

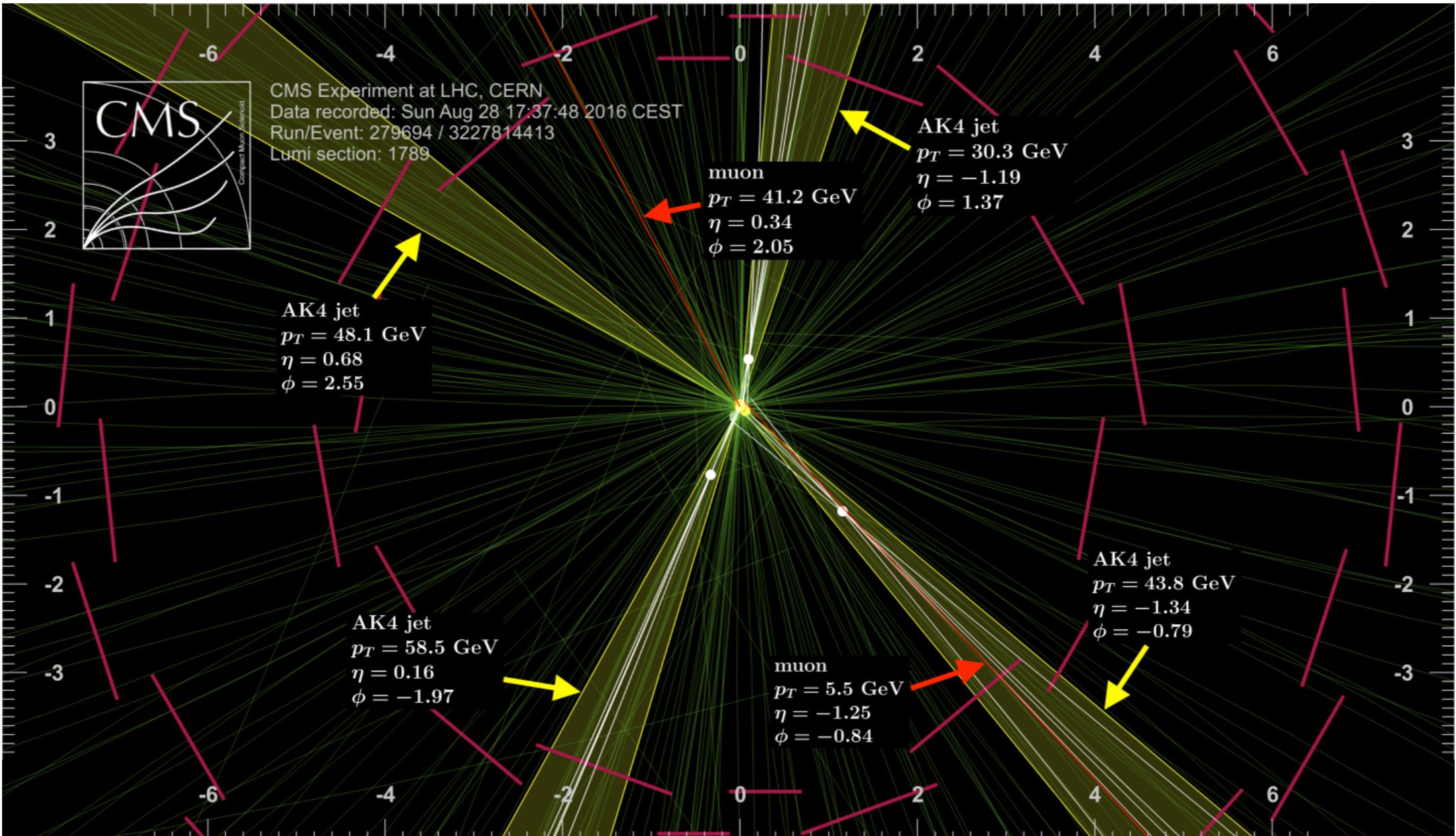
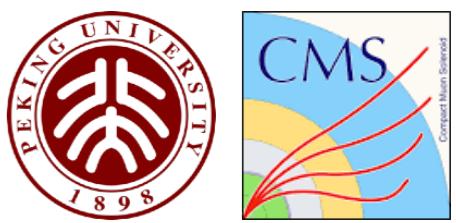
# *Transformer models for Heavy Flavor Jet Identification in CMS*



Alexandre De Moor, Congqiao Li, Denise Müller, Huilin Qu, **Sitian Qian**  
on behalf of CMS Collaboration

