Jet Flavor Tagging (and Particle Flow) Using AI Tools (for e+e- Higgs factories)

Taikan Suehara / 末原　大幹
(ICEPP, The University of Tokyo)

with L. Gui (Imperial), R. Tagami (Tokyo) (for flavor tagging)
T. Tanabe (MI-6 Co.), L. Gray (Fermilab) (for particle flow)

Deep learning with Higgs factories

- Significant part of reconstruction is “pattern recognition”
  - Cut-based method should have limitation
  - DNN should take more information than human-tuning
- “Big data” detector for Higgs factories
  - Much more detector elements than before
  - Should fit with modern network with many learning weights
  - Also good for detector design
- Sensor → objects → physics
  should be more seamless with deep learning techniques
  - Event reconstruction is the heart of the chain

Today's topics

All works done with ILD full simulation (and FCCee Delphes for comparison)

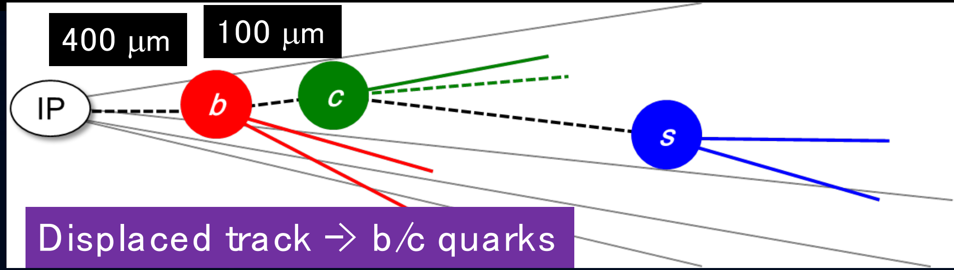
Flavor tagging with Particle Transformer (ParT)

- Modern DNN-based jet flavor tagging originally developed for LHC
- Much better performance than current algorithm (LCFIPlus(2013))
  - Reported by FCCee colleagues earlier, comparison done
- Big impact on Higgs studies
  - Including self coupling

Particle flow with DNN (ongoing work, no conclusion)

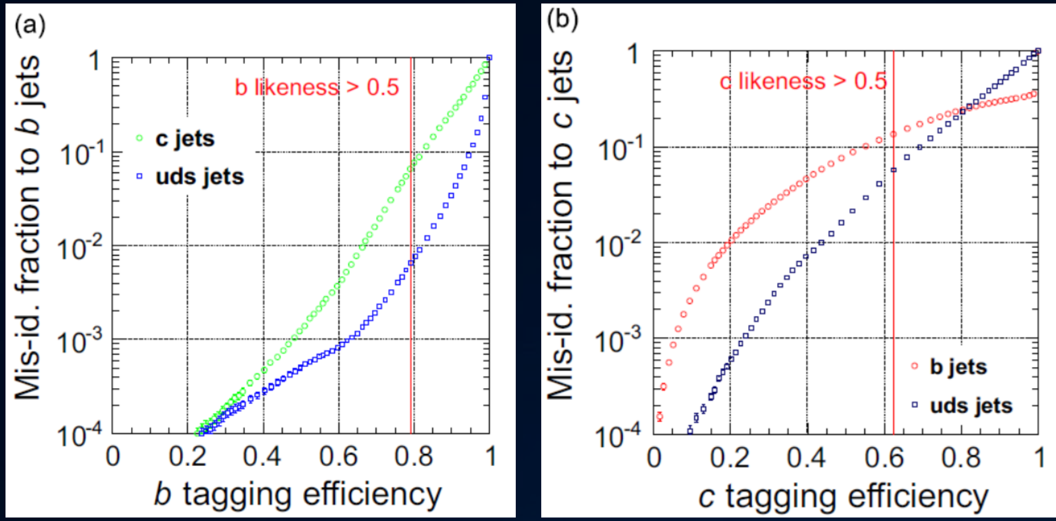
- Based on GNN developed for CMS HGCAL clustering
  - GravNet
  - Object condensation loss function
  - Timing information can be included → detector optimization
- Implementing track-cluster matching

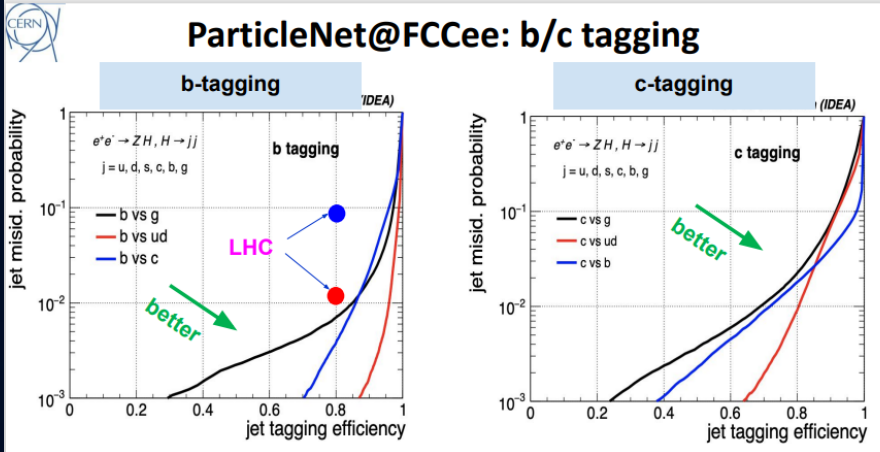
Flavor tagging for Higgs factories



- Jet flavor tagging is essentially important for Higgs studies (including self coupling)
- LCFIPlus (published 2013)[1] was long used for flavor tagging
  - b-tag: ~80% eff., 10% c / 1% uds acceptance;
  - c-tag: ~50% eff., 10% b / 2% uds acceptance.
- Recently FCCee reported ~10x better rejection using ParticleNet (GNN)
  - To be confirmed with full simulation (with latest algorithm: Particle Transformer (ParT)

  → If good, consider to apply to physics analyses hopefully with common framework



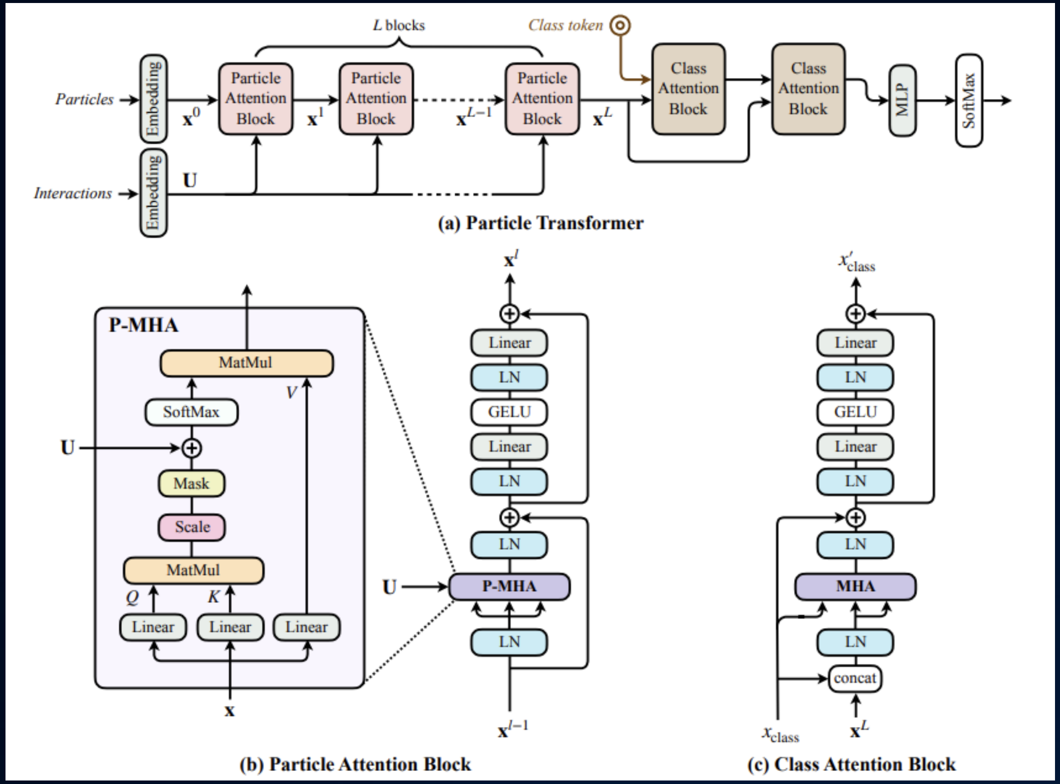


WP	Eff (b)	Mistag (g)	Mistag (ud)	Mistag (c)
Loose	90%	2%	0.1%	2%
Medium	80%	0.7%	<0.1%	0.3%

WP	Eff (c)	Mistag (g)	Mistag (ud)	Mistag (b)
Loose	90%	7%	7%	4%
Medium	80%	2%	0.8%	2%

Particle Transformer (ParT)

- Transformer: self-attention based algorithm intensively used for NLP (e.g. chatGPT)
  - Weak biasing: possible to train big samples efficiently (with more learnable weights)
    but demanding big training sample for high performance
- ParT is a new Transformer-based architecture for Jet tagging, published in 2022[2].
- Surpasses the performance of ParticleNet
  - ParticleNet (or other GNNs) only looks “neighbor” particles while Transformer judges where to look by training

