RAISE All-Hands Meeting in Iceland
Task 4.1:
Event reconstruction and classification at the CERN HL-LHC

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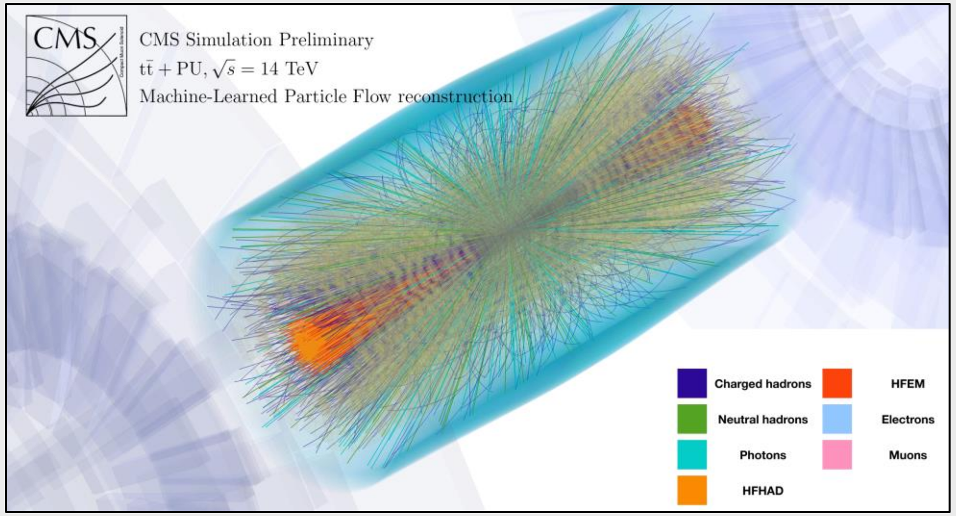
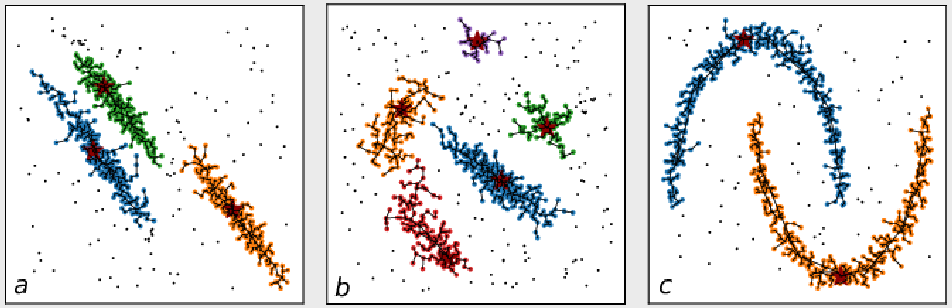
Introduction

- Task 4.1: Event reconstruction and classification at the CERN HL-LHC

- We work on four different but related efforts
  - AI–based particle flow reconstruction algorithm, *MLPF (Machine-learned Particle-Flow)* [1] (in collaboration with CMS)
  - Traditional GPU-accelerated clustering algorithm, *CLUE (CLUstering of Energy)* (in collaboration with CMS)
  - HW benchmarking based on AI-models for HEP
  - Data challenges for the Exascale era



Using MLPF in CMSSW.



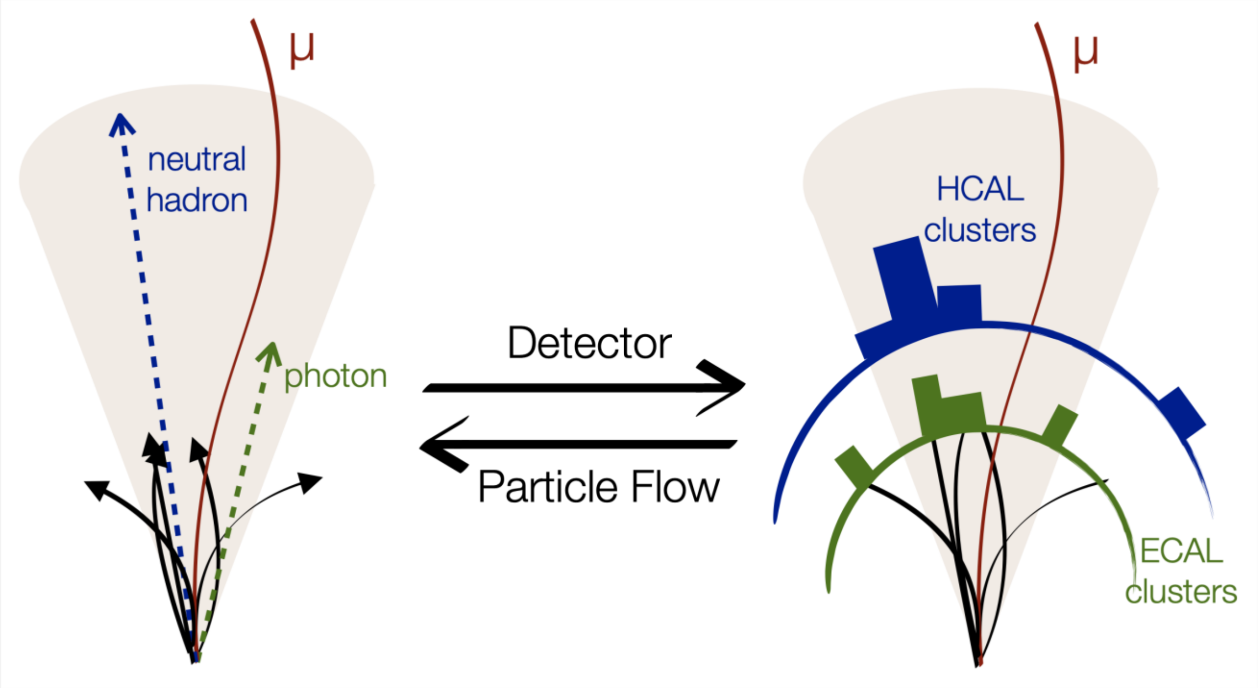
CLUE clustering on synthetic data. [2]

[1] J. Pata et al. Eur. Phys. J. C (2021) 81: 381 (https://link.springer.com/article/10.1140/epjc/s10052-021-09158-w)
[2] https://doi.org/10.3389/fdata.2020.591315

Event reconstruction using MLPF

What is event reconstruction?