ML4Jets 2022 @ Rutgers University, 2022/11/01

# INTRODUCTION: JET TAGGING



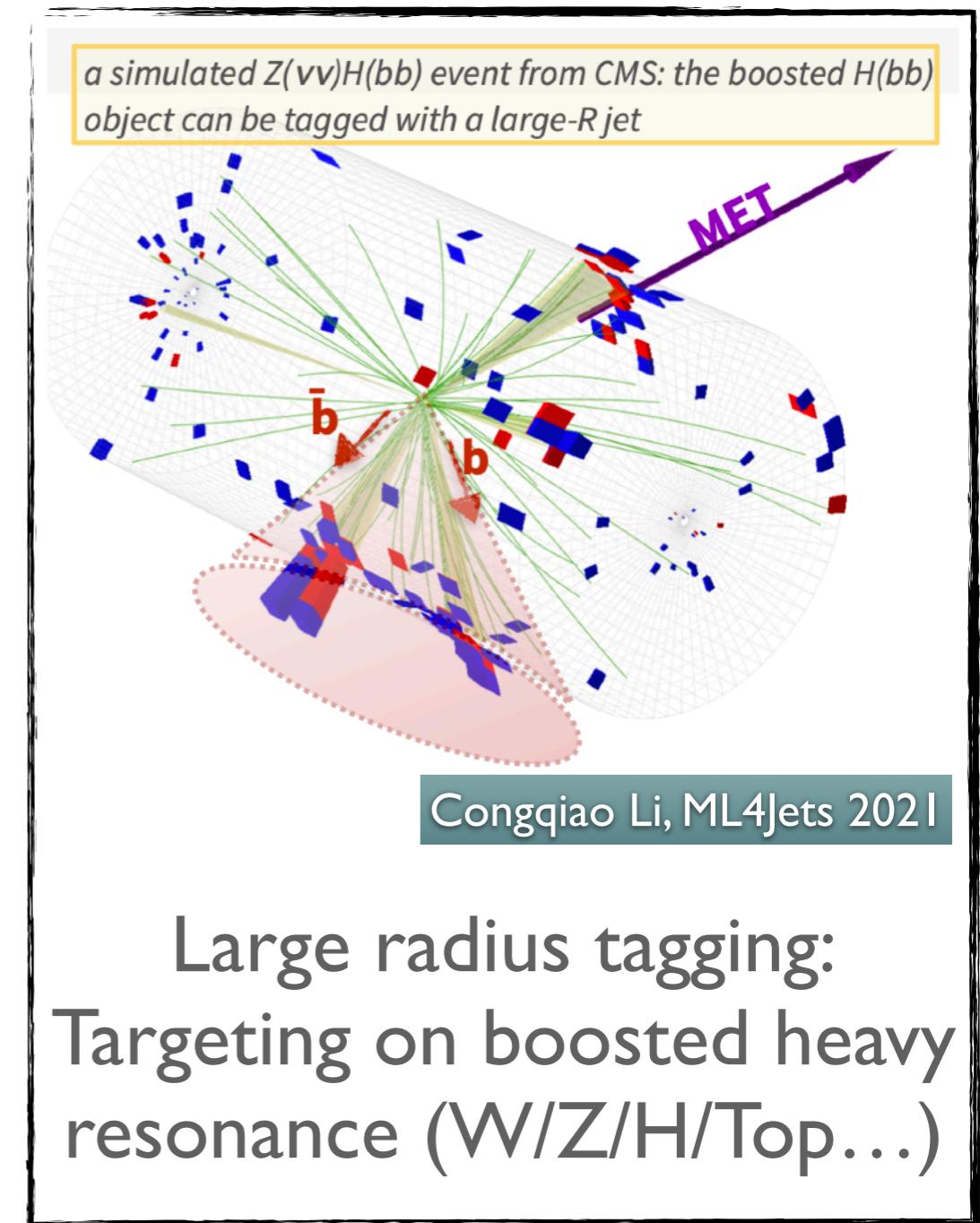
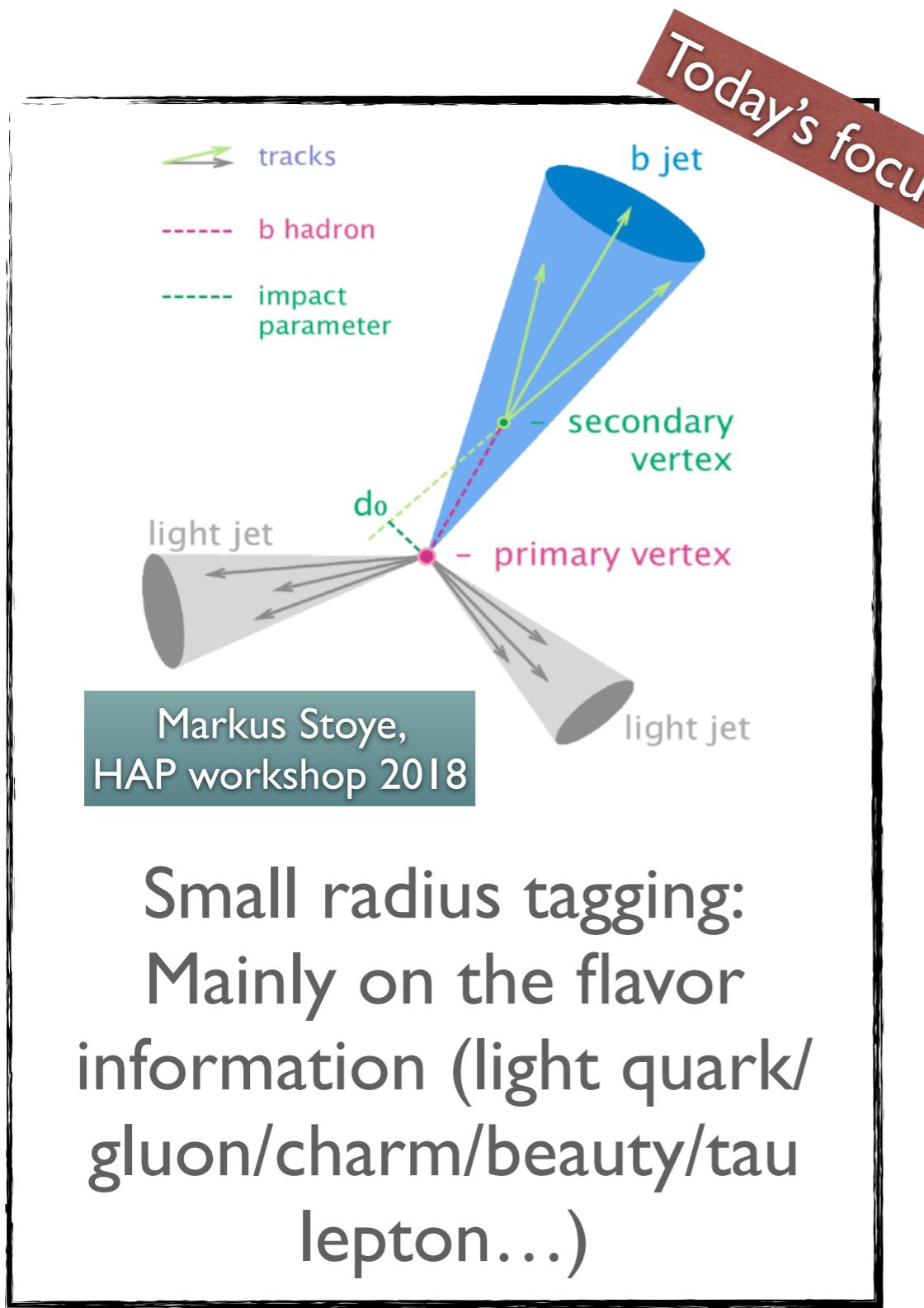
## Jet tagging:

Identifying the particle that initiates the jet with  
experimentally observed quantities

# INTRODUCTION: JET TAGGING



## Different types of jet tagging



# HEAVY FLAVOR TAGGING



- Problem setup of heavy flavor (HF) tagging:
  - Focus on small radius jet (in CMS: anti-kT with R=0.4)
  - Usually 3 cases:
    - Tagged as “b”
    - Tagged as “c”
    - Tagged as light flavor (“udsg”)
    - Can involve more categories including hadronic tau, “uds” vs “gluon” etc.
  - Key features of HF tagging:
    - Track displacement is of vital importance
      - Due to longer life of heavy flavor hadrons!

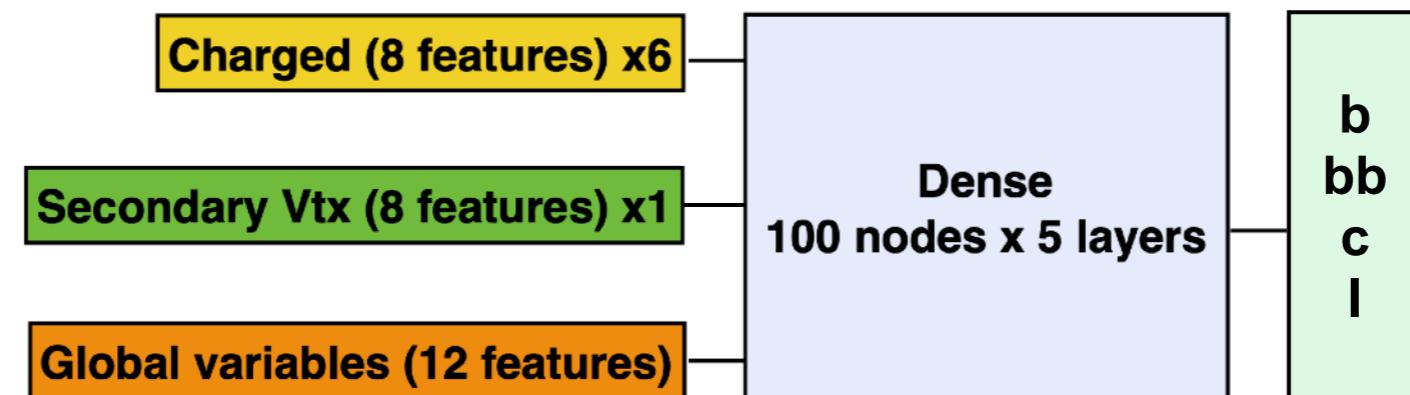
# HEAVY FLAVOR TAGGING @ CMS



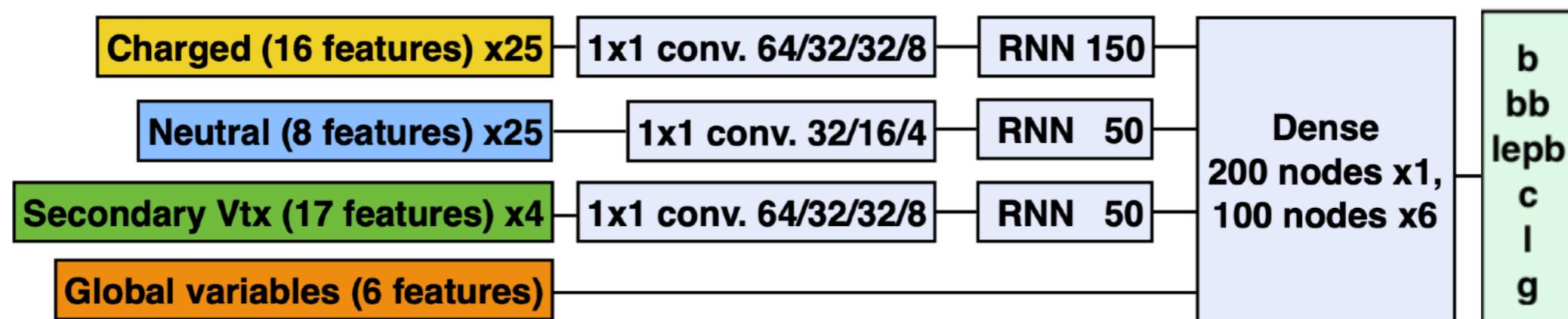
## Brief review of CMS HF tagging evolution:

