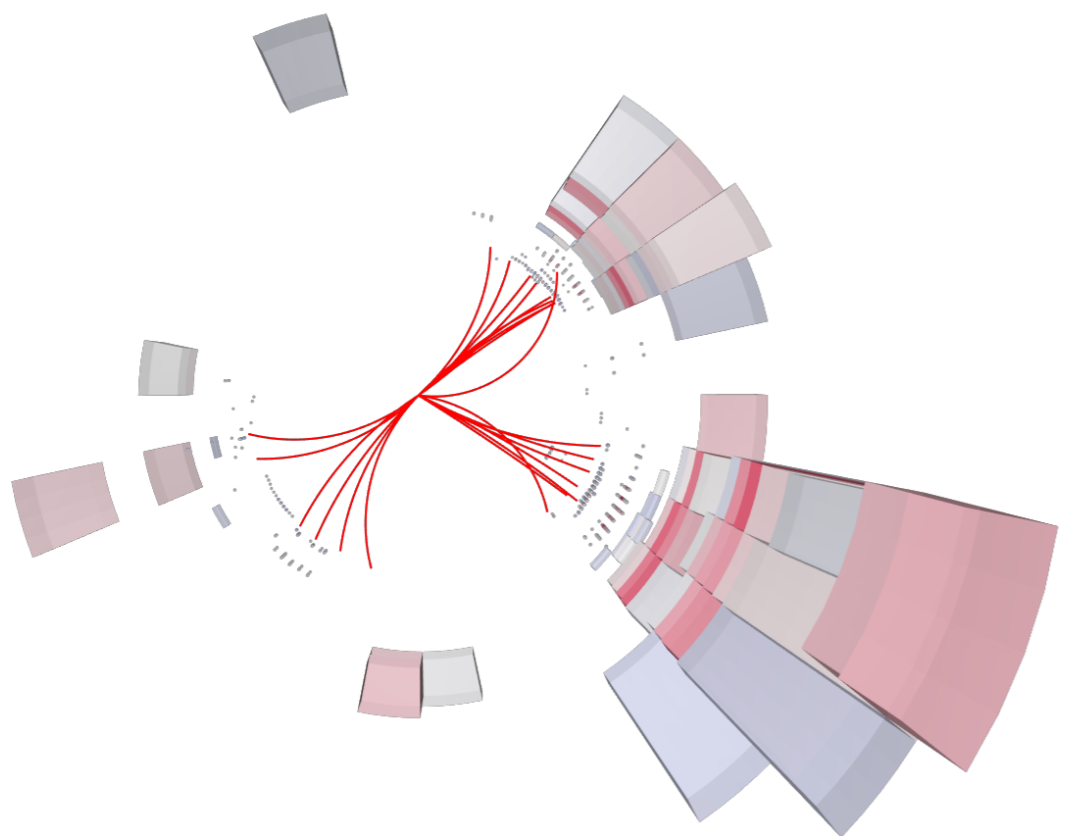


ATLAS bound : $|\kappa_c| < 8.5$
CMS bound : $1.1 < |\kappa_c| < 5.5$

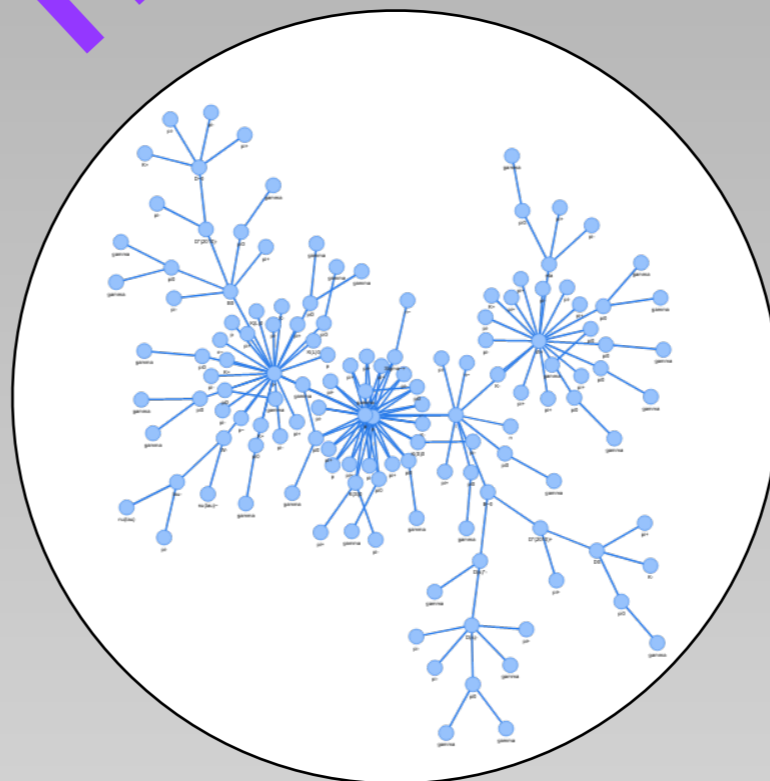
- Future direction of tagger improvement:**
1. Explainable taggers on heterogeneous pc
 2. A systematic uncertainty extraction.
 3. How much universal taggers can be made across topologies?



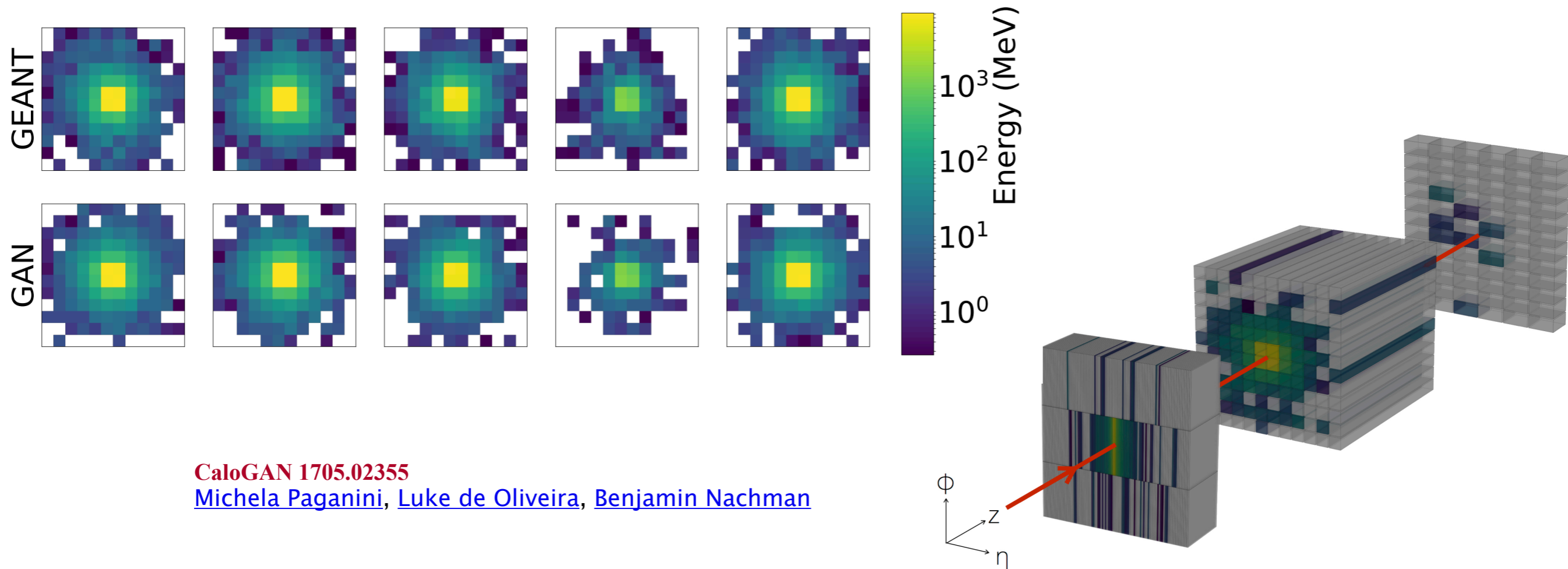
Generative models for calorimeter simulations



$$f_{\{\theta\}} (\text{ } , z)$$

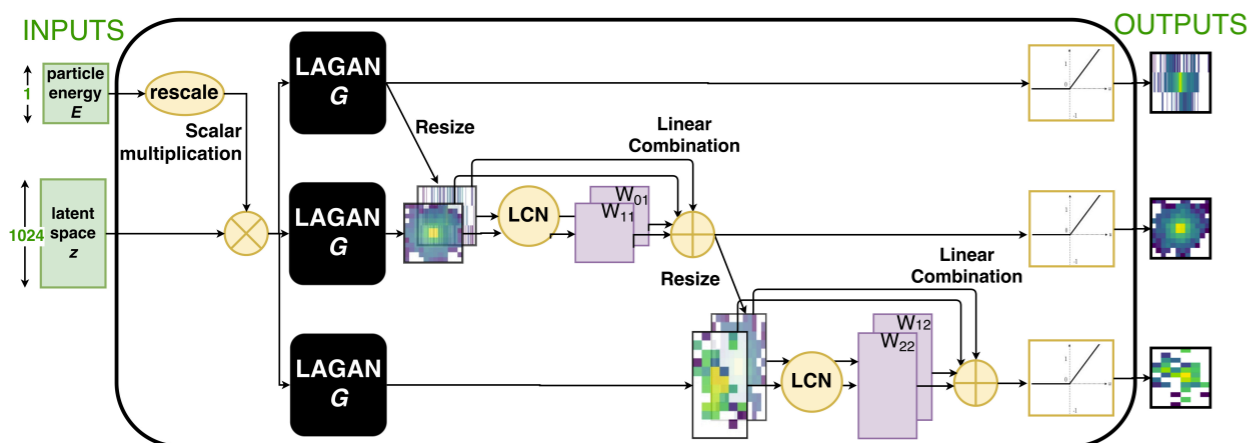


Detector simulation using ML

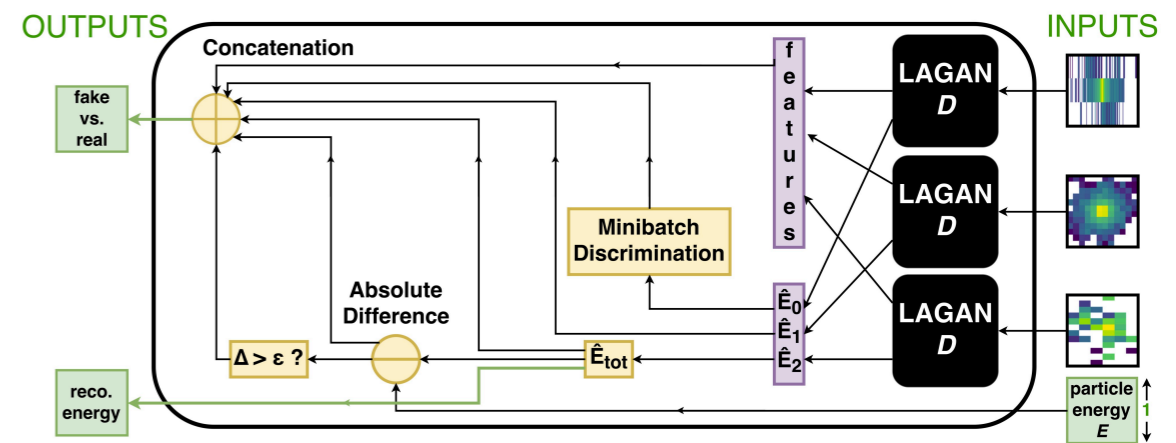


CaloGAN 1705.02355

[Michela Paganini](#), [Luke de Oliveira](#), [Benjamin Nachman](#)

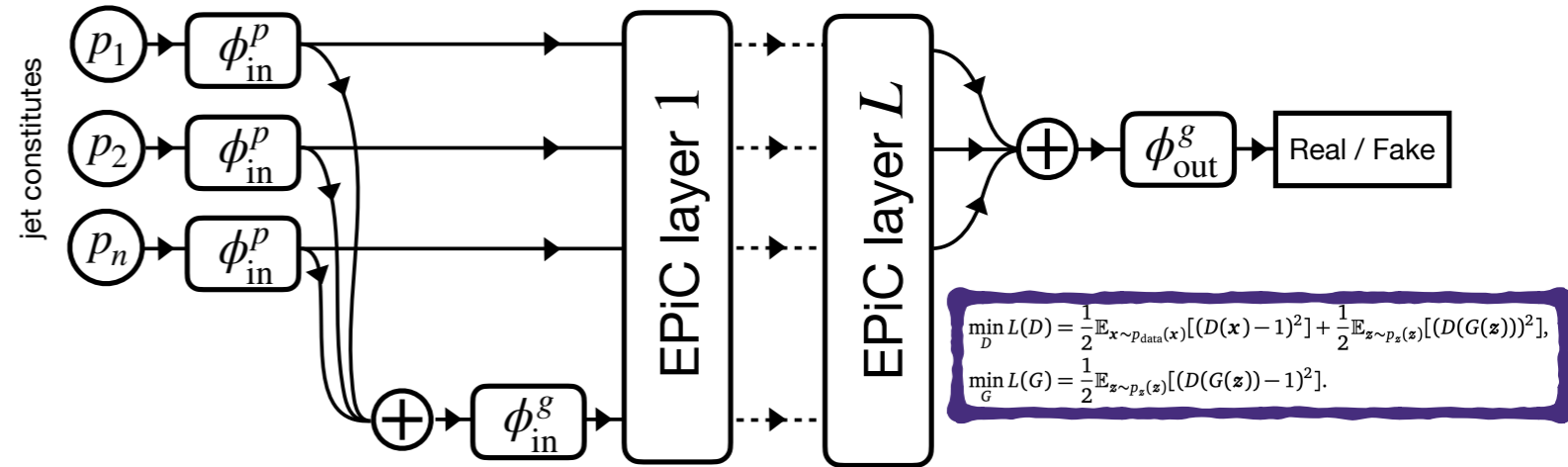
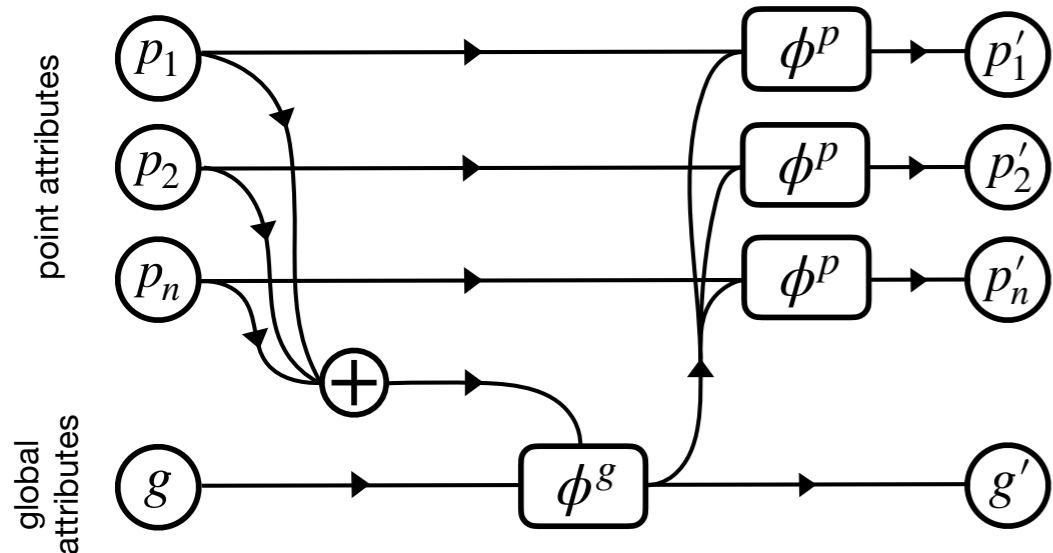