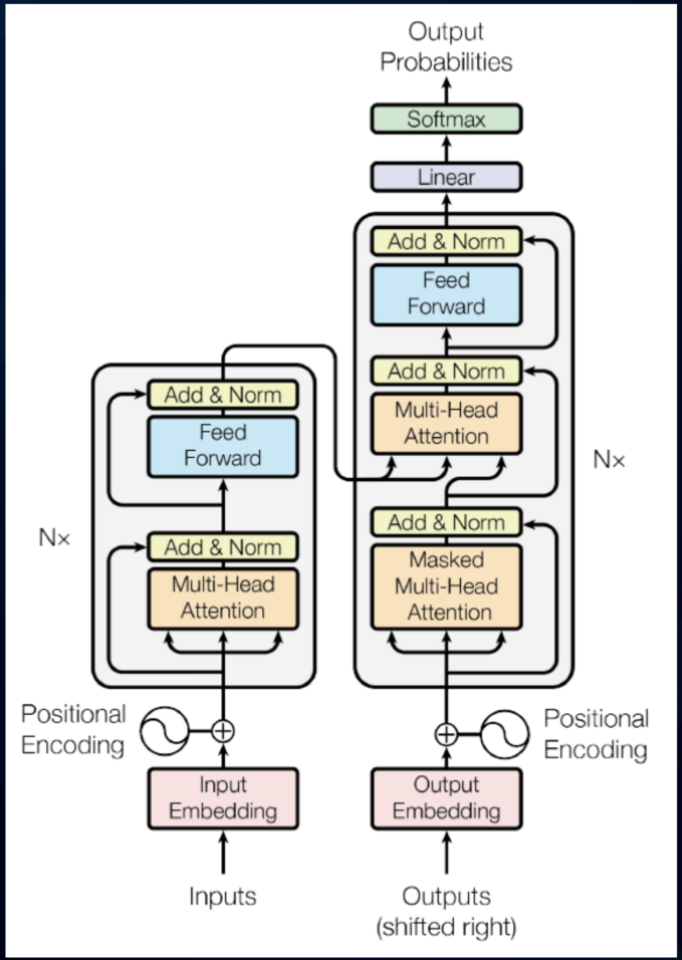


(a) Particle Transformer
(b) Particle Attention Block
(c) Class Attention Block

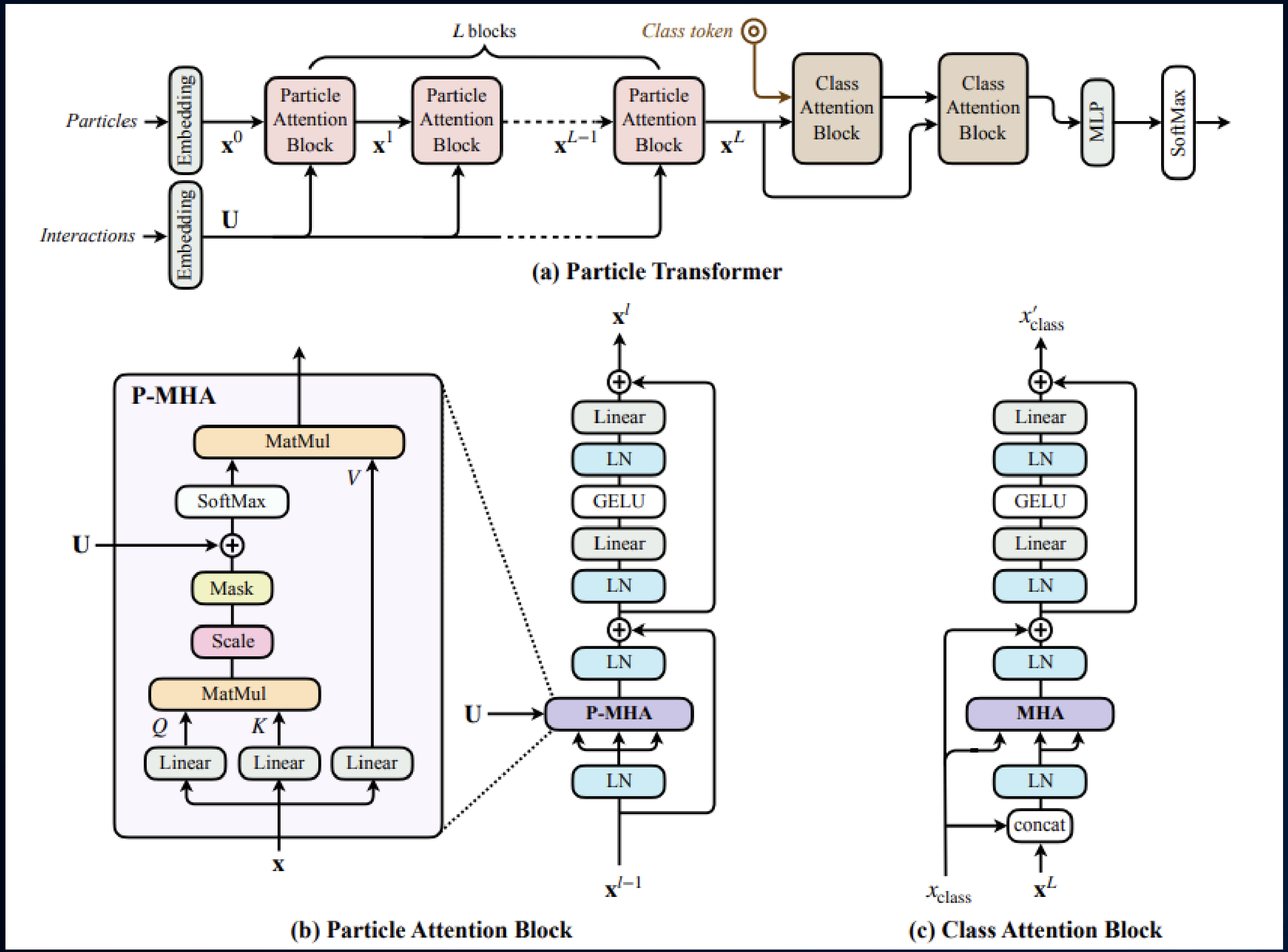
Performance on event categorization (ie. not direct flavor tagging but flavor information is essential for the categorization)

	All classes		$H \to b\bar{b}$	$H \to c\bar{c}$	$H \to gg$	$H \to 4q$	$H \to \ell\nu qq'$	$t \to bqq'$	$t \to b\ell\nu$	$W \to qq'$	$Z \to q\bar{q}$
	Accuracy	AUC	$\mathrm{Rej}_{50\%}$	$\mathrm{Rej}_{50\%}$	$\mathrm{Rej}_{50\%}$	$\mathrm{Rej}_{50\%}$	$\mathrm{Rej}_{99\%}$	$\mathrm{Rej}_{50\%}$	$\mathrm{Rej}_{99.5\%}$	$\mathrm{Rej}_{50\%}$	$\mathrm{Rej}_{50\%}$
PFN	0.772	0.9714	2924	841	75	198	265	797	721	189	159
P-CNN	0.809	0.9789	4890	1276	88	474	947	2907	2304	241	204
ParticleNet	0.844	0.9849	7634	2475	104	954	3339	10526	11173	347	283
ParT	**0.861**	**0.9877**	**10638**	**4149**	**123**	**1864**	**5479**	**32787**	**15873**	**543**	**402**
ParT (plain)	0.849	0.9859	9569	2911	112	1185	3868	17699	12987	384	311

Comparison between regular Transformer and Particle Transformer



Regular Transformer



Particle Transformer

Note:
- MHA – MultiHeadAttention
- P-MHA – Augmented version of MHA by Particle Transformer that involves Interactions Embeddings instead of Positional Embeddings

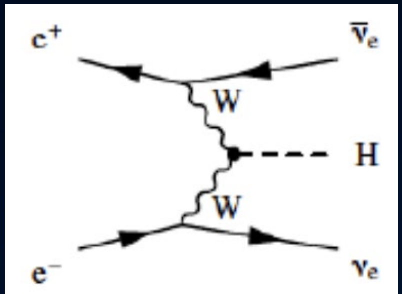
Data Used For Investigation

- ILD full simulation:

  1. e+ e- $\longrightarrow$ qq (at 91 GeV)
     (DBD sample used for initial LCFIPlus study)
  2. e+ e- $\longrightarrow$ νvH $\longrightarrow$ νvqq (at 250 GeV)
     (2020 production, process ID: 410001-410006)

  With 1M jets (500k events) each

$$\left\{ \begin{array}{c} q = b,c,uds \\ \nu = \text{neutrino} \end{array} \right\}$$

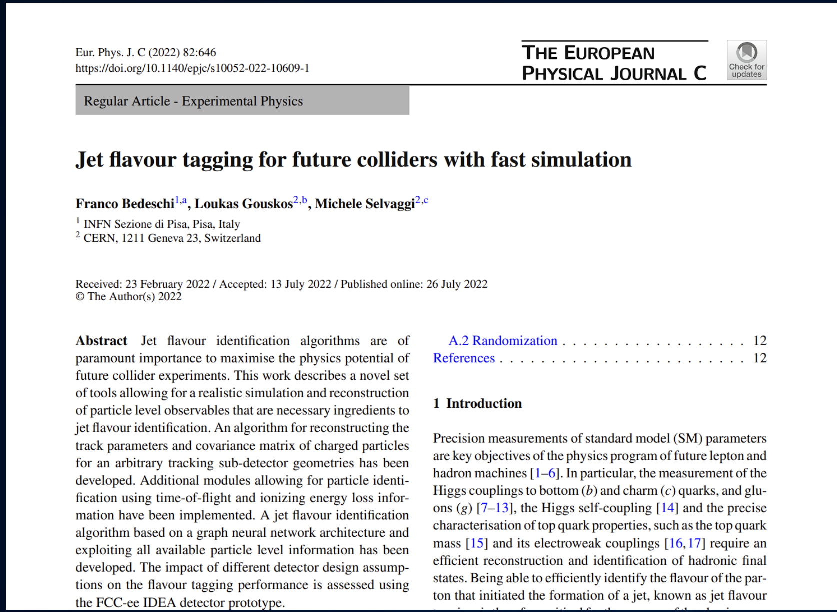


- FCCee fast simulation (Delphes with IDEA detector):

  e+ e- $\longrightarrow$ νvH $\longrightarrow$ νvqq (at 240 GeV)

  With 10M jets (5M events) each

- 80% are used for training, 5% for validation, 15% for test



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Regular Article - Experimental Physics

Jet flavour tagging for future colliders with fast simulation

Franco Bedeschi[1,a], Loukas Gouskos[2,b], Michele Selvaggi[2,c]

[1] INFN Sezione di Pisa, Pisa, Italy
[2] CERN, 1211 Geneva 23, Switzerland

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Abstract Jet flavour identification algorithms are of paramount importance to maximise the physics potential of future collider experiments. This work describes a novel set of tools allowing for a realistic simulation and reconstruction of particle level observables that are necessary ingredients to jet flavour identification. An algorithm for reconstructing the track parameters and covariance matrix of charged particles for an arbitrary tracking sub-detector geometries has been developed. Additional modules allowing for particle identification using time-of-flight and ionizing energy loss information have been implemented. A jet flavour identification algorithm based on a graph neural network architecture and exploiting all available particle level information has been developed. The impact of different detector design assumptions on the flavour tagging performance is assessed using the FCC-ee IDEA detector prototype.

