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REFINING FAST SIMULATION USING MACHINE LEARNING

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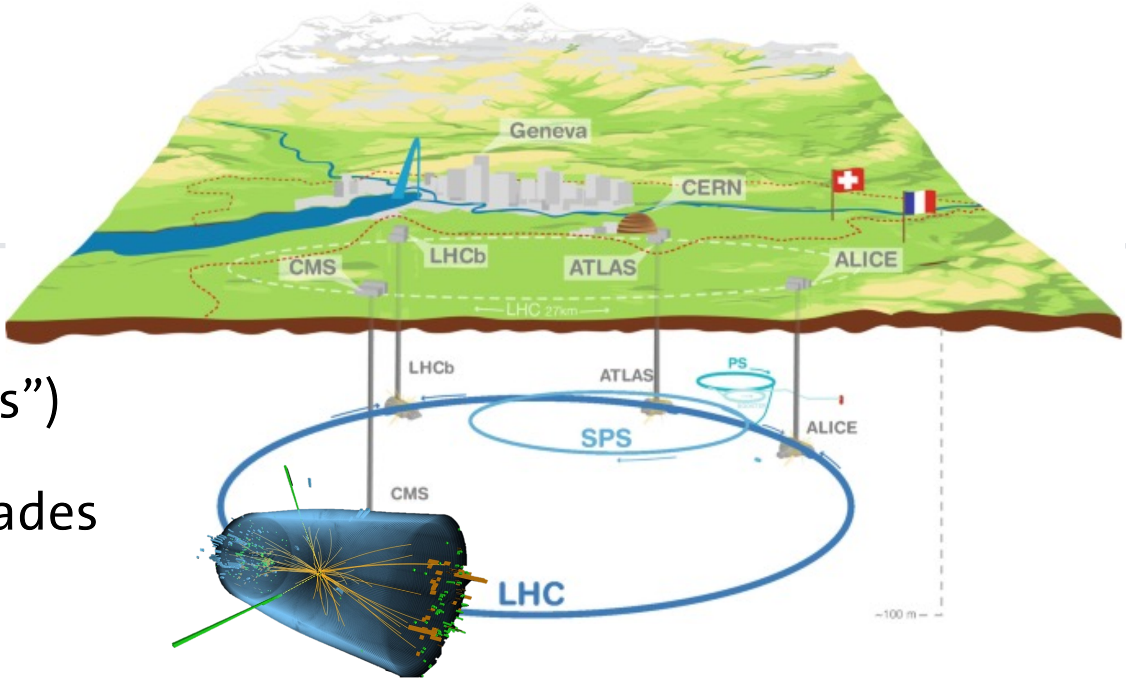
[1]UNIVERSITÄT HAMBURG, [2]FERMI NATIONAL ACCELERATOR LABORATORY

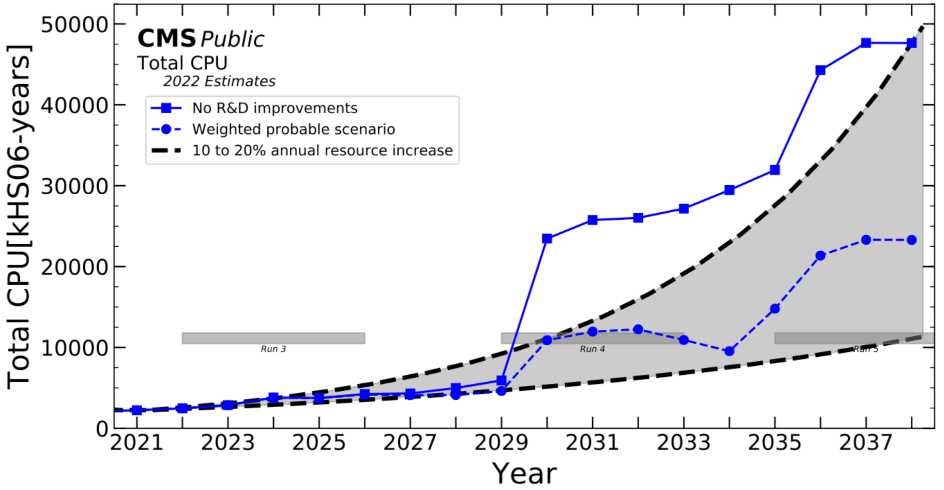
INTRODUCTION



- Most high energy physics analyses rely on a large number of **simulated** proton-proton collisions (= "events")
- Higher **LHC luminosity** (= more events) & detector upgrades (= more complex data) → **fast simulation** techniques and R&D needed to stay within **computing budget**
- In **CMS**, two simulation chains (FullSim/FastSim) are used that produce output of same dimensionality/structure

	GEN → Event generation	**SIM** → Detector simulation	**DIGI** → Digitization	**RECO** Reconstruction
FullSim	same e.g., MadGraph	GEANT4	same	analyze as if data
FastSim ≈ 15% of sim. events		parametrized energy loss x100 faster		use GEN info x2.5 faster

➢ FullSim: ≈ 100 s/event, FastSim: ≈ 10 s/event



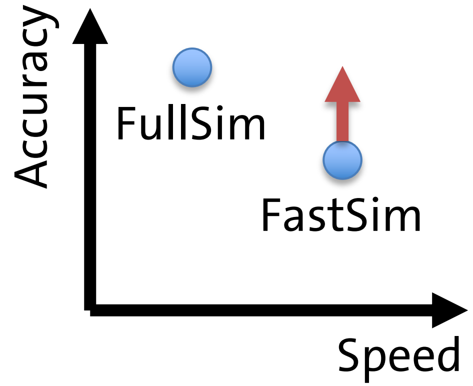
twiki.cern.ch/twiki/bin/view/CMSPublic/CMSOfflineComputingResults

GEN →	SIM →	DIGI →	RECO →	AOD →	NanoAOD
Event generation	Detector simulation	Digitization	Reconstruction	“Analysis Object Data”	further processed analysis format

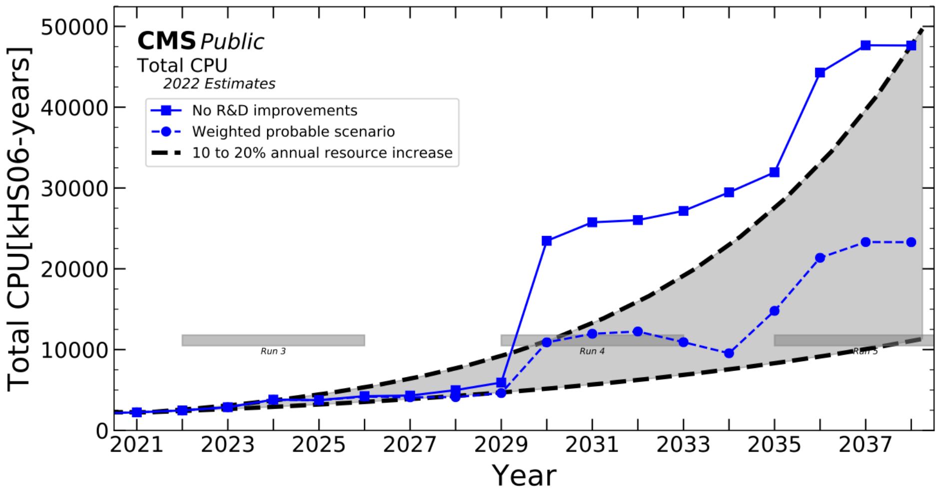
INTRODUCTION

- FastSim advantage in speed comes at the price of **decreased accuracy** in some of the final analysis observables

➢ **Aim**: increase FastSim accuracy to promote its wider usage



- Possible FastSim **tuning** approaches:
  - Internal tuning of functions/parameters (within **SIM/RECO**)
    e.g., denoising showers using ML github.com/cms-denoising/SimDenoising
  - Post-hoc tuning (after **NanoAOD**)
    - **Reweighting** = defining weights for individual events/jets/…
      e.g., DCTR introduced in arXiv:1907.08209
    - **Refining** = changing (high-level) observables
      e.g., Wasserstein-GAN for air showers in arXiv:1802.03325



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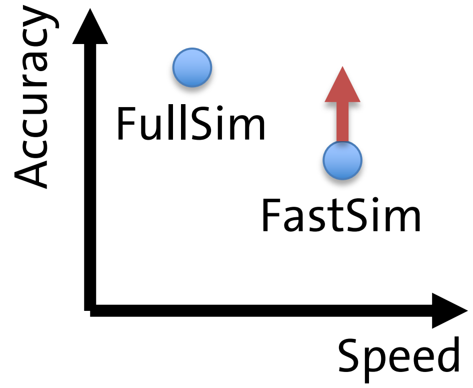

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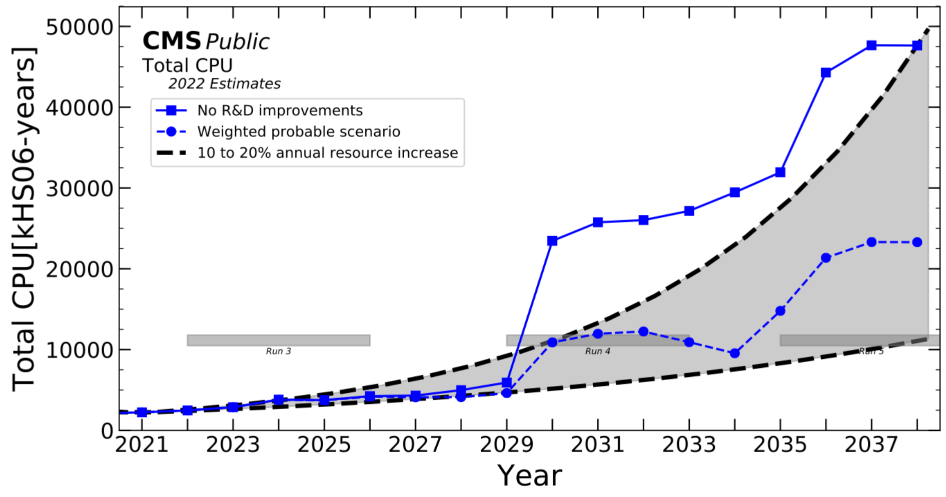

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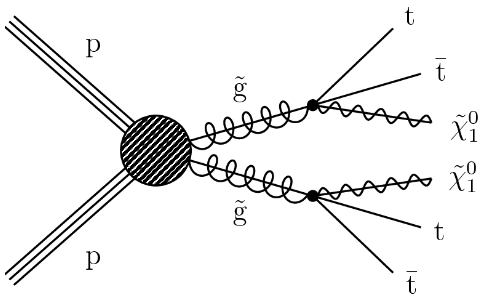
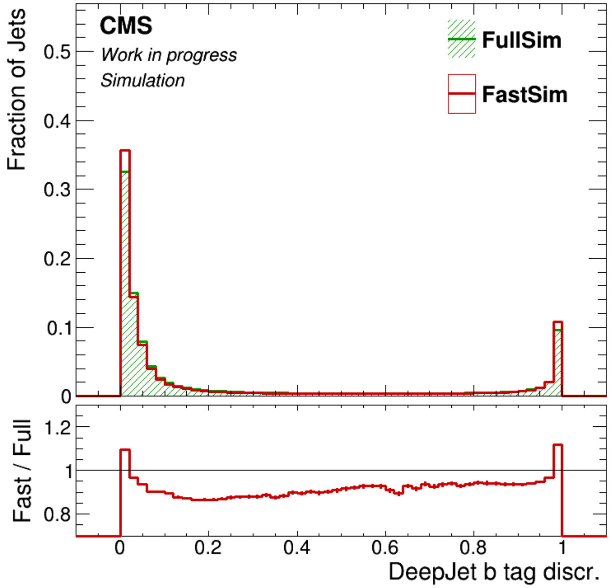
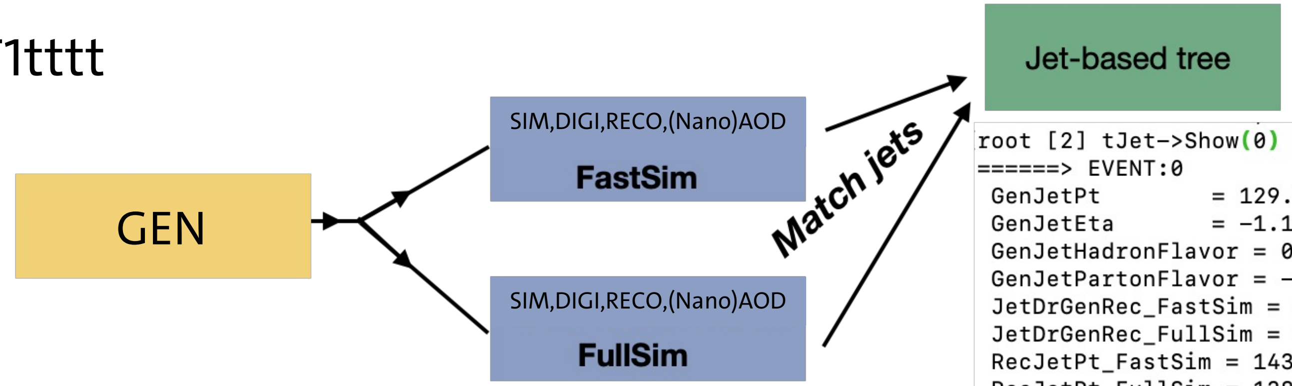
INTRODUCTION

- Focus on refinement of **jet observables** e.g.,
  - Magnitude and direction of momentum:
    $(p_x, p_y, p_z) \rightarrow (p_T, \eta, \varphi)$
  - Jet (sub)structure e.g.,
    - Flavour tagging, here: **DeepJet** algorithm (DNN, arXiv:2008.10519)
    - ➢ 4 output nodes: b, c, uds, g (softmax activated)
    - ➢ 4 discriminators in NanoAOD: b, c vs. b, c vs. uds+g („CvL“), uds vs. g („QG“)