Generator

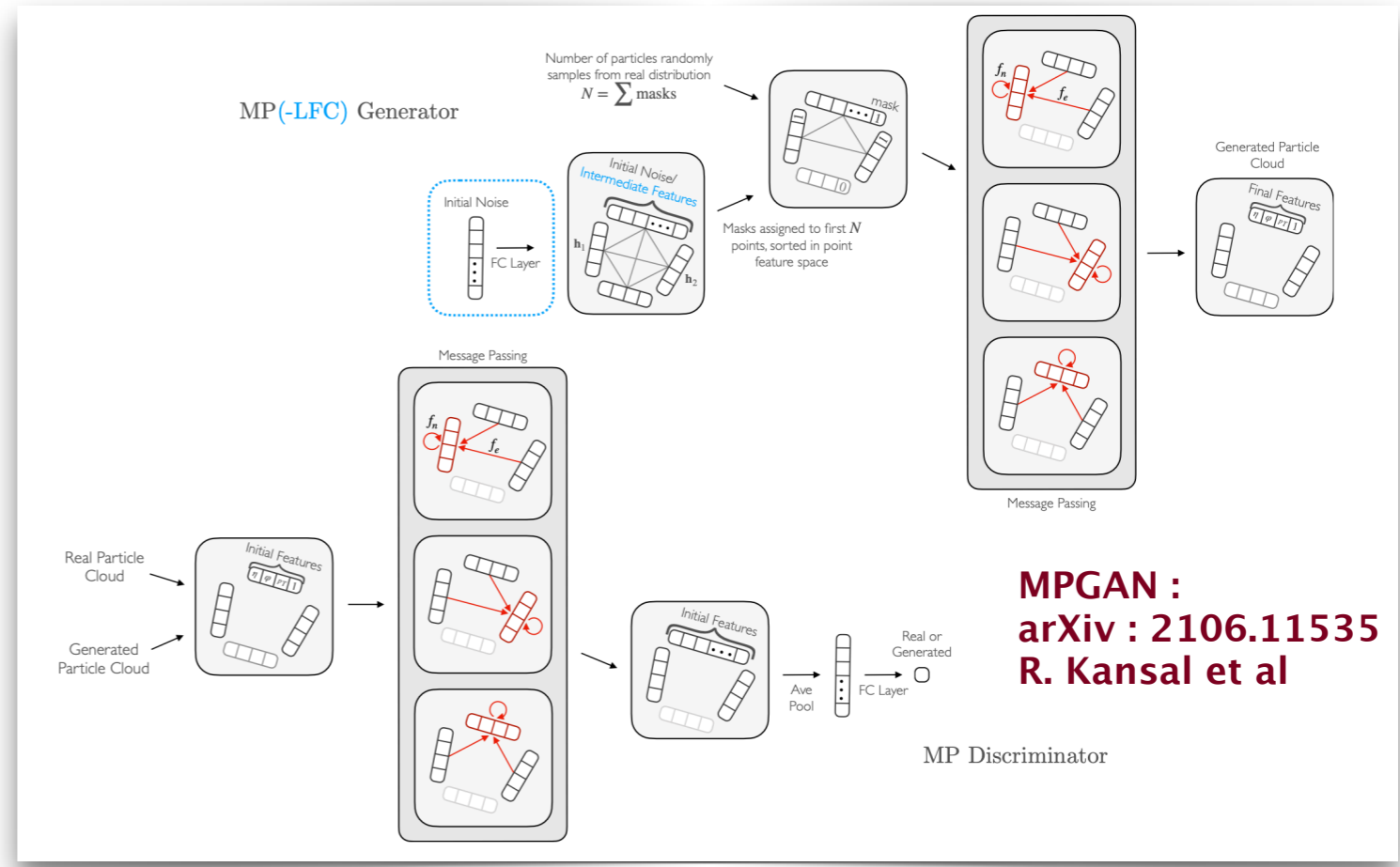
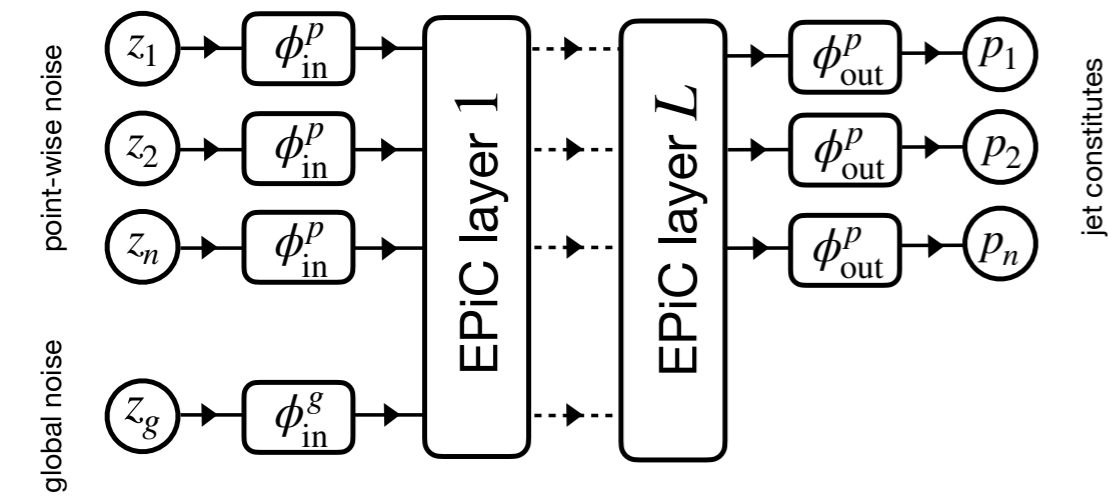


Discriminator

Detector simulation using ML

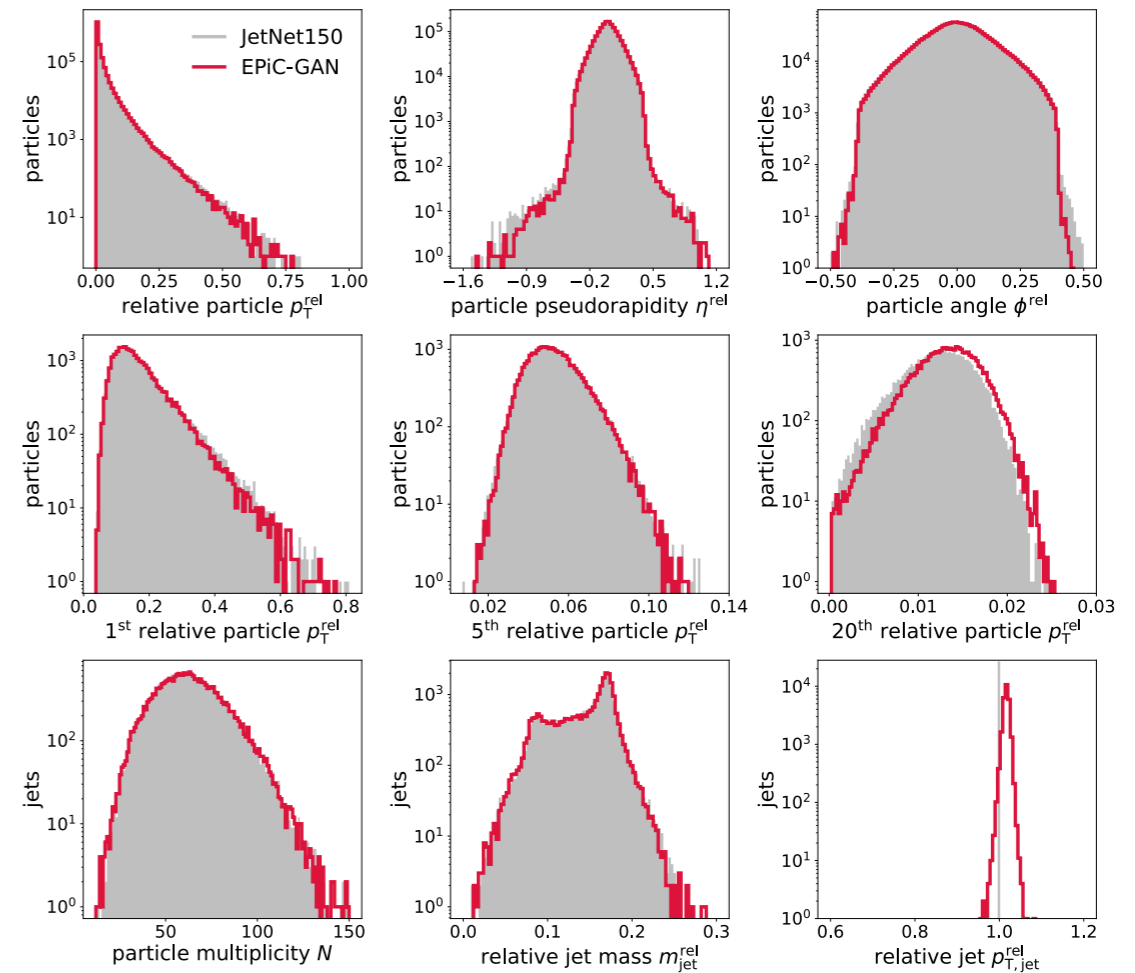
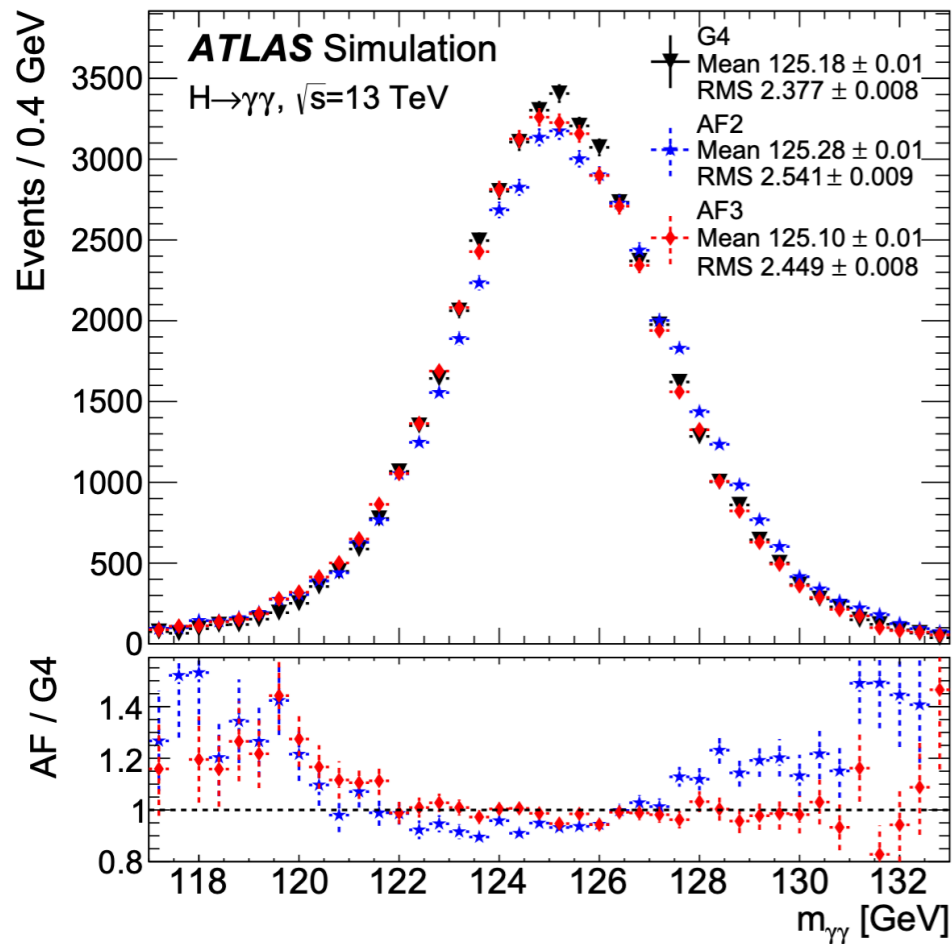


EPiC-GAN : SciPost Phys. 15, 130 (2023) Erik Buhmann, Gregor Kasieczka, Jesse Thaler