- ~ 2016: **CSVv2(NN)** and cMVAv2(BDT)
  - CSVv2 is based on a very simple 1 layer NN
- 2017: deepCSV

ArXiv: 1712.07158  
CSVv2, cMVAv2 & deepCSV



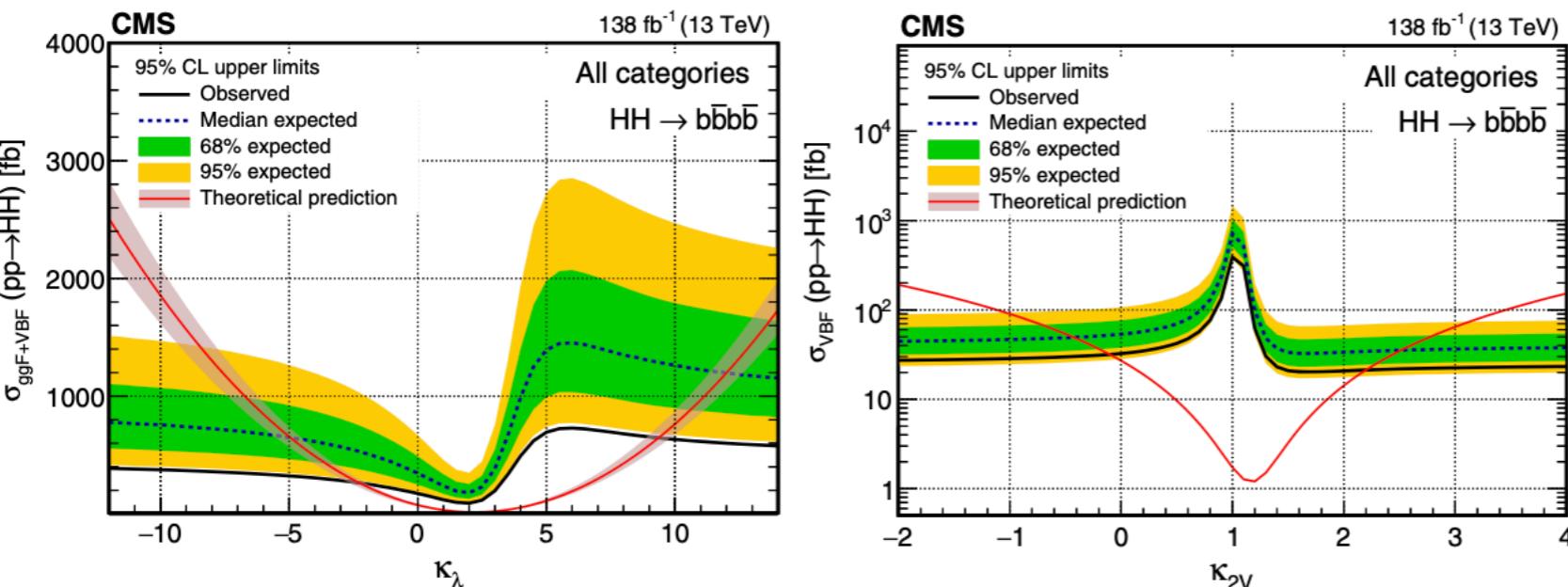
- Mid 2017: deepJet (deepFlavour) ArXiv: 2008.10519



# HEAVY FLAVOR TAGGING @ CMS



- Brief review of CMS HF tagging evolution:
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  - Mid 2017: deepJet (deepFlavour) ArXiv: 2008.10519
- Rich physical results have continuously come out with the help of CMS HF tagging algorithms!

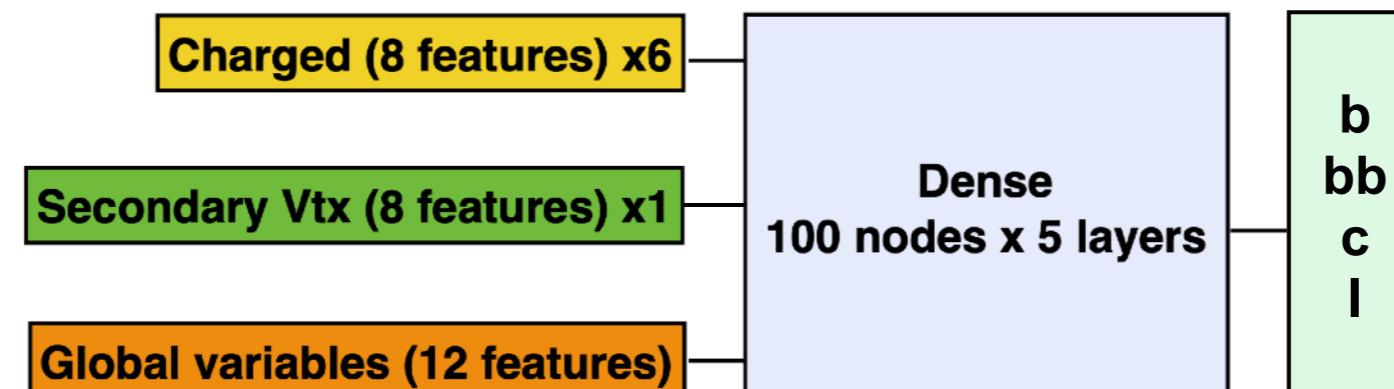
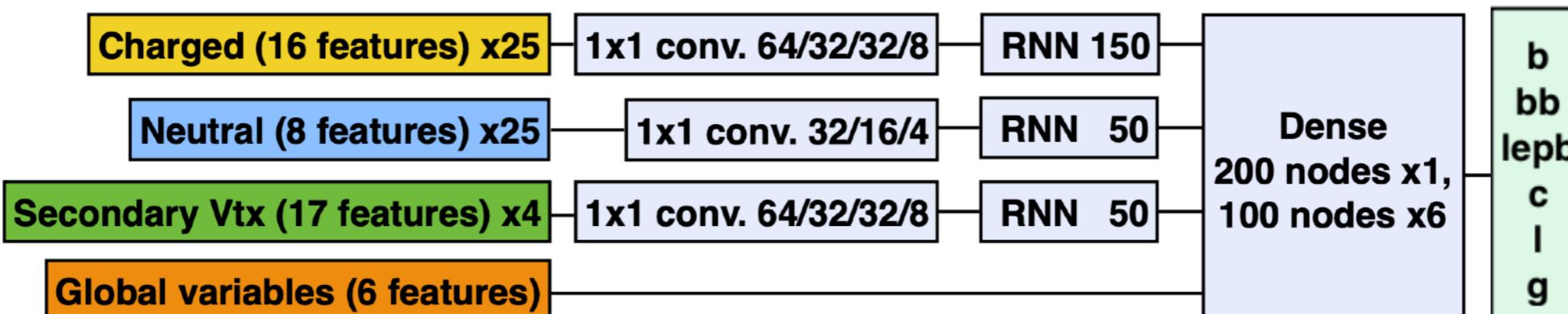


PhysRevLett.129.081802

Exciting result from  
CMS Full Run2  
nonresonant HH4b  
measurement, b  
tagging is based on  
DeepJet algorithm