- **Training sample**: SUSY simplified model T1tttt simulated with FastSim and FullSim (same GEN events, 0 PU)
  - ➢ Match jets using ΔR angular criterion
  - ➢ Jet **triplets**: (GEN, FastSim, FullSim)




```
root [2] tJet->Show(0)
======> EVENT:0
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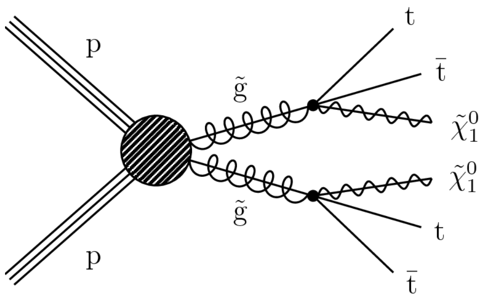

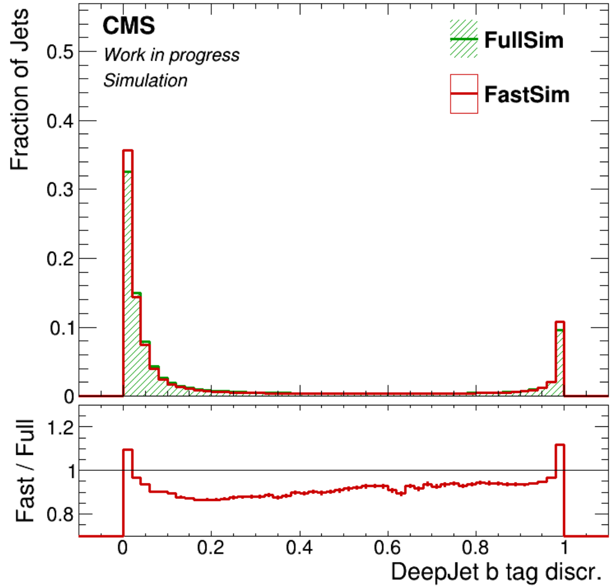

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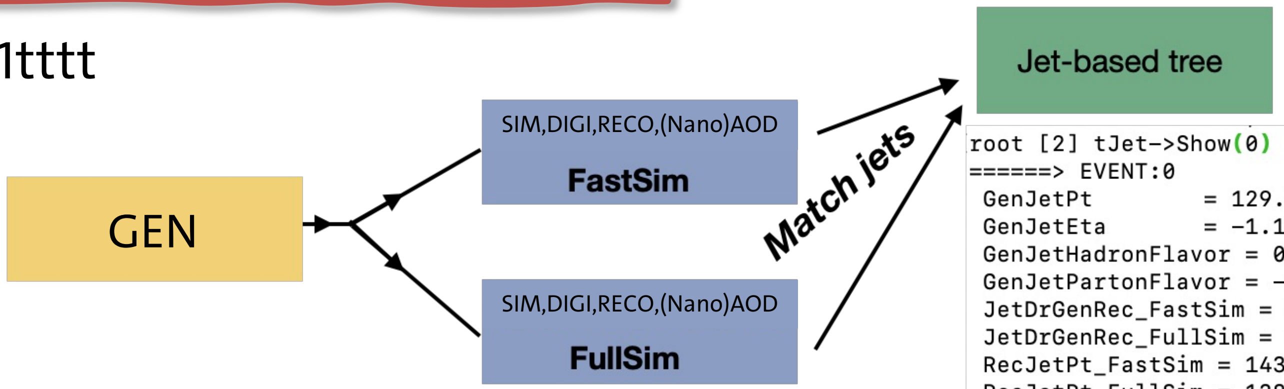


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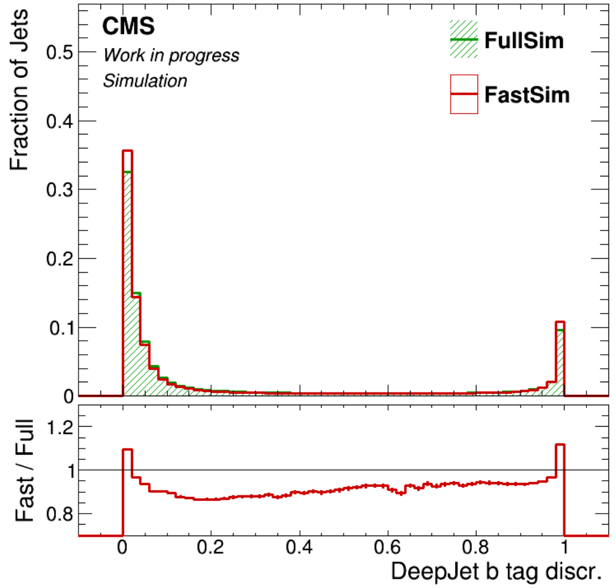
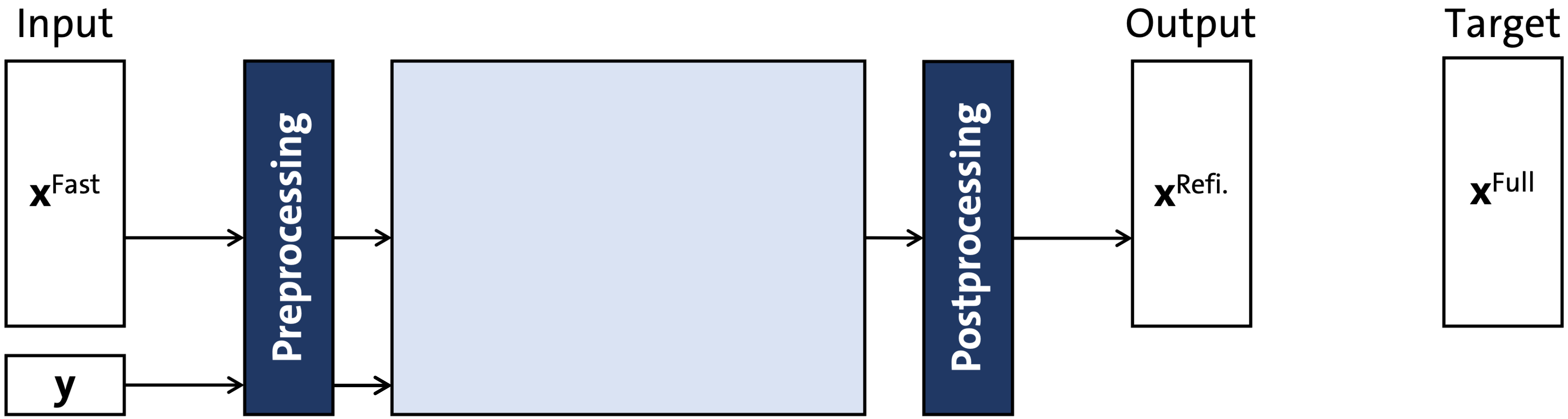
REFINING (REGRESSION) – GENERAL IDEA



Employ **regression neural network** to refine FastSim:

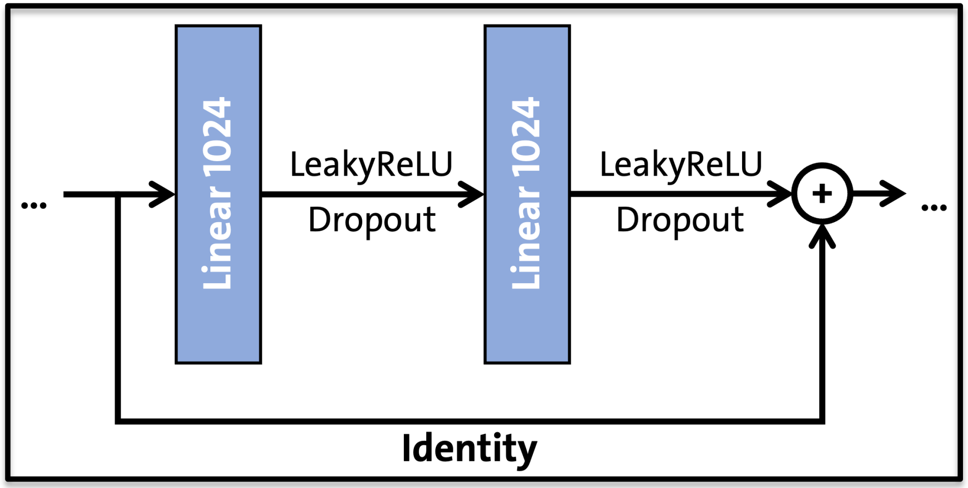
- Input: **FastSim** variables $\mathbf{x}^{\mathrm{Fast}}$ = 4 DeepJet discriminators

  Parameters $\mathbf{y}$ = p_T^{GEN}, η^{GEN}, true hadron flavor (b, c, or light quark/gluon)
- Output: **Refined** variables $\mathbf{x}^{\mathrm{Refined}}$ = 4 DeepJet discriminators
- Target: **FullSim** variables $\mathbf{x}^{\mathrm{Full}}$ = 4 DeepJet discriminators

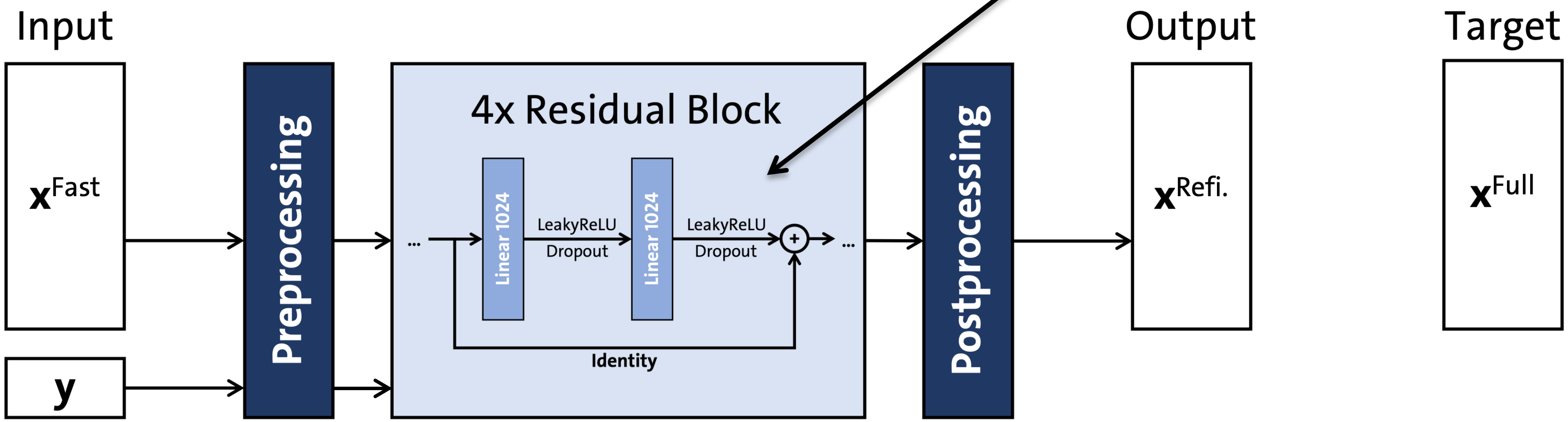


REFINING (REGRESSION) – NN ARCHITECTURE

ResNet paper arXiv:1512.03385



- ResNet-like **skip connections** → learn only residual corrections
- **Preprocessing**: transform input variables/parameters (logit-transform in order to center around 0, transform to original DeepJet output values, one-hot-encode true hadron flavour)
- **Postprocessing**: DeepJet softmax constraint + backtransf.



MAE: mean absolute error (jet-jet pairs)
MSE: mean squared error (jet-jet pairs)
MMD: maximum mean discrepancy (ensembles)

REFINING (REGRESSION) – LOSS TERMS

- **MSE**: output-target pair-based
  - Correct for deterministic FastSim biases

use MSE/MAE combination („Huber loss"), less sensitive to outliers

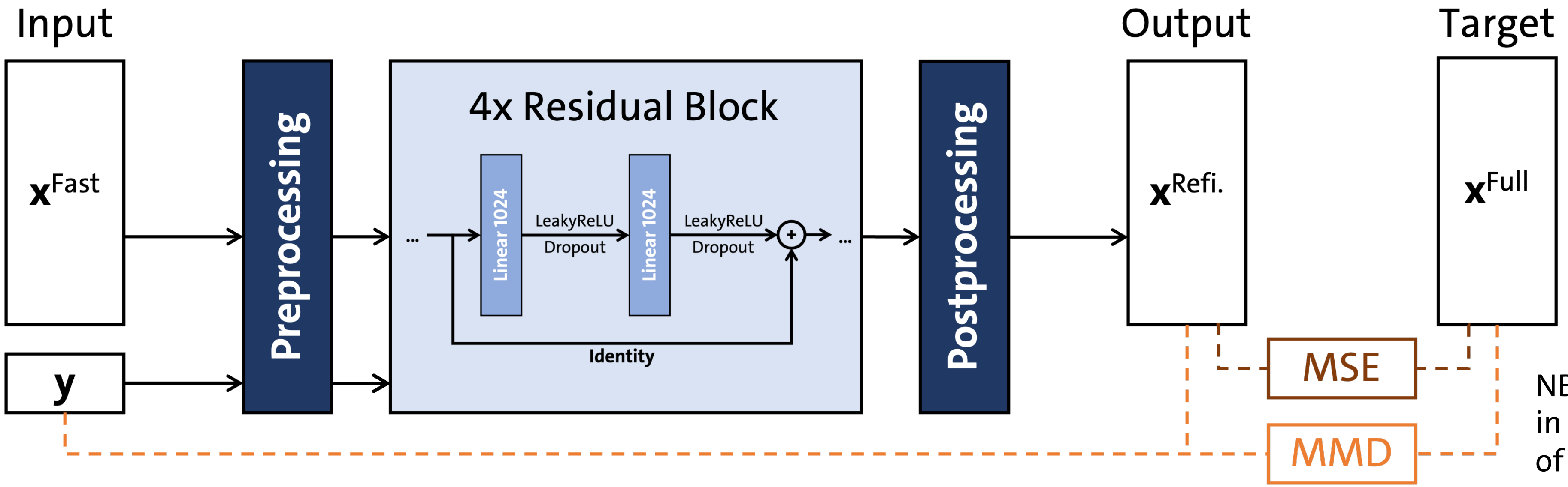