1 Introduction

Precision measurements of standard model (SM) parameters are key objectives of the physics program of future lepton and hadron machines [1–6]. In particular, the measurement of the Higgs couplings to bottom (b) and charm (c) quarks, and gluons (g) [7–13], the Higgs self-coupling [14] and the precise characterisation of top quark properties, such as the top quark mass [15] and its electroweak couplings [16,17] require an efficient reconstruction and identification of hadronic final states. Being able to efficiently identify the flavour of the parton that initiated the formation of a jet, known as jet flavour

https://link.springer.com/article/10.1140/epjc/s10052-022-10609-1

Input Variables - Features

*Naming follows FCCee scheme – may not express exact meaning

- Impact Parameter (6):

pfcand_dxy
pfcand_dz
pfcand_btagSip2dVal
pfcand_btagSip2dSig
pfcand_btagSip3dVal
pfcand_btagSip3dSig

*d0/z0 and 2D/3D impact parameters, 0 for neutrals

- Jet Distance (2):

pfcand_btagJetDistVal
pfcand_btagJetDistSig

*Displacement of tracks from line passing IP with direction of jet
0 for neutrals

- Particle ID (6):

pfcand_isMu
pfcand_isEl
pfcand_isChargedHad
pfcand_isGamma
pfcand_isNeutralHad
pfcand_type

* Not including strange-tagging related variables (TOF, dE/dx etc.)
* Simple PID for ILD, not optimal

- Kinematic (4):

pfcand_erel_log
pfcand_thetarel
pfcand_phirel
pfcand_charge

*Fraction of the particle energy wrt. jet energy (log is taken)

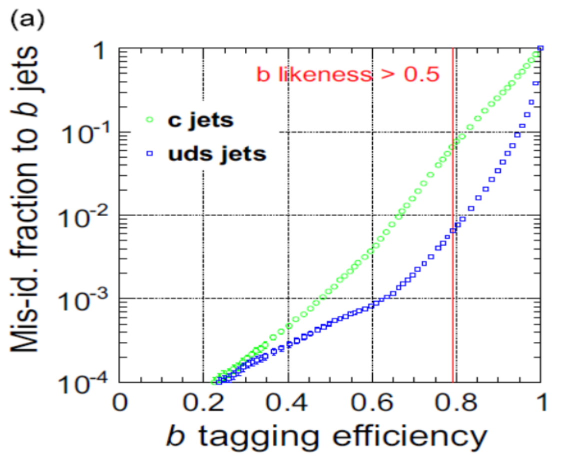
- Track Errors (15):

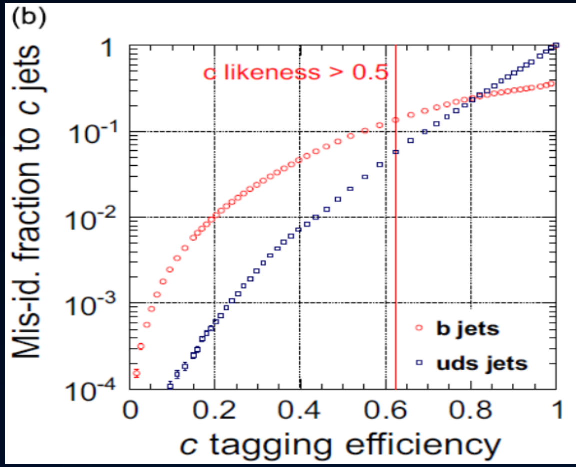
pfcand_dptdpt
pfcand_detadeta
pfcand_dphidphi
pfcand_dxydxy
pfcand_dzdz
pfcand_dxydz
pfcand_dphidxy
pfcand_dlambdadz
pfcand_dxyc
pfcand_dxyctgtheta
pfcand_phic
pfcand_phidz
pfcand_phictgtheta
pfcand_cdz
pfcand_cctgtheta

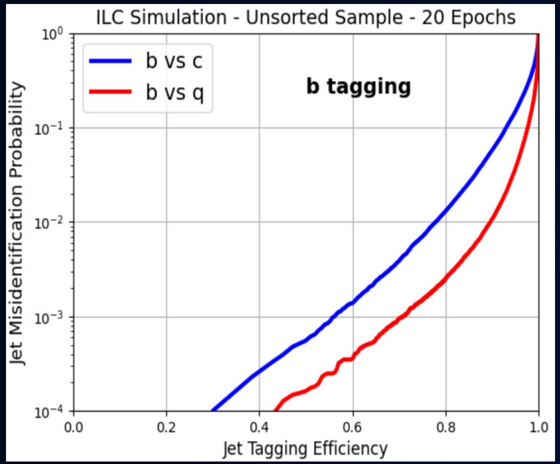
*each element of covariant matrix
0 for neutrals

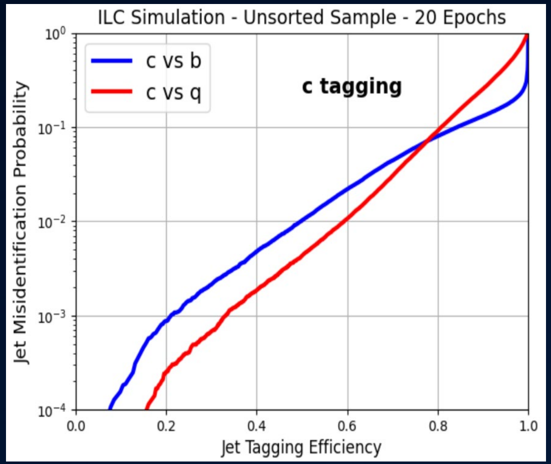
Application of ParT to ILD data
(ILD qq 91 GeV, 0.8M jets for training)

- Jet tagging performance is greatly improved by ParT immediately.
- The performance is improved by 4.05 – 9.80 times compared to LCFIPlus with the same set of data.
- 20 epochs are taken,
  200 epochs do not help improving performance but give overtraining





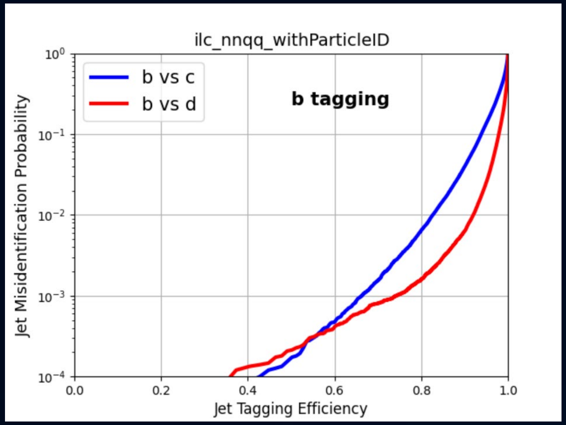


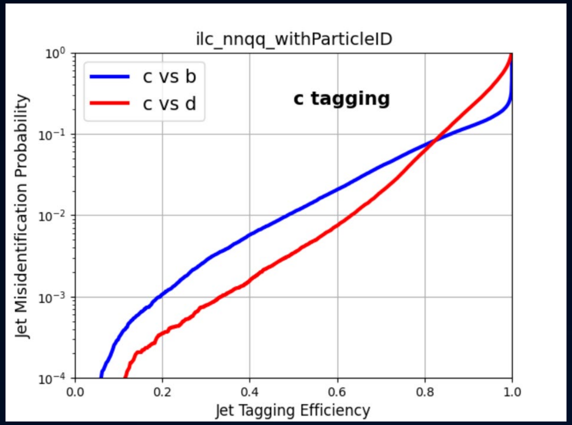


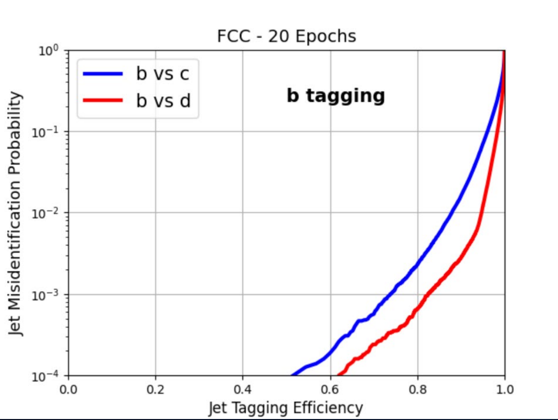
	b-tag 80% eff.		c-tag 50% eff.	
Method	c-bkg acceptance	uds-bkg acceptance	c-bkg acceptance	uds-bkg acceptance
LCFIPlus	10%	1%	10%	2%
ParT	1.29%	0.25%	1.02%	0.43%

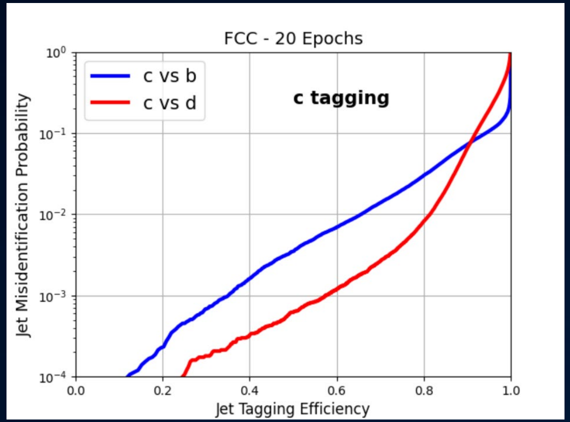
Comparison with FCC data[3]

- Trained with same condition as ILD data for fair comparison. (800k data size, 20 epochs, etc.)
- FCC data has ~ 3 times the performance compared to ILD data.
- Possible cause of the difference:
  - Particle ID: too pessimistic for ILD
  - Definition of some variables
    - Theta, phi etc.
  - Difference on full and fast sim
    - Especially different on tails of distributions
  - Assumed detector resolution (?)









Data	Particle ID	Impact Parameters	Jet Distance	Track Errors	c-bkg acceptance @ b-tag 80% eff.	b-bkg acceptance @ c-tag 50% eff.
ILD (vvqq 250 GeV)	●	●	●	●	**0.64%**	**1.09%**
FCC	●	●	●	●	**0.23%**	**0.35%**

ILD (vvqq 250 GeV) vs. FCC with partial variables

800 kjet for training, 20 epochs

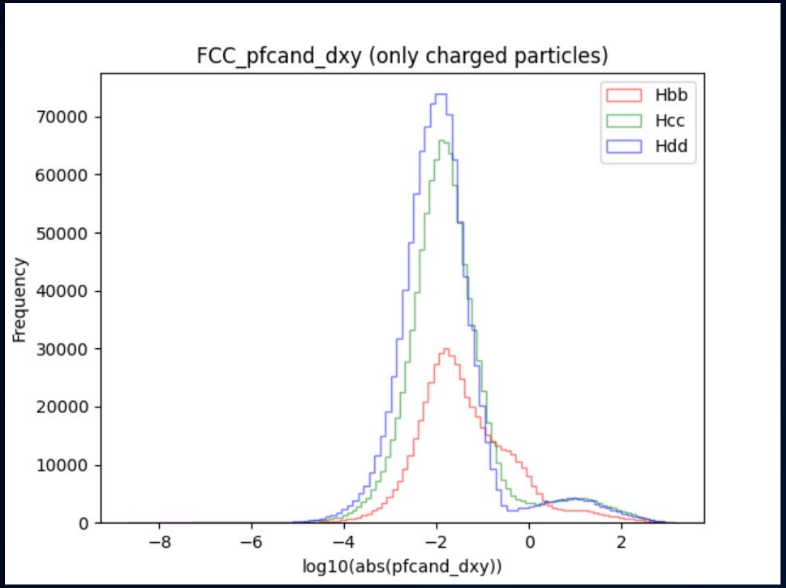
					c-bkg acceptance @ b-tag 80% eff.		b-bkg acceptance @ c-tag 50% eff.	
Plot Index	Particle ID	Impact Parameters	Jet Distance	Track Errors	ILD	FCC	ILD	FCC
(1)	●	●	●	●	0.64%	0.23%	1.09%	0.35%
(2)	✕	●	●	●	0.62%	0.47%	1.14%	0.64%
(3)	✕	●	●	✕	0.71%	0.24%	1.24%	0.35%
(4)	✕	●	✕	●	0.63%	0.75%	1.19%	0.80%
(5)	✕	●	✕	✕	0.79%	0.77%	1.28%	0.80%
(6)	✕	✕	●	●	9.69%	2.64%	6.91%	1.58%