# HEAVY FLAVOR TAGGING @ CMS

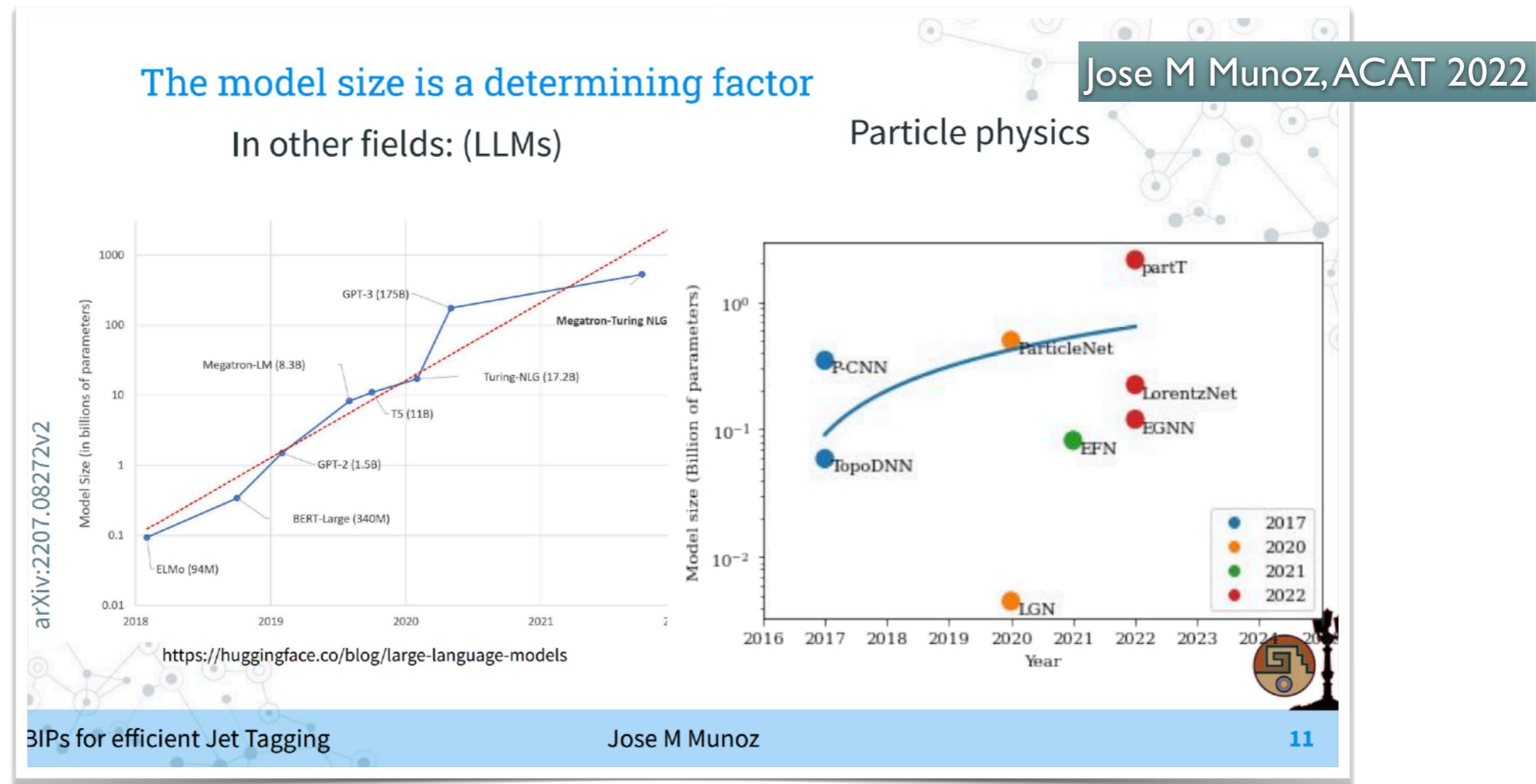


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  - 
  - 
- What about Run3?

# EVOLUTION OF JET TAGGING ALGO.

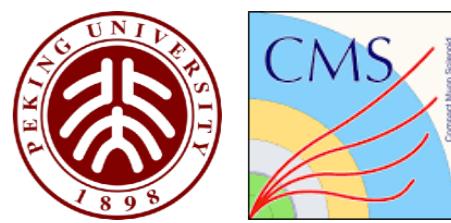


- Observation from CMS HF tagging evolution:
  - Models become larger and larger
  - CMS HF tagging is not alone!



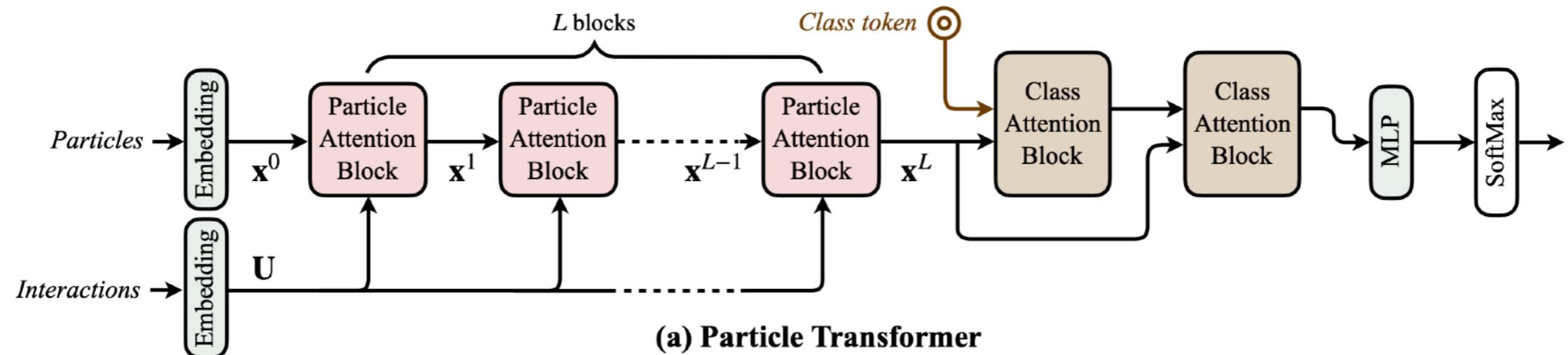
- Larger model is now a trend in not only ML community, but also in HEP! -> Motivates the usage of largest model :)  
-> Particle Transformer (ParT)