$$l_n = \begin{cases} 0.5(x_n - y_n)^2, & \text{if } |x_n - y_n| < delta \\ delta * (|x_n - y_n| - 0.5 * delta), & \text{otherwise} \end{cases}$$

- **MMD**: distribution-based (**primary loss**)
  - Correct for stochastic FastSim biases

given two samples from P(X) and Q(Y):

$$\widehat{\mathrm{MMD}}(P,Q) = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} k(x_i,x_j) + \frac{1}{m^2}\sum_{i=1}^{m}\sum_{j=1}^{m} k(y_i,y_j) - \frac{2}{nm}\sum_{i=1}^{n}\sum_{j=1}^{m} k(x_i,y_j)$$

n = m = batch size = 4096,
k: Gaussian kernel (adaptive σ)

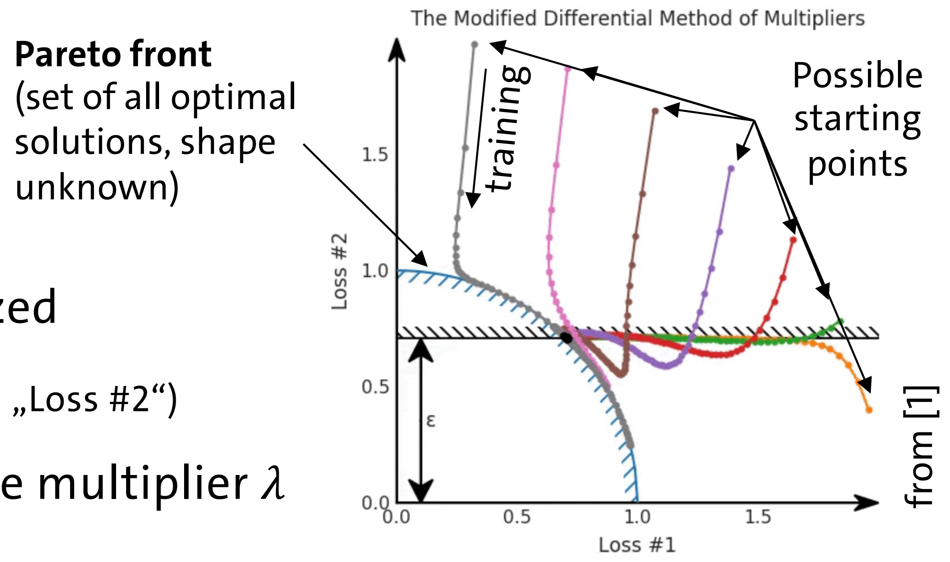


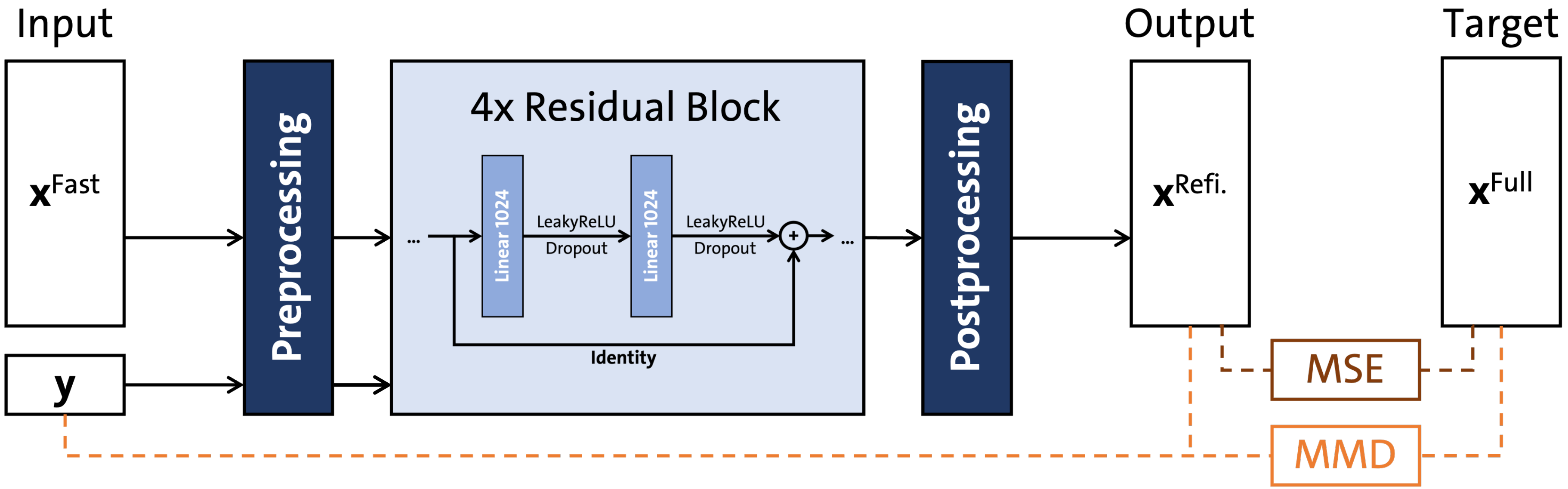
NB: include parameters in MMD to take account of correlations

REFINING (REGRESSION) – LOSS TERMS

Combine loss terms via **MDMM algorithm**:

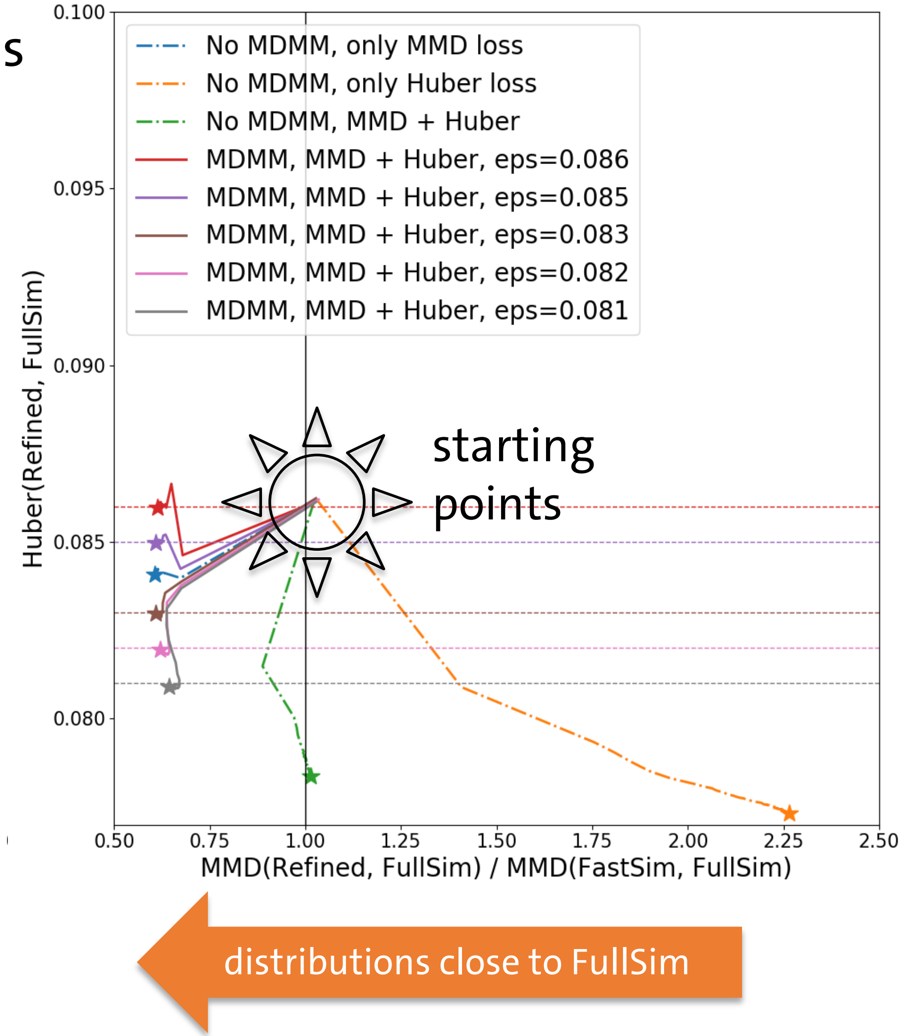
- Reframe problem as **constrained optimization** using **Lagrangian**:
  $\mathcal{L} = f(\theta) - \lambda * (\varepsilon - g(\theta))$ → convergence mathematically formalized
- Minimize $f(\theta)$ (primary loss, „Loss #1") subject to $g(\theta) = \varepsilon$ (additional loss, „Loss #2")
- Gradient descent for NN parameters θ, gradient ascent for Lagrange multiplier λ





REFINING (REGRESSION) – LOSS TERMS

- **Pareto plot**: training history in plane of the two loss terms
  - Primary loss: **MMD(Refined, FullSim)** (horizontal axis)
    normalized to MMD(FastSim, FullSim)
  - Constraint: **Huber(Refined, FullSim)** (vertical axis)
- Trained for 100 epochs with 500 batches
- Simple addition **not optimal**
- **MDMM**: scan of different ε values
  - ➢ If ε is too small it can only be reached by disregarding MMD
  - ➢ If ε is too large MMD also gets worse because jet-jet pairs *have to* change too much
  - ➢ Choose **ε = 0.083**



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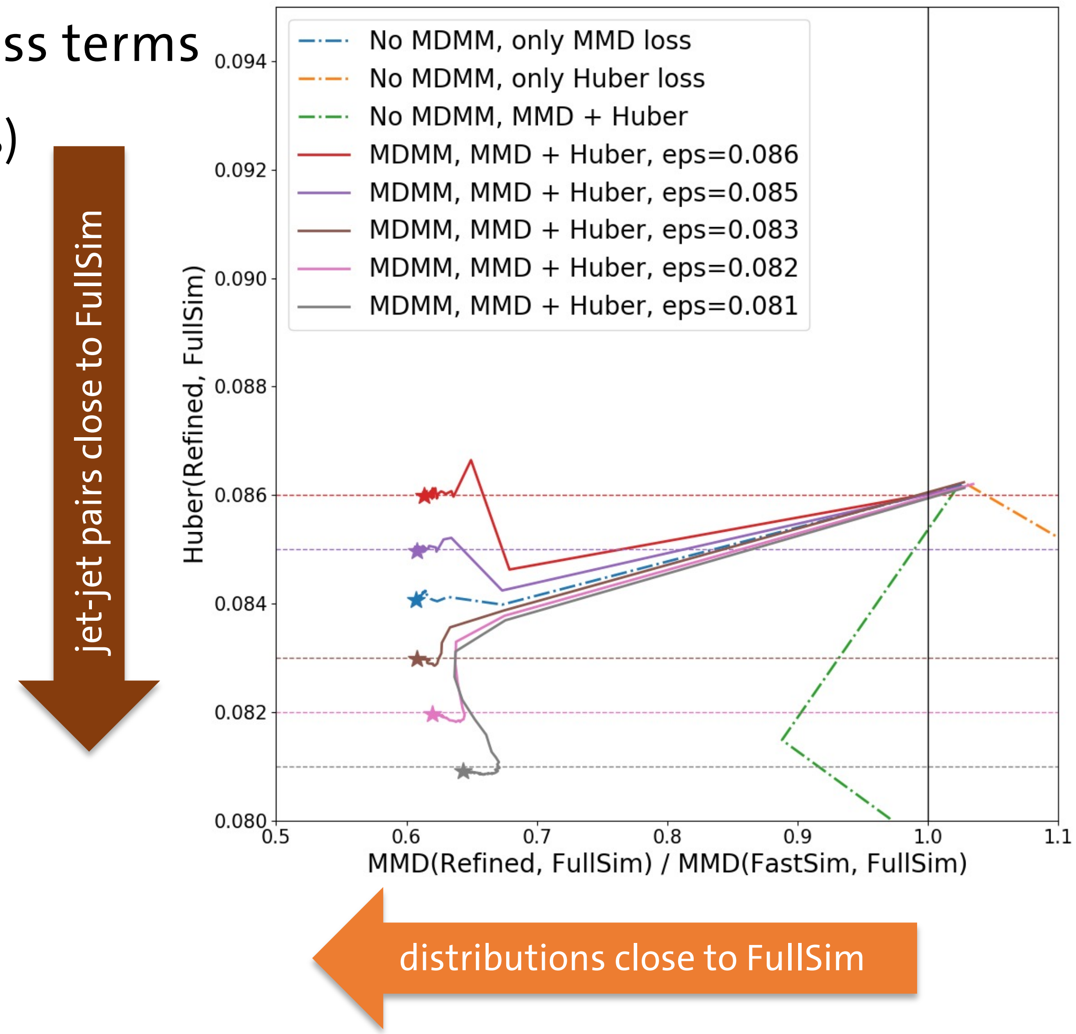
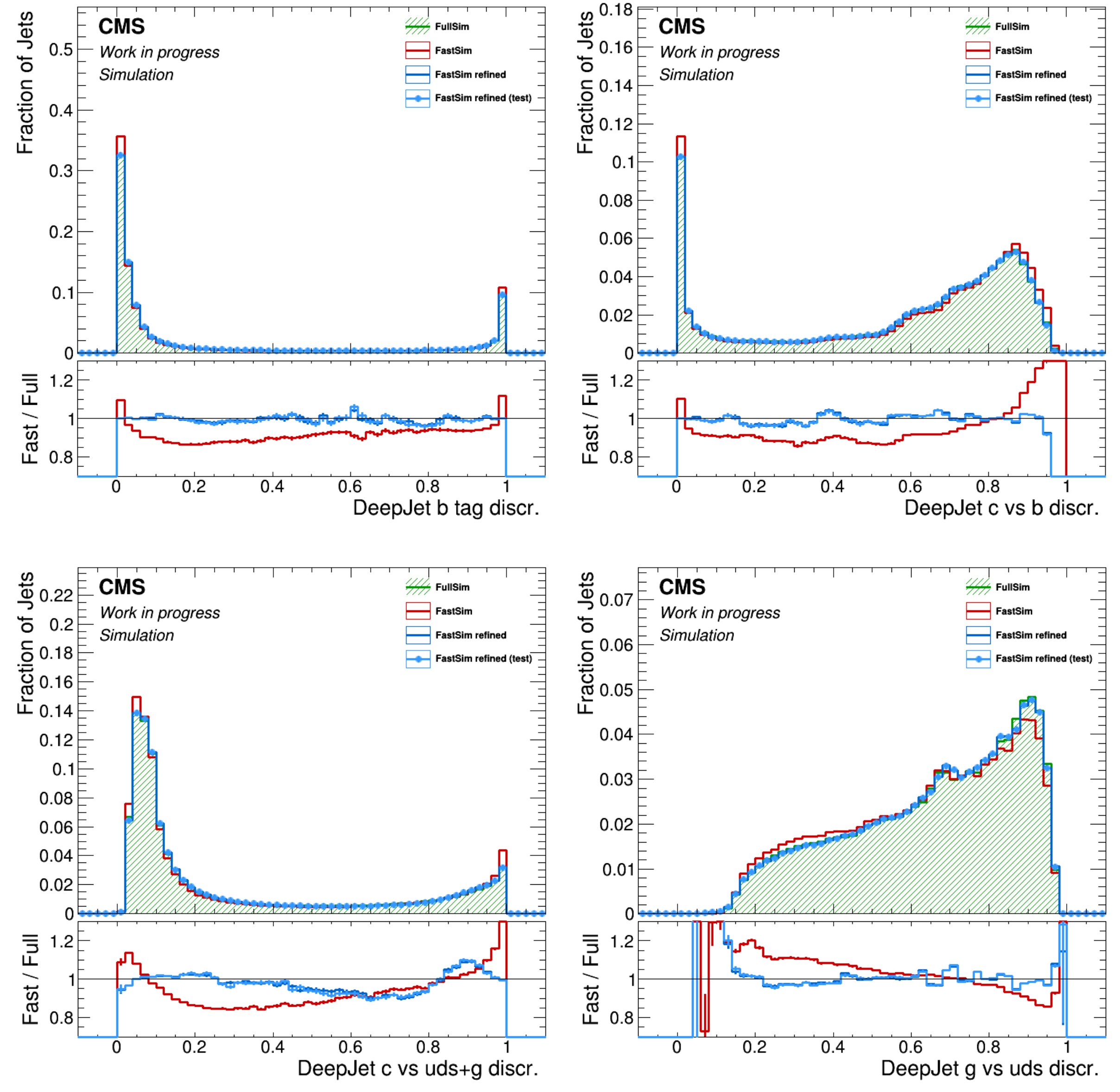
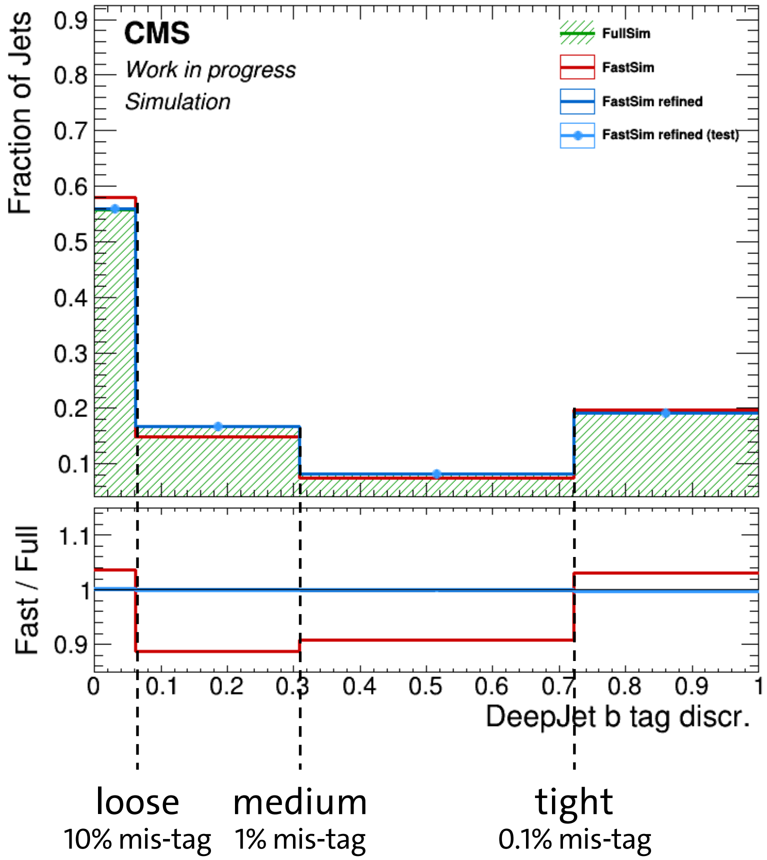