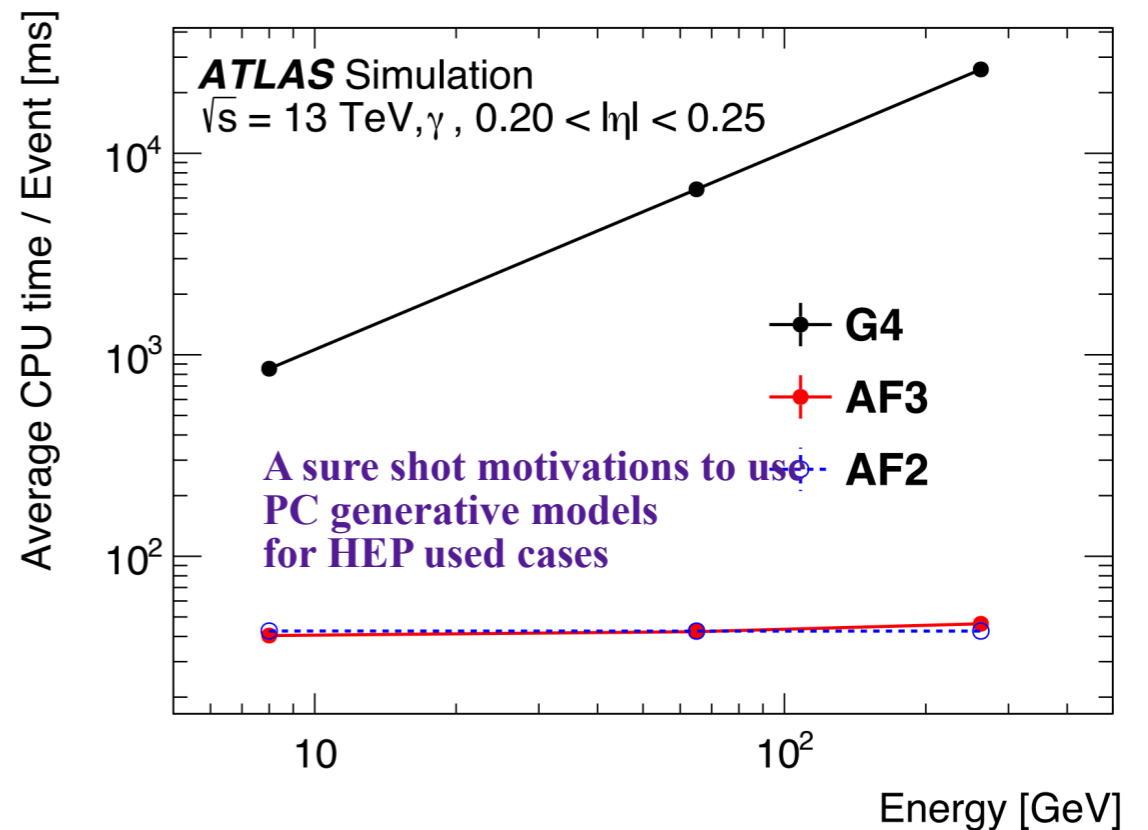
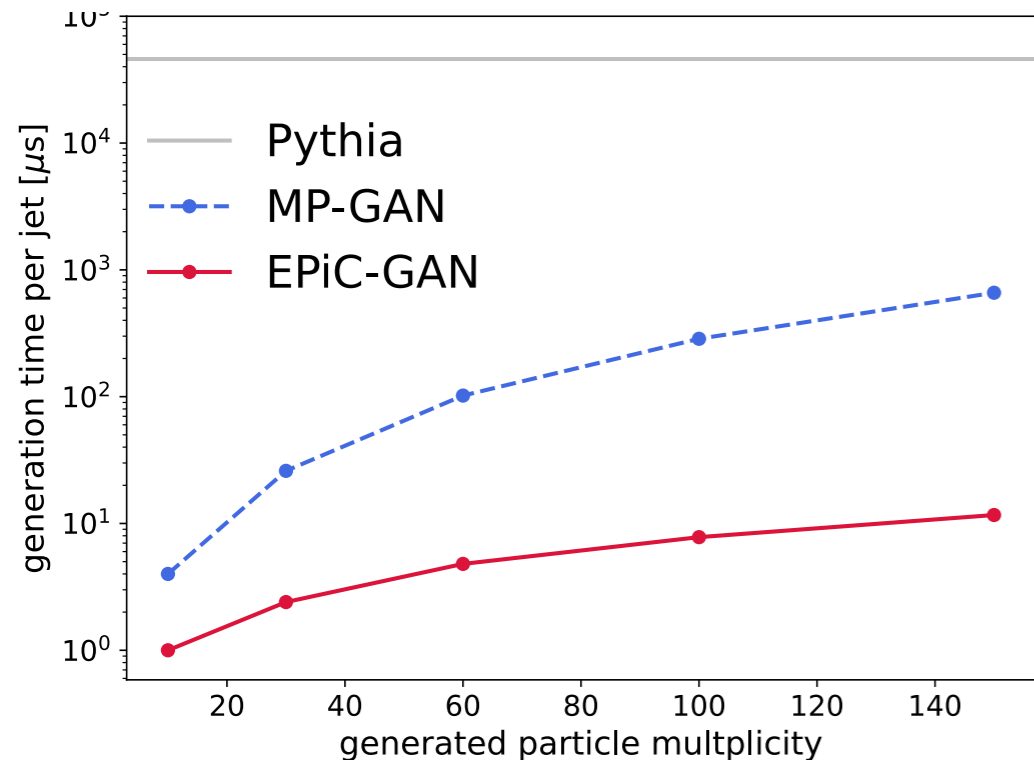


MPGAN : arXiv : 2106.11535 R. Kansal et al

The major gain



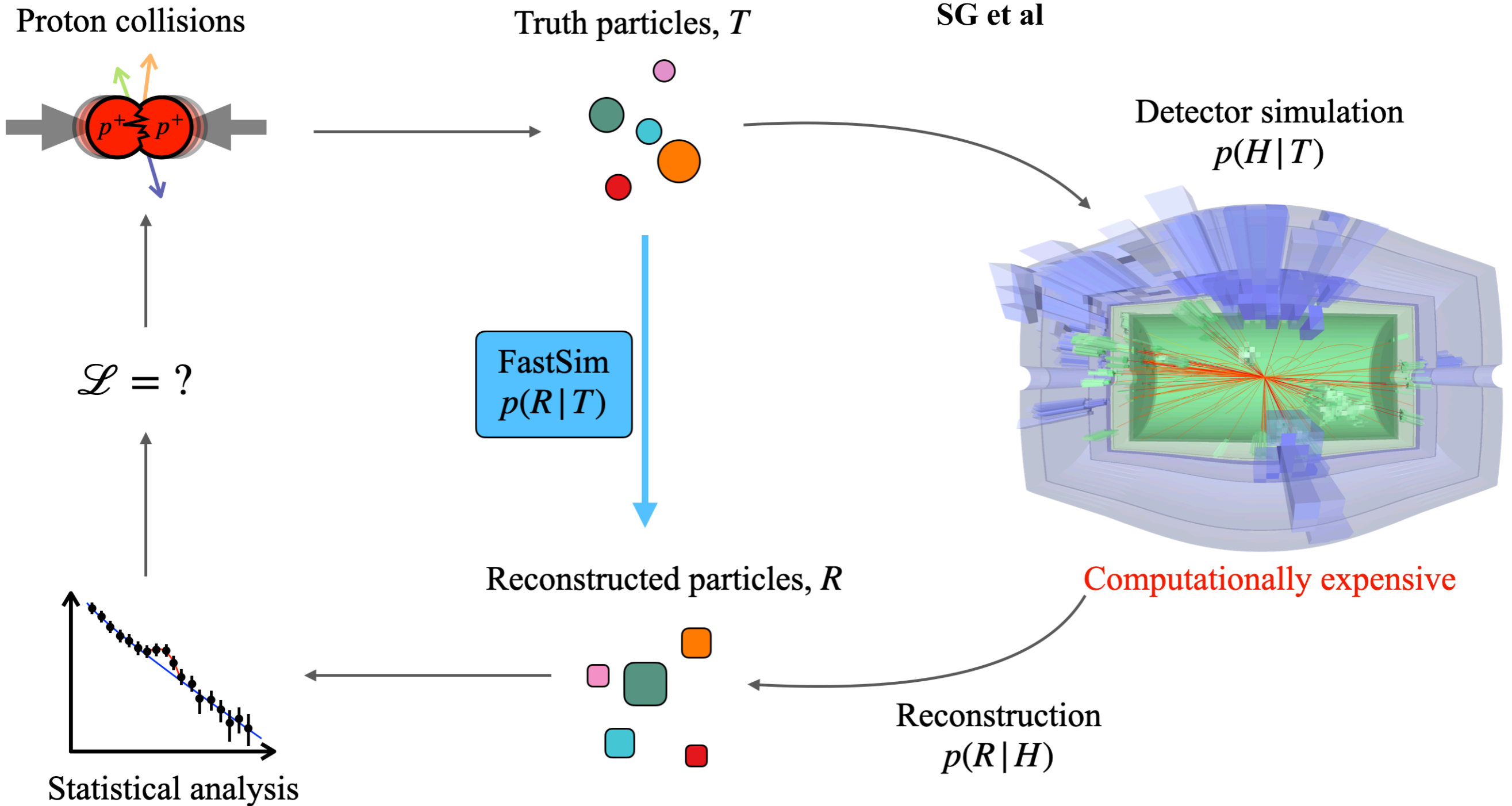
arXiv : 2109.02551



A generative model for Particle-flow

Mach. Learn.: Sci. Technol. 4 (2023) 045036

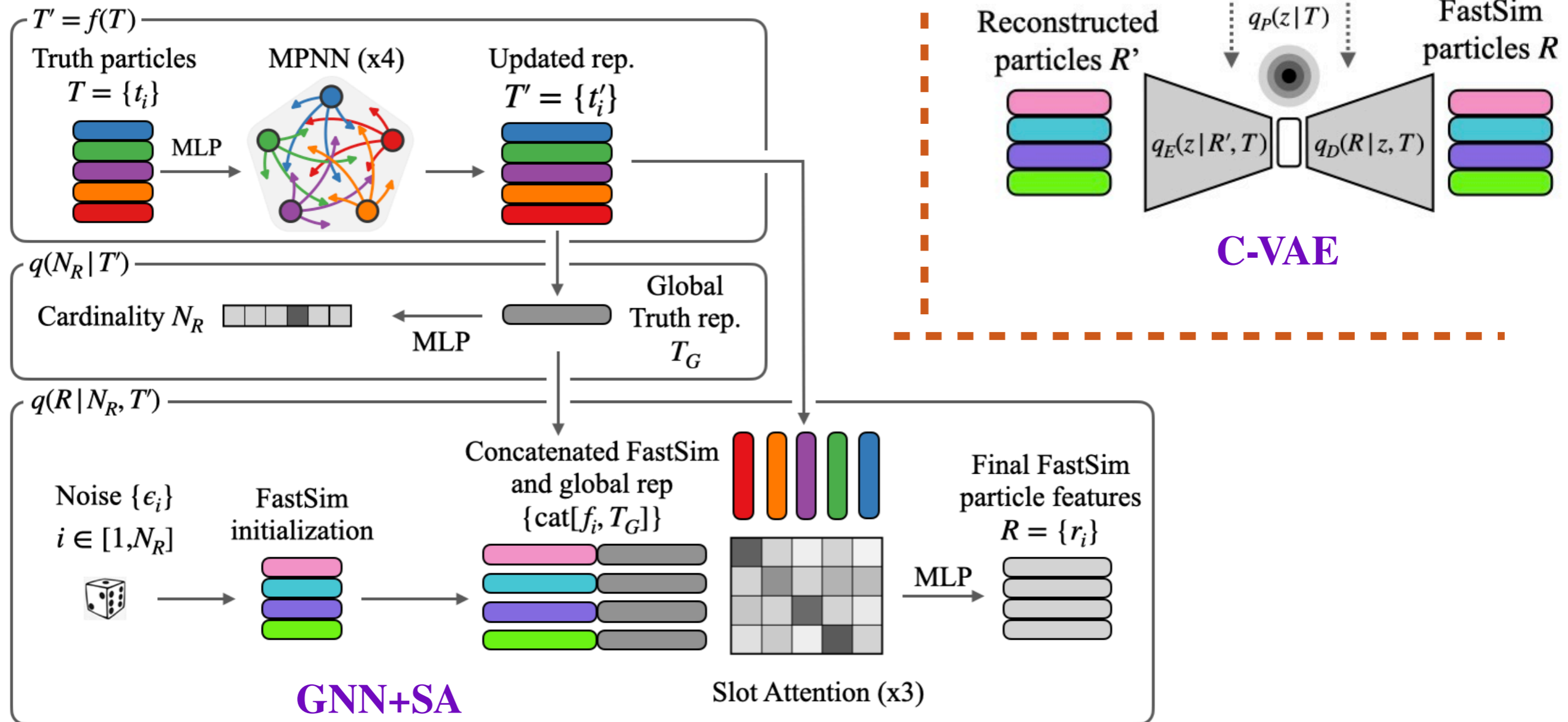
SG et al



$$R \sim p(R|T) = \int dH \delta(R(H) - R) p_{\text{sim}}(H|T).$$

The task of constrained set generation

$$q_{\theta}(\mathbf{R} | \mathbf{T}) \sim q_{\theta_1}(\mathbf{N}_R | \mathbf{T}) q_{\theta_2}(\mathbf{R} | \mathbf{N}_R, \mathbf{T})$$