Observations:

1. PID gives significant effect on FCCee, not ILD (due to easy PID in ILD)
2. Track errors are rather harmful in FCCee
3. Difference on b-tag is small with only impact parameters (5), but still see difference in c-tag
4. (of course) significantly losing performance without impact parameter (but still ~ LCFIPlus)

Potential Improvement: log(abs)

Particle ID	Impact Parameters	Jet Distance	Track Errors	c-bkg acceptance @ b-tag 80% eff.	b-bkg acceptance @ c-tag 50% eff.
✗	●	●	●	0.62%	1.14%
✗	● +log(abs)	● +log(abs)	● +log(abs)	0.54%	1.06%
✗	●	● +log(abs)	● +log(abs)	0.79%	1.33%
✗	●	● +log(abs)	●	0.78%	1.36%
✗	● +log(abs)	●	●	0.47%	1.03%
✗	log(abs)	log(abs)	log(abs)	0.82%	1.32%
✗	●	log(abs)	log(abs)	0.80%	1.37%
✗	●	●	log(abs)	0.82%	1.38%

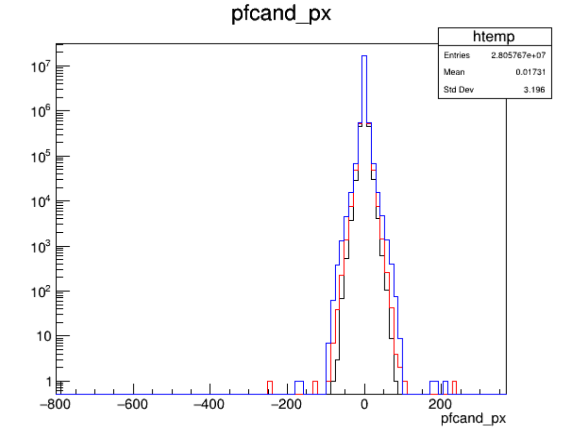


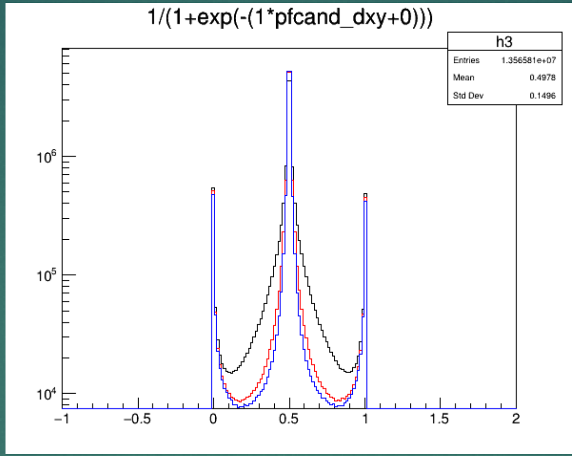
Impact Parameter

ML prefers “gaussian-like” distribution
Not sensitive to small values
(because of linear weighting)

Track errors or impact parameters should convert with e.g. log function
→ slightly improving performance
(but not much as expected…)

Sigmoid





data	sigmoid	b vs c 0.8 score
llc_nnqq	×	0.00647±0.00054
llc_nnqq	O	0.00535±0.00032

Each of the score is the average of 3 times training with standard variation

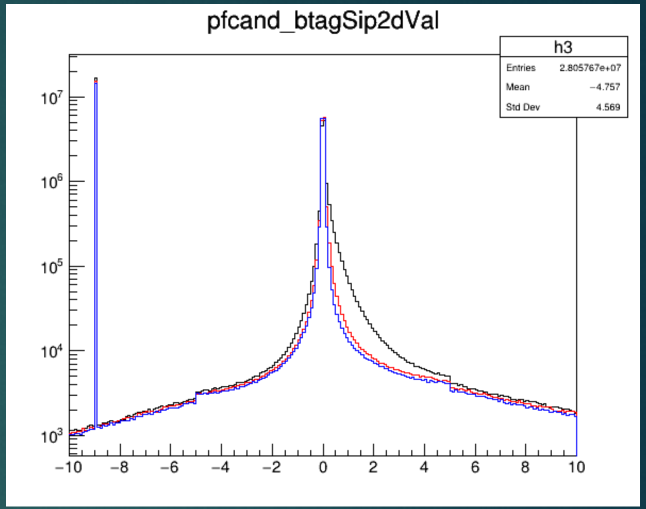
- Applying Sigmoid function to the variables with wide distribution
- The score is better than that of not applying sigmoid.

- Processed variables (8)

pfcand_dxy
pfcand_dz
pfcand_btagSip2dVal
pfcand_btagSip2dSig
pfcand_btagSip3dVal
pfcand_btagSip3dSig
pfcand_dxydz
pfcand_dphidxy

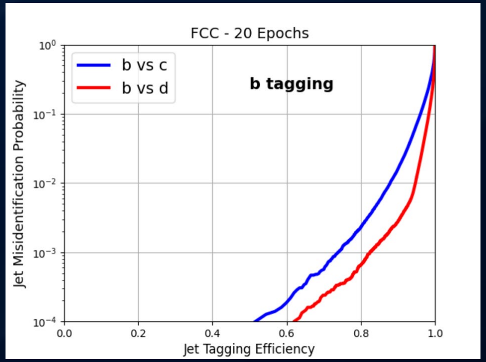
Different Networks for Neutrals

- Currently tracks and neutrals are passing same embedding layer
  - For parameters not available in neutrals, "-9" is set (right figure)
  - Without neutrals, performance is significantly degraded
    - b/c separation (b selection eff. = 80%) in ILC nnqq sample (1M jets):
      - With neutrals: rejection ratio = 123 (acceptance: 0.647%)
      - Without neutrals: rejection ratio = 62.5 (acceptance: 1.28%)
- Tracks and neutrals have flags (like "charge")
- At the initial stage of transformer, they should be separated and going through different embedding network
  - But variables like energy/momentum are common: need some treatment?
- Combine tracks and neutrals
  - Should keep some flags to discriminate tracks and neutrals?

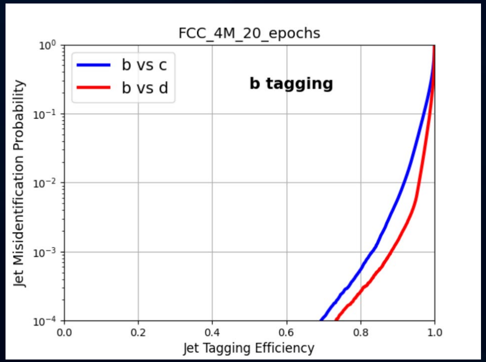


Sample size affects performance (FCCee sample)

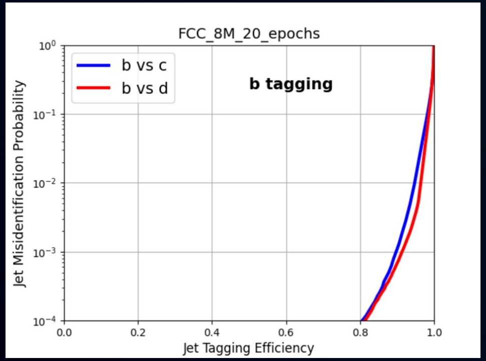
(1)



(2)



(3)



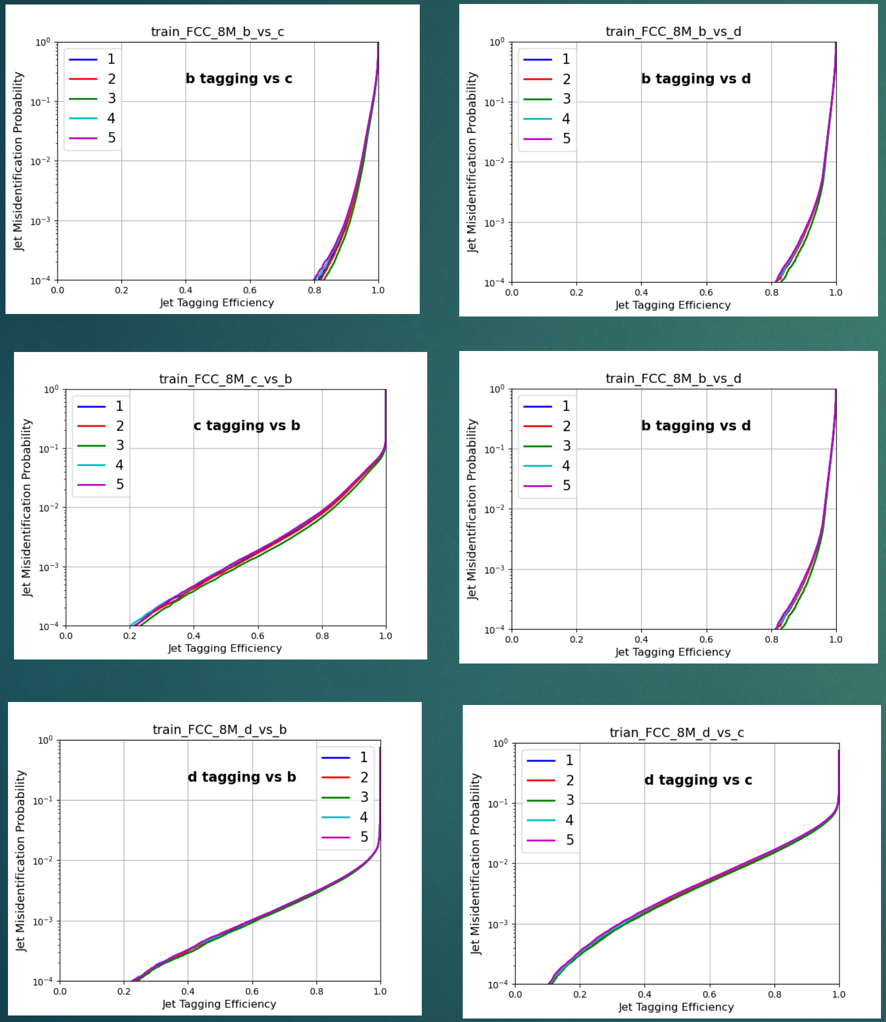
Plot Index	Particle ID	Impact Parameters	Jet Distance	Track Errors	Training Sample size	c-bkg acceptance @ b-tag 80% eff.	b-bkg acceptance @ c-tag 50% eff.
(1)	●	●	●	●	800k	0.23%	0.35%
(2)	●	●	●	●	4M	0.054%	0.20%
(3)	●	●	●	●	8M	Unreasonably good, TBC	

- Training performance significantly improved with bigger data sample size
- Training sample size change of FCC data:

  800k -> 4M : 4 times better performance (b-tagging)

  4M -> 8M: 5 times better performance (b-tagging)
- This non-linearity of increase in performance should be further investigated.
- Bigger data size of ILD should be obtained for better performance, as well as comparison with FCC data for further investigation on its behaviour.