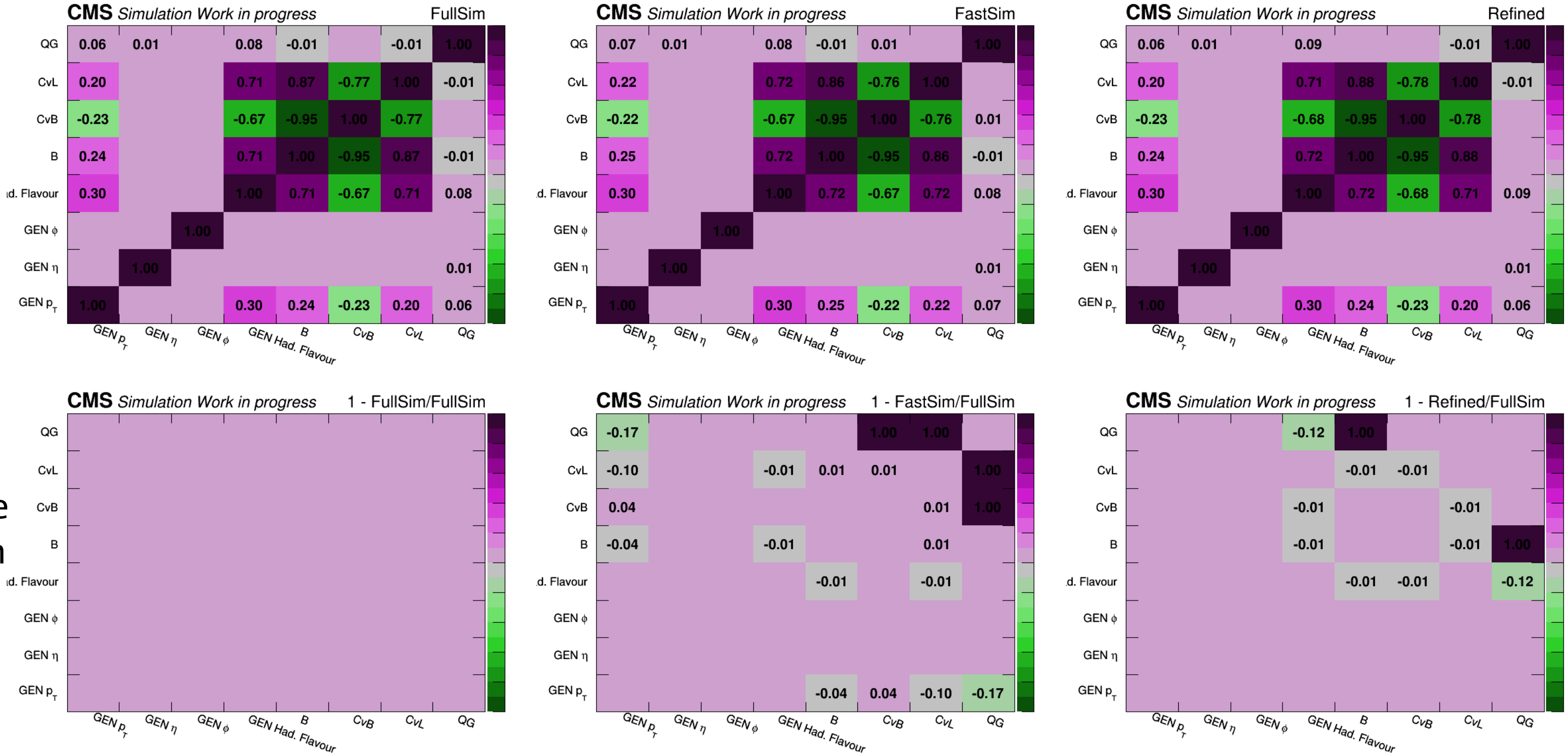
REFINING (REGRESSION) – RESULTS



b tag binned by working point

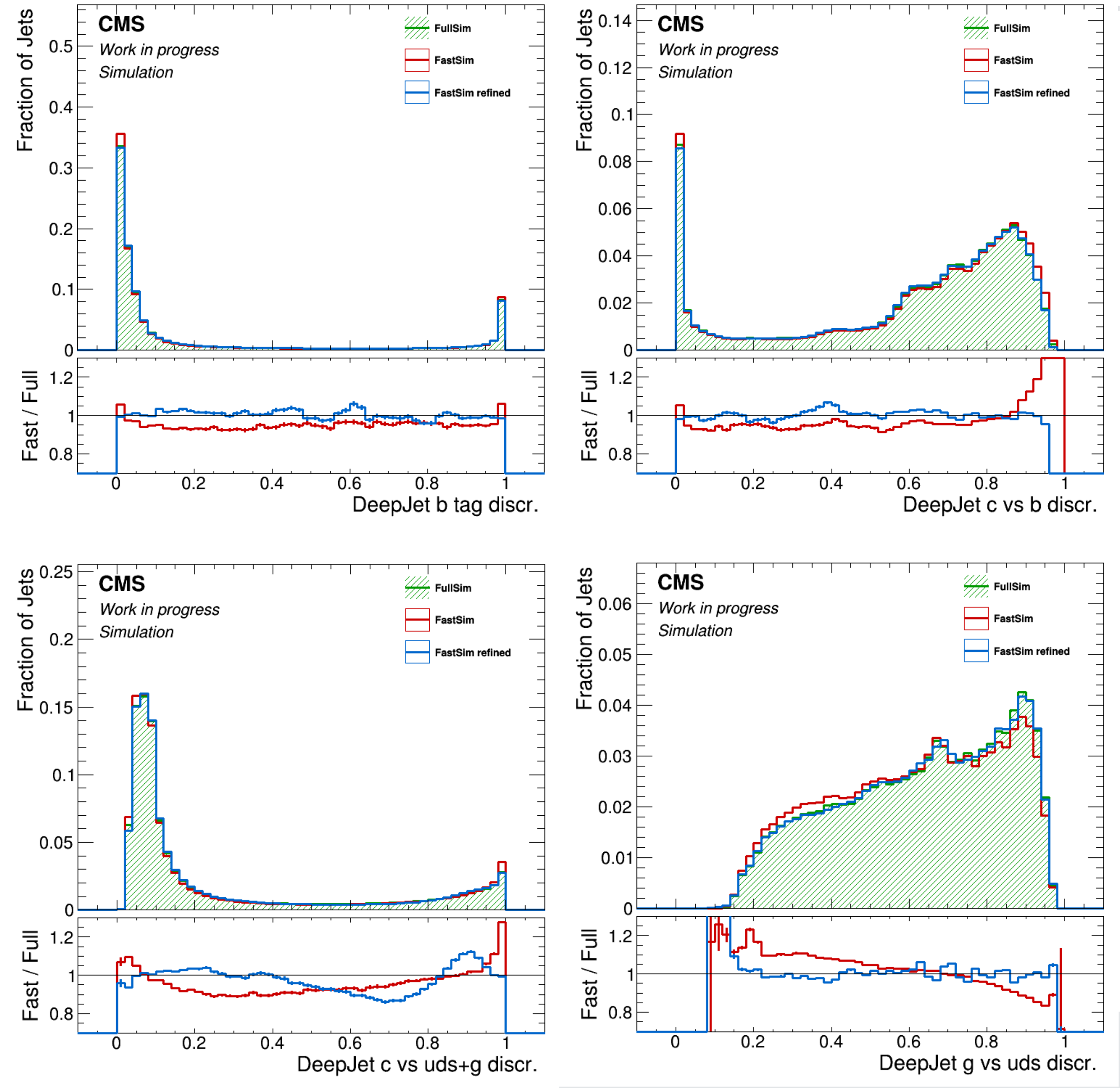


REFINING (REGRESSION) – LINEAR CORRELATION COEFFICIENTS



difference to FullSim

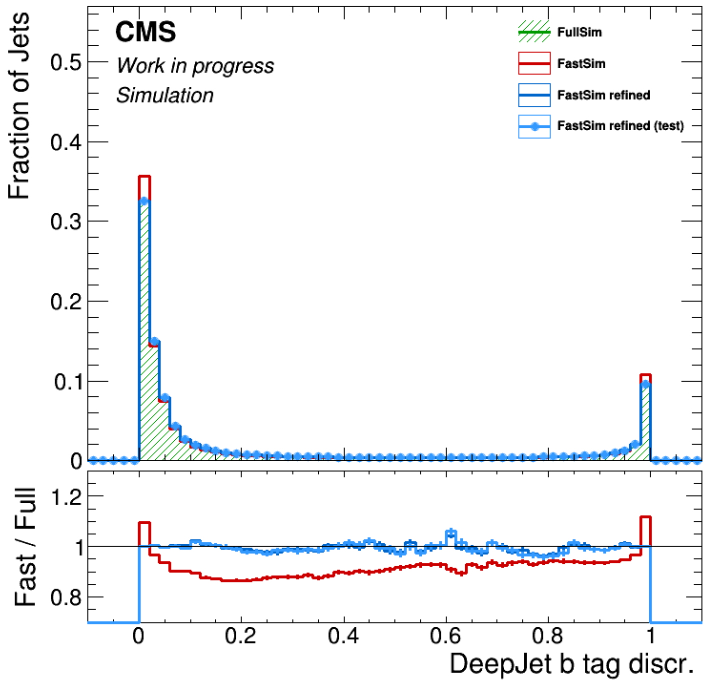
REFINING (REGRESSION) – VALIDATION IN TTBAR



- Good performance for evaluation on **TTbar** (NN trained on T1tttt SUSY dataset)

SUMMARY

- **Fast simulation** techniques needed to face computing challenges
- High **accuracy** of simulation required for most physics analyses
- Applying ML-based **post-hoc refinement** to CMS FastSim output (ResNet-like regression NN)
  - ➢ Considerably improved agreement with FullSim output
  - ➢ Improvement in correlations among output observables and external parameters
- Integration into CMS software framework (CMSSW) in the works (via **ONNX** format)
- Possible extension to other variables/physics objects (e.g., FatJet substructure)



BACKUP

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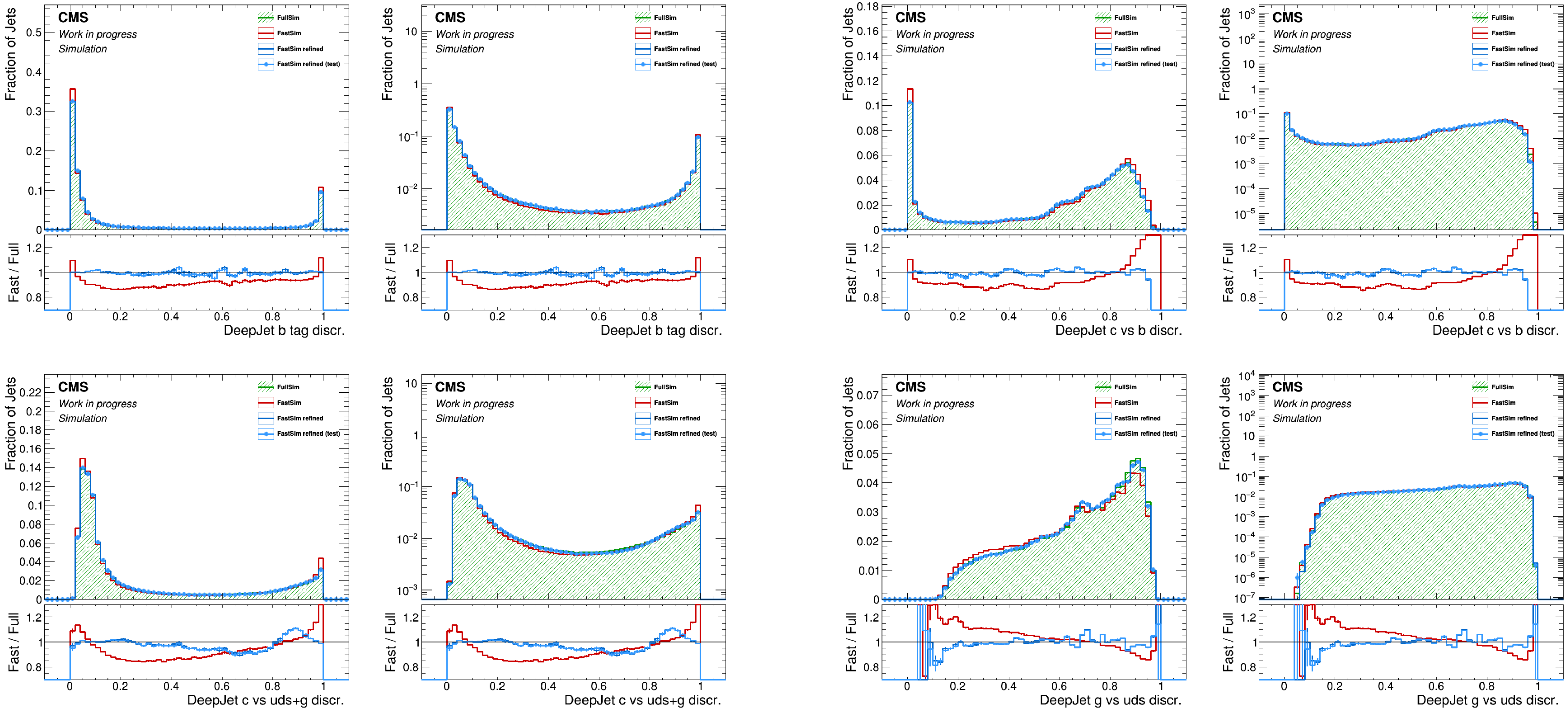
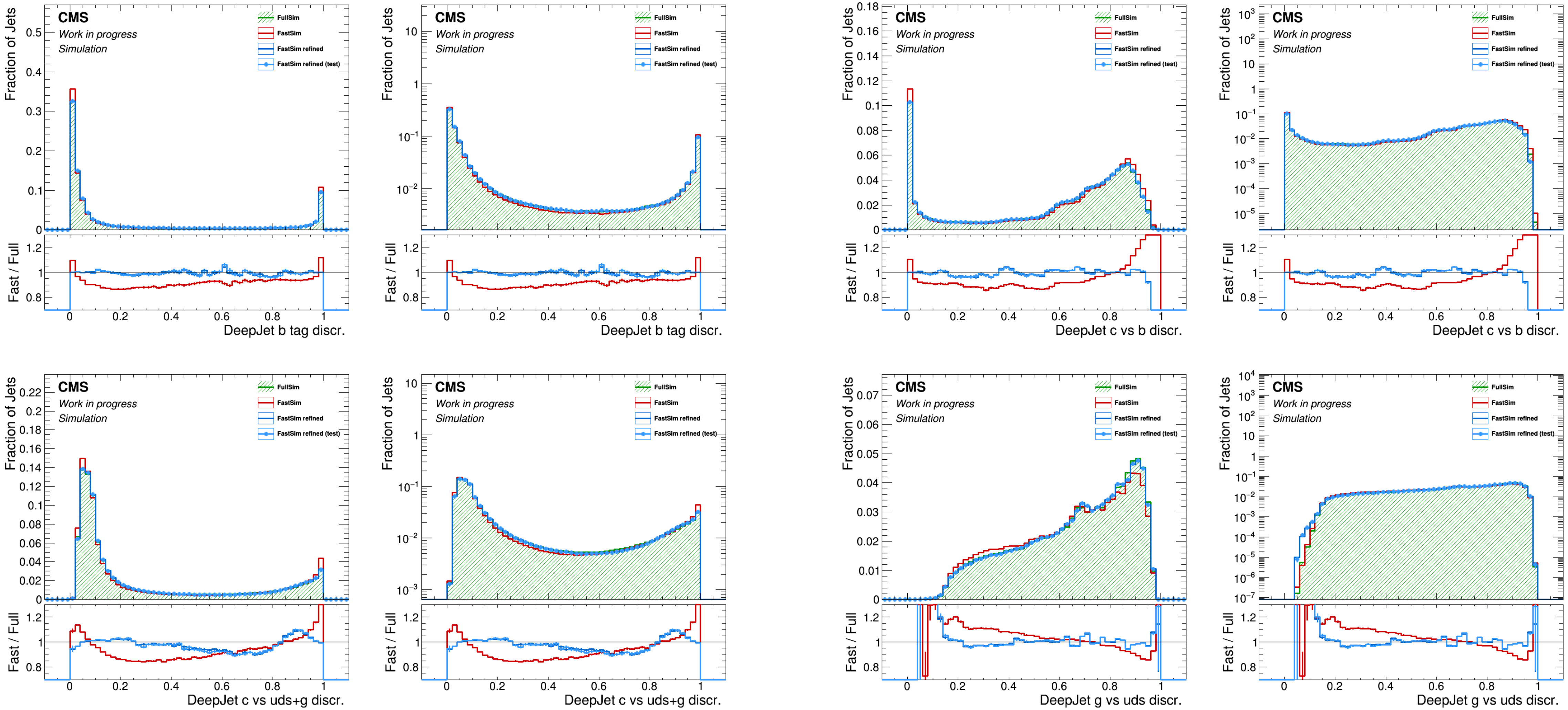


REFINING (REGRESSION) – EPS=0.083



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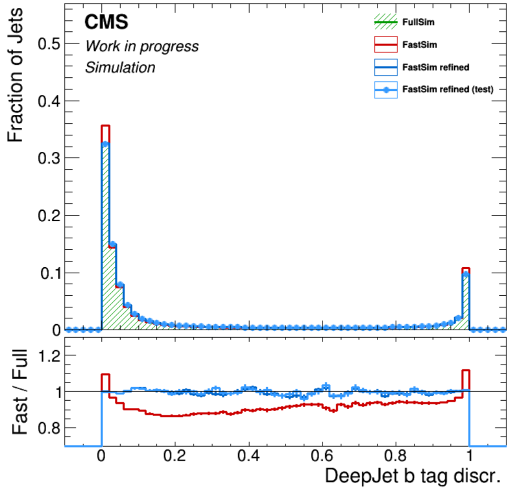

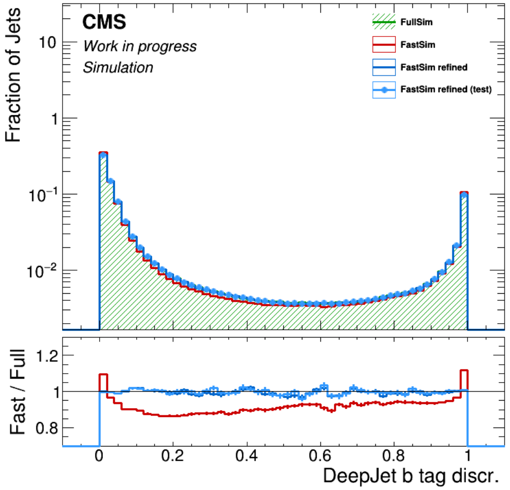

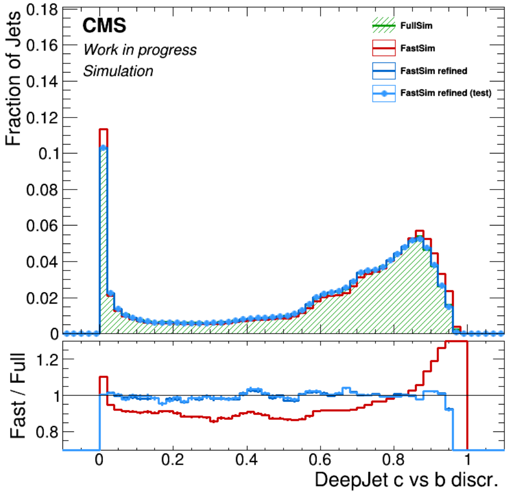

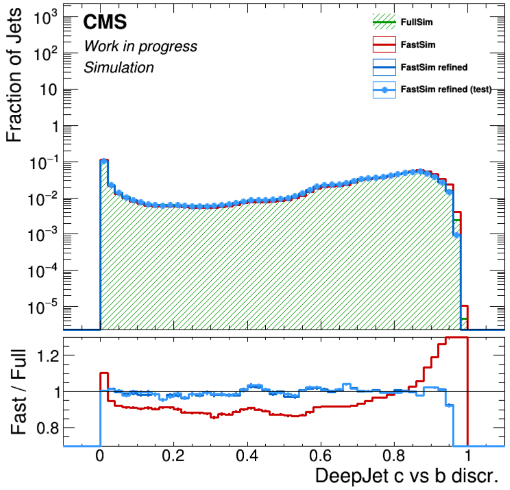

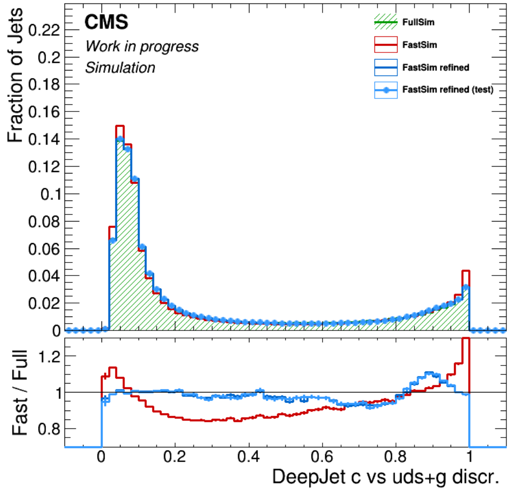

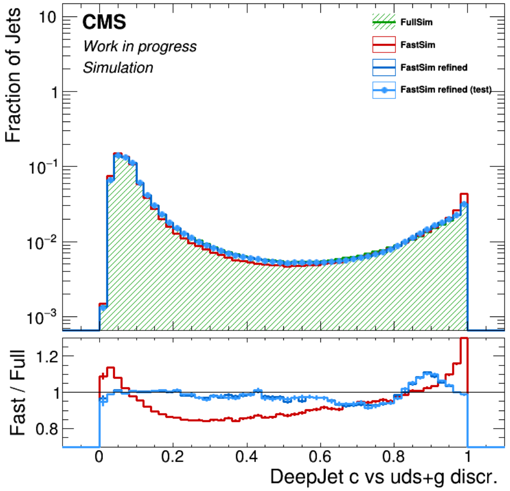

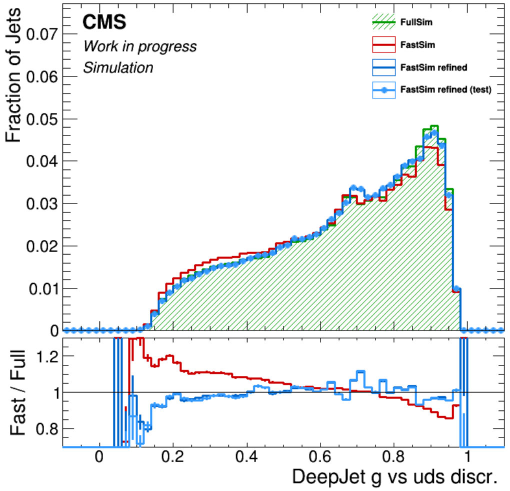

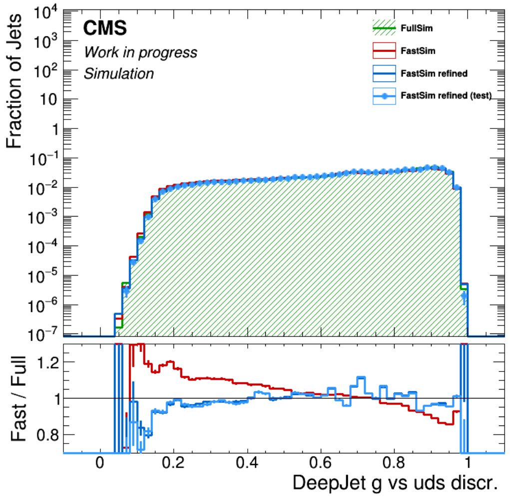

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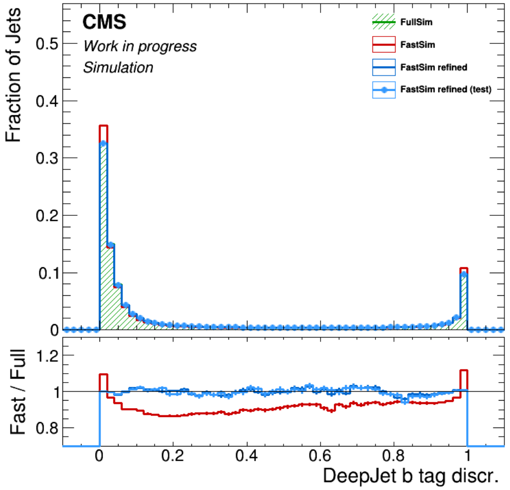

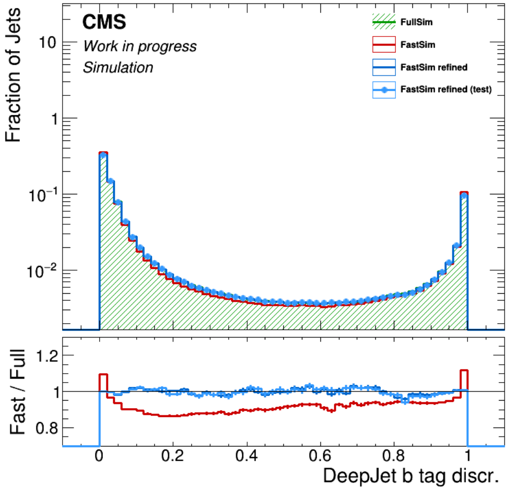

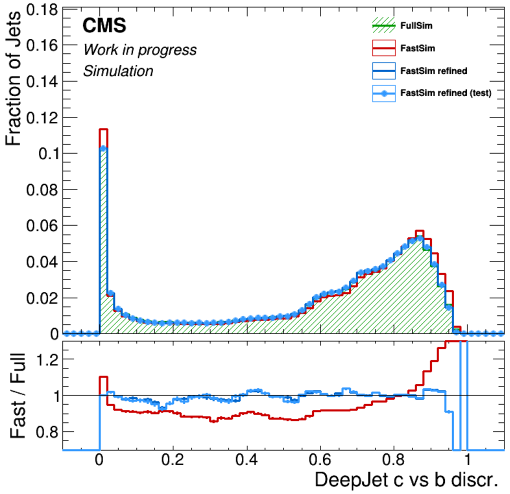

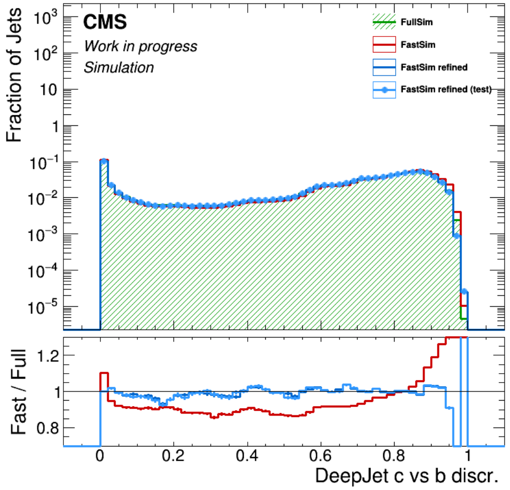

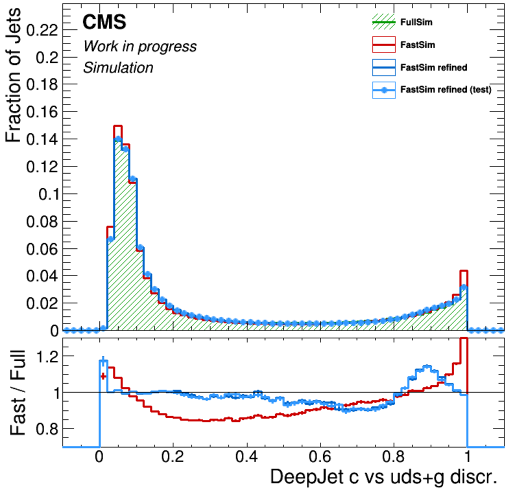

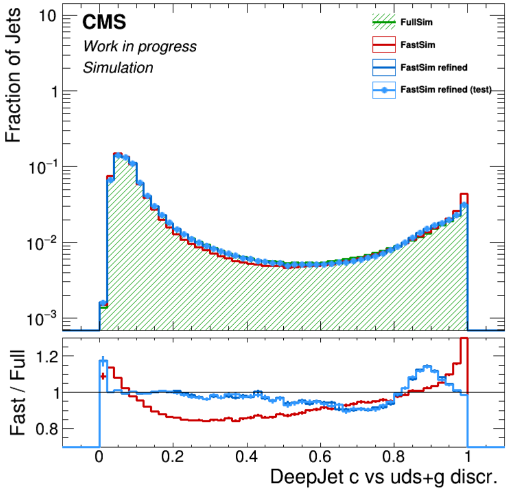

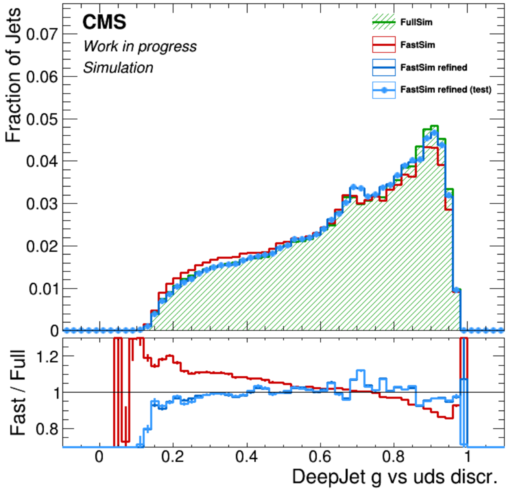