The task of constrained set generation

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

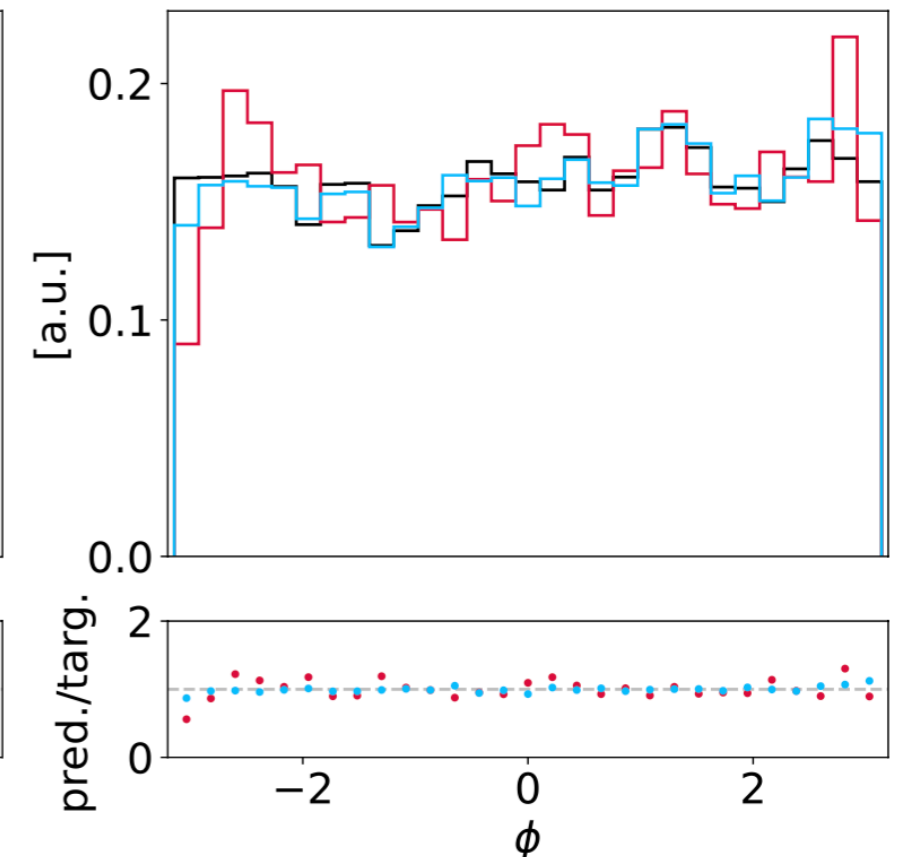
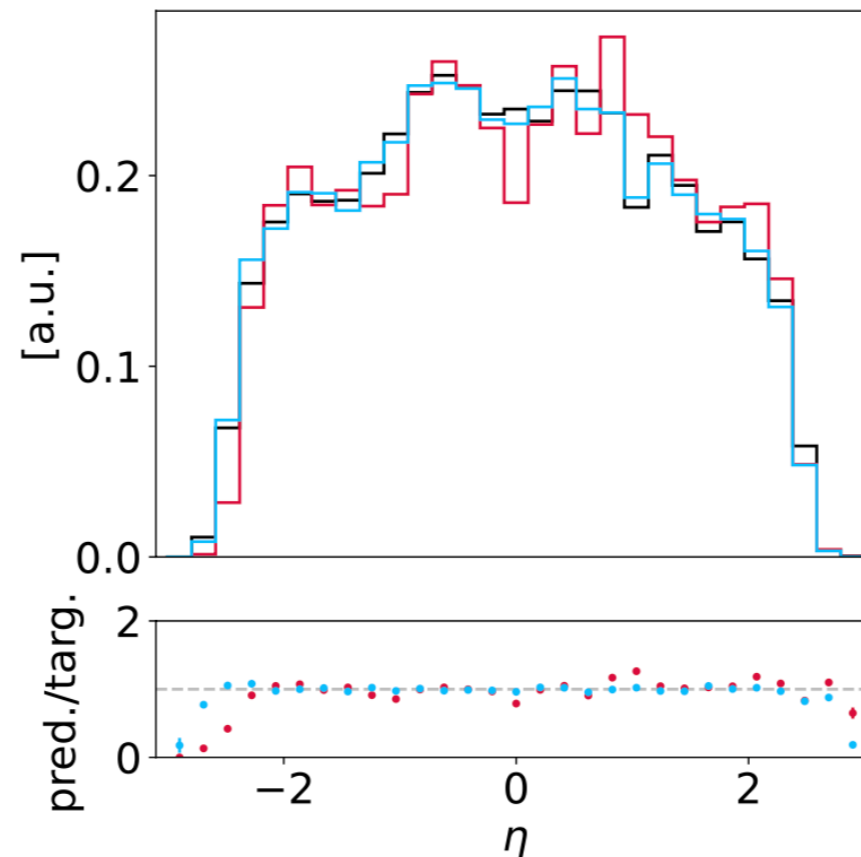
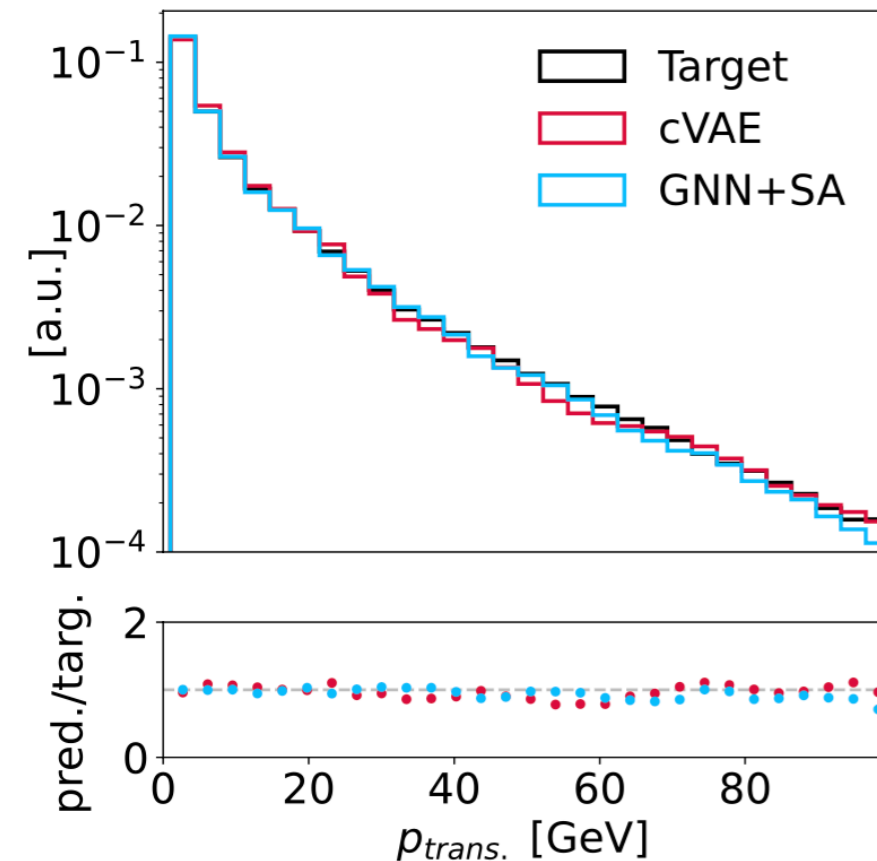
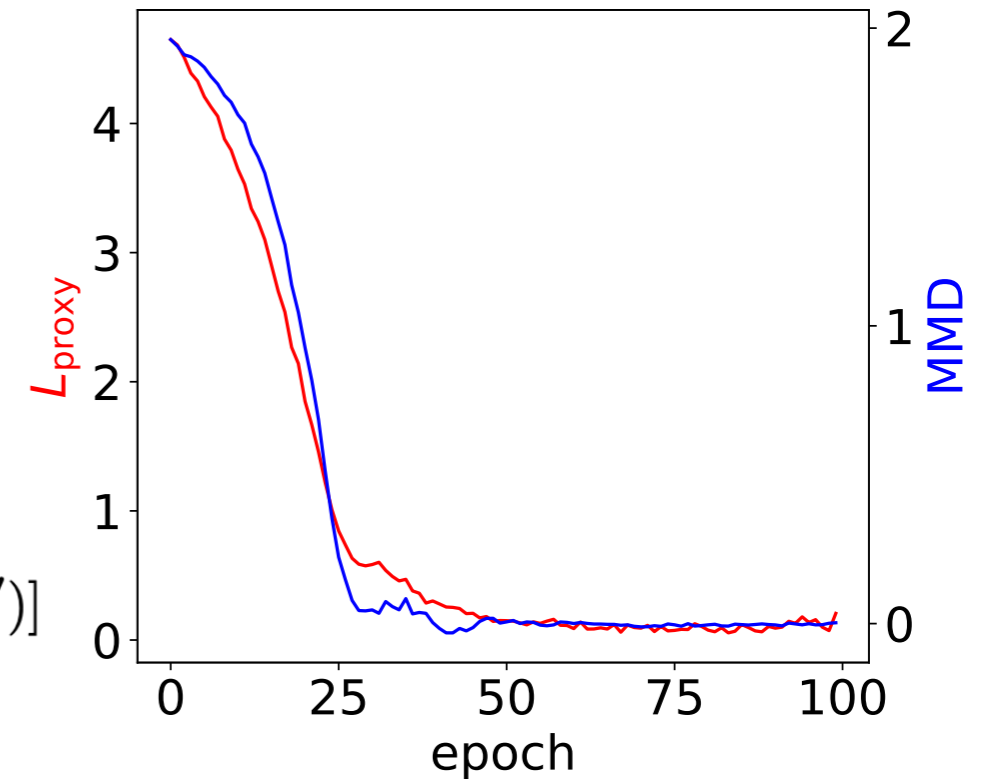
loss :

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

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

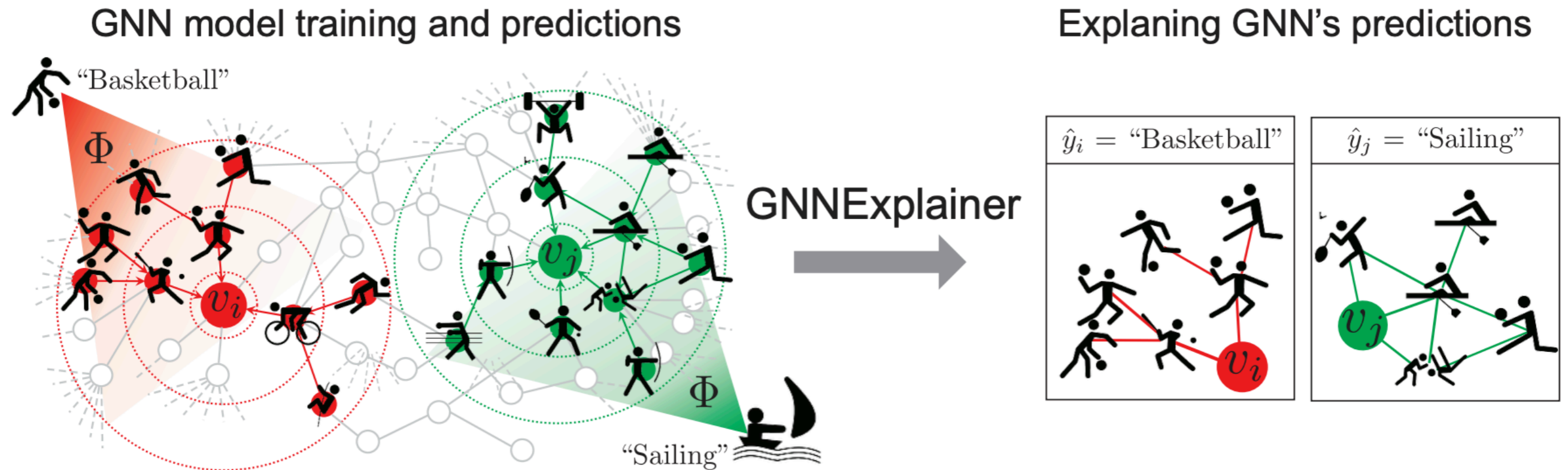
For GNN+SA, we try a regular Hungarian loss and also MMD (maximum mean discrepancy) :

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



What's brewing now?

Major thrust in immediate future : Interpretability



Interpretability is a key issue and efforts are ongoing to map the NN explainability to first principle physics intuition

Interpretability : an example attempt

$$\mathbf{R}_j^{(l)} = \sum_k \frac{x_j A_{jk}}{\sum_m x_m A_{mk}} \mathbf{R}_k^{(l+1)} \quad (3)$$

Neur IPS 2021. F. Mokhtar, R. Kansal et al

where $\mathbf{R}_j^{(l)}$ represent the R -scores of the features of node j at layer l , while the quantity $x_j A_{jk}$ models the extent to which node j at layer l , with activation x_j , contributes to the relevance of node k at layer $l + 1$, where A is the adjacency matrix.

Explainability for MLPF

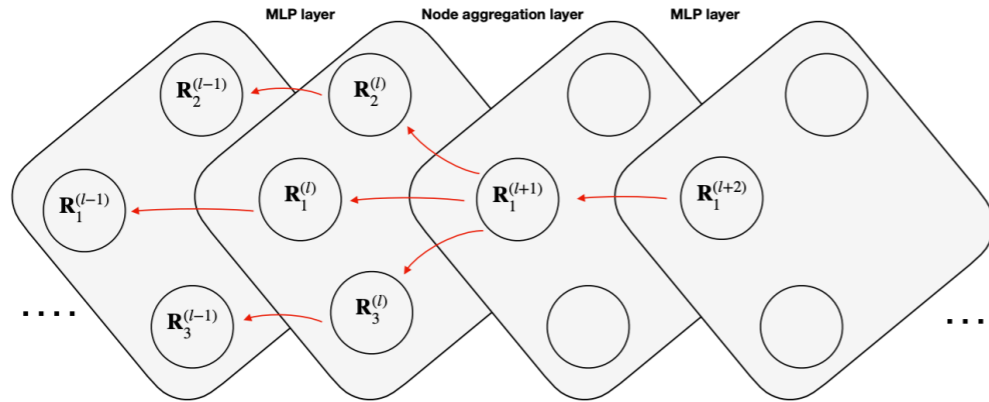
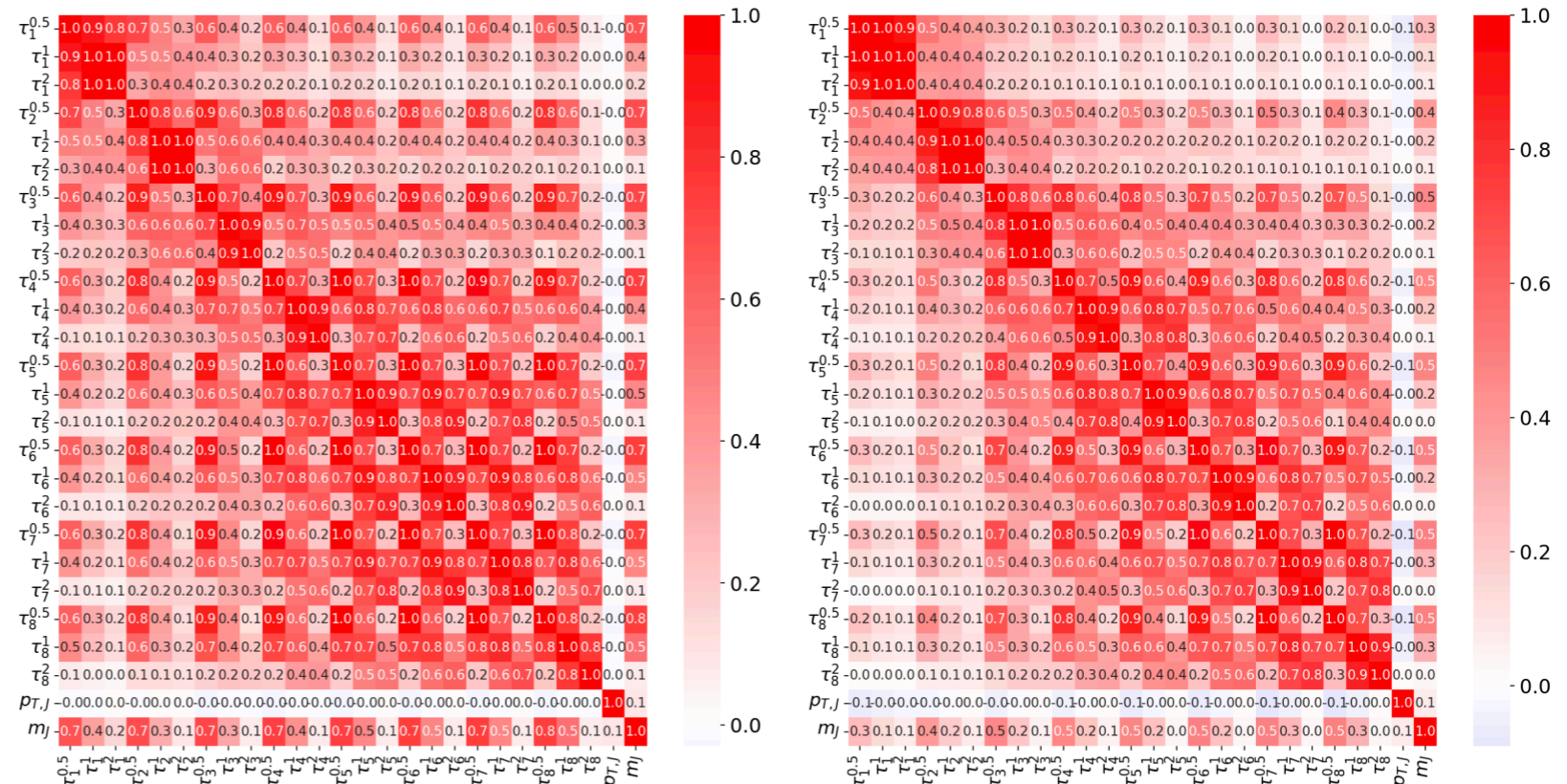


Figure 1: The flow of R -scores of node 1 across the different layers in MLPF. For MLP layers, the redistribution of R -scores follows the standard LRP rules [35, 36]. For the aggregation step in the message passing layer, the redistribution follows Equation 3. We only show three nodes for simplicity.