# PART 101



- Particle Transformer:  
■ the transformer designed for particle physics

ArXiv: 2202.03772



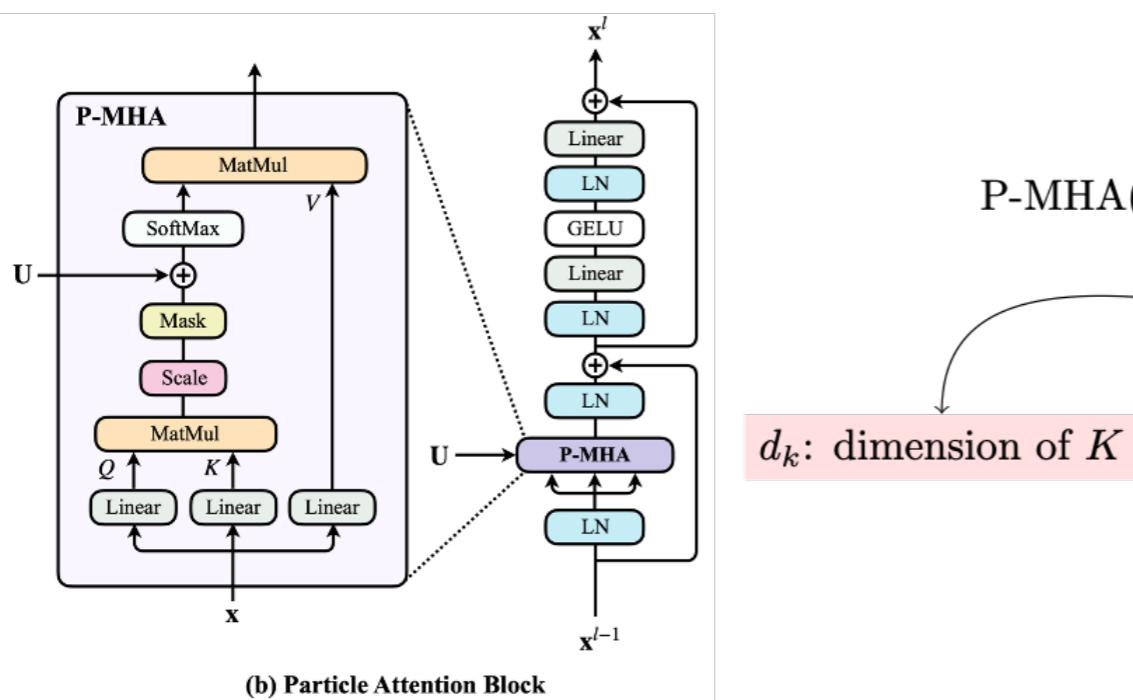
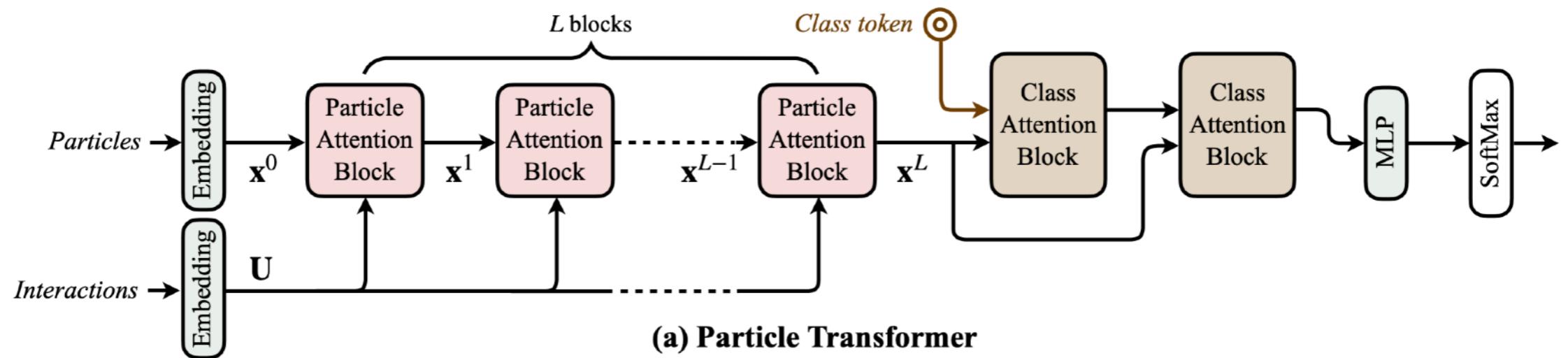
- Input embedding: Not only inject single particle information, but also include pair-wise features
- Particle Attention Block: Multi-Head Attention (MHA)
  - Pair-wise feature are introduced as the attention mask (P-MHA)
- Class Attention Block: Multi-Head Attention
  - Class token is used for the MHA calculation

# PART 101



- Particle Transformer:
  - the transformer designed for particle physics

[ArXiv: 2202.03772](https://arxiv.org/abs/2202.03772)



$$\text{P-MHA}(Q, K, V) = \text{SoftMax}(QK^T / \sqrt{d_k}) + \mathbf{U}V$$

$d_k$ : dimension of  $K$

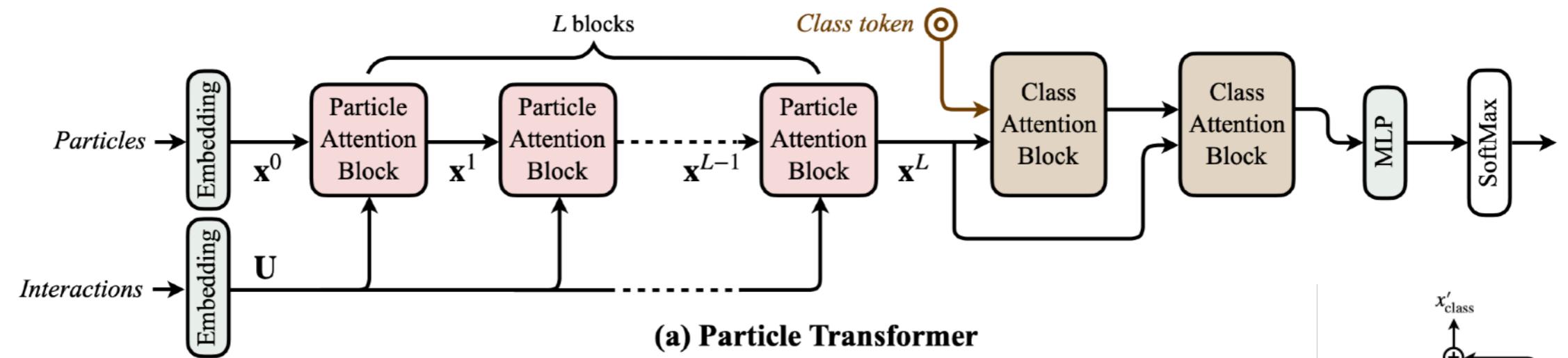
Choice of the pair-wise features: from [LundNet](#)

$$\begin{aligned}\Delta &= \sqrt{(y_a - y_b)^2 + (\phi_a - \phi_b)^2} \\ k_T &= \min(p_{T,a}, p_{T,b}) \cdot \Delta \\ z &= \min(p_{T,a}, p_{T,b}) / (p_{T,a} + p_{T,b}) \\ m^2 &= (E_a + E_b)^2 - \|\mathbf{p}_a + \mathbf{p}_b\|^2\end{aligned}$$