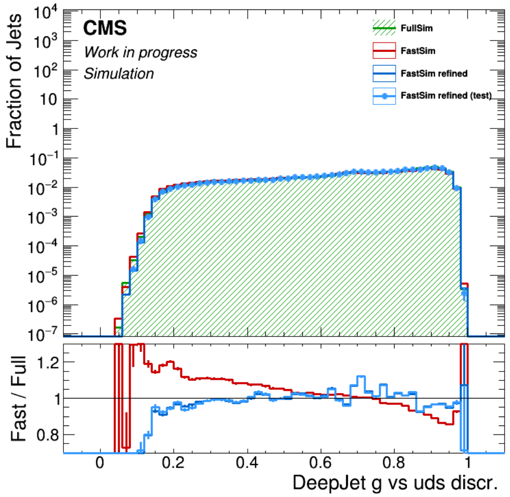

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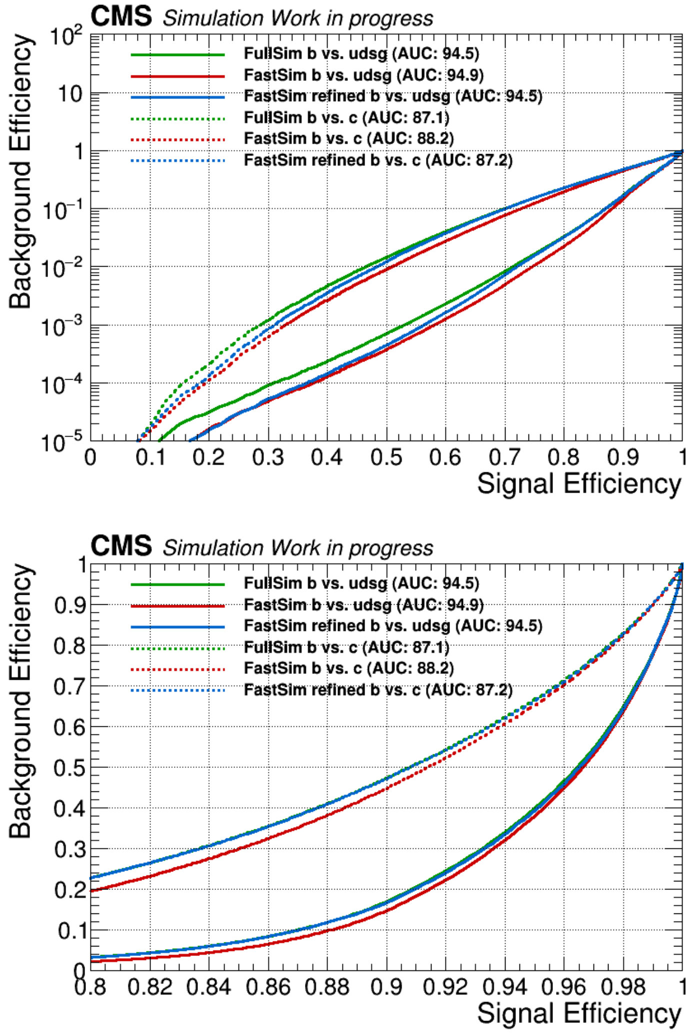
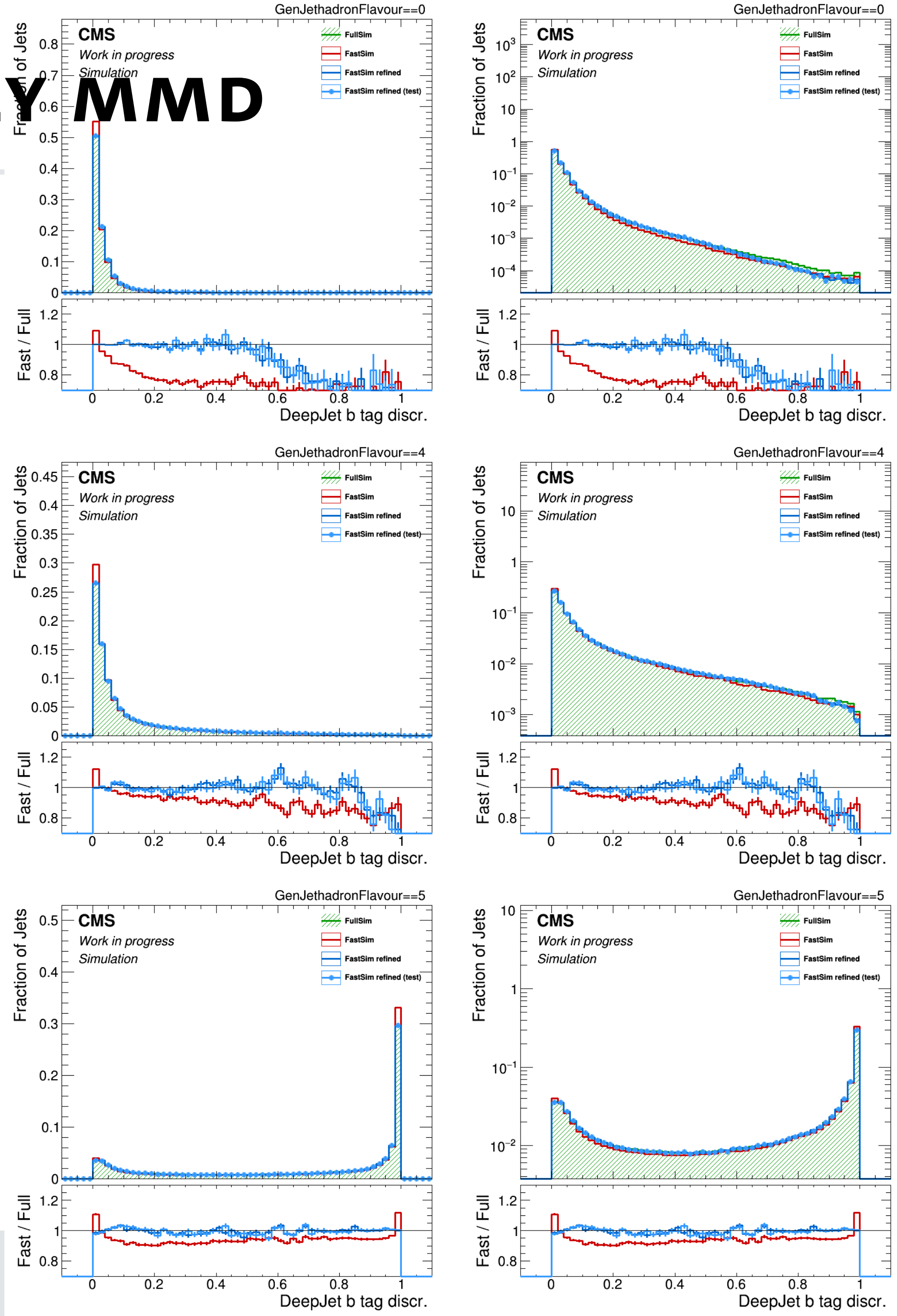
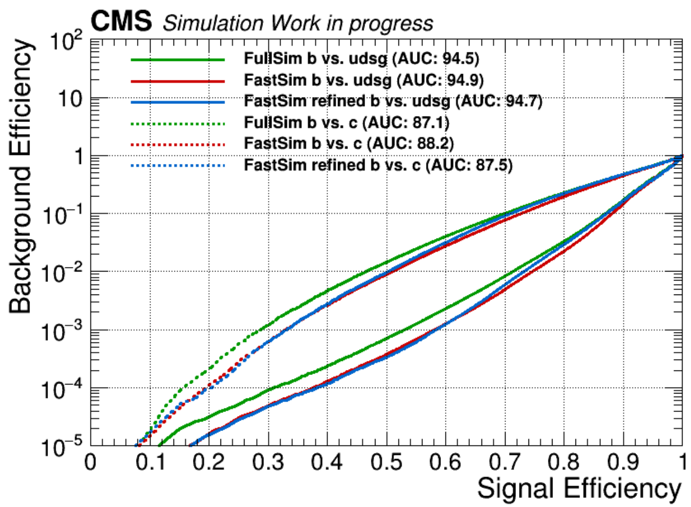
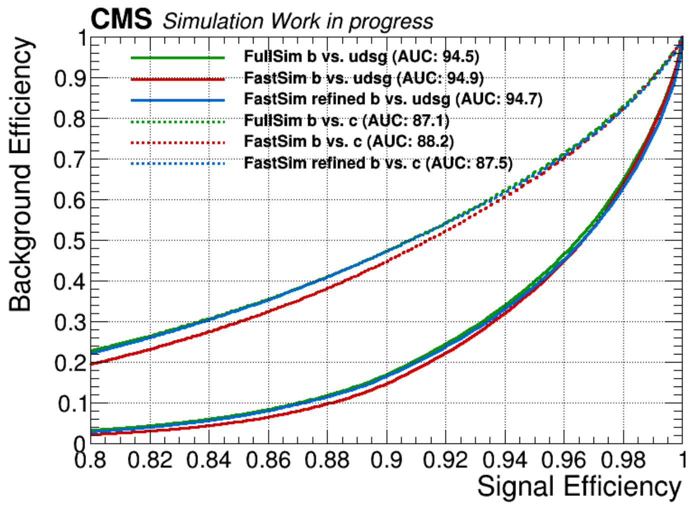
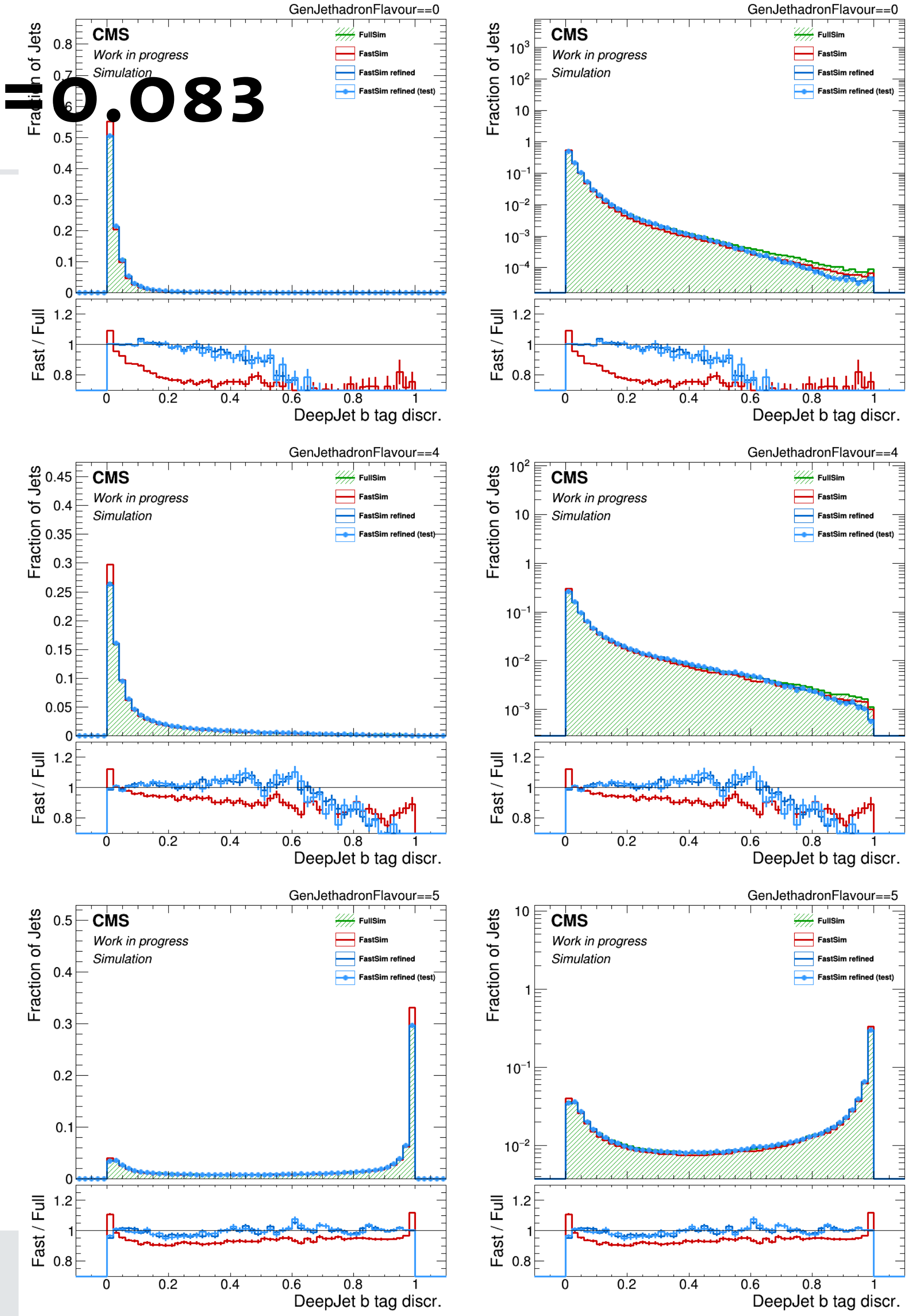




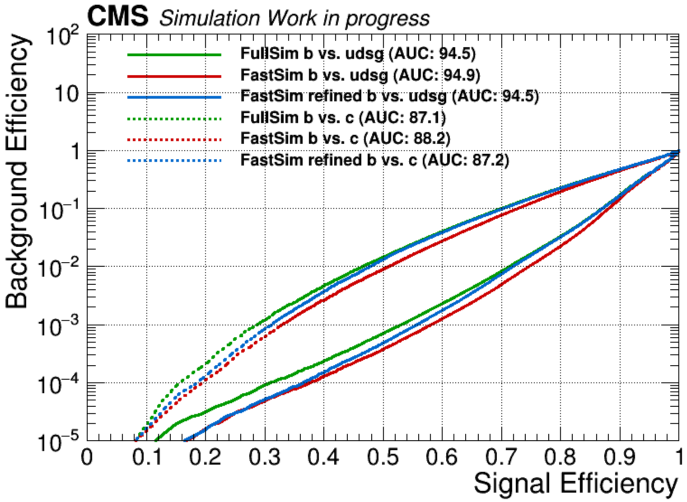
REFINING (REGRESSION) – EPS=0.083

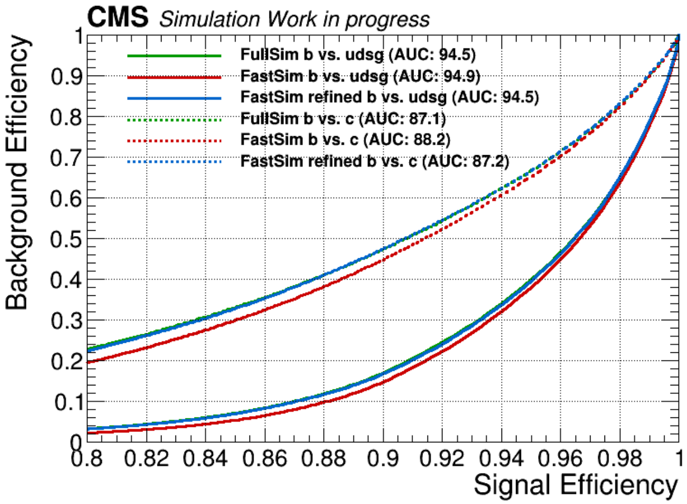


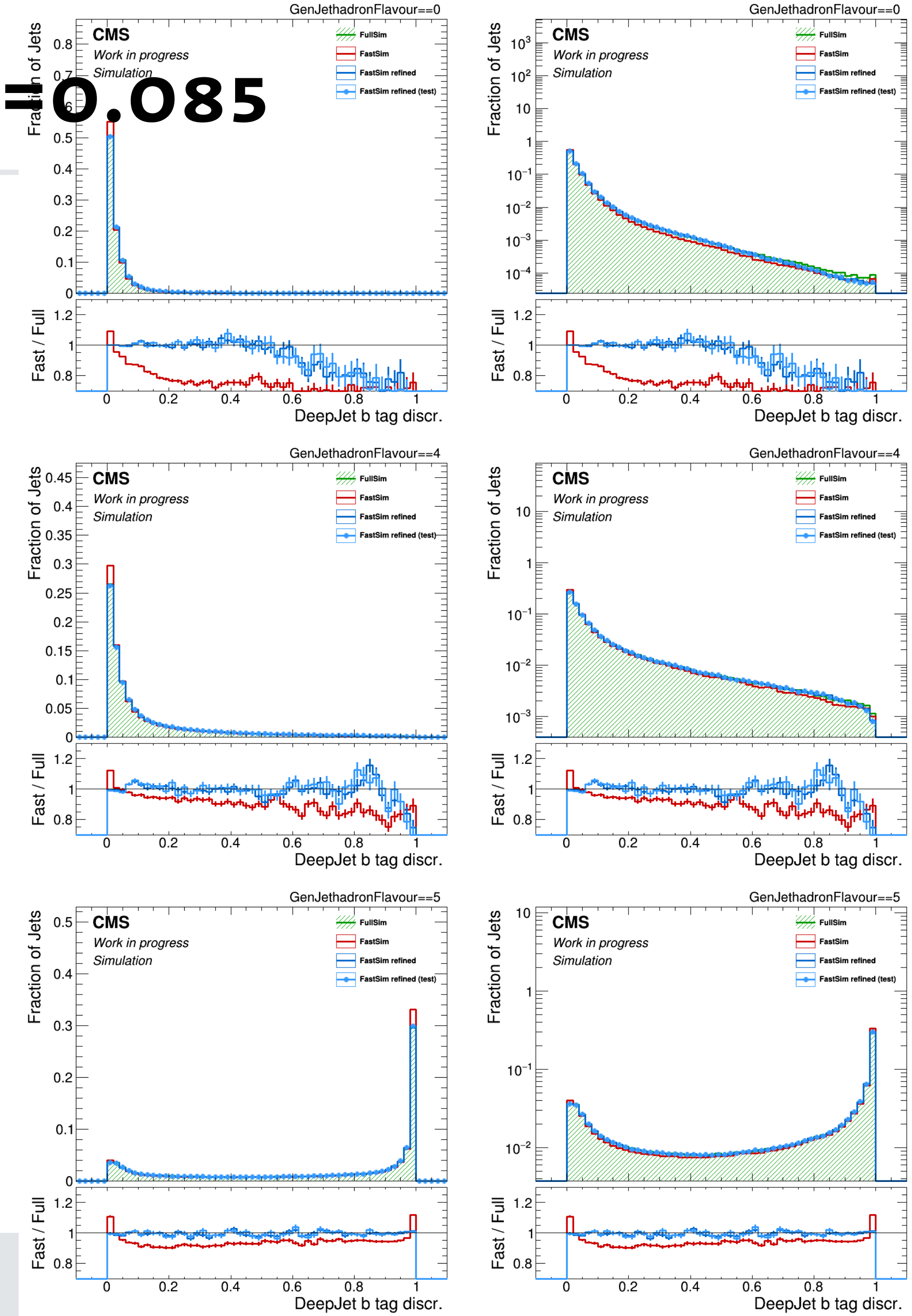




Refining (regression) – EPS=0.085







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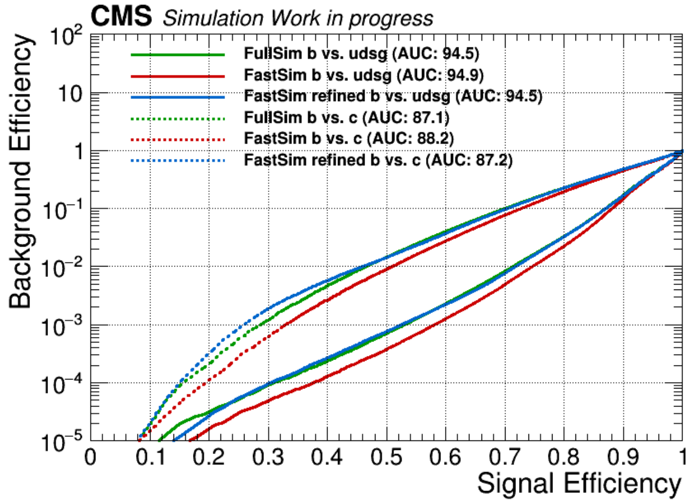
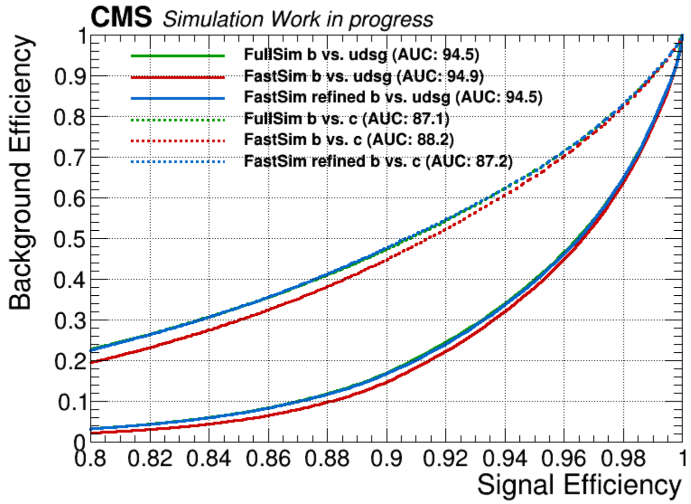
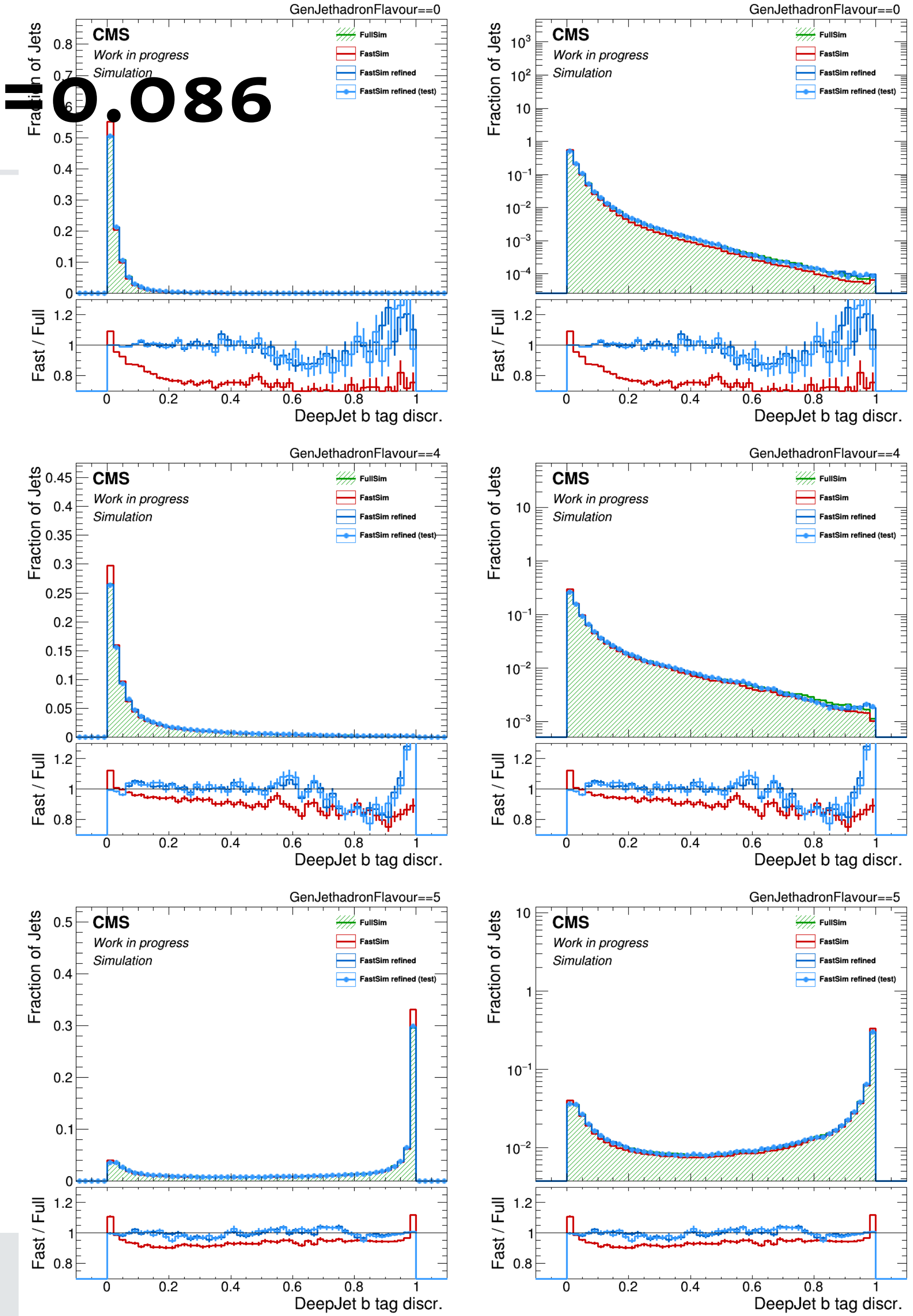
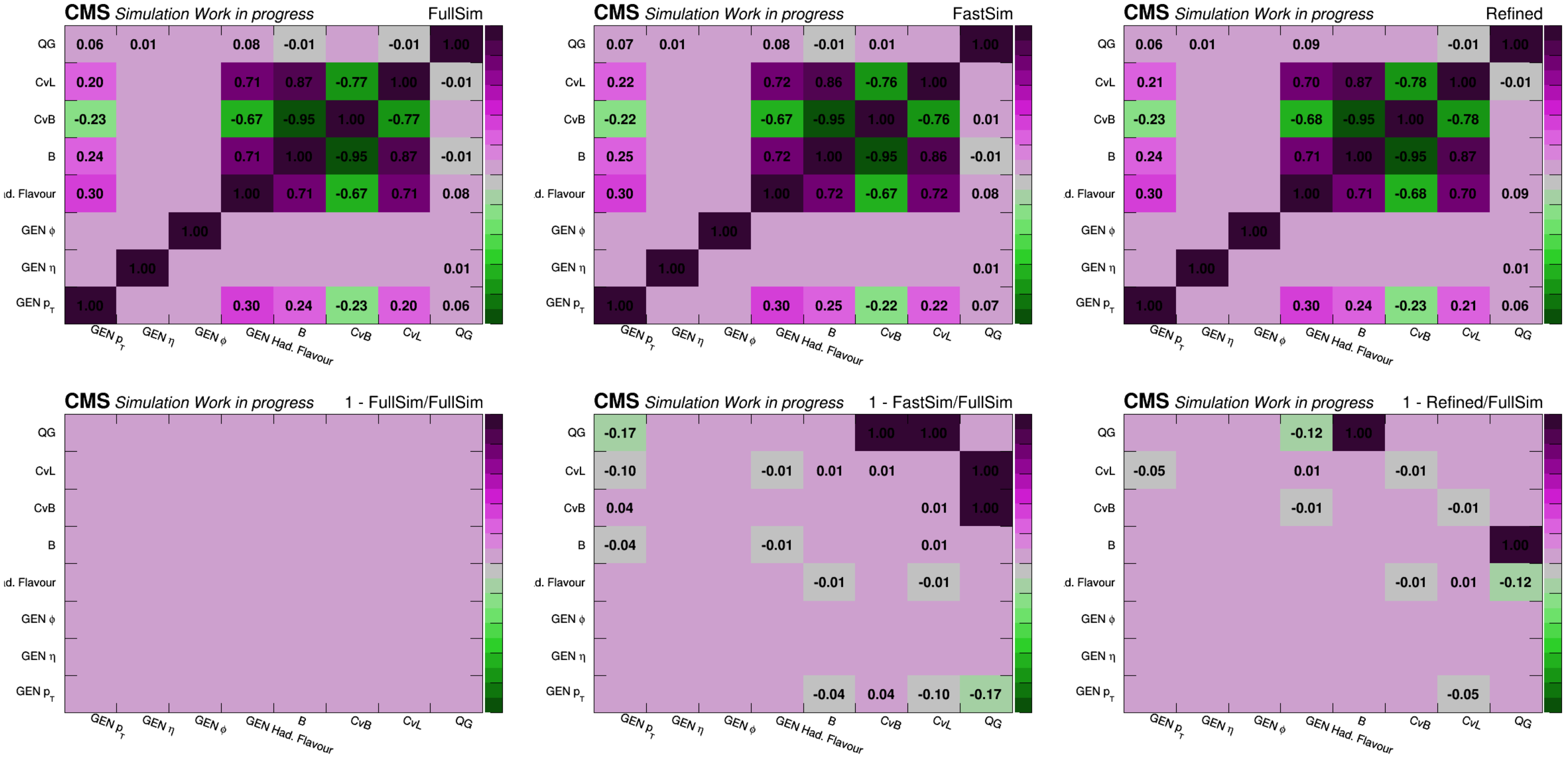






REFINING (REGRESSION) – ONLY MMD



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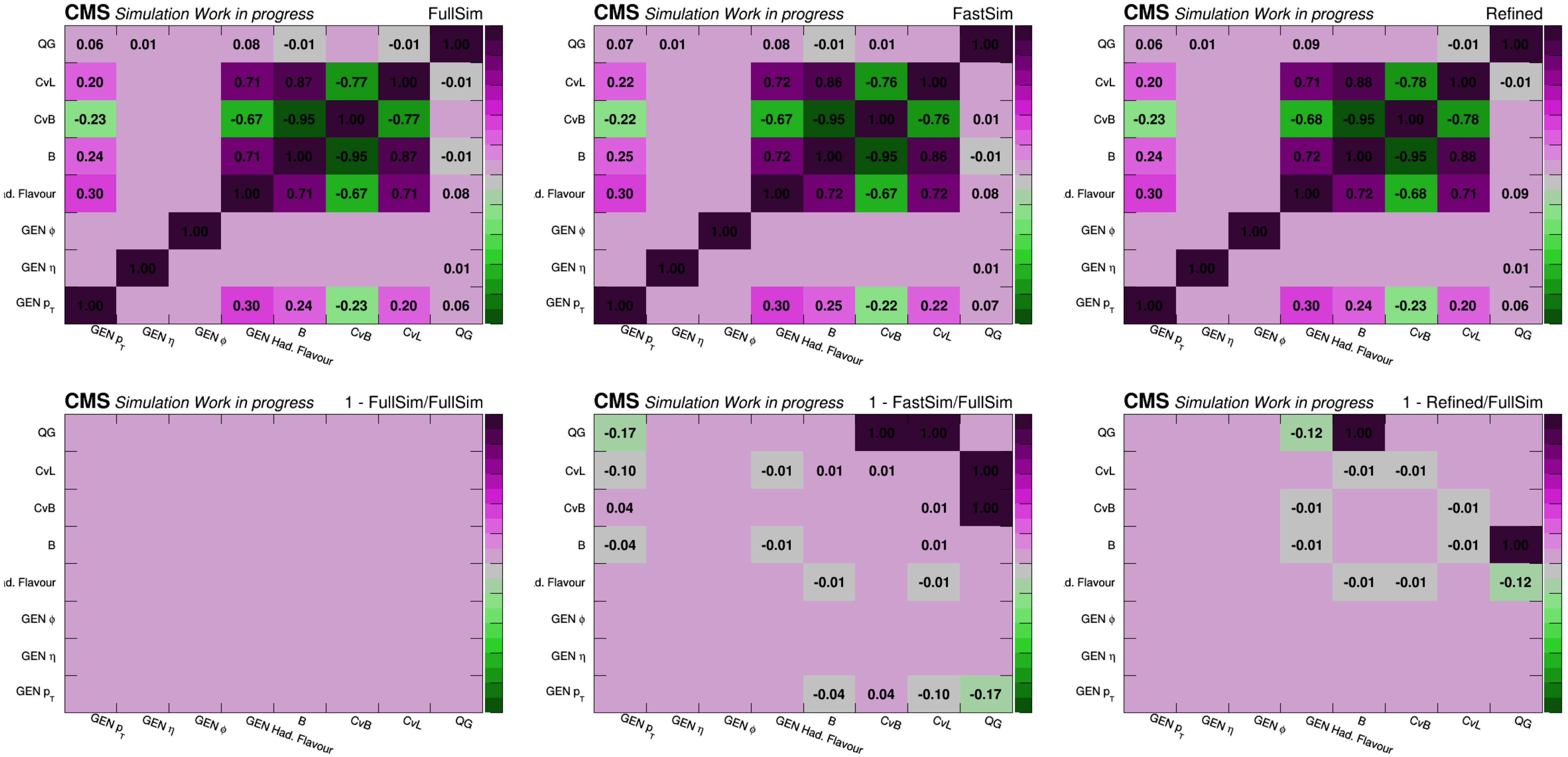

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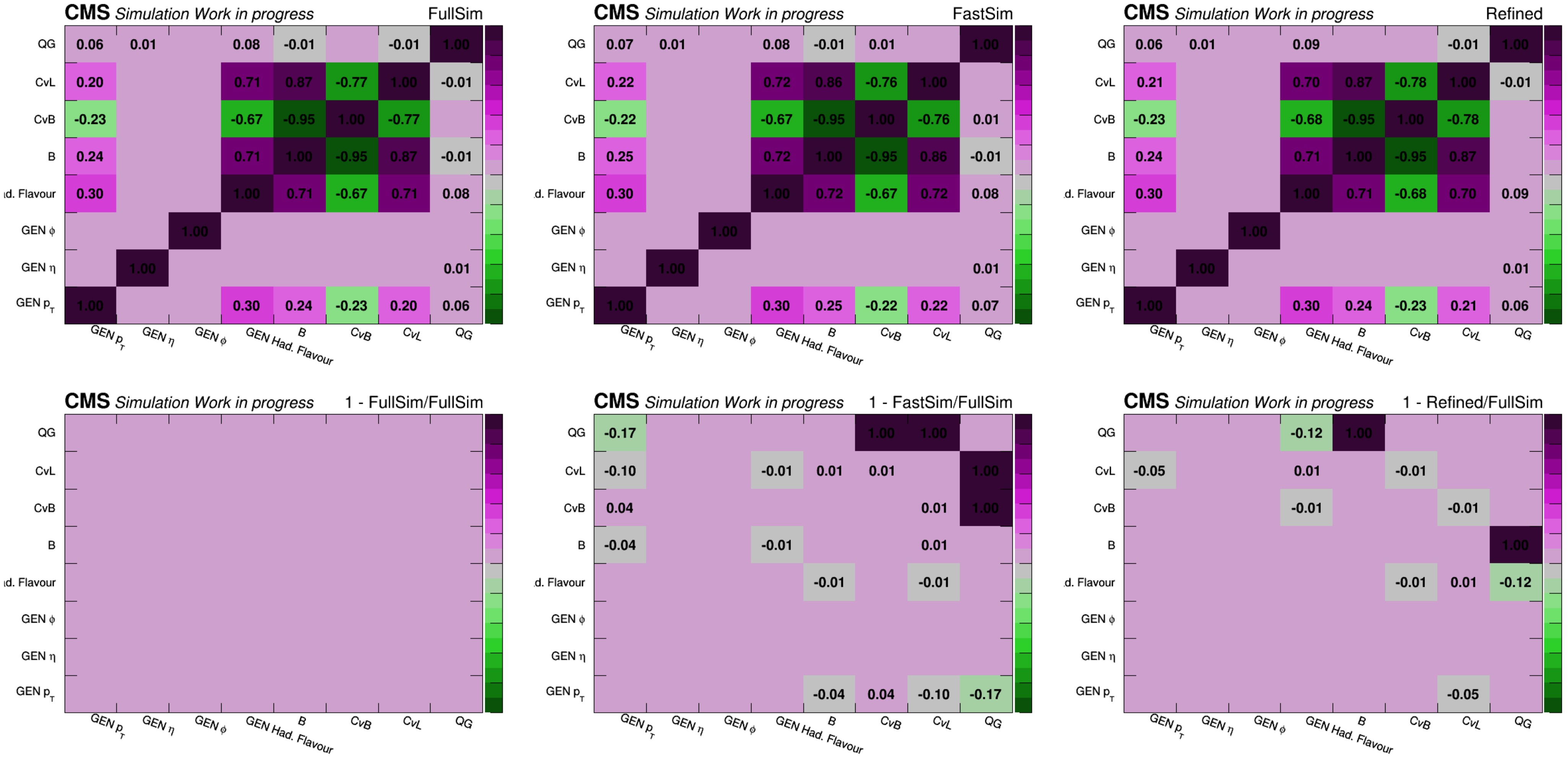

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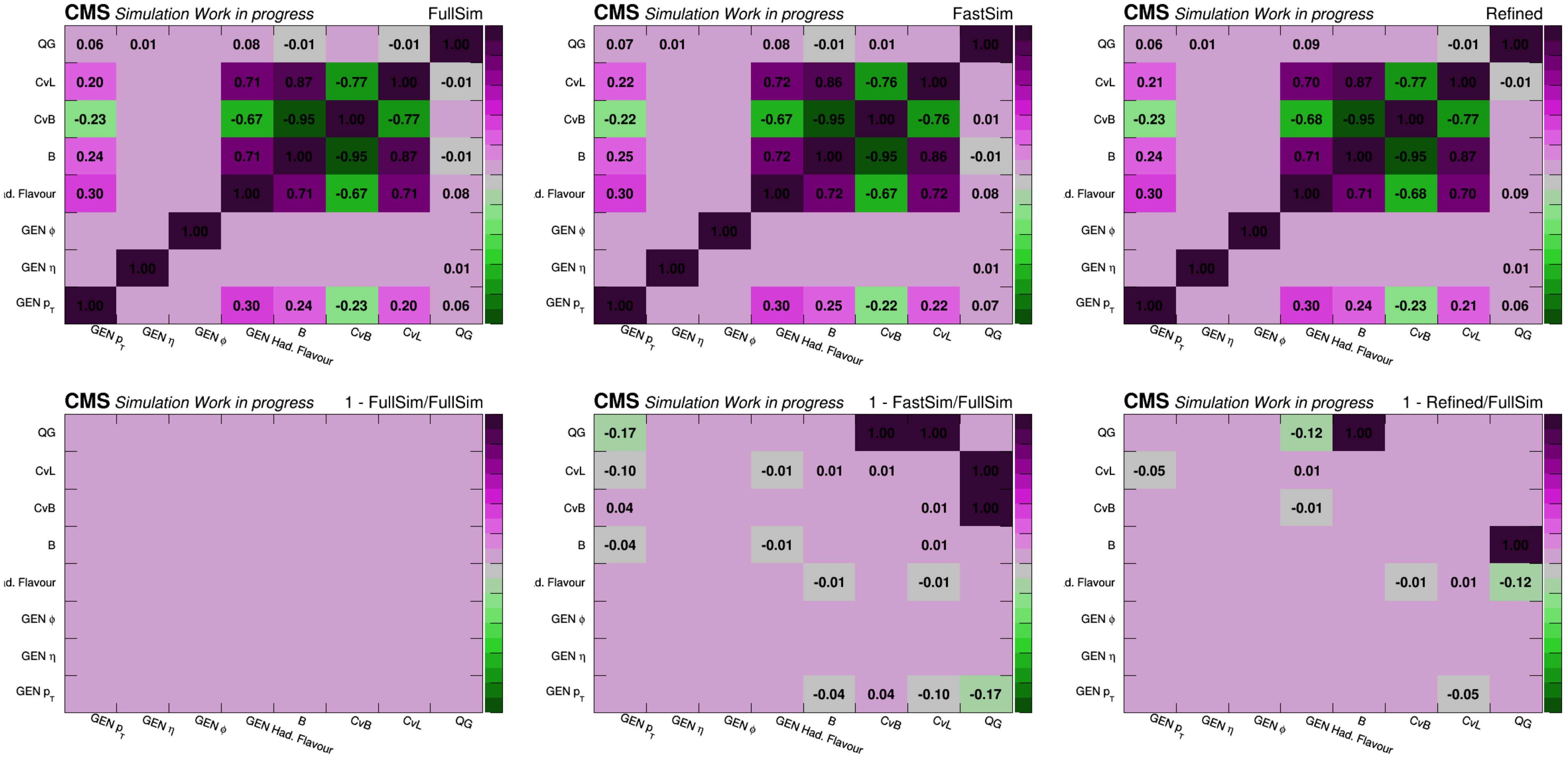
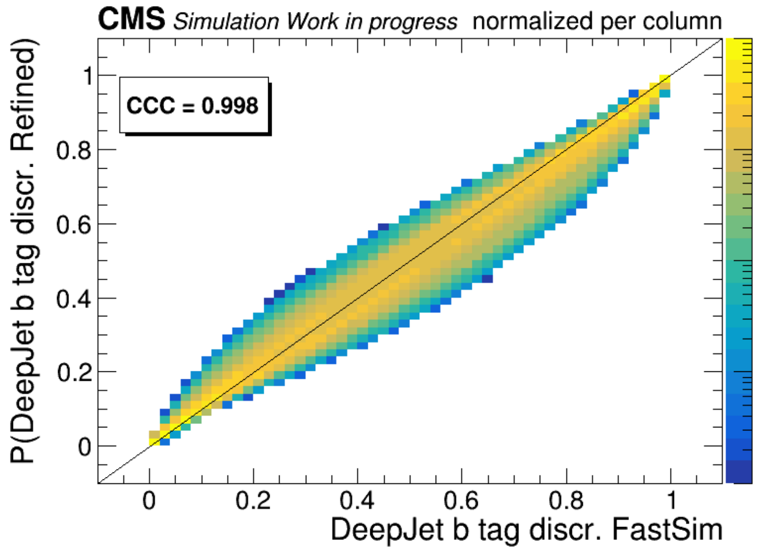
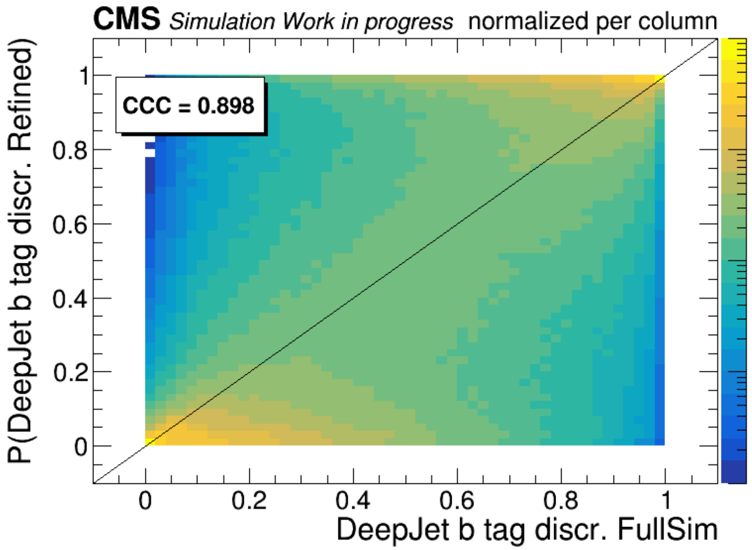


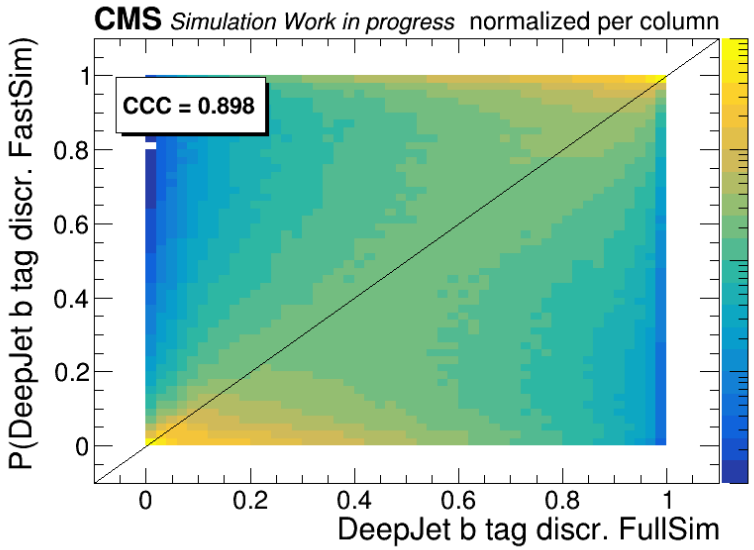
CCC = concordance correlation coefficient
“measures the agreement between two variables”

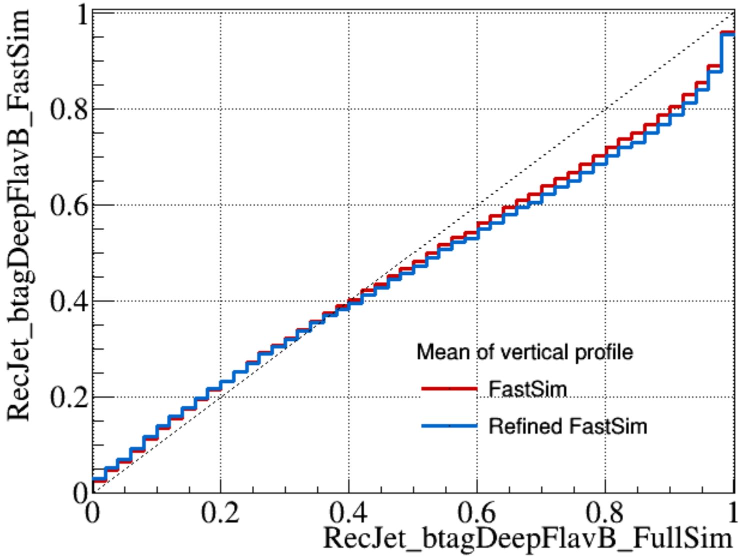
$$\rho_c = \frac{2\rho\sigma_x\sigma_y}{\sigma_x^2 + \sigma_y^2 + (\mu_x - \mu_y)^2}$$

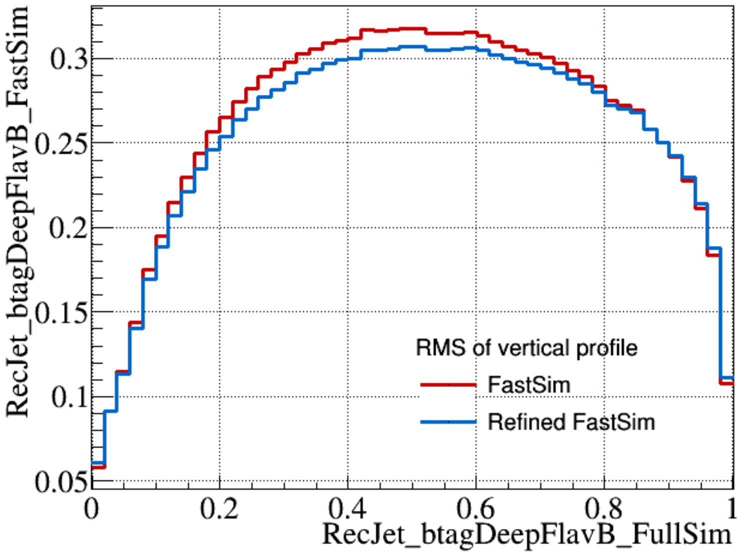
REFINING (REGRESSION) – ONLY MMD











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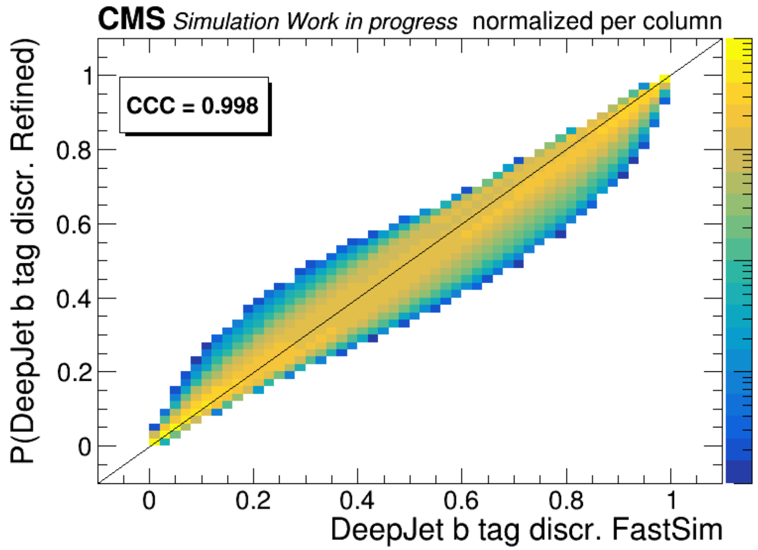

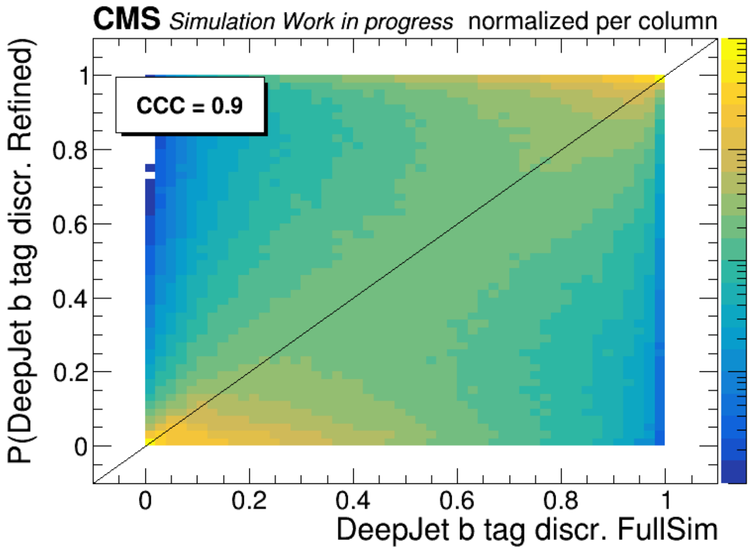

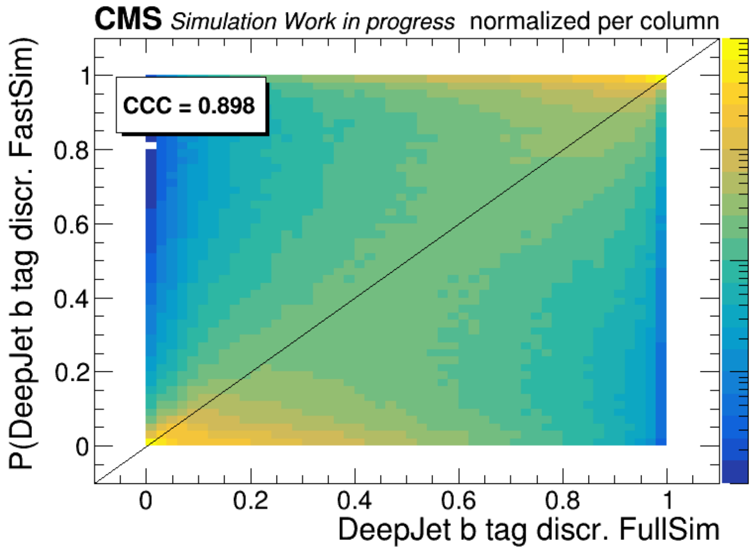

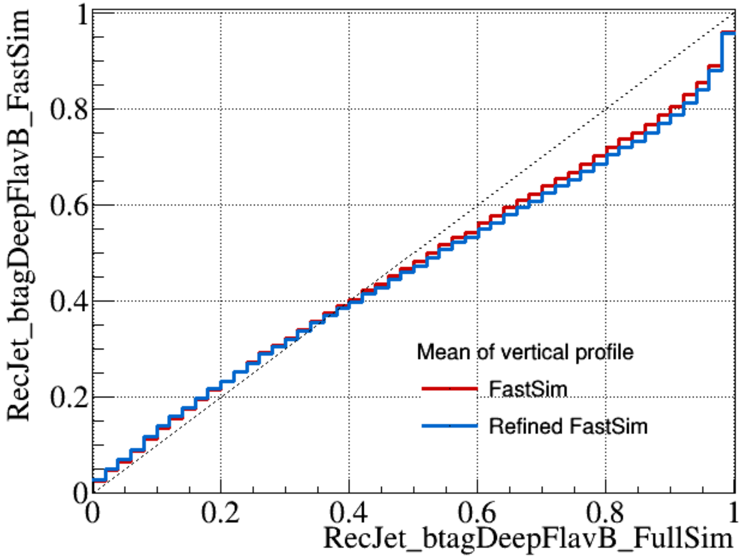

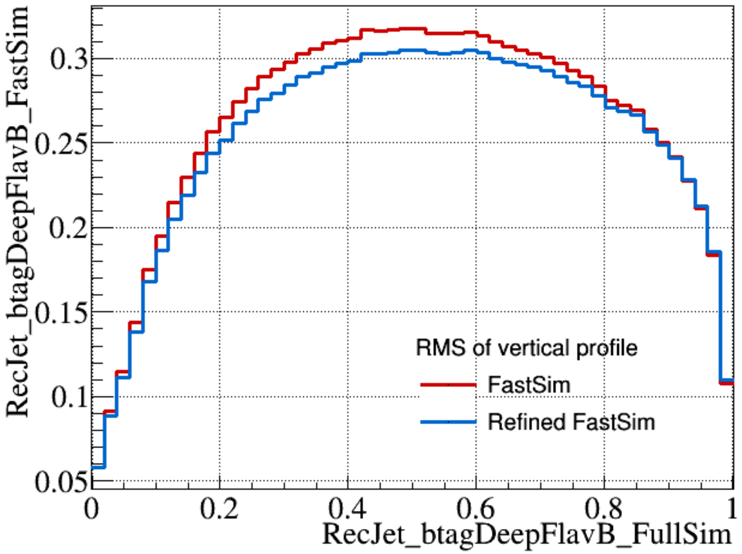

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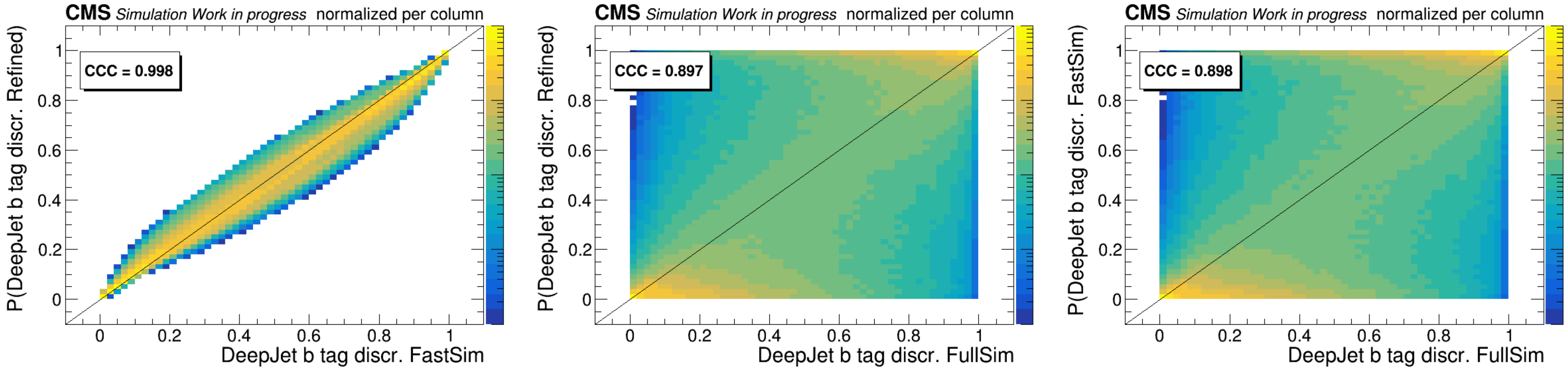

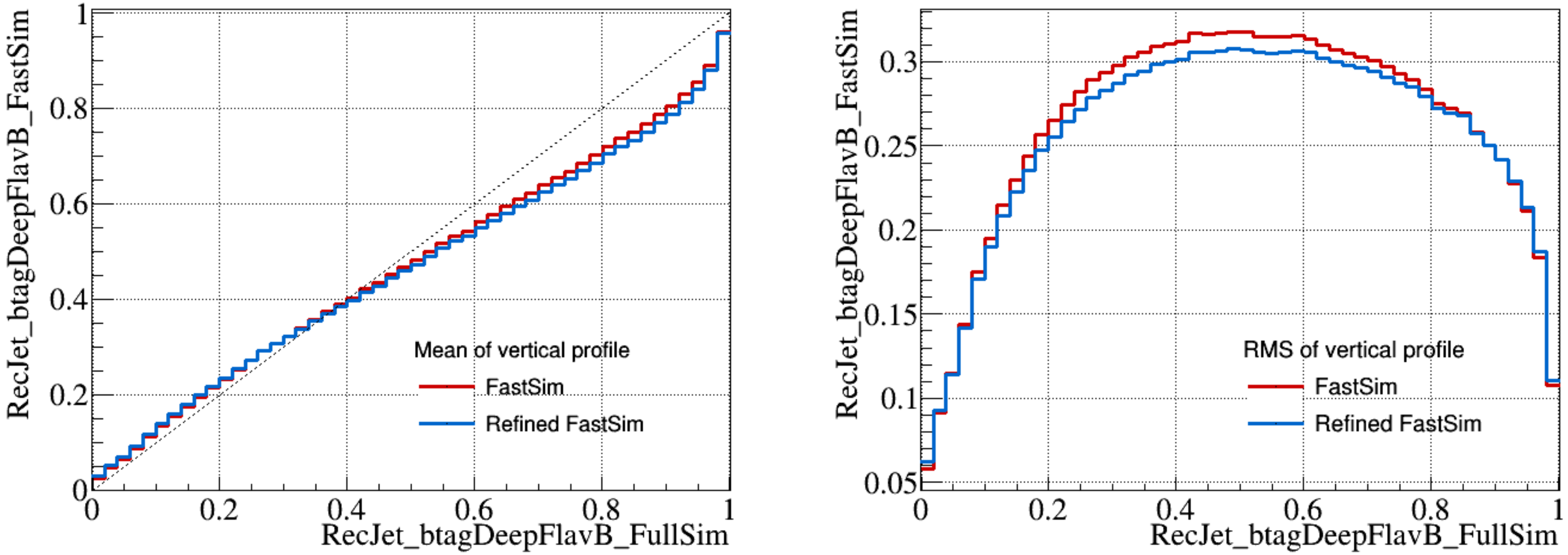

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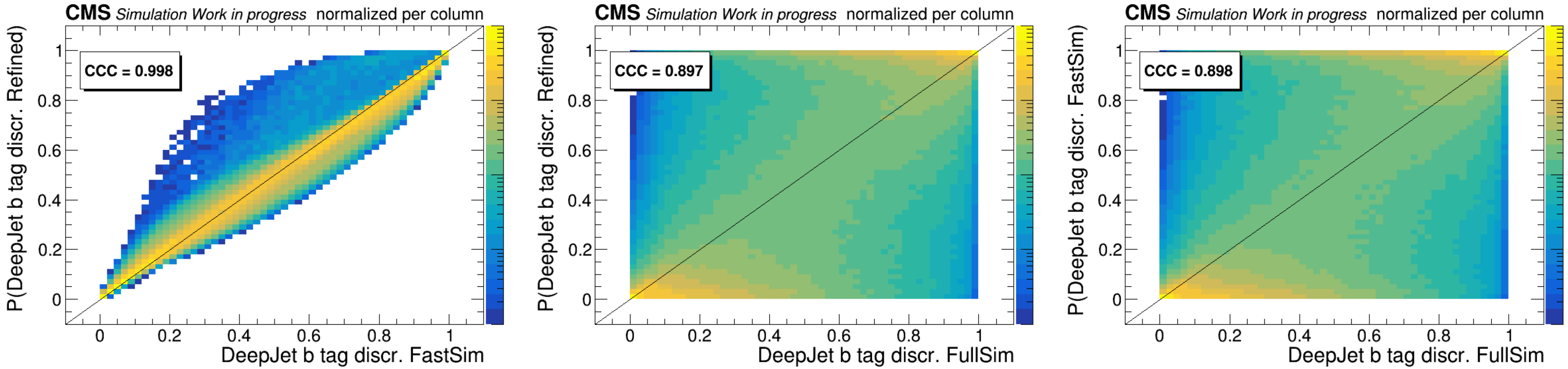