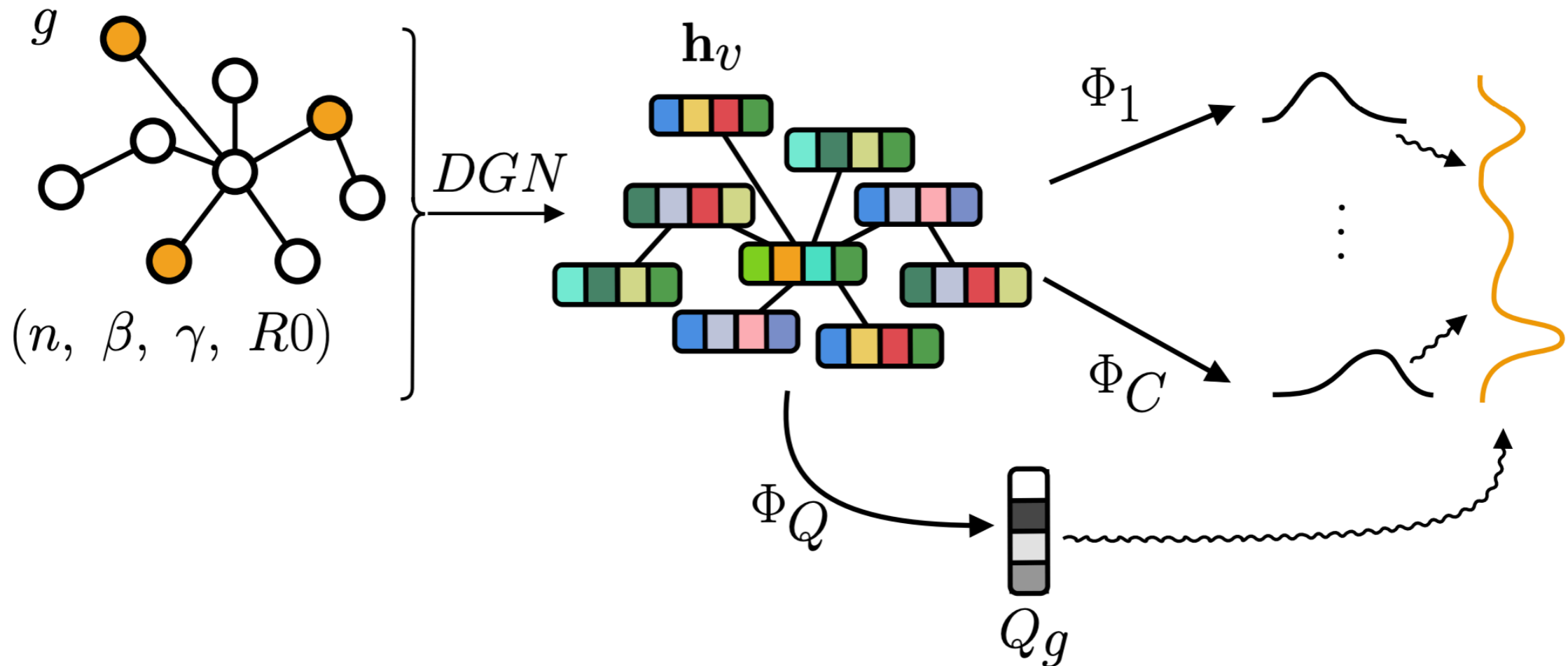
Feature correlation for top tagging.

arXiv 2210.04371

Ayush Khot, Mark S. Neubauer, Avik Roy



Major thrust in immediate future : Uncertainty

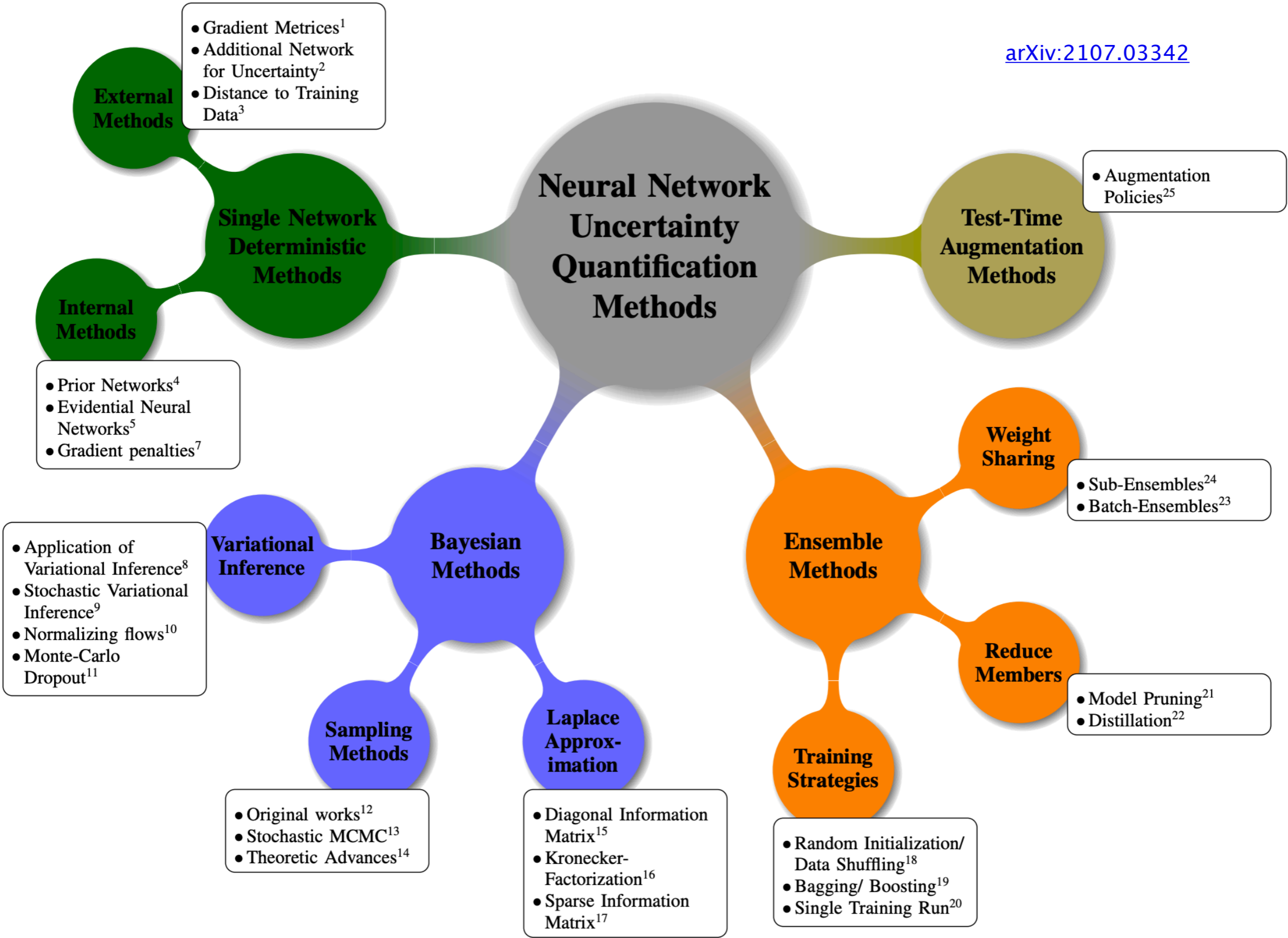


Reliable uncertainty estimation on ML based predictions are crucial for HEP
Only few Bayesian methods have been tested naively.

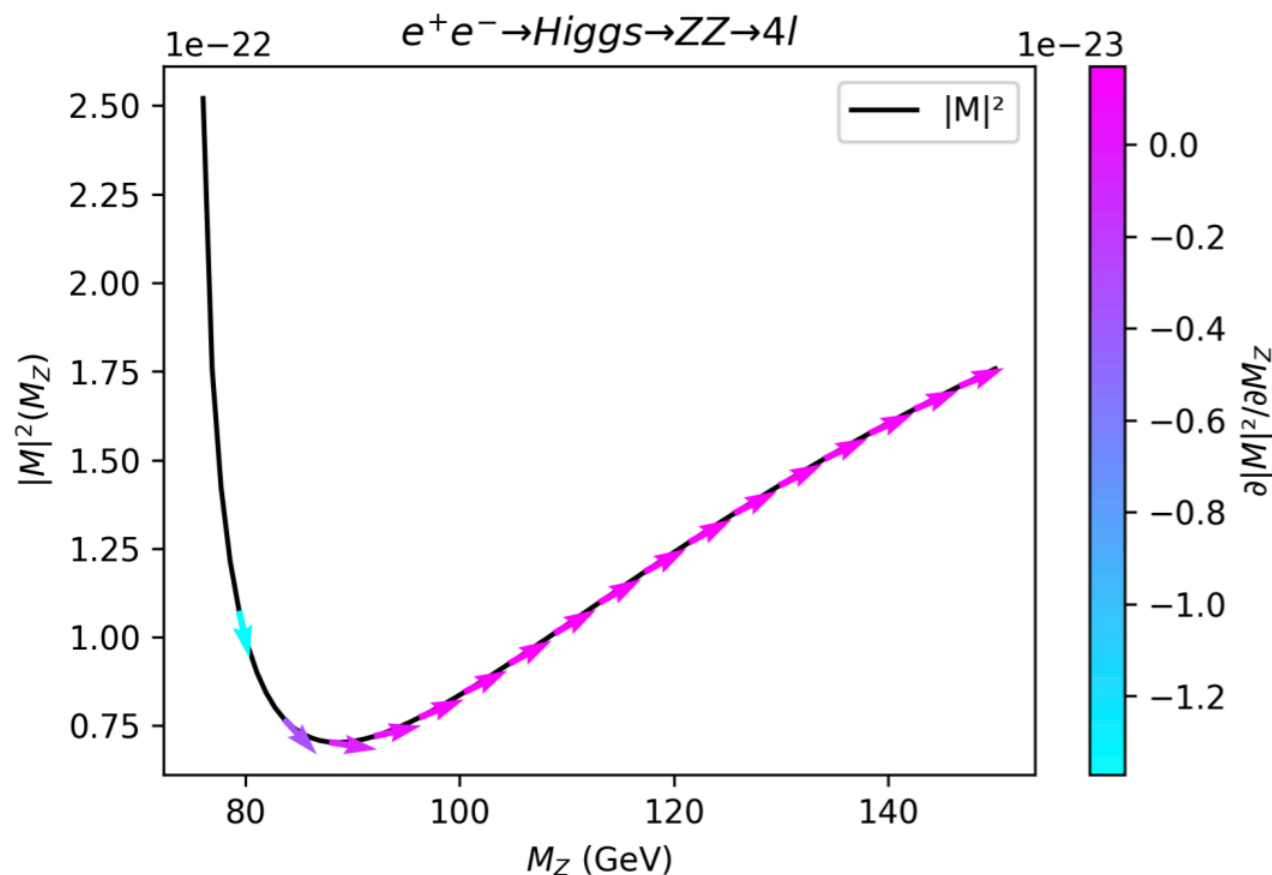
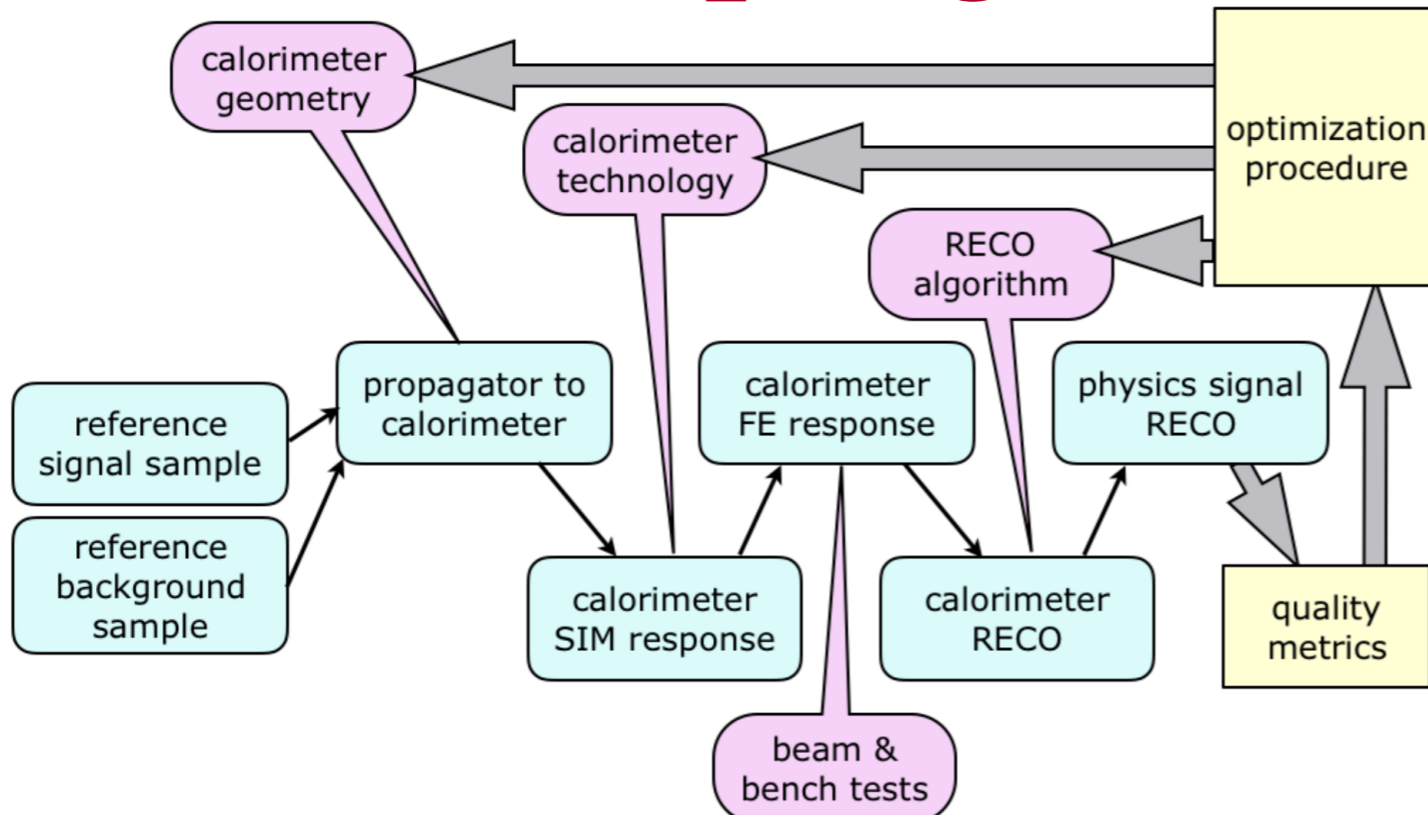
Can we decompose and correlate the aleatoric and epistemic uncertainties with the underlying physics?