# PART 101



- Particle Transformer:
  - the transformer designed for particle physics



$$\text{MHA}_C(Q_C, K_C, V_C) = \text{SoftMax}(Q_C K_C^T / \sqrt{d_{kC}}) V_C$$

$$Q_C = W_{qC}x_{\text{class}} + b_{qC}$$

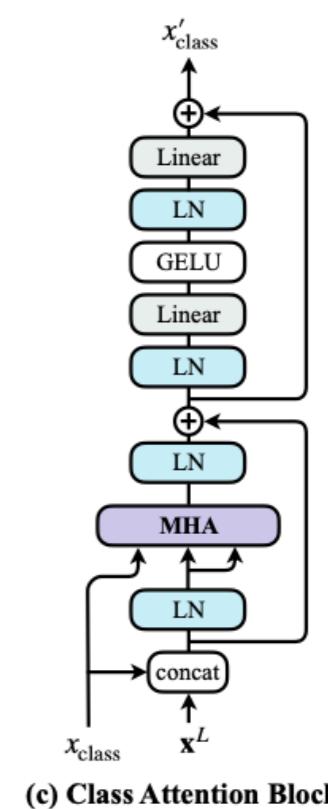
$$K_C = W_{kC}\mathbf{z} + b_{kC}$$

$$V_C = W_{vC}\mathbf{z} + b_{vC}$$

$$d_{kC}: \text{dimension of } K_C$$

$$\mathbf{z} = [x_{\text{class}}, \mathbf{x}^L]$$

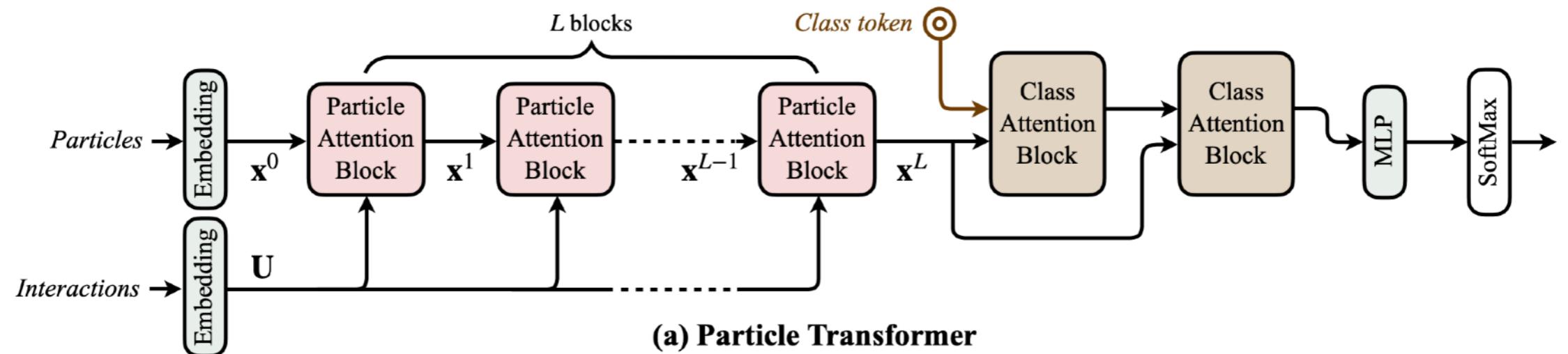
Concatenate class information and particle embedding



# PART @ CMS FOR HF TAGGING



- The debut of ParT in CMS: Run3 HF tagging [ArXiv: 2202.03772](#)



- ParT Architect for CMS HF tagging:
  - 3 Particle Attention Blocks + 1 Class Attention Block
  - GELU as activation for attention blocks, ReLU as attention for initial embedding + final MLP
  - Number of “Heads” in MHA: 8
  - Number of feature: 128 (for  $\mathbf{x}^l$ s)
    - For initial embedding the MLPs are (128-512-128) and (64-64-64-8) for *Particles* and *Interactions* respectively.

# PART @ CMS FOR HF TAGGING



- ParT @ CMS:
  - The input features are almost identical with DeepJet inputs
    - (+): 4 momenta of the constituents; (-): global features.
  - FLOPs: ~117M, #Params: ~1.4M
    - Inference time is similar with ParticleNet's
- Training details:
  - Dataset: ~65M jet from  $t\bar{t}$  and QCD multi-jets
  - Ranger optimizer
  - LR initially set to 1e-3 and will decay linearly after 70% of training to reach 1e-5 in the end
  - Batch size: 512
  - Loss function: cross entropy
  - Model with best loss performance on validation set will be kept

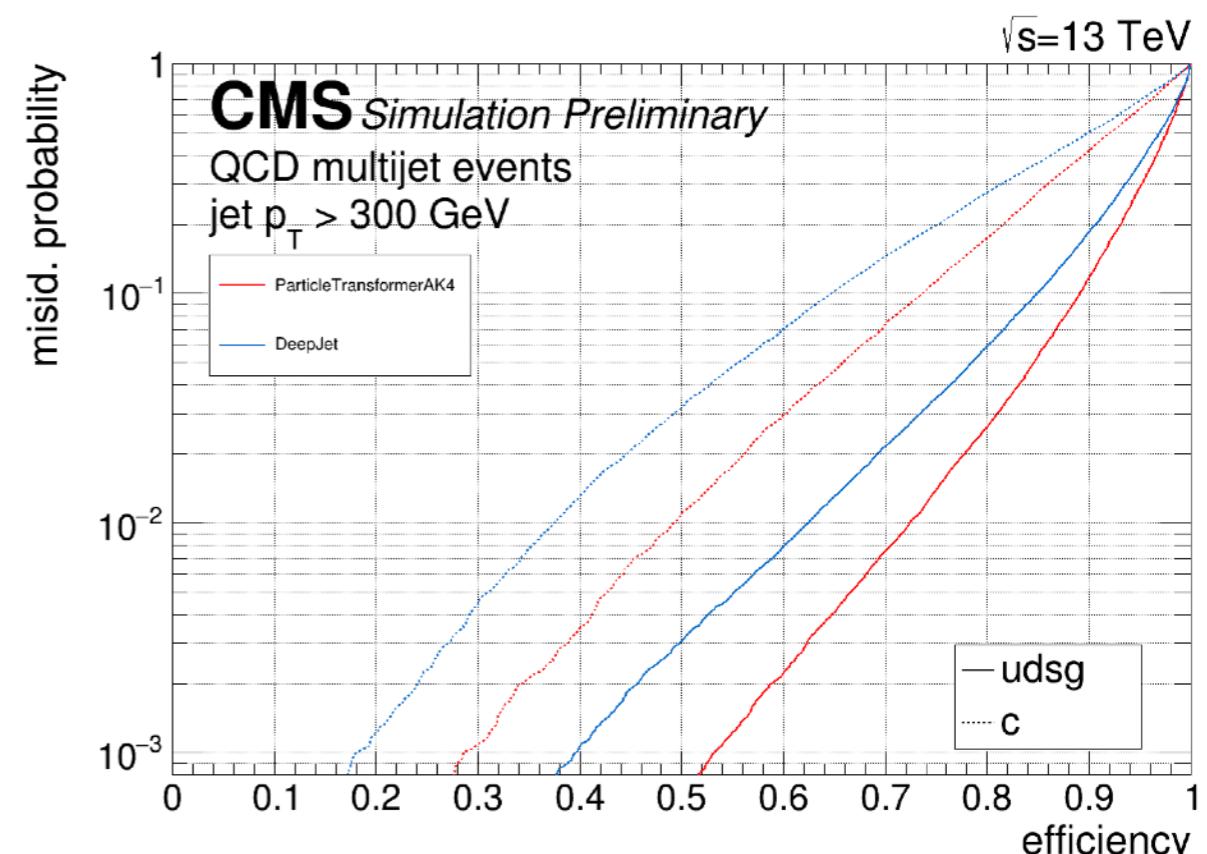
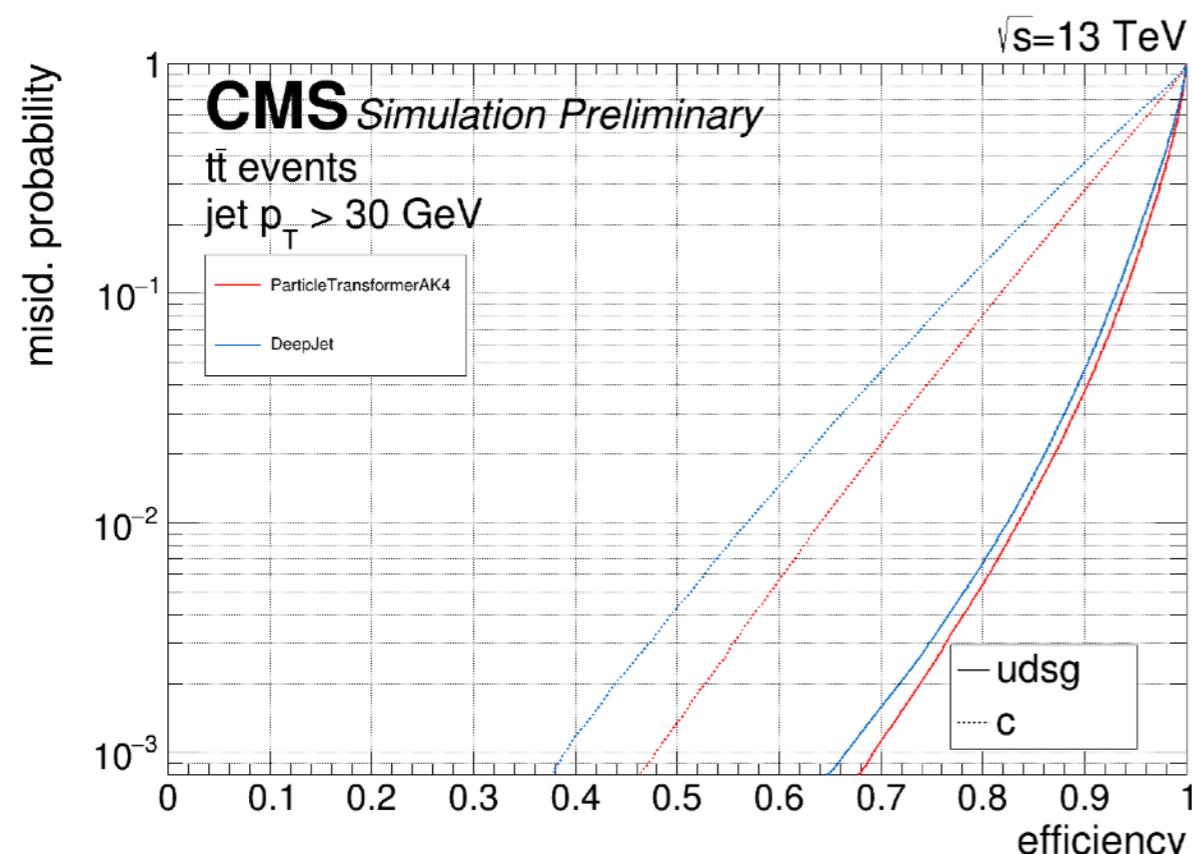
# PART @ CMS FOR HF TAGGING