Multiple Training Runs

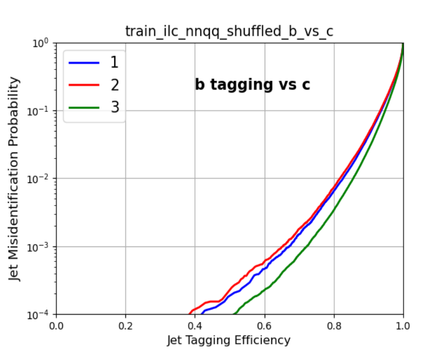


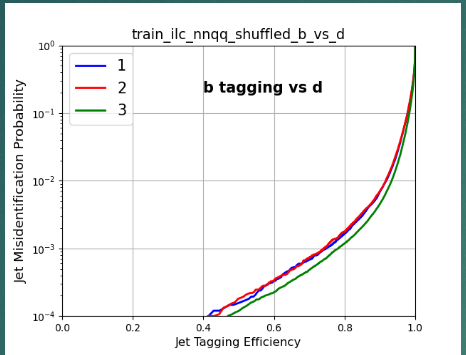
5 times training of FCC_8M data

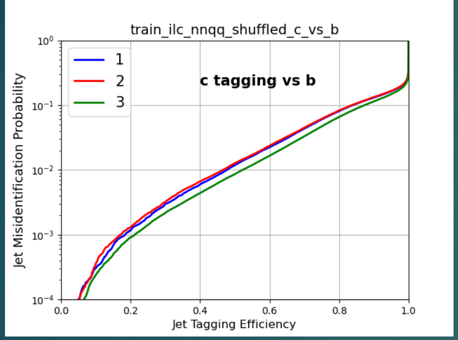
- Multiple training runs don't give significant impacts on results.
- The smaller data size is, the bigger impacts on results multiple runs give.
- The results of no Particle ID trainings varies more than those of with Particle ID.

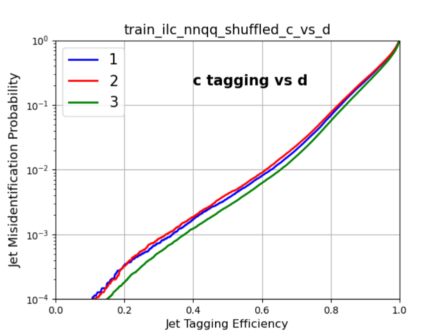
data	Particle ID	b vs c 0.8 Score	variation
FCC 4M	O	4.82e-4	0.43e-4
FCC 8M	O	8.14e-5	1.58e-5
FCC 4M	×	1.69e-3	0.14e-3
FCC 8M	×	7.04e-4	3.49e-4

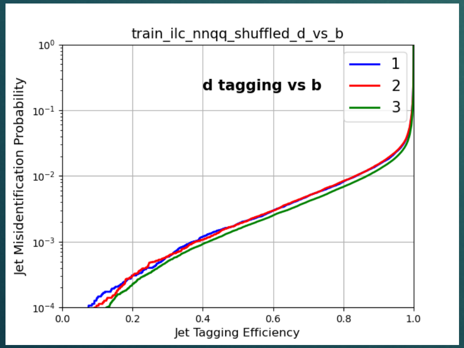
Data Shuffled

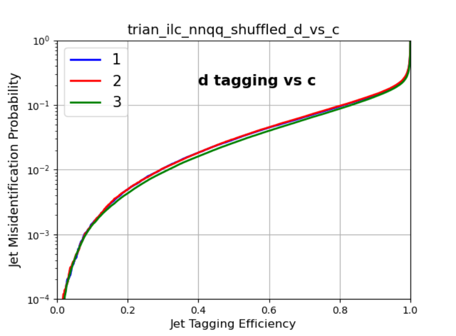












- ILC nnqq dataset
  - 80% training, 5% validation, 15% test
- Shuffled the order of train/test/val making root files
  - Pattern 1: train/val/test
  - Pattern 2: val/train/test
  - Pattern 3: train/test/val
- Will do more comprehensive study

data	b vs c 0.8 score
Shuffle pattern 1	0.00647
Shuffle pattern 2	0.00734
Shuffle pattern 3	0.00338

Fine tuning

Two objectives
- Pretrained with fast sim and fine-tune with full sim
- Pretrained with large central production and fine-tune with dedicated physics samples in each analysis

							c-bkg acceptance @ b-tag 80% eff.		b-bkg acceptance @ c-tag 50% eff.	
Particle ID	**Impact Parameters**	**Jet Distance**	**Track Errors**	**Fine-Tuning Sample**	**Training Sample**	**Similar theta/phi ?**	**No Fine-Tuning**	**With Fine-Tuning**	**No Fine-Tuning**	**With Fine-Tuning**
✗	●	●	●	FCC 240 GeV (8M)	ILD 250 GeV (800k)	✗	0.62%	1.37%	1.14%	1.95%
✗	●	●	●	FCC 240 GeV (8M)	ILD 250 GeV (800k)	●	1.77%	1.32%	2.22%	2.01%
●	●	●	●	ILD 250 GeV (800k)	ILD 91 GeV (80k)	●	4.49%	0.97%	3.79%	1.53%

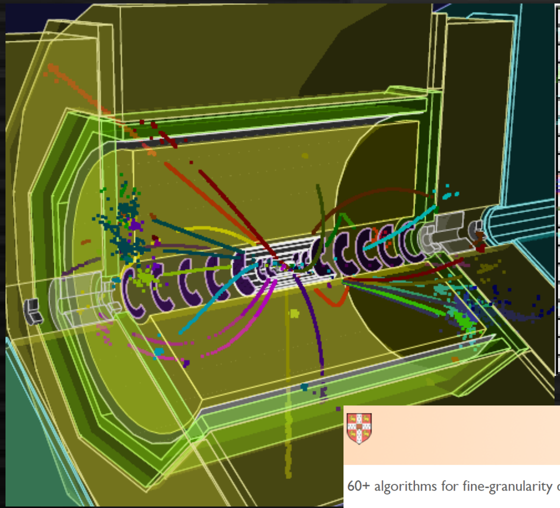
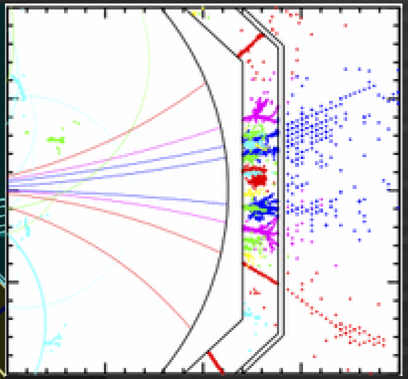
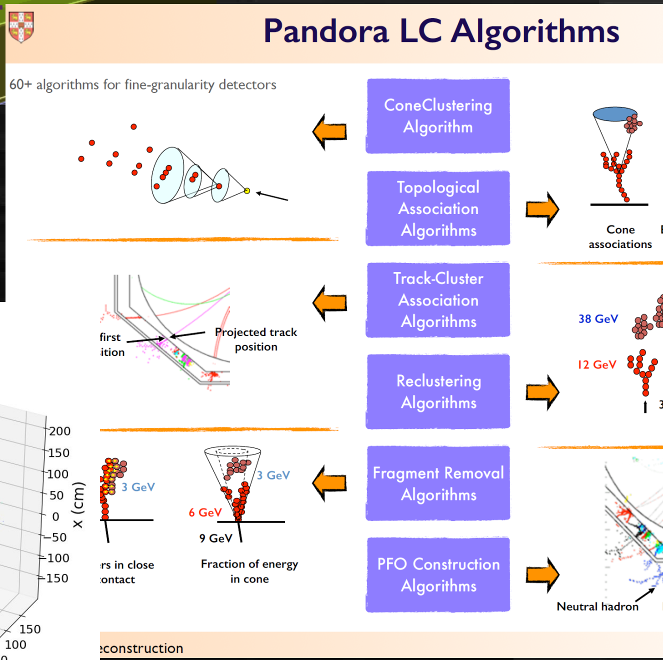
- Use result of 8M FCC data to train ILD 800k data
- Improves performance only when setups are similar
- Training of same setup (pretrain ILD 91 GeV data with ILD 250 GeV data) gives best performance
- Further investigation should be conducted on how to maximise the outcome for fine-tuning between different data sets

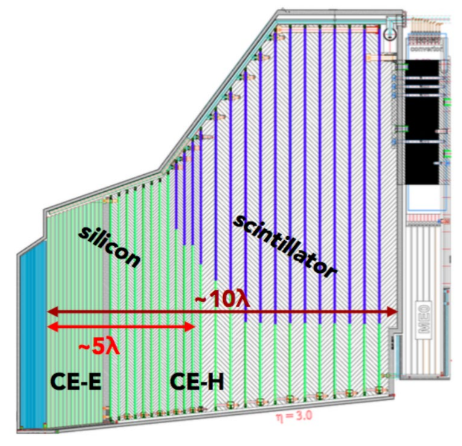
Plans for flavor tagging

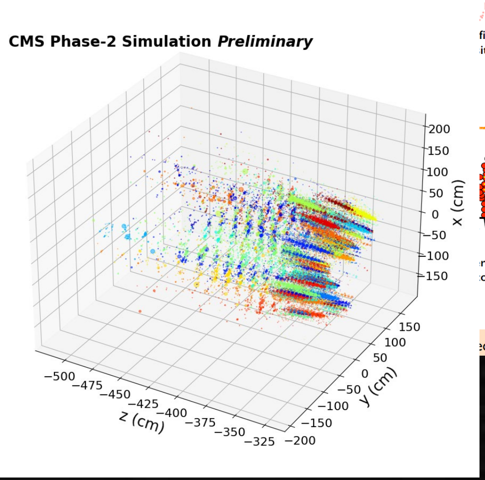
- Optimizing network and inputs
  - Embedding of neutral particles
  - Improve variables (especially on interaction)
  - Hyperparameter tuning
- Strange tagging
  - Preparing PID variables (by dE/dx and TOF) ongoing
- Inference to be used for physics analyzes
  - Importing trained network to reconstruction framework
    - Interfacing to LCFIPlus planned
    - Also to native key4hep/Gaudi framework
- Collaboration with CEPC group being discussed