Major thrust in immediate future : Uncertainty

[arXiv:2107.03342](https://arxiv.org/abs/2107.03342)



Differential programming in HEP



```
generate p p > t t~, t > b udsc udscx , t~ > b~ udsc udscx
output madjax generated_ttbar
```

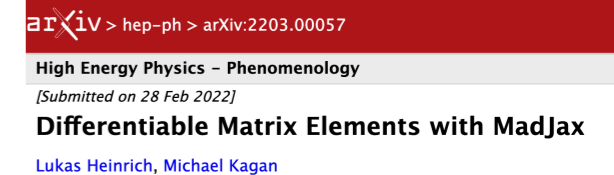
```
set auto_update 0
```

2. Evaluation:

```
import madjax
mj = madjax.MadJax('generated_ttbar')
E_cm = 14000 #GeV
process = 'Matrix_1_gg_ttx_t_budx_tx_bxdx'
matrix_element = mj.matrix_element(E_cm, process)
```

```
parameters = ('mass', 6): 173.0 #set top mass
phasespace_coords = [0.1]*14 #14D phasespace
```

```
val, grad = matrix_element(parameters, phasespace_coords)
grad[('mass', 6)] #gradient wrt top mass
```

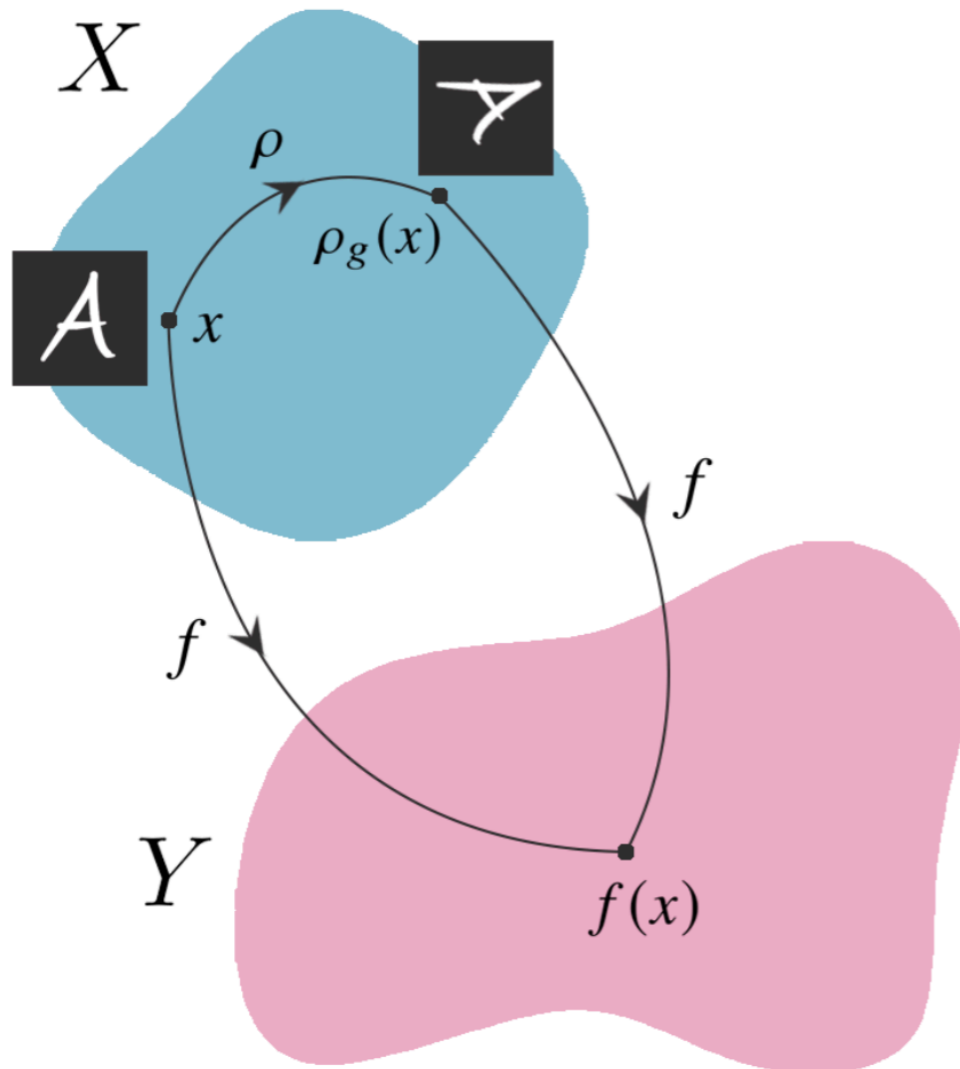


Symmetry equivariant networks

[arXiv:2203.06153](https://arxiv.org/abs/2203.06153) : SG et al

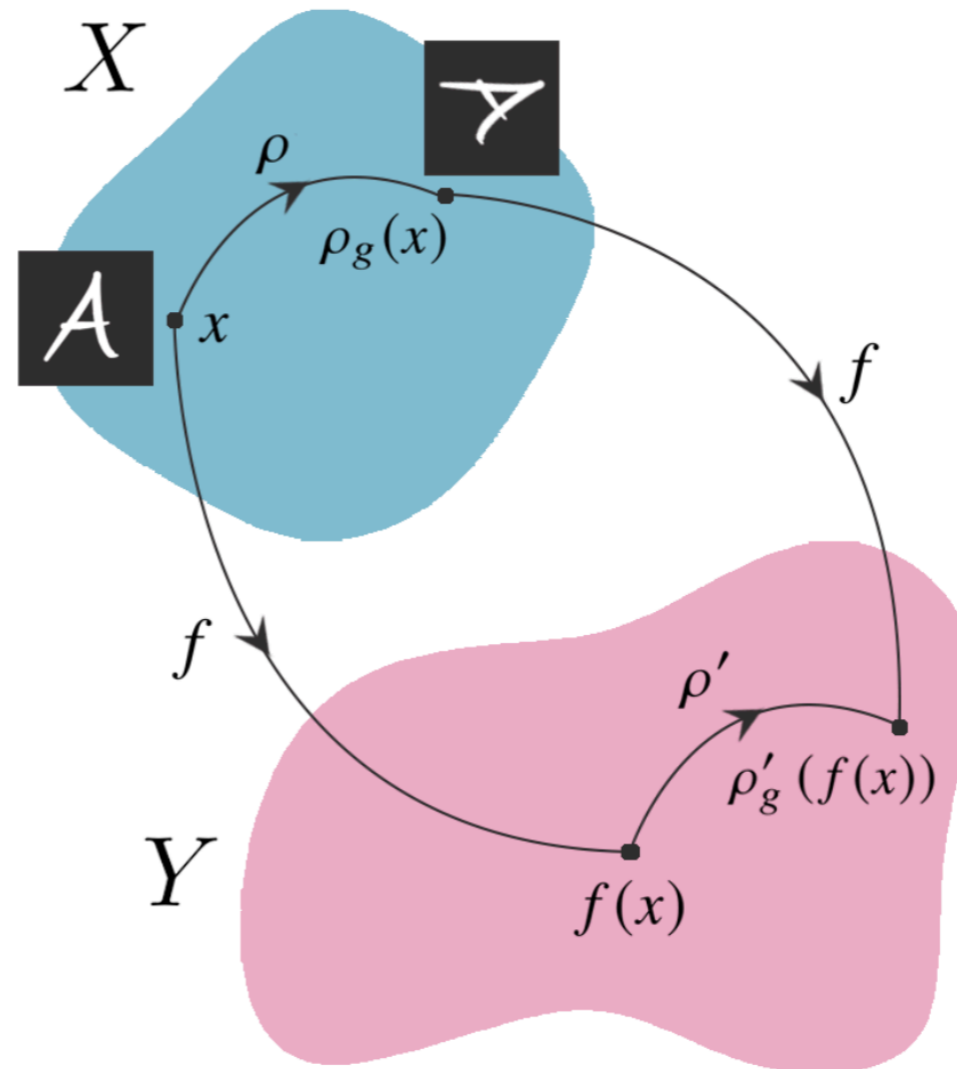
Invariance

$$f(\rho_g(x)) = f(x)$$



Equivariance

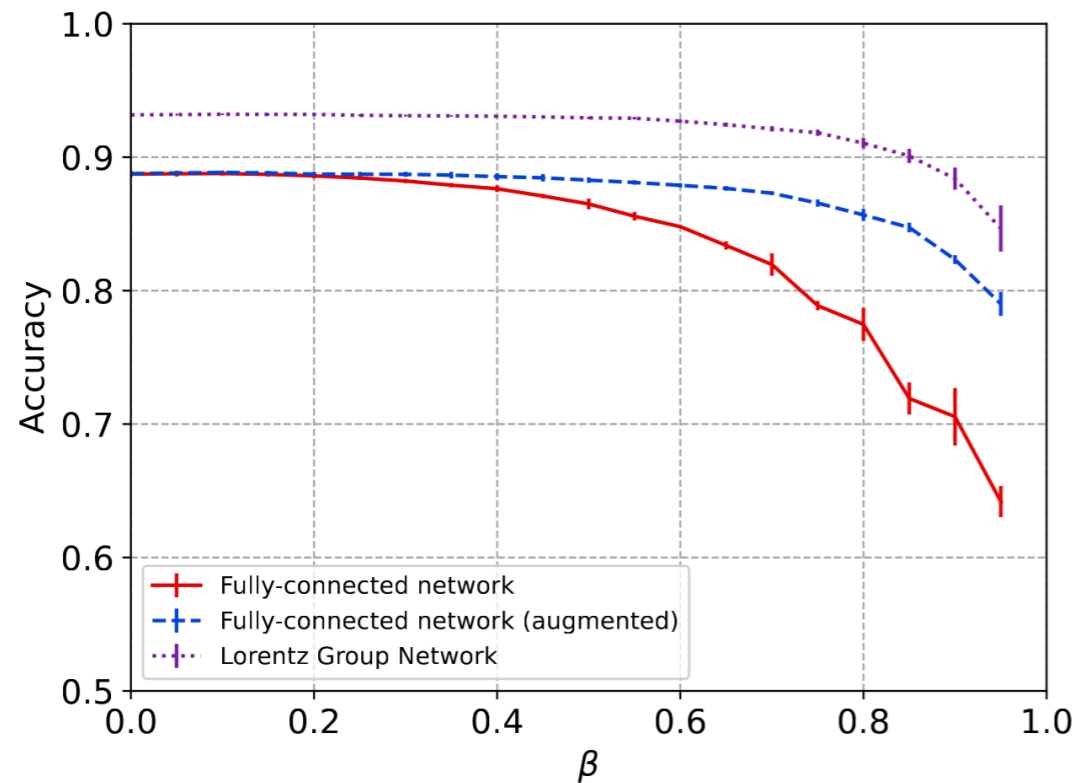
$$f(\rho_g(x)) = \rho'_g(f(x))$$



Symmetry equivariant networks

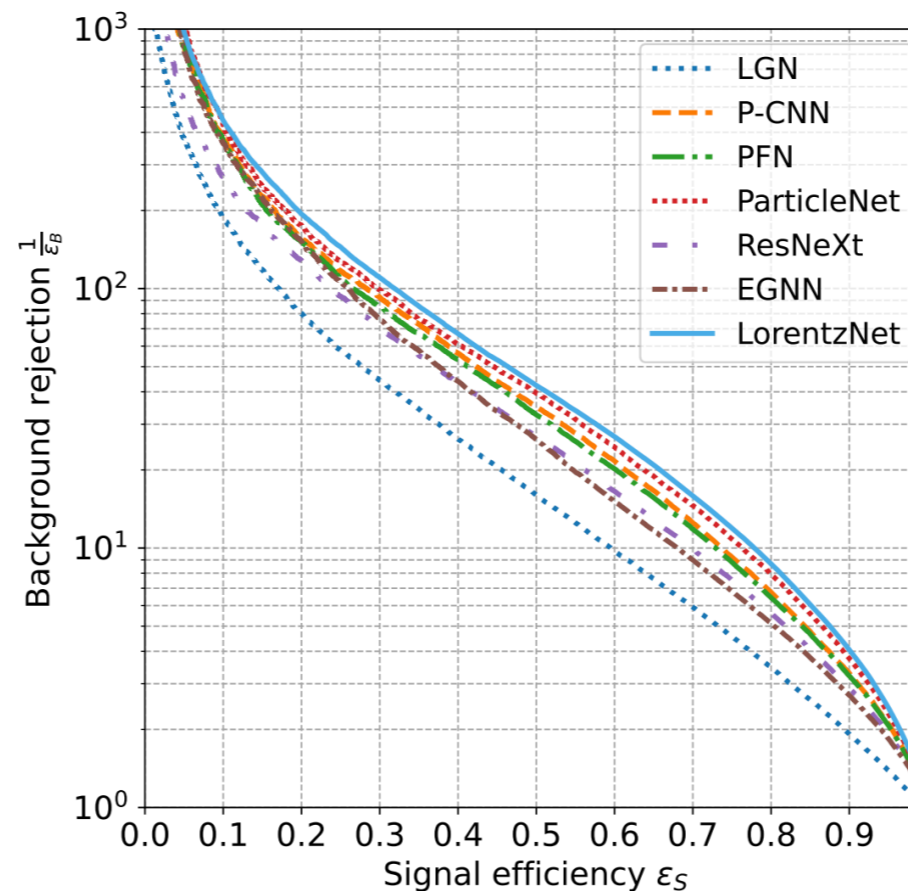
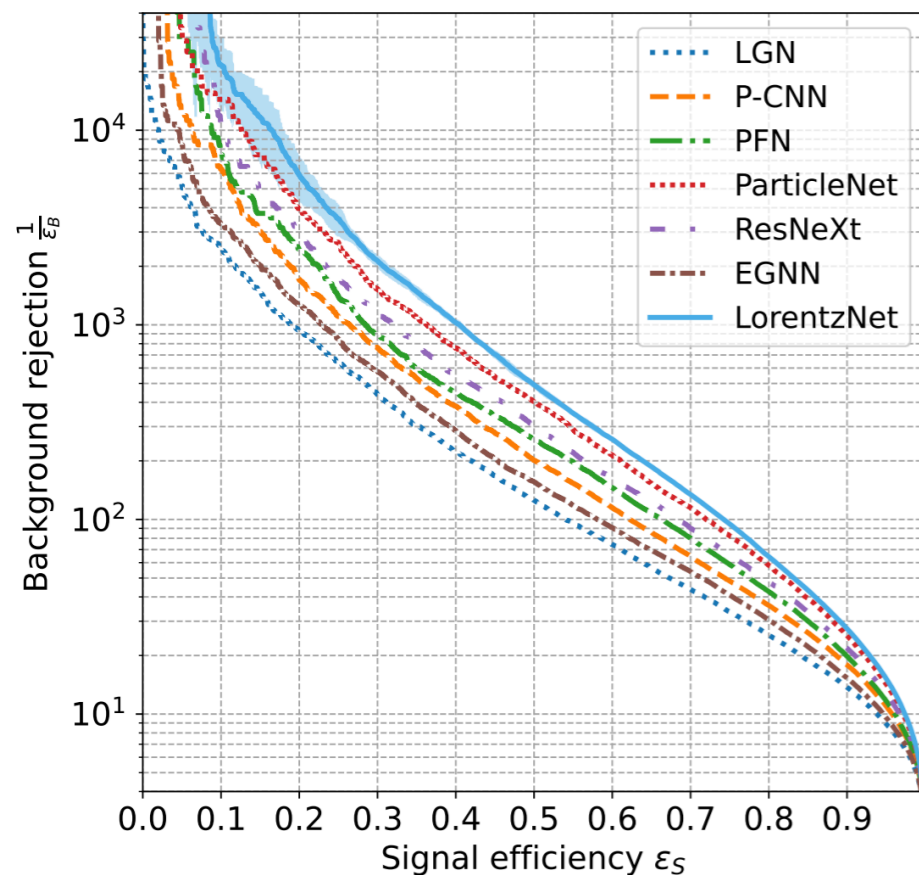
[arXiv:2006.04780](#) : A Bogatskiy et al

[arXiv:2203.06153](#) : SG et al



$$m_{ij}^l = \phi_e \left(h_i^l, h_j^l, \psi(\|x_i^l - x_j^l\|^2), \psi(\langle x_i^l, x_j^l \rangle) \right)$$

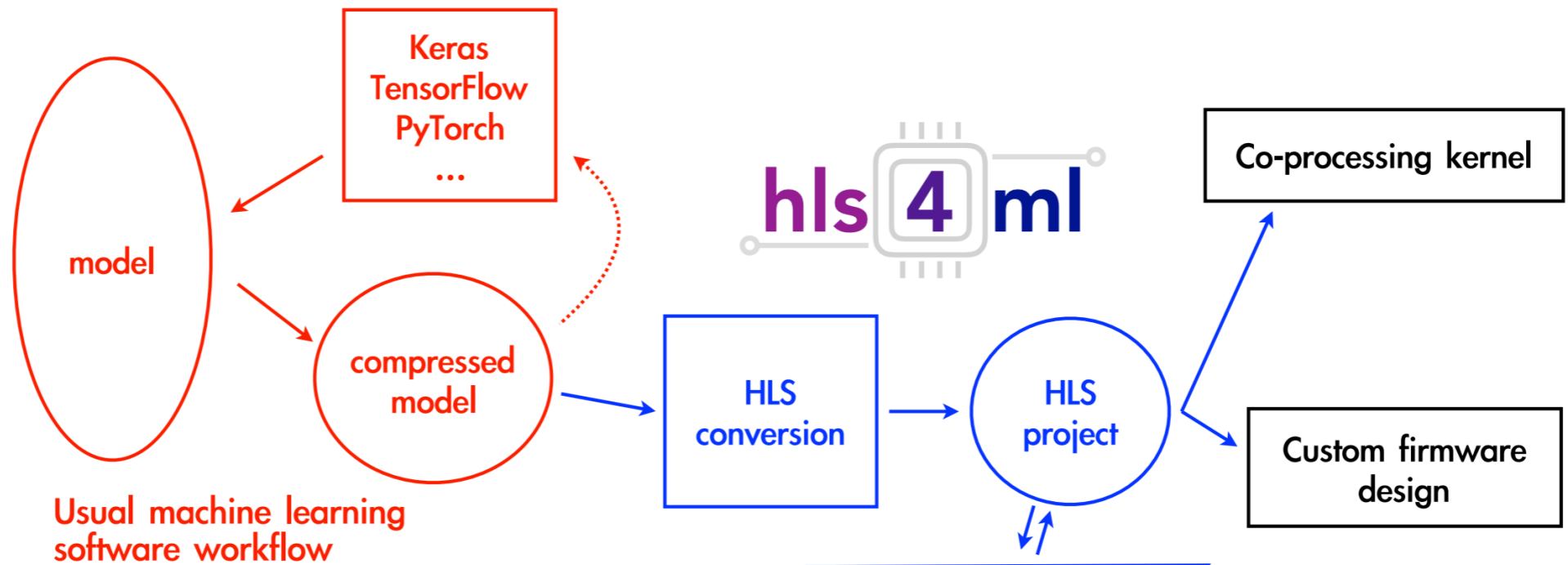
$$h_i^{l+1} = h_i^l + \phi_h \left(h_i^l, \sum_{j \in [N]} w_{ij} m_{ij}^l \right),$$