## ■ Performance: b tagging

DP-2022/050

Left:  $t\bar{t}$  events, Right: QCD multijets



Performance on b tagging of ParT @ CMS:  
Solid(dashed) ROC curves indicate the mistagging rates for  
“udsg”(“c”) jet at given b tagging signal efficiency

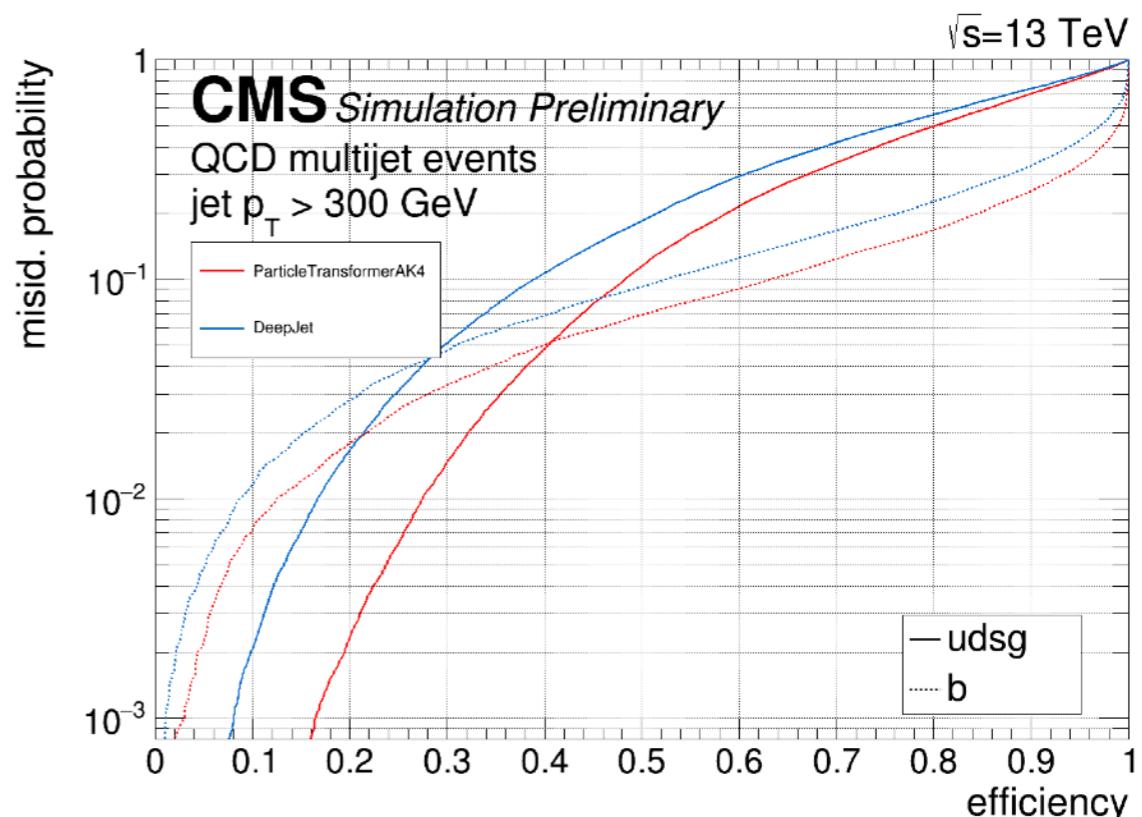
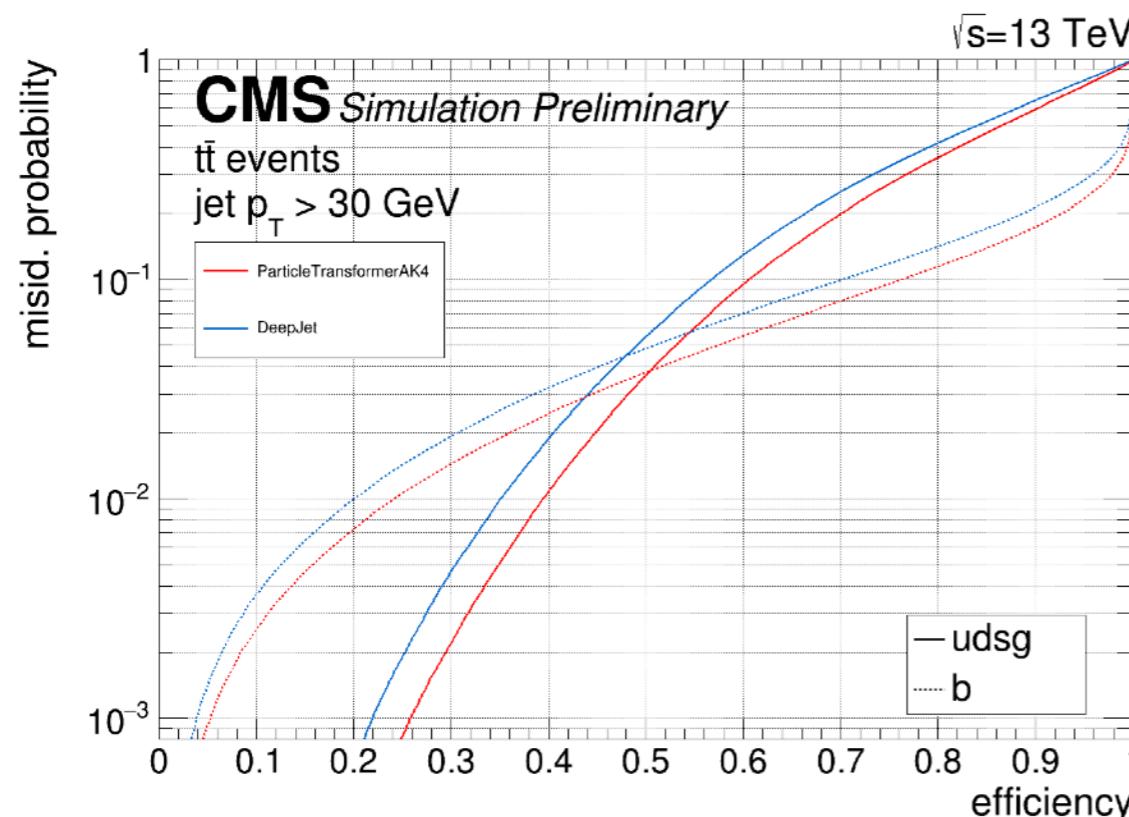
# PART @ CMS FOR HF TAGGING



## ■ Performance: c tagging

DP-2022/050

Left:  $t\bar{t}$  events, Right: QCD multijets



Performance on c tagging of ParT @ CMS:  
Solid(dashed) ROC curves indicate the mistagging rates for  
“udsg”(“b”) jet at given c tagging signal efficiency

# PART @ CMS FOR HF TAGGING



- Summary:
  - Jet tagging is an important yet challenging task in HEP, among which flavor tagging is of vital importance
  - CMS has kept investigating HF tagging with more and more advanced models
  - For Run3, Particle Transformer (ParT) is considered as the official HF tagging algorithm
  - Significant improvement on HF tagging performance is observed from the comparison between ParT and previous CMS State-Of-The-Art model: DeepJet

# BACK UP

# PART vs PARTICLENET ON AK8 JET



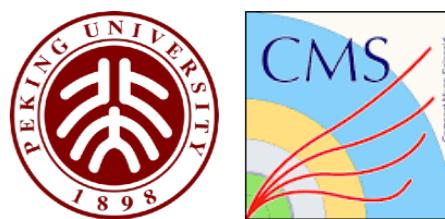
**Table 4.** Number of trainable parameters and FLOPs.