Particle flow with DNN: introduction

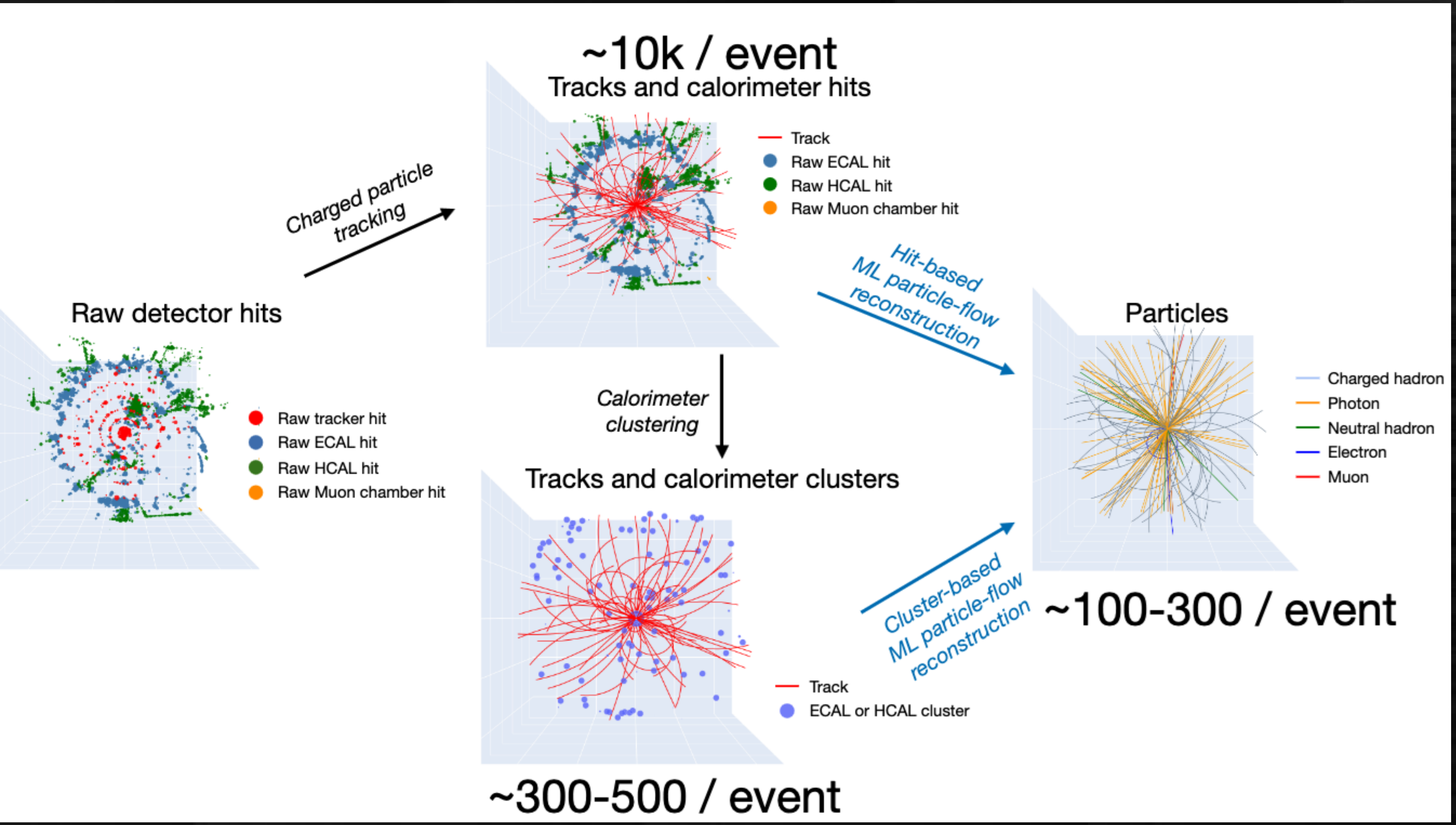
- Separation of cluster at calorimeter
  - Charged or neutral cluster
- Essential for jet energy resolution
- Current algorithm: PandoraPFA
  - Combination of various process
  - Not easy to optimize or adding more info
- CMS HGCal clustering
  - Similar to ILD calo
  - Good for starting point





Two ways for particle flow?



Track-cluster matching from calorimeter hits

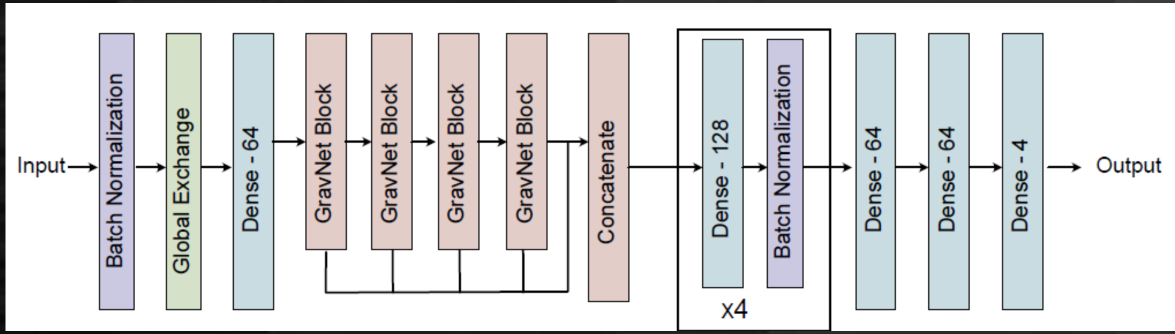
- More freedom
- Distance-based connection more efficient
- We are working this way

Track-cluster matching from subclusters

- Less input
- Transformer-like algorithm can be utilized?
- Additional clustering algorithm needed

PFA: clustering algorithm

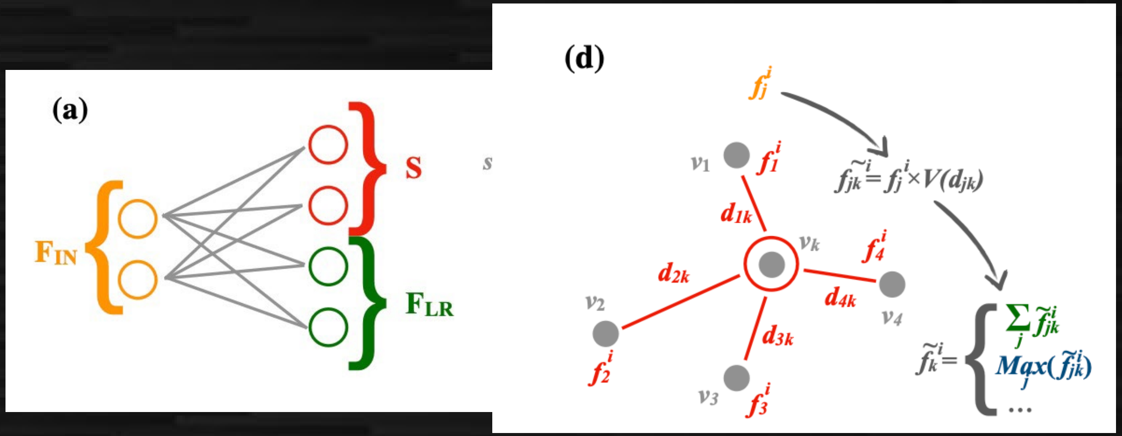
- Input: position/energy/timing of each hit
- Output: virtual coordinate and β for each hit



GravNet

arXiv:1902.07987

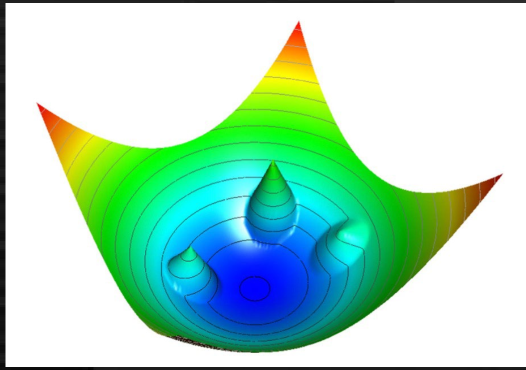
- The virtual coordinate (S) is derived from input variables with simple MLP
- Convolution using "distance" at S (bigger convolution with nearer hits)
- Concatenate the output with MLP



Object Condensation (loss function)

arXiv:2002.03605

$$L = L_p + s_C(L_\beta + L_V)$$

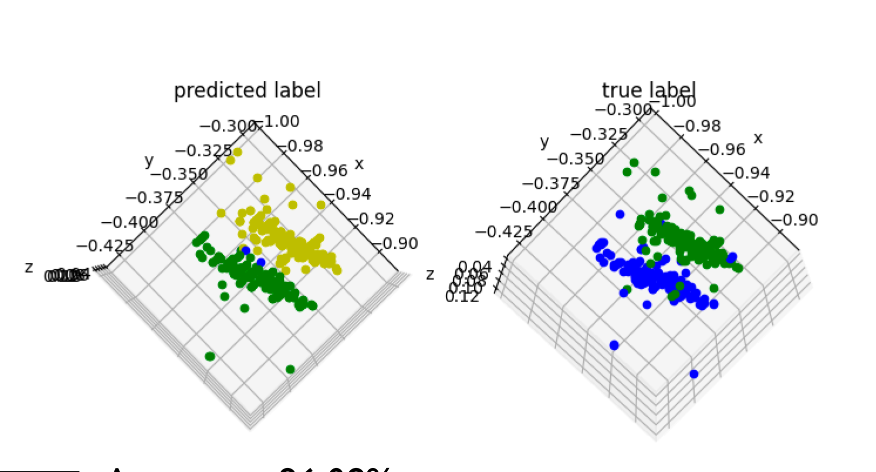


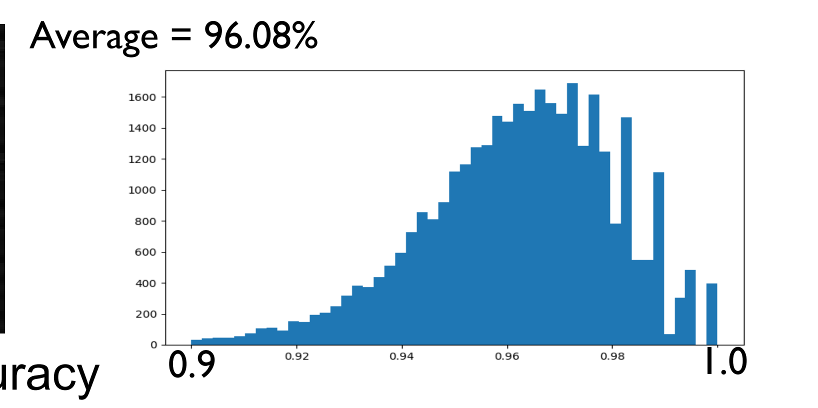
- Condensation point: The hit with largest β at each (MC) cluster
- L_V: Attractive potential to the condensation point of the same cluster and repulsive potential to the condensation point of different clusters
- L_β: Pulling up β of the condensation point
- L_p: Regression to output features