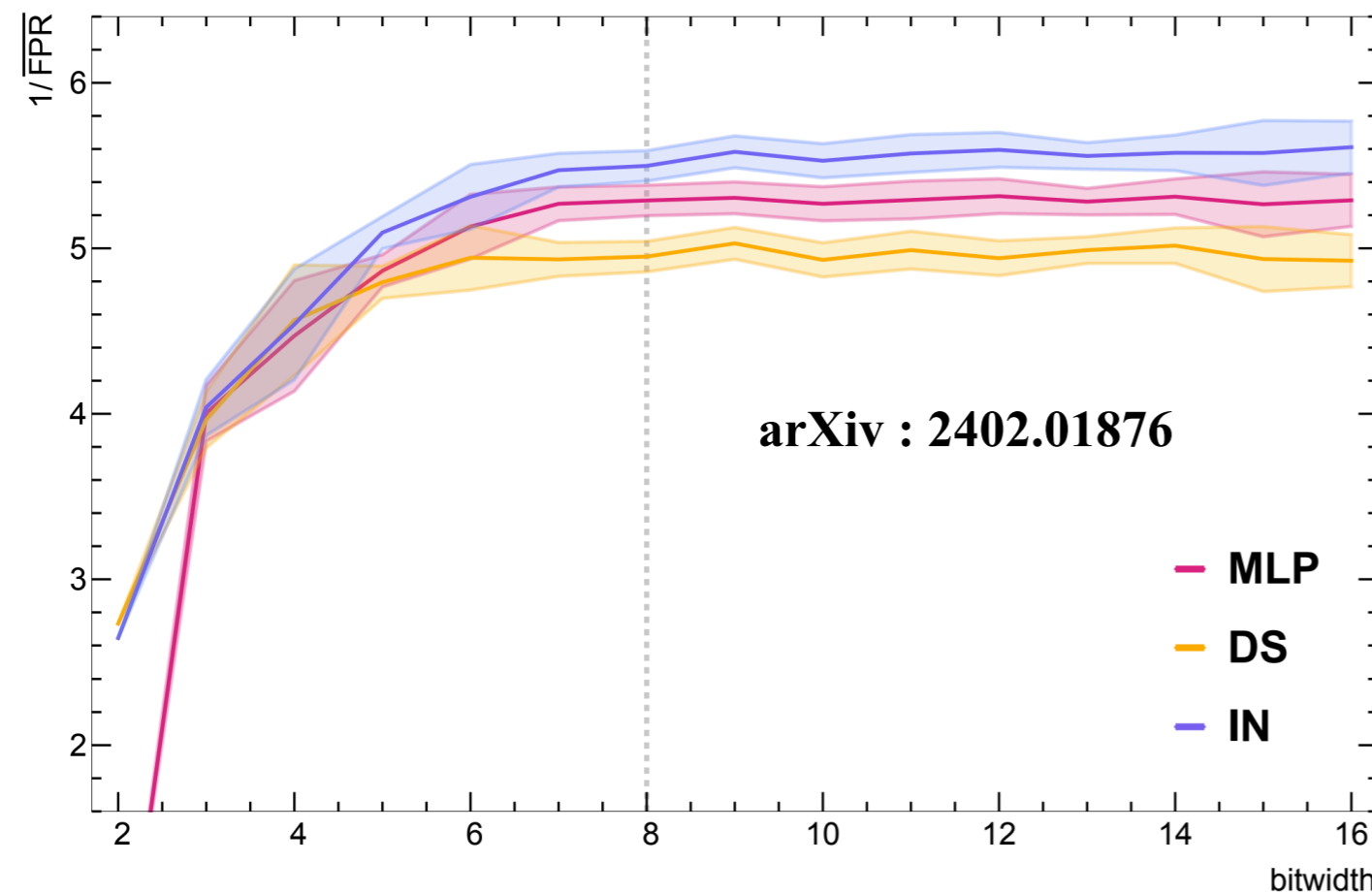
LG equivariant GNN :
[arXiv 2201.08187](#)

ML on FPGA

arXiv : 1804.06913



Usual machine learning software workflow



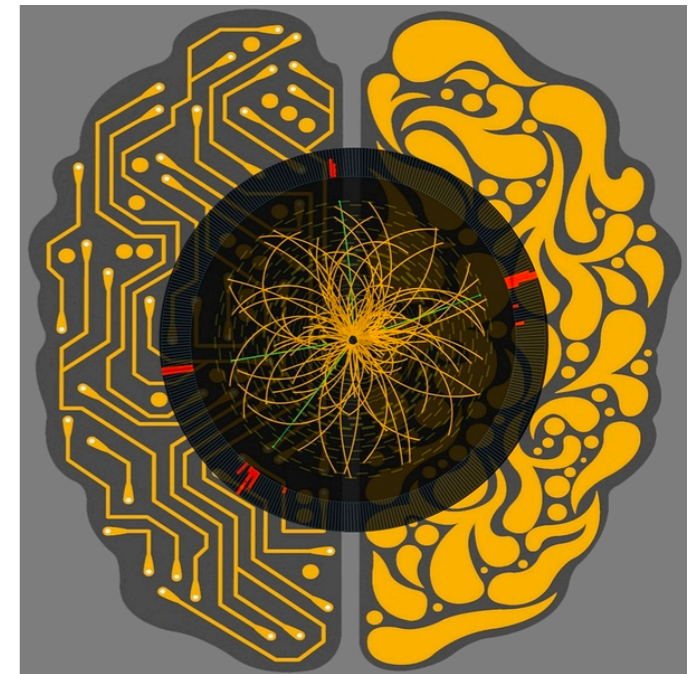
arXiv : 2402.01876

— MLP
— DS
— IN

Architecture	Constituents	Parameters	FLOPs	Accuracy	AUC				
					g	q	W	Z	t
MLP		26,826	53,162	$64.6 \pm 0.1\%$	0.84	0.88	0.90	0.88	0.92
DS	8	3,461	36,805	$64.0 \pm 0.3\%$	0.84	0.88	0.90	0.88	0.92
IN		3,347	37,232	$64.9 \pm 0.2\%$	0.84	0.88	0.91	0.89	0.92
MLP		20,245	40,485	$68.4 \pm 0.3\%$	0.87	0.89	0.91	0.90	0.94
DS	16	3,461	71,109	$69.4 \pm 0.2\%$	0.87	0.89	0.93	0.92	0.94
IN		3,347	140,432	$70.8 \pm 0.2\%$	0.88	0.90	0.94	0.92	0.94
MLP		24,101	48,197	$66.2 \pm 0.2\%$	0.90	0.89	0.89	0.88	0.94
DS	32	3,461	139,717	$75.9 \pm 0.1\%$	0.91	0.91	0.96	0.95	0.95
IN		7,400	109,556	$75.8 \pm 0.3\%$	0.91	0.91	0.96	0.95	0.95

Take away

Image: FermiLab

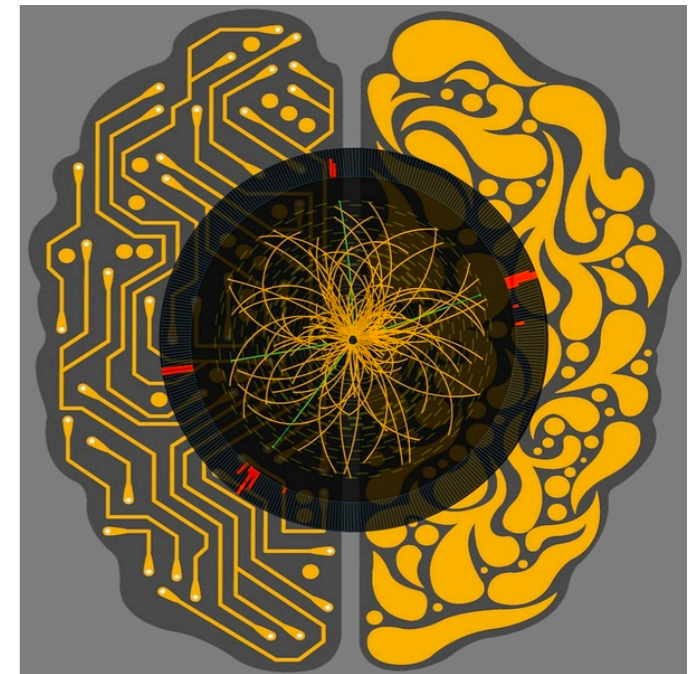


- ✓ **ML is here to stay with HEP.**
- ✓ **When looked through the lens of ML, LHC and EIC are not that far.**
- ✓ **Interpretability and uncertainty estimations are two key aspects where we the HEP-ML people need to emphasize.**
- ✓ **Need to keep a close connection with the comp-sc/math community with the latest developments and contribute if possible.**
- ✓ **Symmetry equivariance and geometric DL methods might play a key role in this field.**
- ✓ **Didn't want to talk about an elephant entering the room : QML (but should track it).**