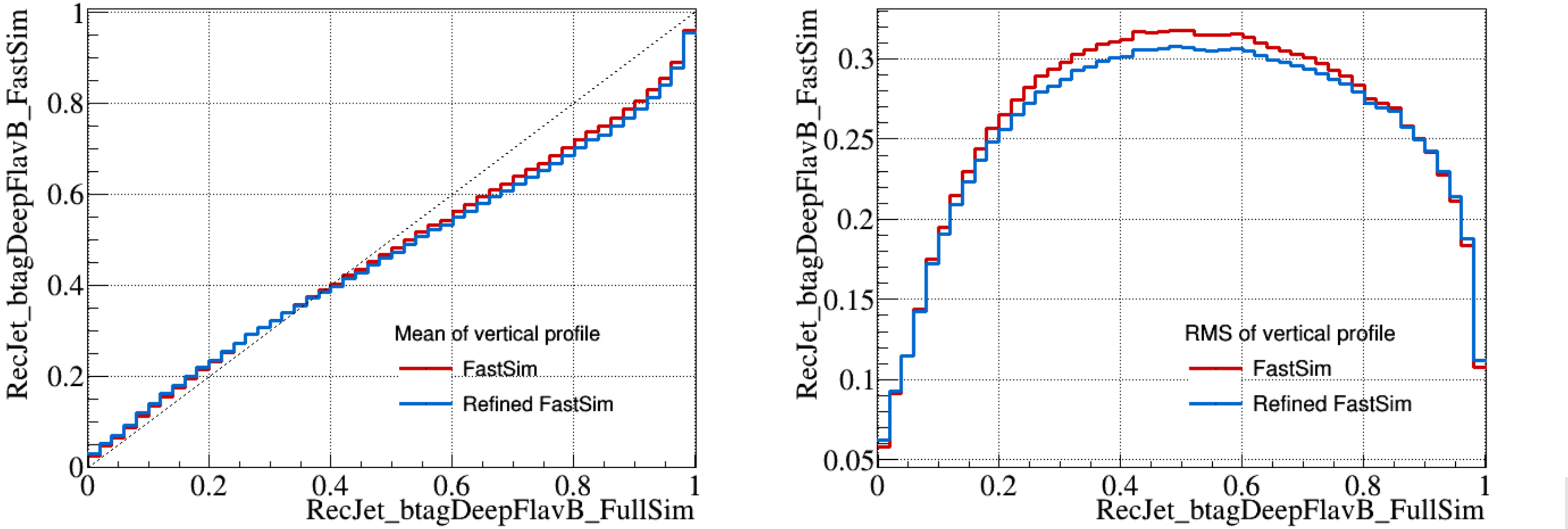
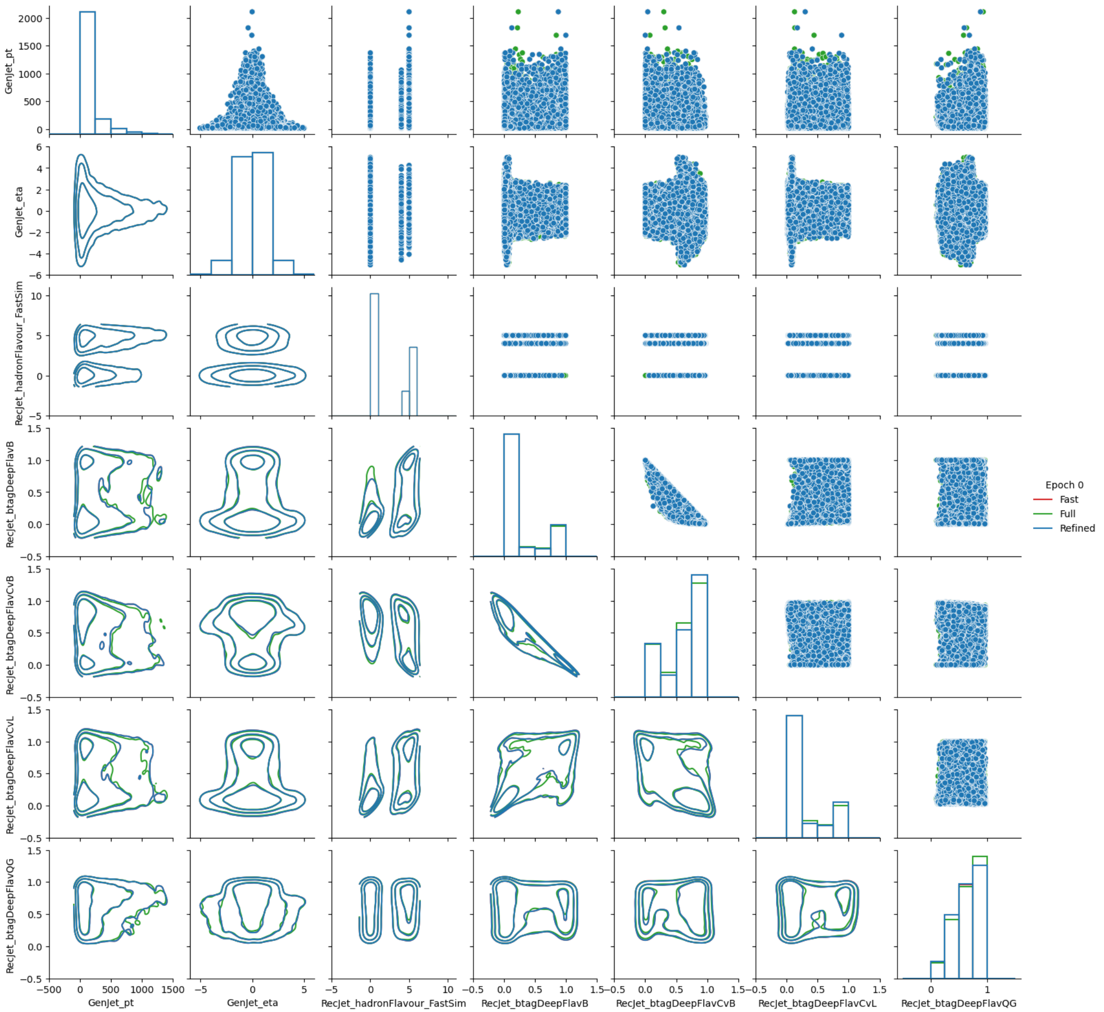




REFINING (REGRESSION) – TRAINING SHAPSHOTS (EPS=0.084)

- Starting point
- Normal space

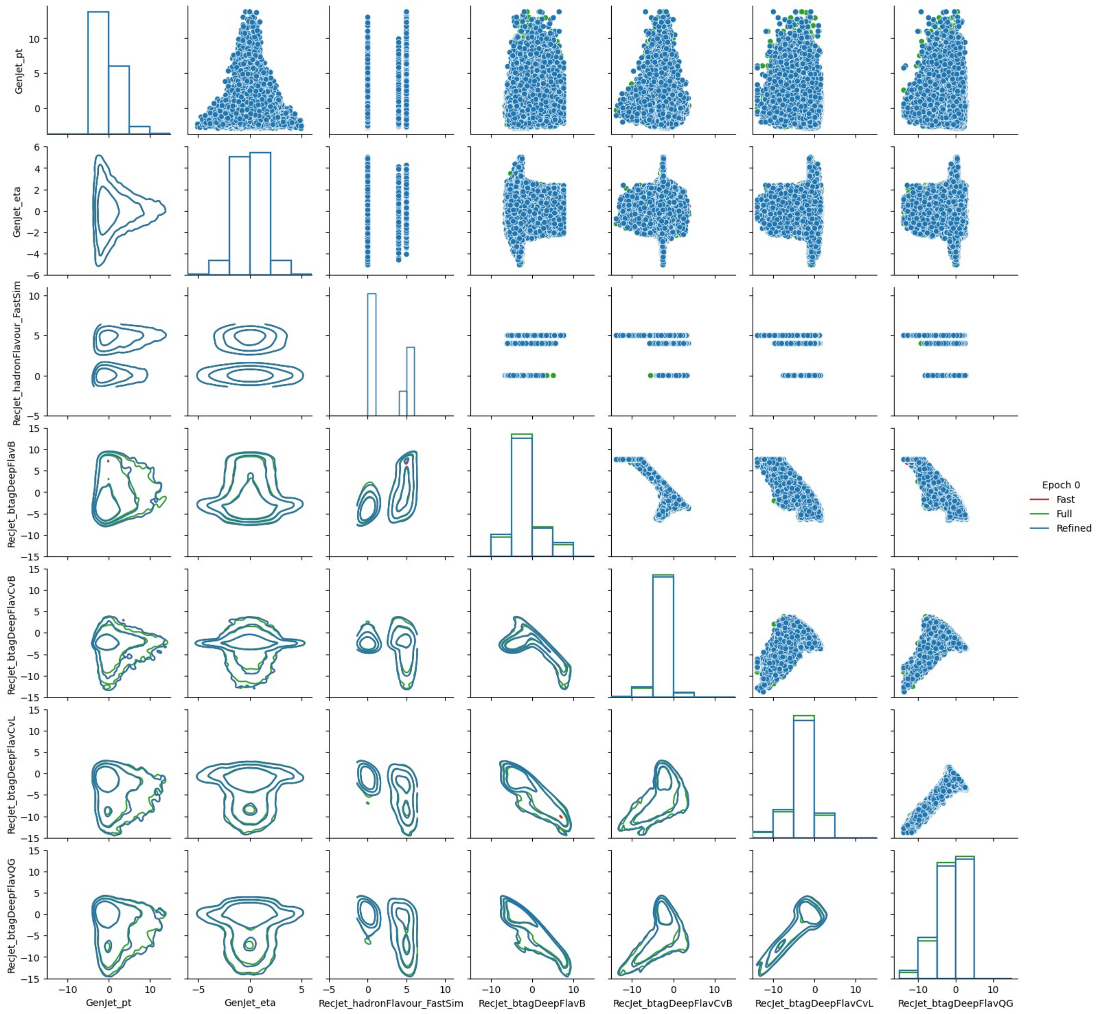


REFINING (REGRESSION) – TRAINING SHAPSHOTS (EPS=0.084)

- After epoch 100
- Normal space

Refining (Regression) – Training shapshots (eps=0.084)

- Starting point
- Transformed space



Refining (regression) – training shapshots (eps=0.084)

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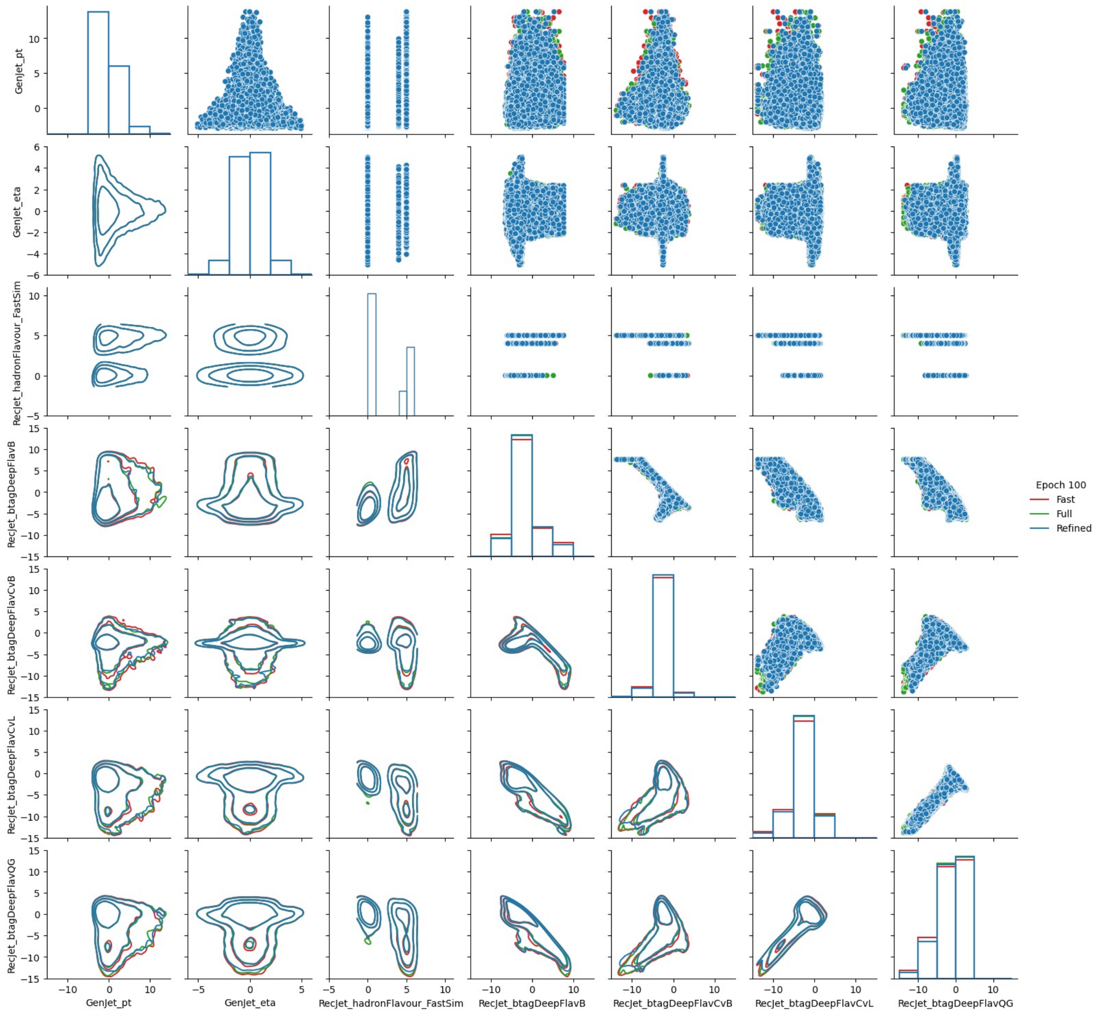
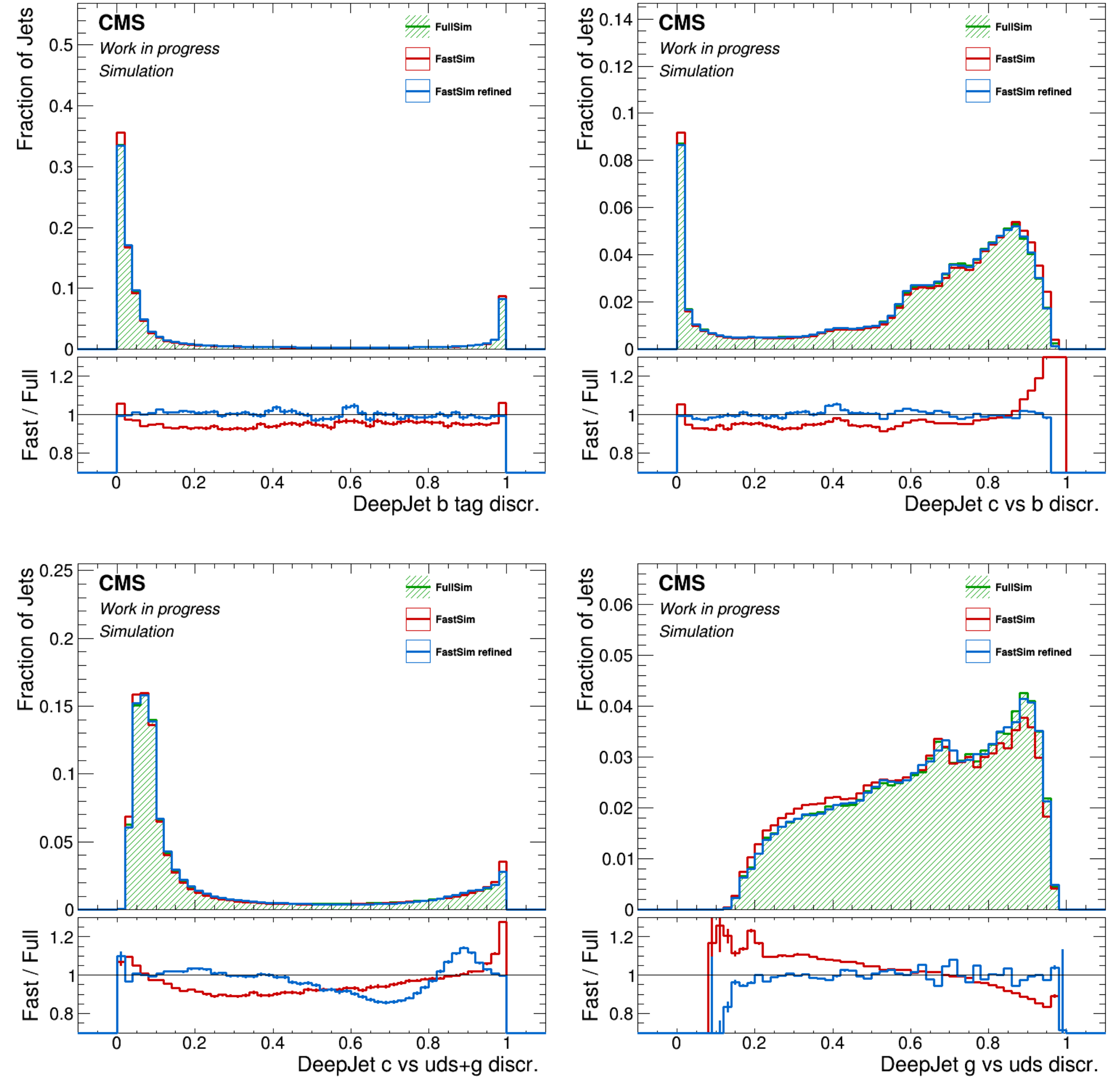
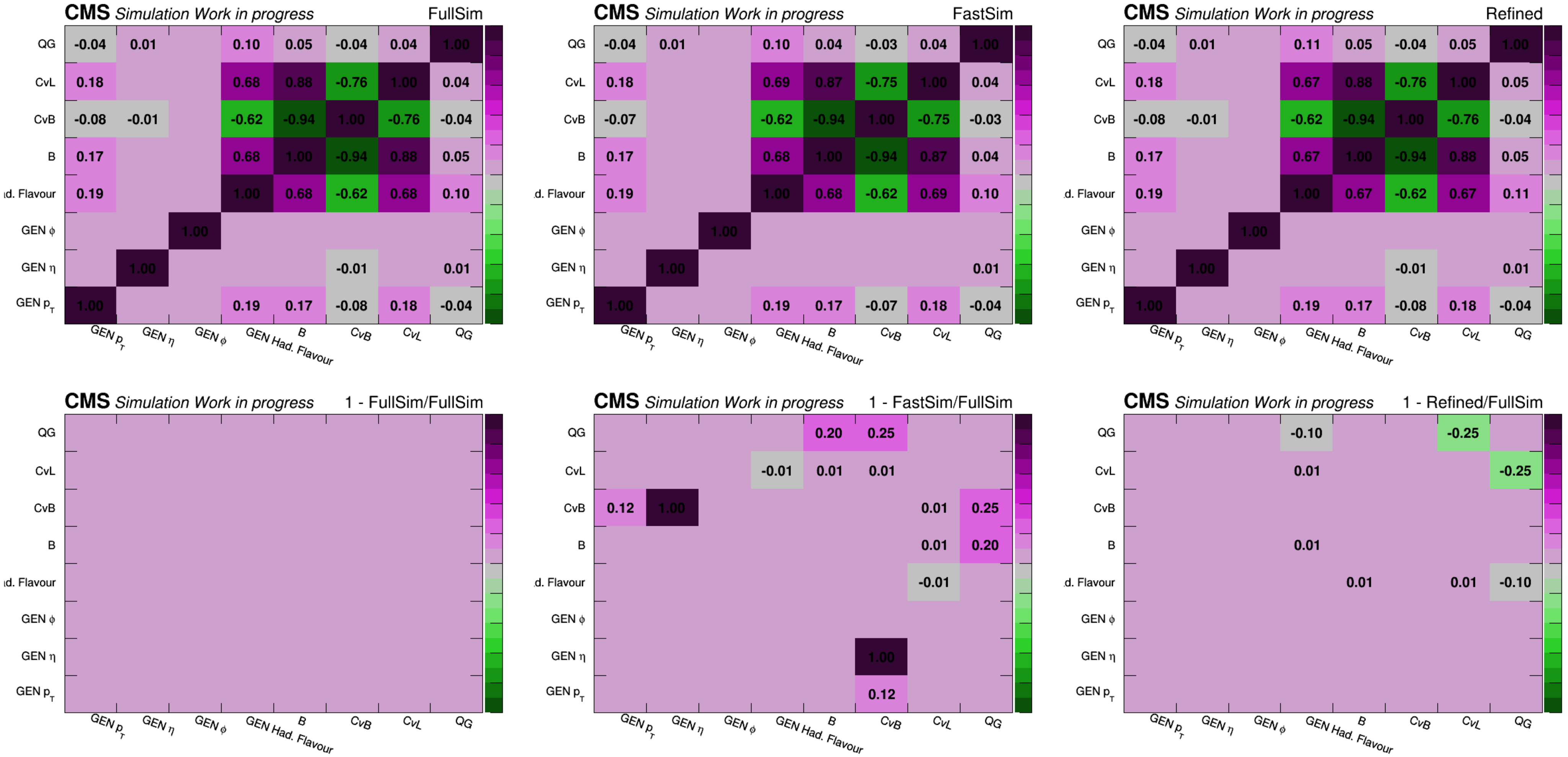


REFINING (REGRESSION) – VALIDATION IN TTBAR (ONLY MMD)

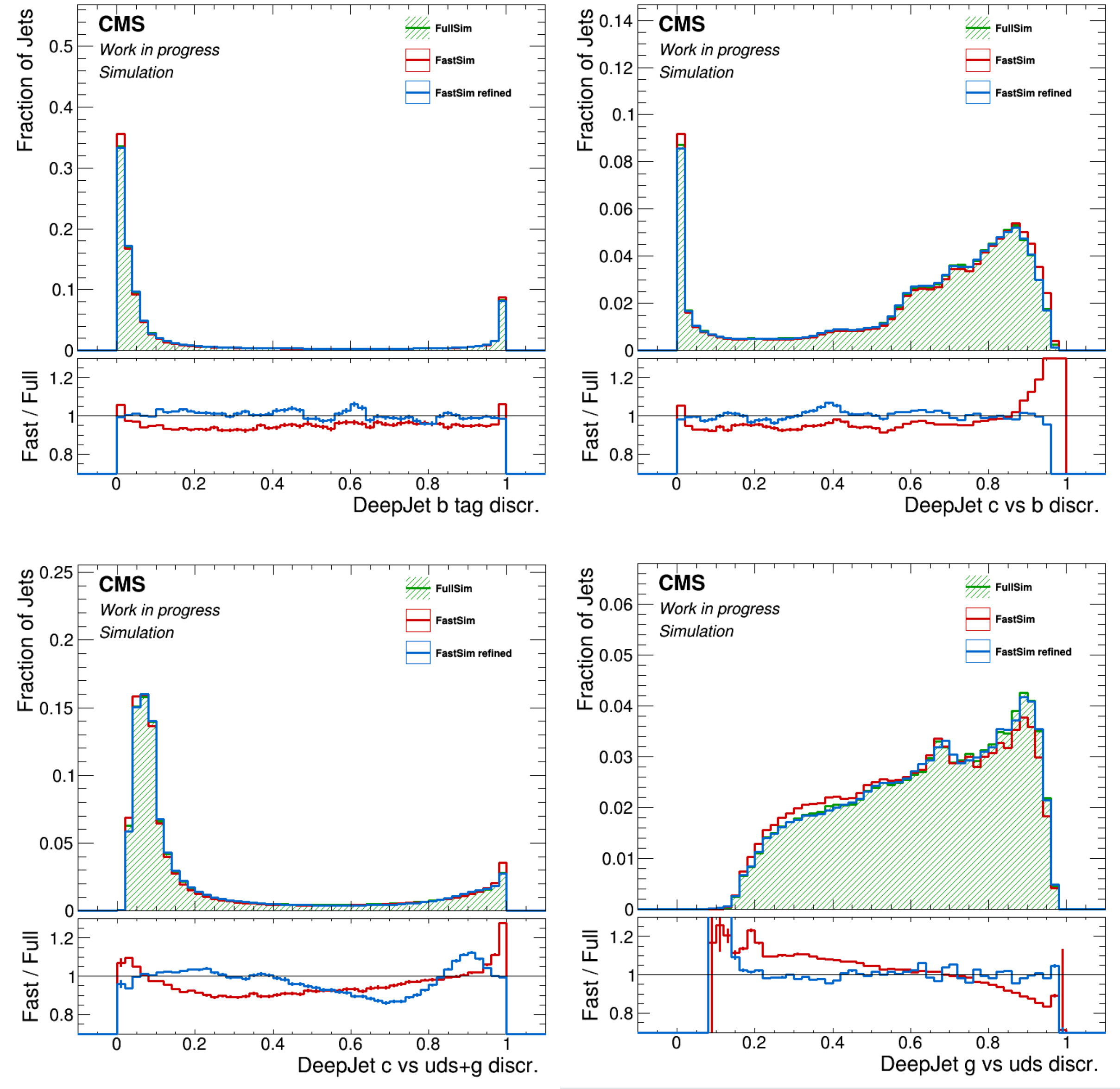


- Good performance for evaluation on **TTbar** (NN trained on T1tttt SUSY dataset)

REFINING (REGRESSION) – VALIDATION IN TTBAR (ONLY MMD)



REFINING (REGRESSION) – VALIDATION IN TTBAR (EPS=0.083)



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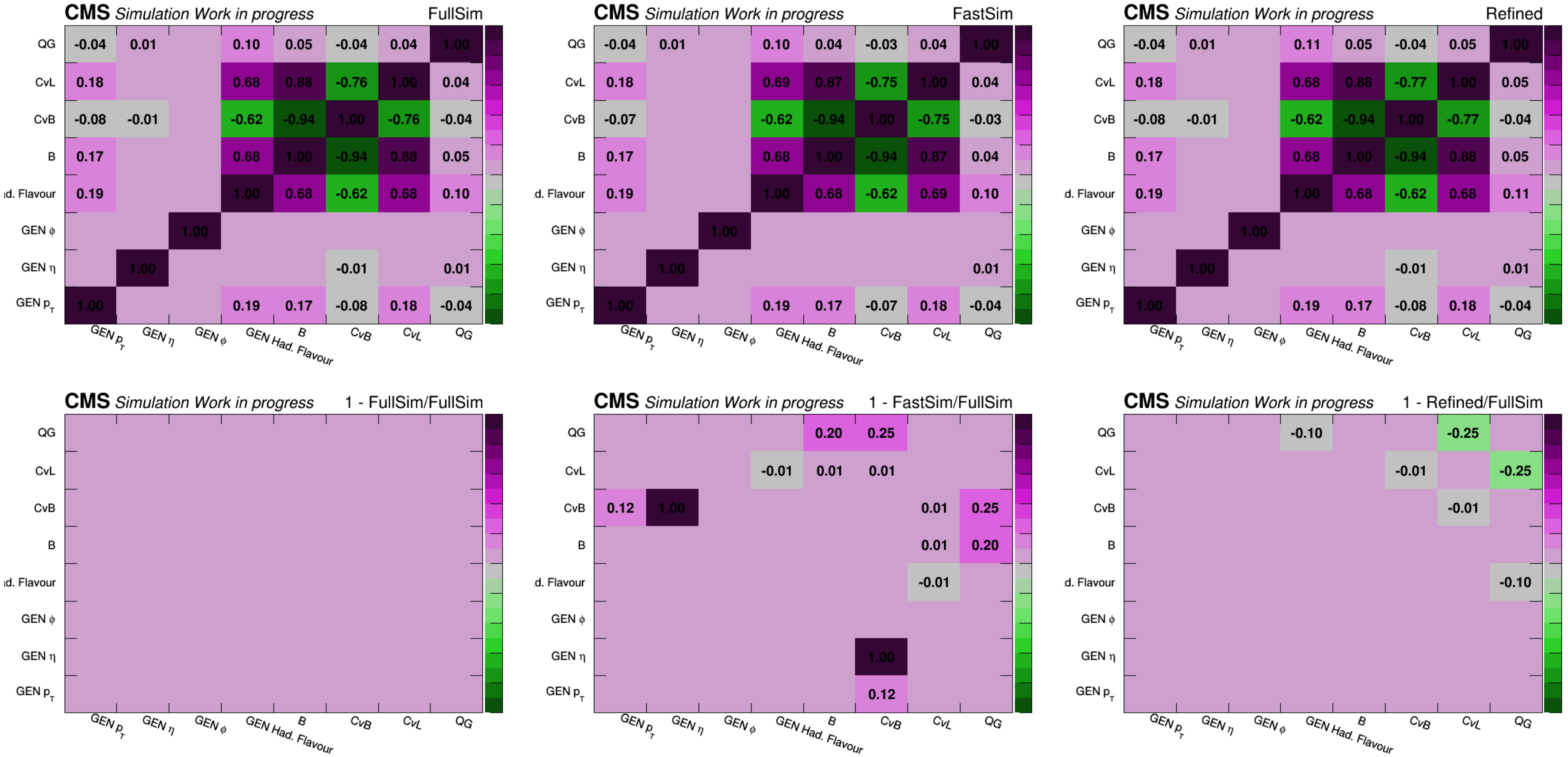
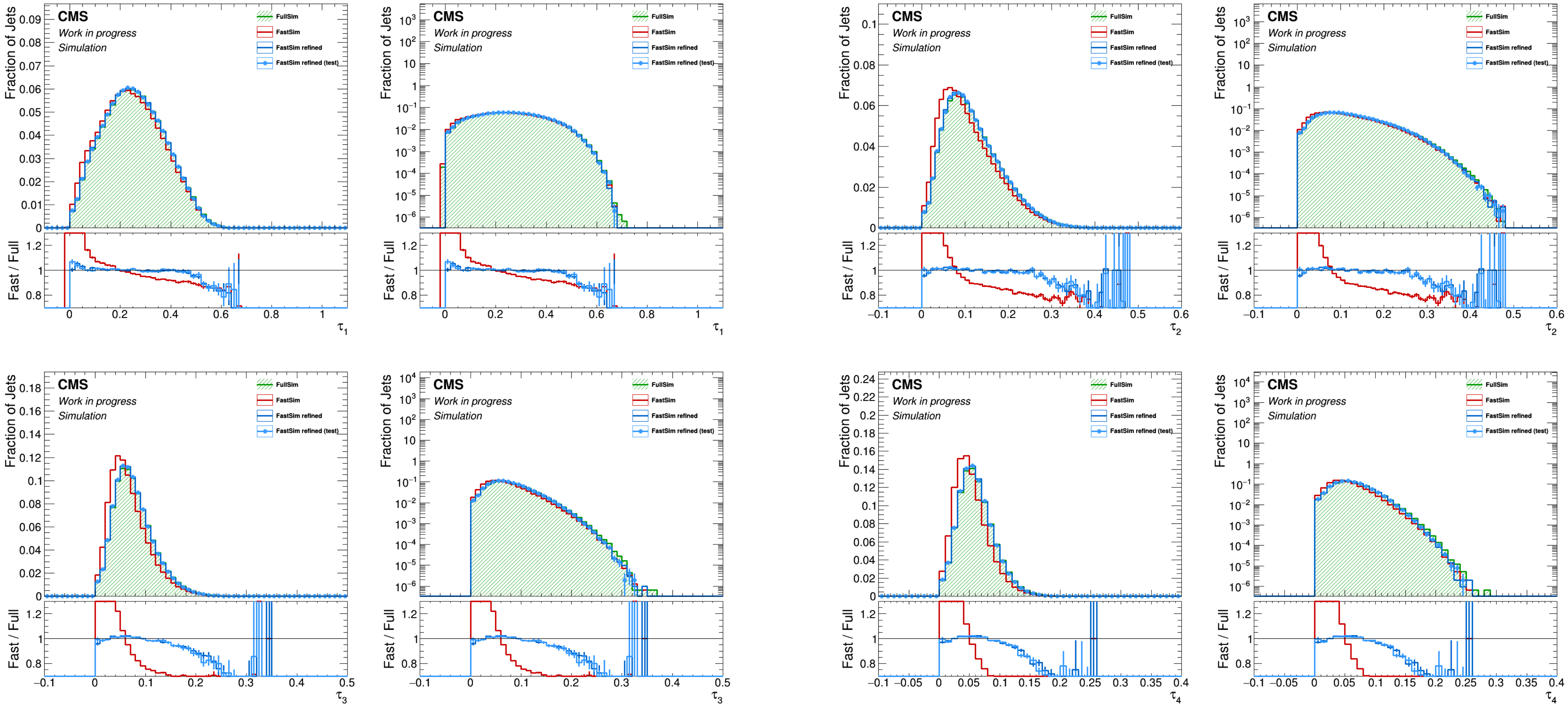


REFINING (REGRESSION) – FATJETS (ONLY MMD)



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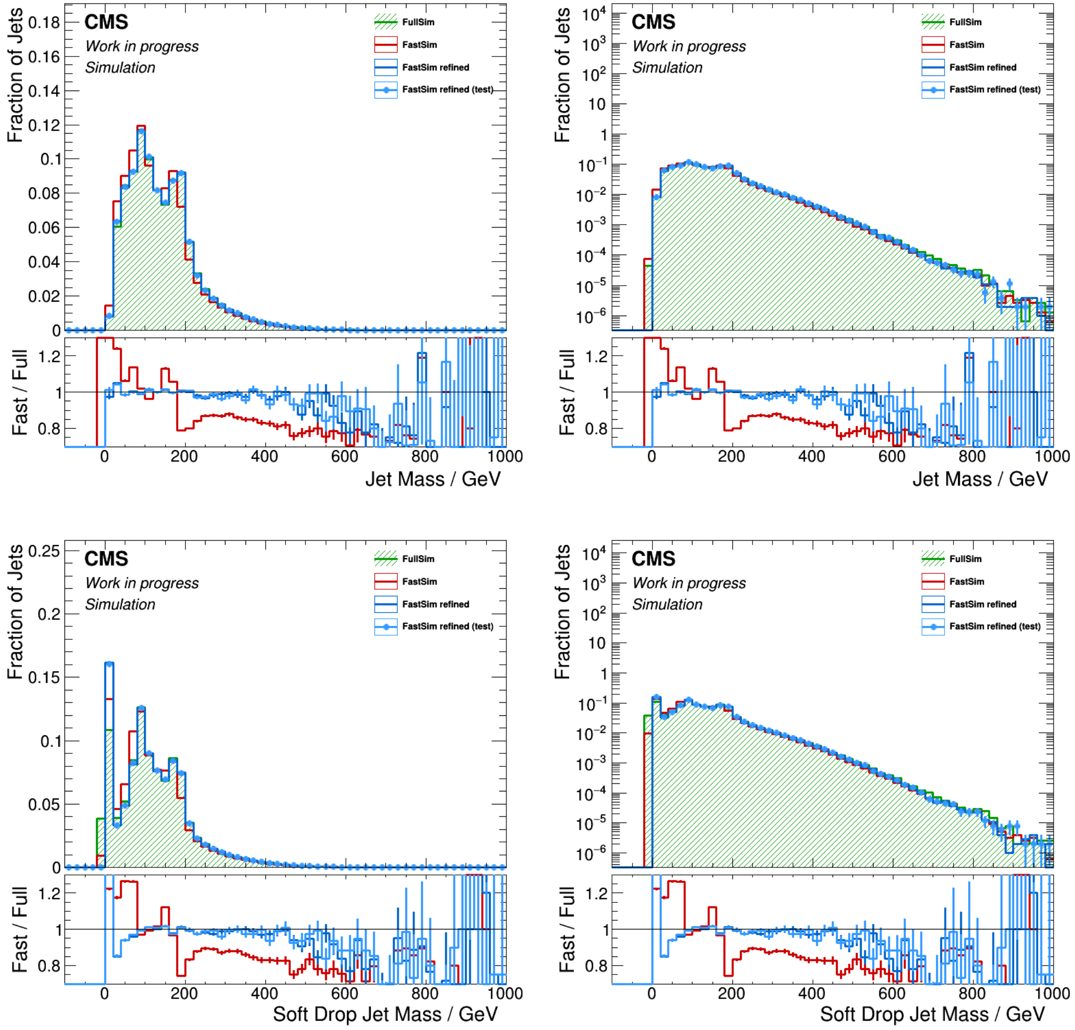

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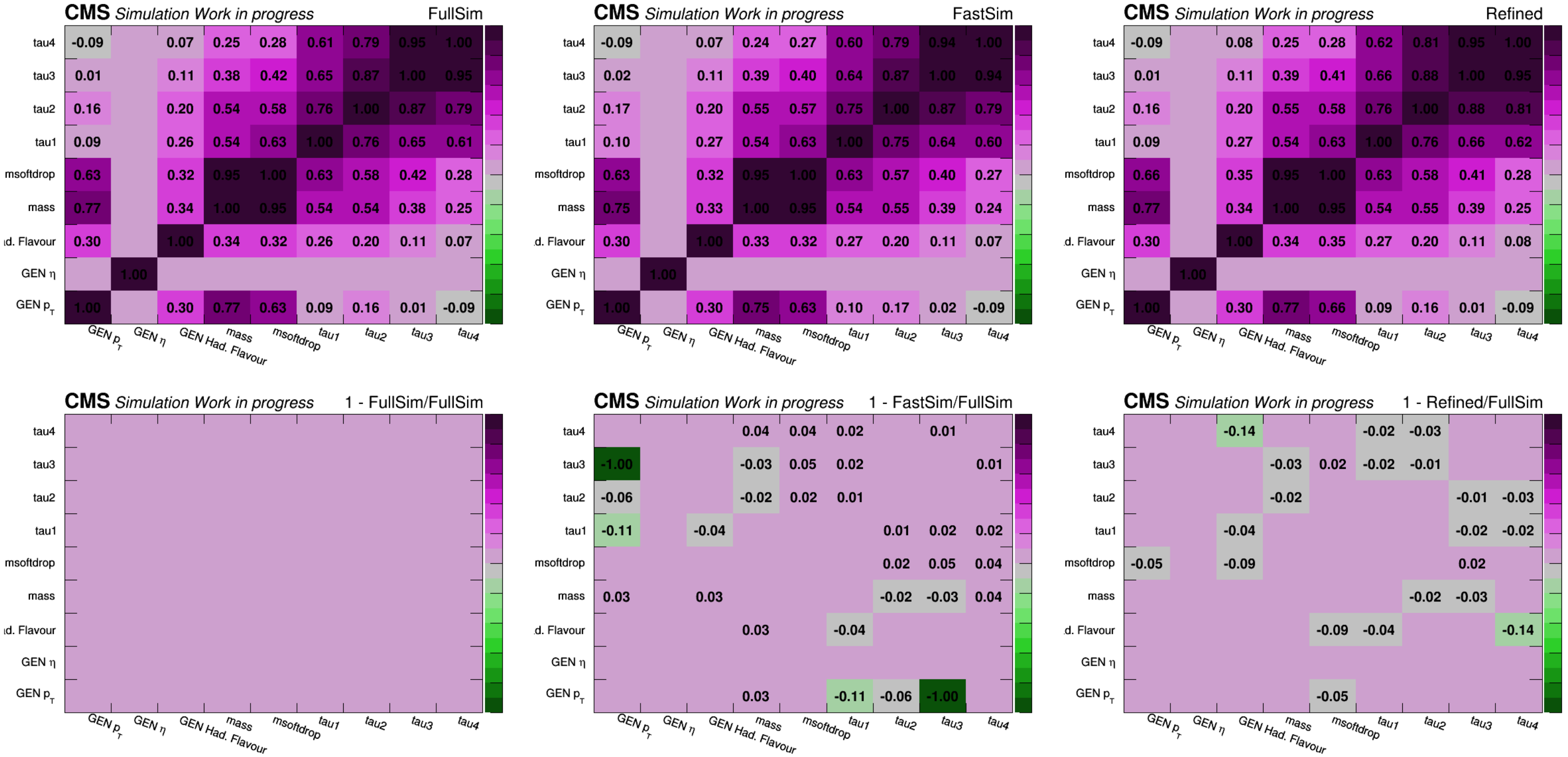
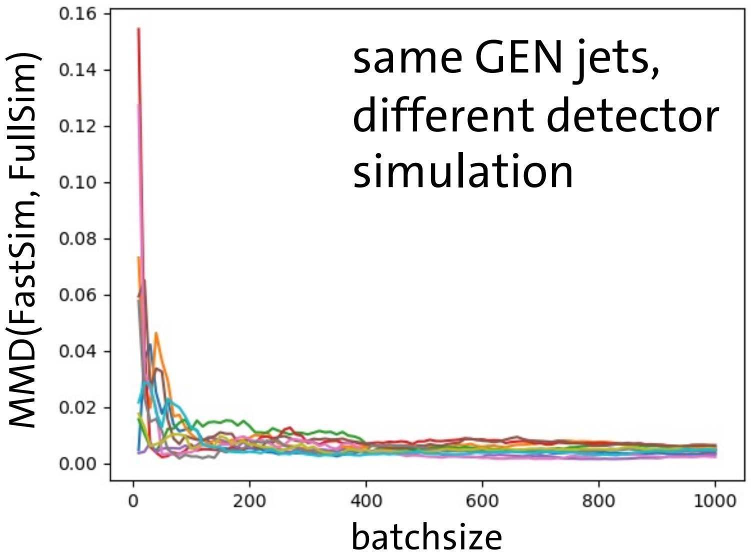


Refining (regression) – network details

- Jet preselection dR(jet, closest jet) > 0.5 (for GEN, FastSim & FullSim jet individually)
- NN architecture
  - LeakyReLU negative slope = 0.01
  - Dropout rate = 0.5
- Loss terms
  - Huber delta = 0.1
  - MMD calculated individually for each class of hadron flavour: $\mathrm{MMD} = \sum_{i\,\epsilon\,had.\,flav.} MMD_i$
  - MMD Gaussian kernel bandwidth adaptive: $\mathrm{MMD} = \sum_{\sigma\,\epsilon\,\{\frac{\sigma_0}{100},\frac{\sigma_0}{10},\sigma_0,10\sigma_0,100\sigma_0\}} MMD_\sigma$, $\sigma_0 = \overline{\mathrm{L2\ dist.}}$