Importing to ILD full simulation

- Prepare features from ILD full simulation
  - With recent versions (> v02-02)
- Input features: (x, y, z, edep)
- True cluster info
  from MCParticle and LCRelation
- Produced events
  - Two photons
    (5/10 GeV, fixed opening angles)
  - (n x) taus (5/10 GeV)
- Evaluation
  - Fraction of hits associated to the correct cluster (accuracy)

Example of a two-photon event
(5 GeV, 30 mrad)





Reasonable
performance seen

Angle[mrad]	30	60	90	120	150
Accuracy[%]	96.08	98.64	99.30	99.68	99.56

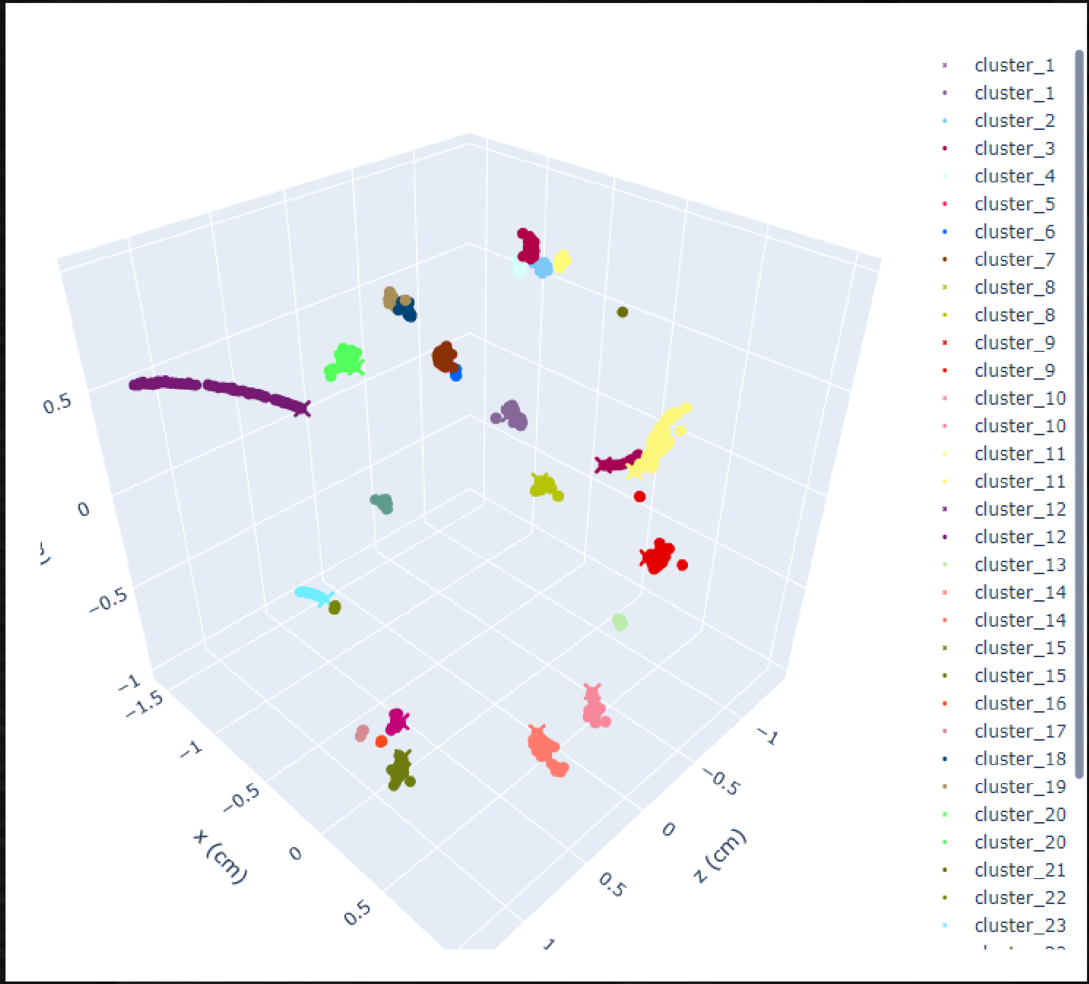
For details, refer eg. https://indico.slac.stanford.edu/event/7467/contributions/5948/attachments/2887/8032/230517-lcws2023-hlreco-suehara.pdf

Work in Progress: track-cluster matching

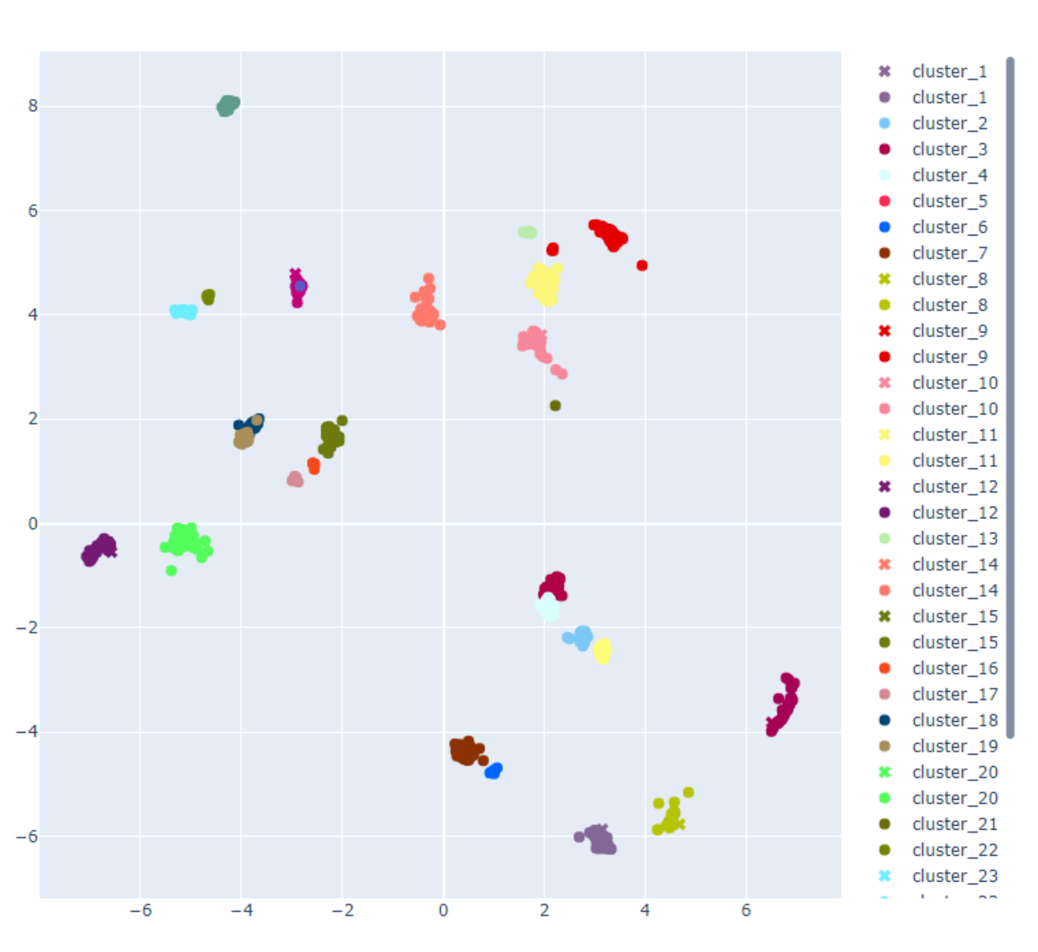
- PFA is essentially a problem "to subtract hits from tracks"
- HGCAL algorithm does not utilize track information
  - Only calorimeter clustering exists
- Simple extension to include track information
  - Adding "virtual hits" derived from track information
    - Hits at position where the track enters the calorimeter (from LCIO StackState)
  - Add a term to the object condensation loss function
    - Pulling up β of tracks (virtual hits) to promote them to condensation points