<https://iml-wg.github.io/HEPML-LivingReview/>

Take away

Image: FermiLab



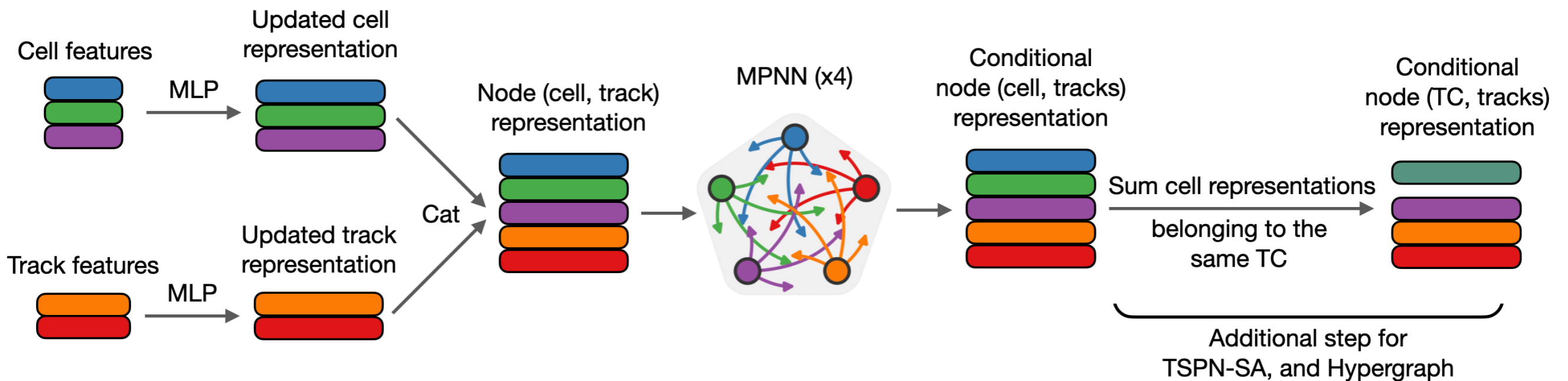
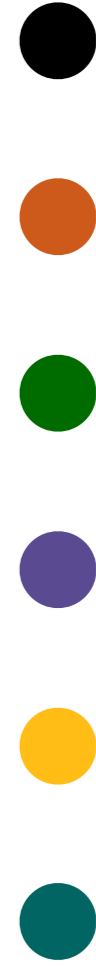
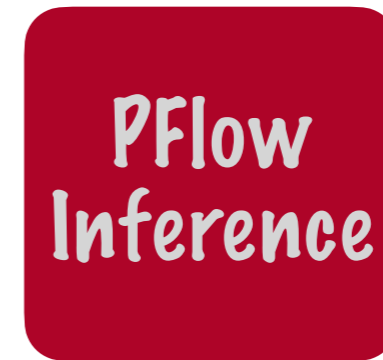
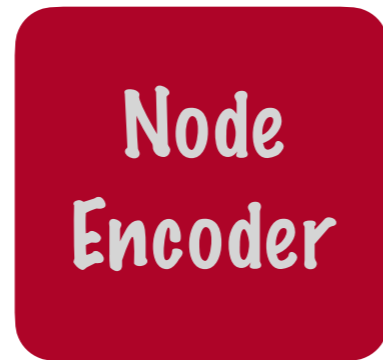
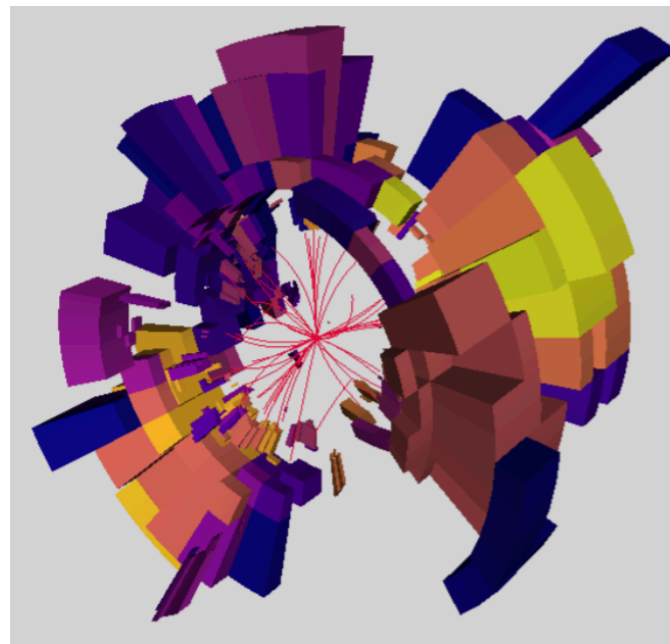
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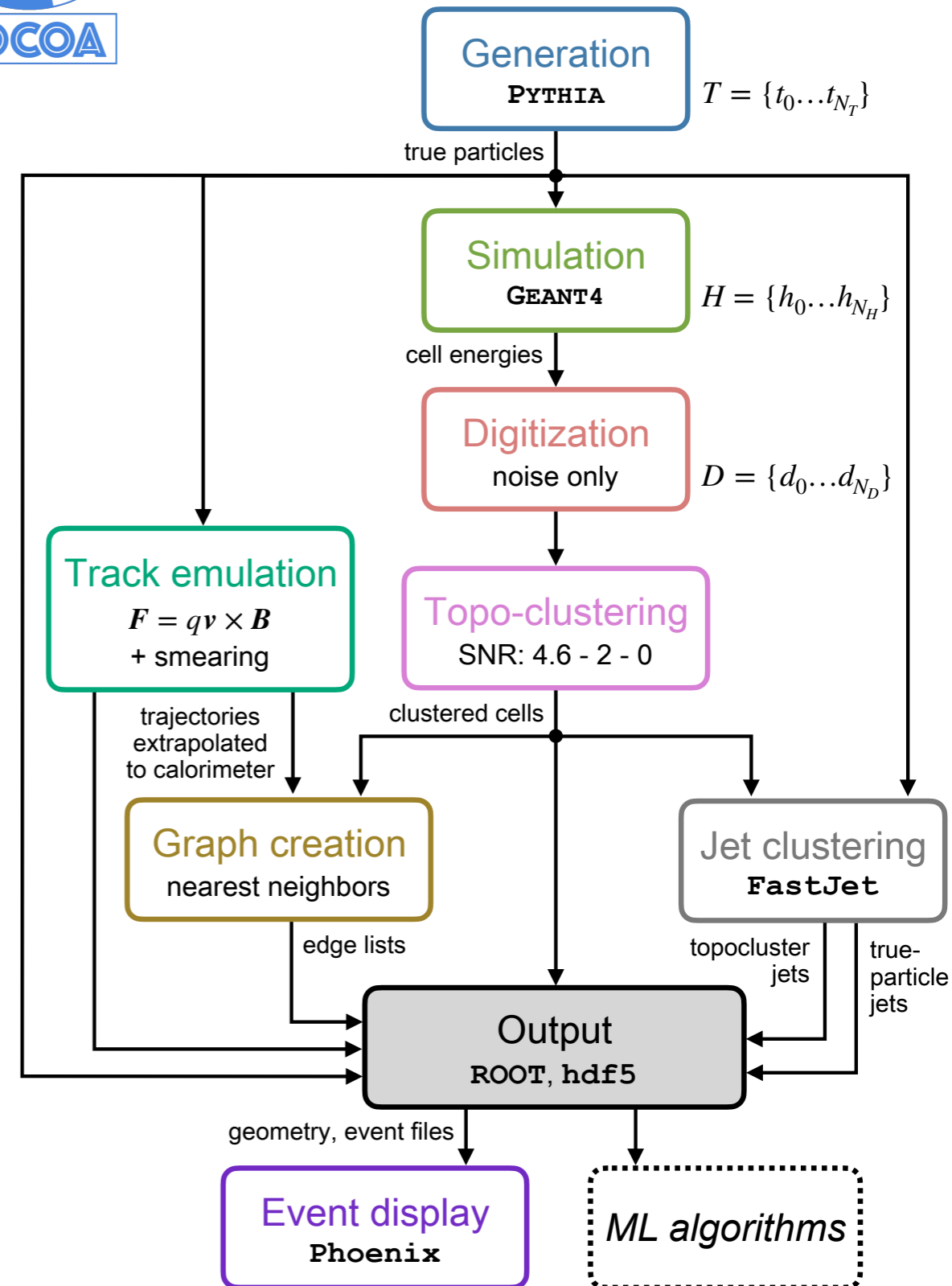
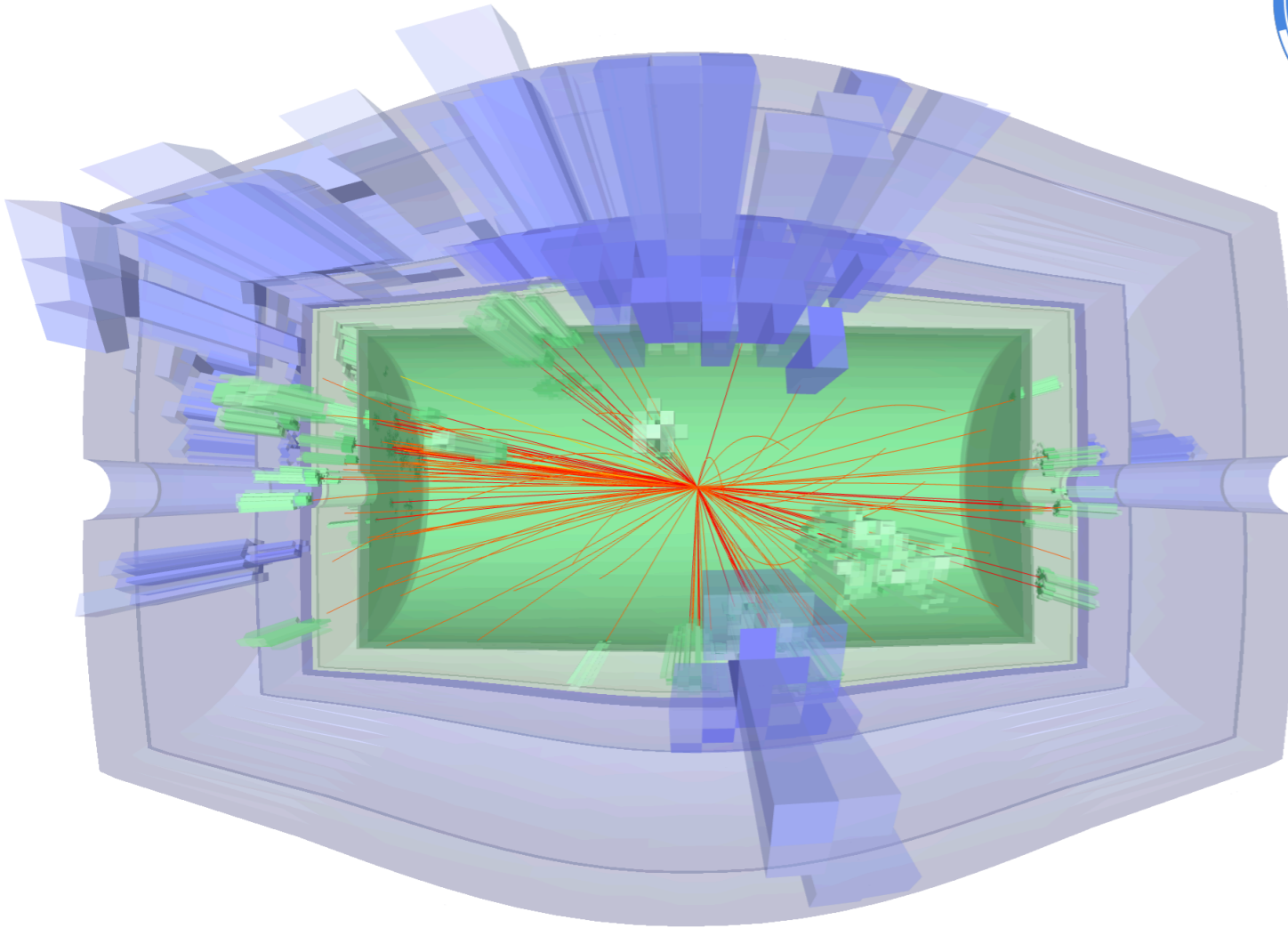
THANK YOU



The general workflow



The COCOA

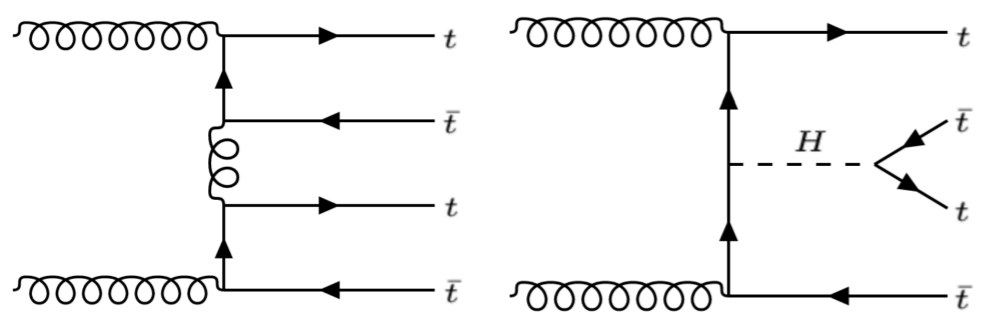


COnfigurable Calorimeter simulation for AI

- ✓ A complete hermetic geometry with full GEANT simulation.
- ✓ PYTHIA-8 based ME/PS & Hadronization
- ✓ FASTJET integration is inbuilt.
- ✓ Comes with an ATLAS style pPFlow.



Event construction using NN



$$\sigma_{t\bar{t}t\bar{t}} = 22.5^{+4.7}_{-4.3} (\text{stat})^{+4.6}_{-3.4} (\text{syst}) \text{ fb} = 22.5^{+6.6}_{-5.5} \text{ fb.}$$

Eur. Phys. J. C 83 (2023) 496

Operators	Expected C_i/Λ^2 [TeV ⁻²]	Observed C_i/Λ^2 [TeV ⁻²]
O_{QQ}^1	[-2.4, 3.0]	[-3.5, 4.1]
O_{Qt}^1	[-2.5, 2.0]	[-3.5, 3.0]
O_{tt}^1	[-1.1, 1.3]	[-1.7, 1.9]
O_{Qt}^8	[-4.2, 4.8]	[-6.2, 6.9]