	Accuracy	# params	FLOPs
PFN	0.772	86.1 k	4.62 M
P-CNN	0.809	354 k	15.5 M
ParticleNet	0.844	370 k	540 M
<b>ParT</b>	<b>0.861</b>	2.14 M	340 M
ParT (plain)	0.849	2.13 M	260 M

**Table 1.** Jet tagging performance on the JETCLASS dataset. ParT is compared to PFN (Komiske et al., 2019b), P-CNN (CMS Collaboration, 2020b) and the state-of-the-art ParticleNet (Qu & Gouskos, 2020). For all the metrics, a higher value indicates better performance. The ParT architecture using plain MHAs instead of P-MHAs, labelled as ParT (plain), is also shown for comparison.

	All classes		$H \rightarrow b\bar{b}$	$H \rightarrow c\bar{c}$	$H \rightarrow gg$	$H \rightarrow 4q$	$H \rightarrow \ell\nu qq'$	$t \rightarrow bqq'$	$t \rightarrow b\ell\nu$	$W \rightarrow qq'$	$Z \rightarrow q\bar{q}$
	Accuracy	AUC	Rej <sub>50%</sub>	Rej <sub>50%</sub>	Rej <sub>50%</sub>	Rej <sub>50%</sub>	Rej <sub>99%</sub>	Rej <sub>50%</sub>	Rej <sub>99.5%</sub>	Rej <sub>50%</sub>	Rej <sub>50%</sub>
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
<b>ParT</b>	<b>0.861</b>	<b>0.9877</b>	<b>10638</b>	<b>4149</b>	<b>123</b>	<b>1864</b>	<b>5479</b>	<b>32787</b>	<b>15873</b>	<b>543</b>	<b>402</b>
ParT (plain)	0.849	0.9859	9569	2911	112	1185	3868	17699	12987	384	311

# PART VS PARTICLENET ON AK8 JET



**Table 3.** Impacts of the training dataset size. Entries in bold correspond to the training using the full 100 M training dataset.

	All classes		$H \rightarrow b\bar{b}$	$H \rightarrow c\bar{c}$	$H \rightarrow gg$	$H \rightarrow 4q$	$H \rightarrow \ell\nu qq'$	$t \rightarrow bqq'$	$t \rightarrow b\ell\nu$	$W \rightarrow qq'$	$Z \rightarrow q\bar{q}$
	Accuracy	AUC	Rej <sub>50%</sub>	Rej <sub>50%</sub>	Rej <sub>50%</sub>	Rej <sub>50%</sub>	Rej <sub>99%</sub>	Rej <sub>50%</sub>	Rej <sub>99.5%</sub>	Rej <sub>50%</sub>	Rej <sub>50%</sub>
ParticleNet (2 M)	0.828	0.9820	5540	1681	90	662	1654	4049	4673	260	215
ParticleNet (10 M)	0.837	0.9837	5848	2070	96	770	2350	5495	6803	307	253
<b>ParticleNet (100 M)</b>	<b>0.844</b>	<b>0.9849</b>	<b>7634</b>	<b>2475</b>	<b>104</b>	<b>954</b>	<b>3339</b>	<b>10526</b>	<b>11173</b>	<b>347</b>	<b>283</b>
ParT (2 M)	0.836	0.9834	5587	1982	93	761	1609	6061	4474	307	236
ParT (10 M)	0.850	0.9860	8734	3040	110	1274	3257	12579	8969	431	324
<b>ParT (100 M)</b>	<b>0.861</b>	<b>0.9877</b>	<b>10638</b>	<b>4149</b>	<b>123</b>	<b>1864</b>	<b>5479</b>	<b>32787</b>	<b>15873</b>	<b>543</b>	<b>402</b>

**Table 6.** Comparison between ParT and existing models on the quark-gluon tagging dataset. ParT refers to the model trained from scratch on this dataset. ParticleNet-f.t. and ParT-f.t. denote the corresponding models pre-trained on JETCLASS and fine-tuned on this dataset. Results for other models are quoted from their published results: P-CNN and ParticleNet (Qu & Gouskos, 2020), PFN (Komiske et al., 2019b), ABCNet (Mikuni & Canelli, 2020), PCT (Mikuni & Canelli, 2021), rPCN (Shimmin, 2021), and LorentzNet (Gong et al., 2022). The subscript “exp” and “full” distinguish models using partial or full particle identification information.

	Accuracy	AUC	Rej <sub>50%</sub>	Rej <sub>30%</sub>
P-CNN <sub>exp</sub>	0.827	0.9002	34.7	91.0
PFN <sub>exp</sub>	—	0.9005	34.7 ± 0.4	—
ParticleNet <sub>exp</sub>	0.840	0.9116	39.8 ± 0.2	98.6 ± 1.3
rPCN <sub>exp</sub>	—	0.9081	38.6 ± 0.5	—
ParT <sub>exp</sub>	0.840	0.9121	41.3 ± 0.3	101.2 ± 1.1
ParticleNet-f.t. <sub>exp</sub>	0.839	0.9115	40.1 ± 0.2	100.3 ± 1.0
<b>ParT-f.t.<sub>exp</sub></b>	<b>0.843</b>	<b>0.9151</b>	<b>42.4 ± 0.2</b>	<b>107.9 ± 0.5</b>
PFN <sub>full</sub>	—	0.9052	37.4 ± 0.7	—
ABCNet <sub>full</sub>	0.840	0.9126	42.6 ± 0.4	118.4 ± 1.5
PCT <sub>full</sub>	0.841	0.9140	43.2 ± 0.7	118.0 ± 2.2
LorentzNet <sub>full</sub>	0.844	0.9156	42.4 ± 0.4	110.2 ± 1.3
ParT <sub>full</sub>	0.849	0.9203	47.9 ± 0.5	129.5 ± 0.9
<b>ParT-f.t.<sub>full</sub></b>	<b>0.852</b>	<b>0.9230</b>	<b>50.6 ± 0.2</b>	<b>138.7 ± 1.3</b>

**Table 5.** Comparison between ParT and existing models on the top quark tagging dataset. ParT refers to the model trained from scratch on this dataset. ParticleNet-f.t. and ParT-f.t. denote the corresponding models pre-trained on JETCLASS and fine-tuned on this dataset. Results for other models are quoted from their published results: P-CNN and ParticleNet (Qu & Gouskos, 2020), PFN (Komiske et al., 2019b), JEDI-net (Moreno et al., 2020), PCT (Mikuni & Canelli, 2021), LGN (Bogatskiy et al., 2020), rPCN (Shimmin, 2021), and LorentzNet (Gong et al., 2022).

	Accuracy	AUC	Rej <sub>50%</sub>	Rej <sub>30%</sub>
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
<b>ParT-f.t.</b>	<b>0.944</b>	<b>0.9877</b>	<b>691 ± 15</b>	<b>2766 ± 130</b>