Preliminary results – looks working

10 Taus @ 10 GeV each

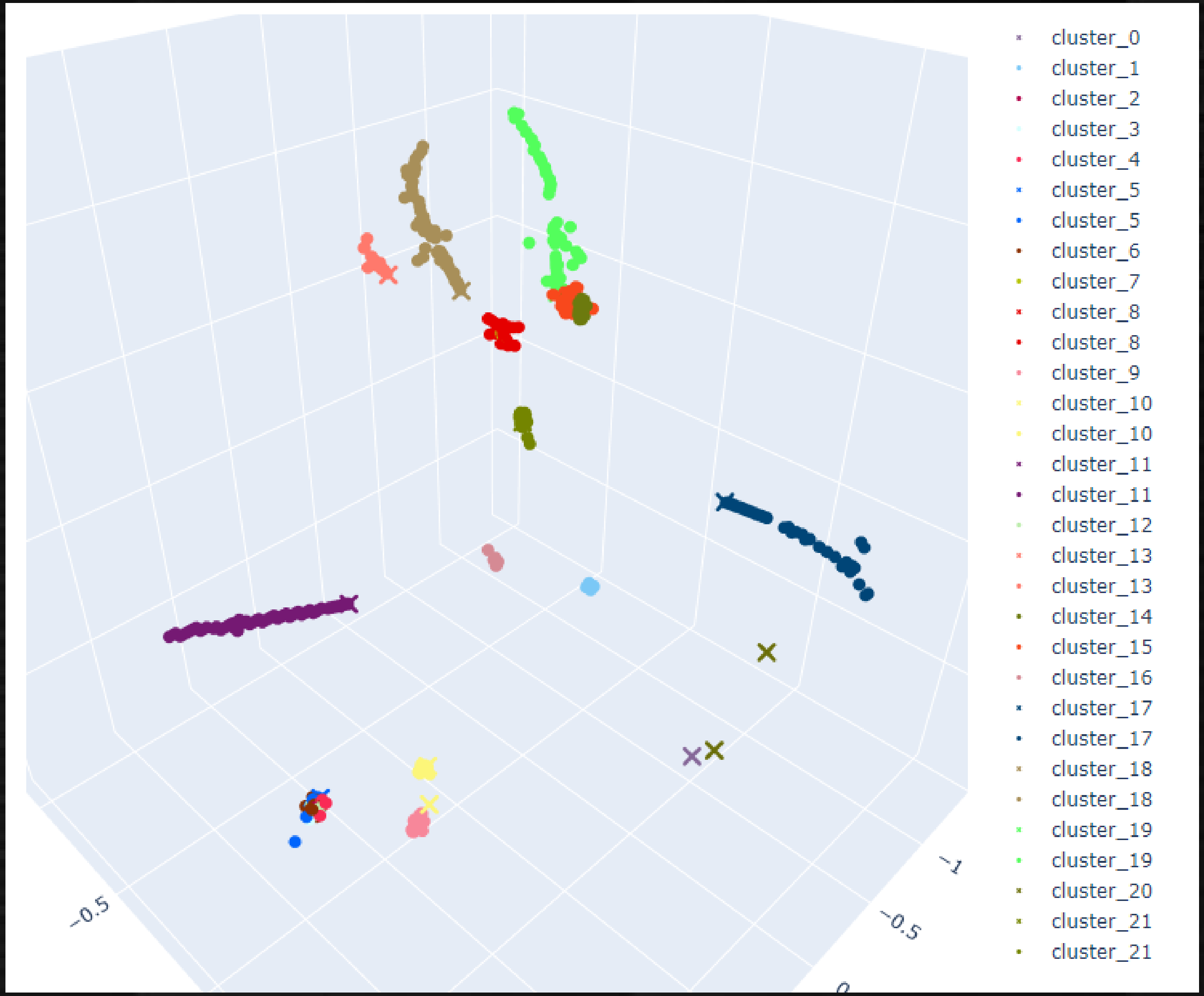


Real 3D coordinate

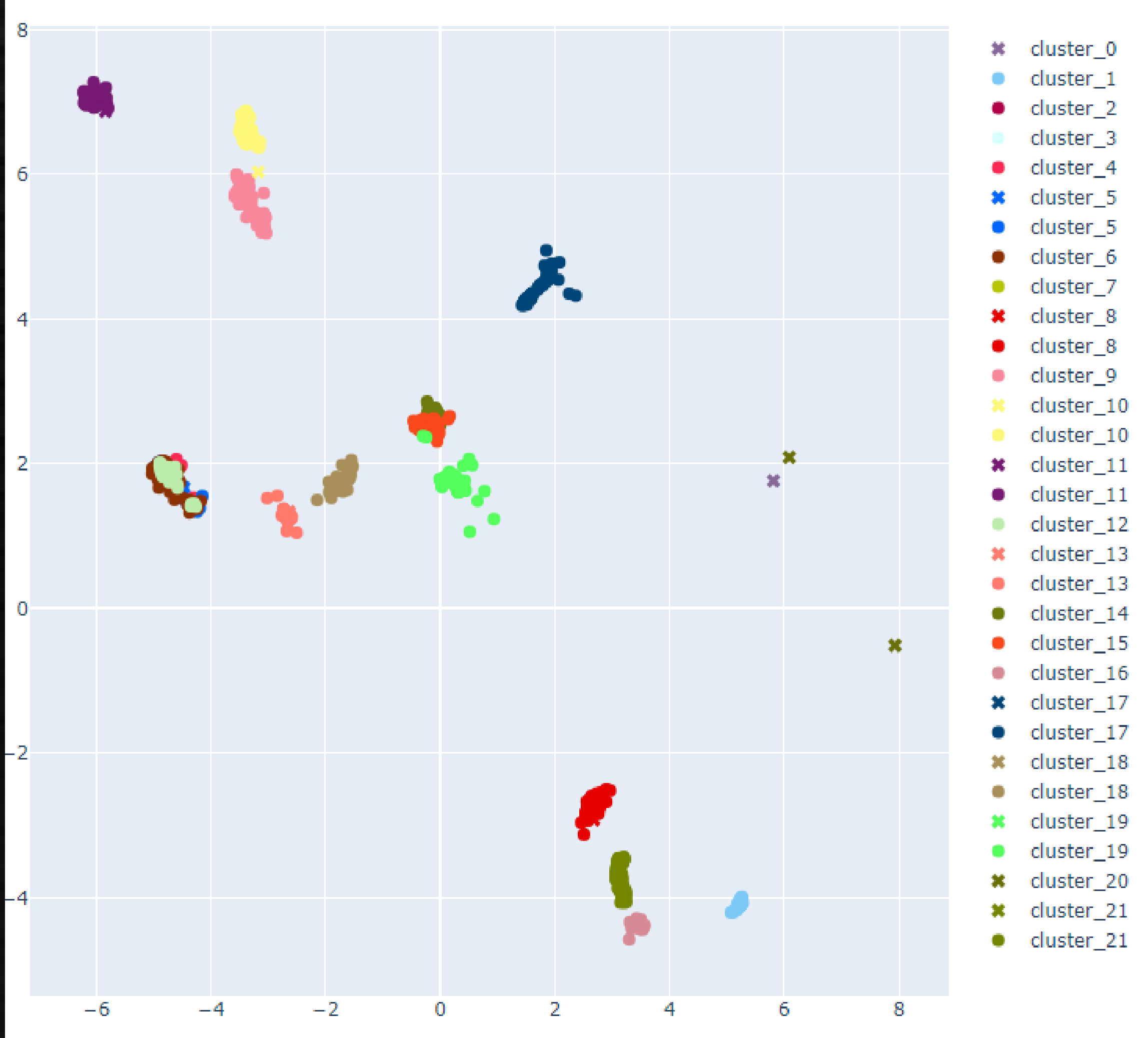


Output from GNN

Preliminary results – labeling need to improve?



Real 3D coordinate



Output from GNN

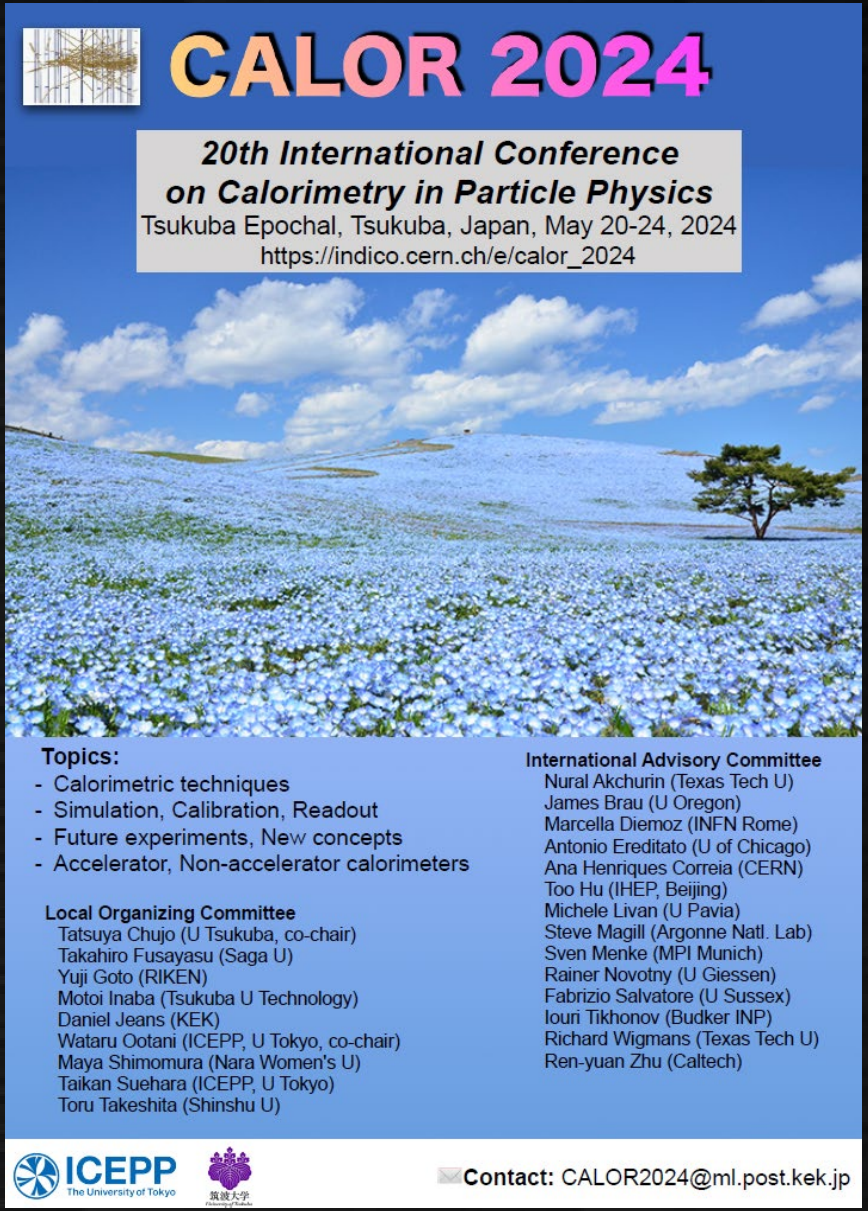
Things to do for PFA

- Labeling (MC cluster) is a non-trivial task
  - Tracks emit secondary particles often labeled as different
  - Need cluster corresponding to the track with reasonable matching of track momentum and cluster energy
- Quantitative comparison
  - With traditional PFA (e.g. PandoraPFA)
  - Jet energy resolution
  - Other measures?
- Regression of cluster energy?
- Detector effect to be studied
  - Especially effect of timing

Summary of all

- DNN-based PFA and flavor tagging are being investigated
- For flavor tagging:
  - ParT based flavor tagging gives ~10x better performance than LCFIPlus → need to replace
  - Optimization still being done, investigation of sample size needed
  - Incorporation to analysis framework desired
  - Fine-tuning is powerful: to investigate how to use it for analysis
- For PFA:
  - First implementation of track-cluster matching done, comparison with existing PFA to be done
  - Other methods (pre-clustering + transformer) can be investigated

Advertisements



CALOR 2024: https://indico.cern.ch/e/calor_2024
LCWS 2024: https://agenda.linearcollider.org/e/lcws2024

Summary / long-term plans

- New DNN-based particle flow algorithm is under development based on clustering at CMS HGCAL study
- Track-cluster matching is being implemented, statistical results will come soon
  - Energy regression with track momentum information will be the next step of implementation
- Medium/long term plans (or just hopes)
  - Can be extended to any analyses using cluster/jet information using the PFA as "a foundation model"
    - Such as Particle ID, Jet clustering, even physics analyses directly
  - "Differentiate" detector parameters/designs for optimization

Summary

- Particle Transformer seems very promising in quark flavour tagging.
- Its performance can be further improved by adjusting the input parameters.
- Bigger data set is required for better training outcomes.
- Fine-tuning is effective with the model, but only for similar data setups.
- It’s maybe time to start thinking of how to apply to physics analyses.
- Its application on other reconstruction algorithms should be explored.