- Training
  - Learning rate = 1e-4 (exponential decay with $\gamma = 0.96$ each epoch)
  - Adamax optimizer

REFINING (REGRESSION) – MMD



- Training on jet$^{\text{FastSim}}$-jet$^{\text{FullSim}}$ pairs problematic (stochasticity in simulations)
  → instead use measure that compares **distributions**
- From Wikipedia:

Kernel two-sample test [edit]

Given *n* training examples from $P(X)$ and *m* samples from $Q(Y)$, one can formulate a test statistic based on the empirical estimate of the MMD

$$\widehat{\mathrm{MMD}}(P,Q) = \left\| \frac{1}{n}\sum_{i=1}^{n}\varphi(x_i) - \frac{1}{m}\sum_{i=1}^{m}\varphi(y_i) \right\|_{\mathcal{H}}^2$$

$$= \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}k(x_i,x_j) + \frac{1}{m^2}\sum_{i=1}^{m}\sum_{j=1}^{m}k(y_i,y_j) - \frac{2}{nm}\sum_{i=1}^{n}\sum_{j=1}^{m}k(x_i,y_j)$$

to obtain a **two-sample test** [12] of the null hypothesis that both samples stem from the same distribution (i.e. $P=Q$) against the broad alternative $P \neq Q$.

- Gaussian kernel: $k(x,x') = \exp\left(-\frac{1}{2\sigma^2}\|x-x'\|^2\right)$
- Plot: MMD of different FastSim/FullSim jet batches with varying size (jets defined by p_T, η, DeepCSV)
  - **Batchsize** must be large enough to get a good estimate

REFINING (REGRESSION) – MDMM ALGORITHM

- Simple approach: add with constant weights
- Better: **Modified Differential Method of Multipliers** algorithm: [1] original paper, [2] explanatory blog post
  reframe problem as **constrained optimization** using a **Lagrangian**: $\mathcal{L} = f(\theta) - \lambda * (\varepsilon - g(\theta))$
  - Minimize $f(\theta)$ („primary loss") subject to $g(\theta) = \varepsilon$ („additional loss")
  - Convergence mathematically formalized, steady states are saddle points
  - Lagrange multiplier λ is adapted in the training along with NN parameters θ
  - $f(\theta)$ and $g(\theta)$ depend on each other
    → both can't be arbitrarily small at the same time
    → have to choose ε (point along Pareto front)

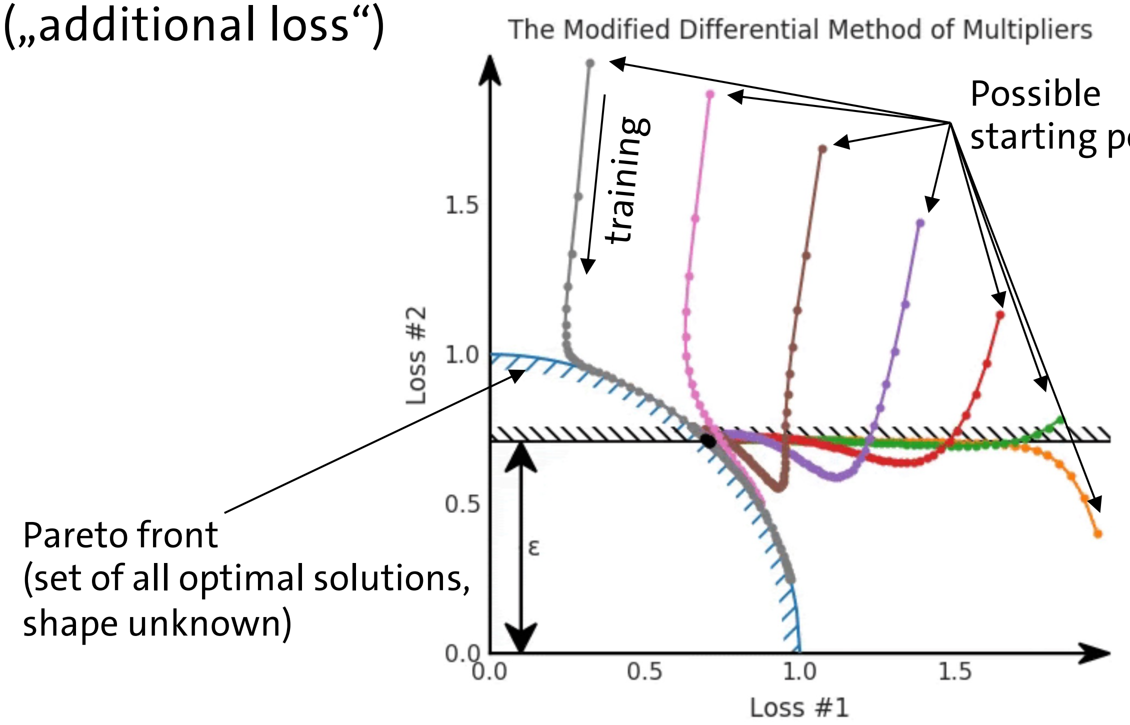
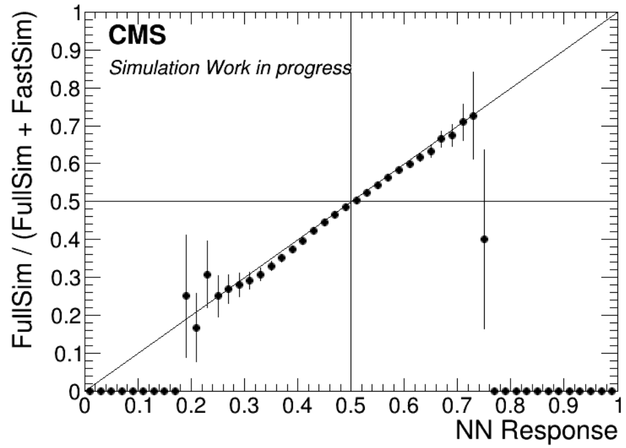


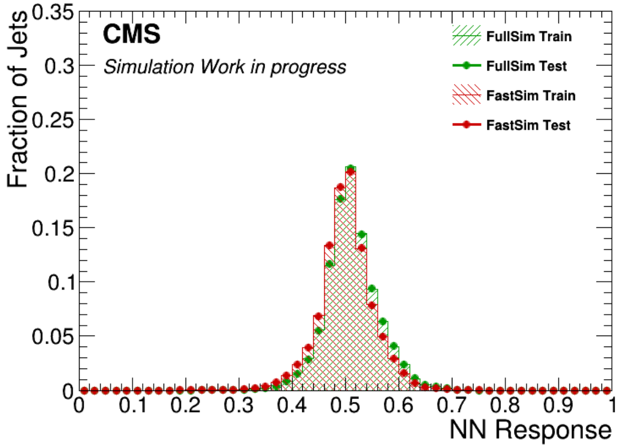
image from [2]

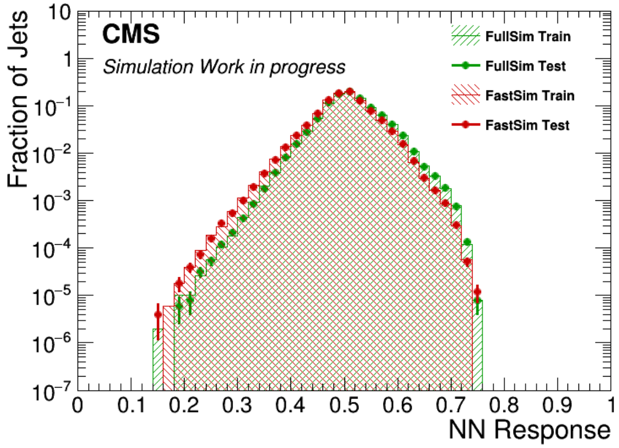
REWEIGHTING (DCTR)

- **DCTR** approach (*Deep neural networks using Classification for Tuning and Reweighting,* arXiv:1907.08209)
  1. Train calibrated NN classifier f(x) to distinguish FastSim from FullSim
  2. Define weight $w(x) = f(x) / (1 – f(x)) \approx p_{\text{FullSim}}(x) / p_{\text{FastSim}}(x)$
  3. Reweight FastSim by w(x)

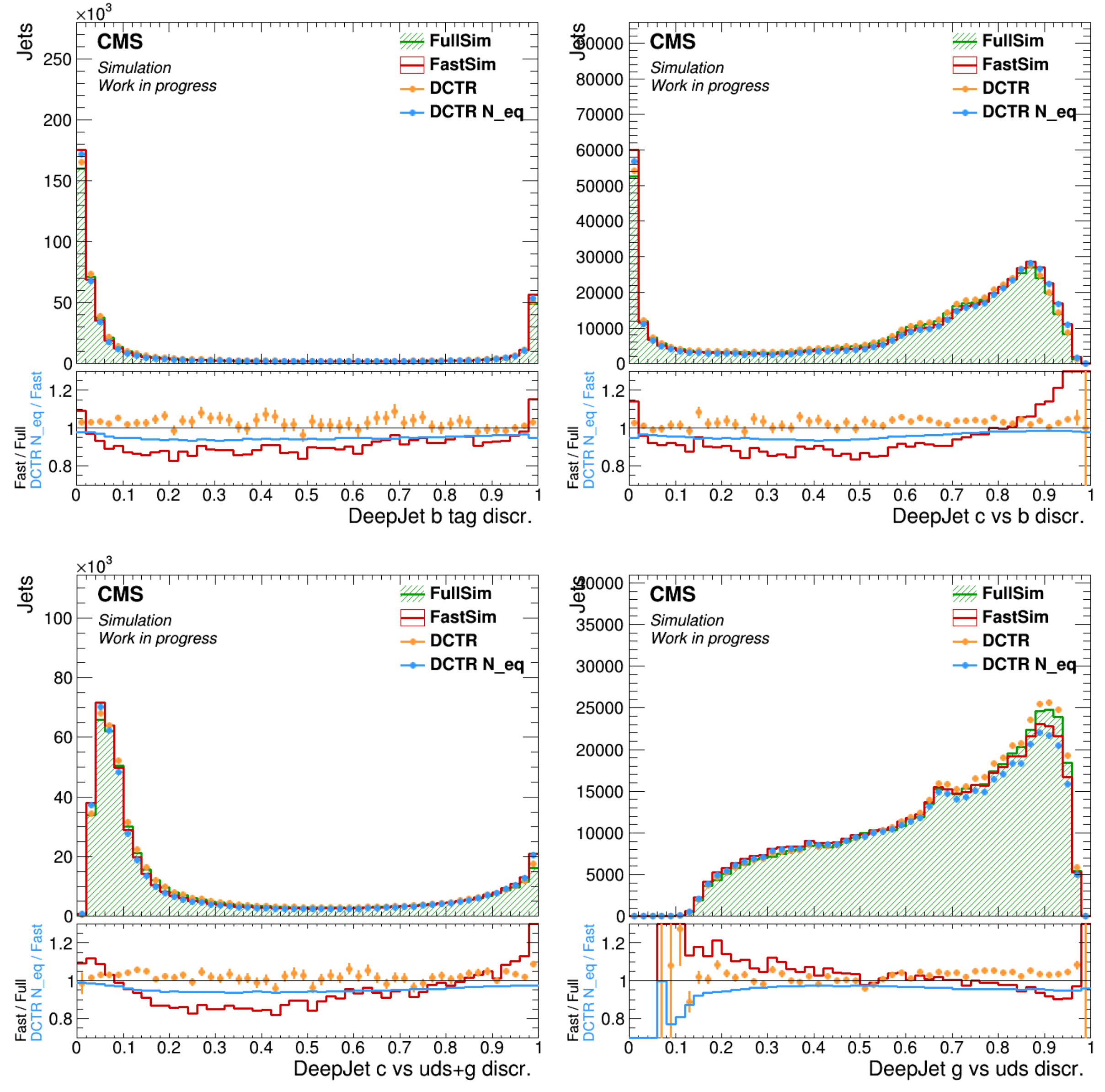


- Input **variables**: 4 DeepJet discriminator values
- GEN parameters: p_T^{GEN}, η^{GEN}, true hadron flavor
- Simple **fully-connected NN**:
  - 3 hidden layers with 64 nodes
  - Binary cross entropy loss
- Training with 1M jet triplets





REWEIGHTING (DCTR)



- **Good agreement** after reweighting
- Weights limit statistical power of FastSim

  → How to quantify?
- For a sample with N jets with weights $\sum_{i=1}^{N} w_i$
  - Error: $\delta Fast_{DCTR} = \sqrt{\sum_i w_i^2} = \sqrt{N * (RMS^2 + \overline{w}^2)}$

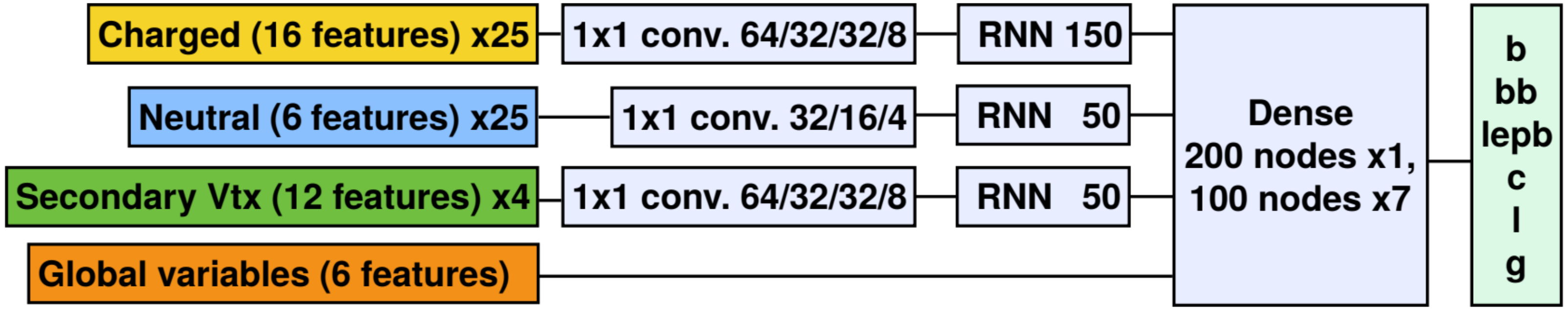
    with $RMS = \frac{1}{N} \sum_{i=1}^{N} (w_i - \overline{w})^2$
  - Equivalent events: $N_{eq} = \frac{(\sum_i w_i)^2}{\sum_i w_i^2} = \frac{N}{1+\left(\frac{RMS}{\overline{w}}\right)^2}$

    → N_{eq} events with weight=1 would have same relative statistical fluctuation

➢ Loss of **max. 5 – 10 %**

DEEPJET

- DeepJet architecture: 6 output nodes with **softmax** activation function → sum = 1 (arXiv:2008.10519)



- However, in NanoAOD: 4 (composite) discriminators:
  - btagDeepFlavB := b + bb + lepb
  - btagDeepFlavCvB := c / (c + b + bb + lepb)
  - btagDeepFlavCvL := c / (c + l + g)
  - btagDeepFlavQG := g / (g + l)

→ sum != 1