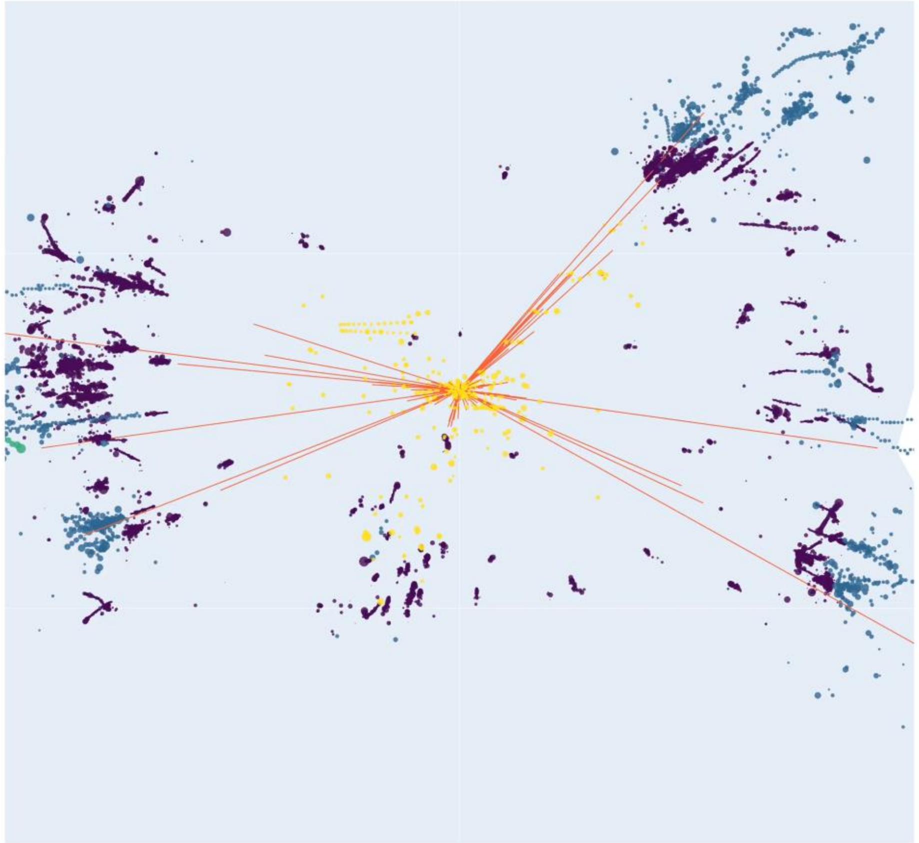
- Event reconstruction attempts to solve the inverse problem of particle-detector interactions, i.e., going from detector signals back to the particles that gave rise to them
- Particle-flow (PF) reconstruction takes tracks and clusters of energy deposits as input and gives particle types and momenta as output



New CoE RAISE Open Data

- https://www.coe-raise.eu/od-pfr
- An extensive open dataset of physics events with full GEANT4 [1] simulation, suitable for PF reconstruction, available in the EDM4HEP [2] format
- ~2.5 TB before pre-processing
- The dataset contains
  - Reconstructed tracks, calorimeter hits and clusters
    - We use these as inputs
  - All generator particles
    - We use these as targets
  - Reconstructed particles by the Pandora algorithm [3,4,5]
    - We use these as a baseline for comparison
- A mixture of $t\bar{t}$, $q\bar{q}$, ZH and WW events

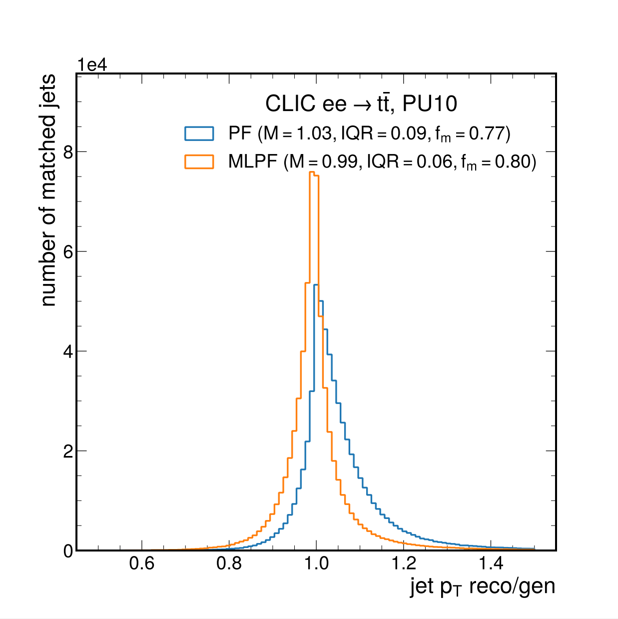
3D visualization of a single event

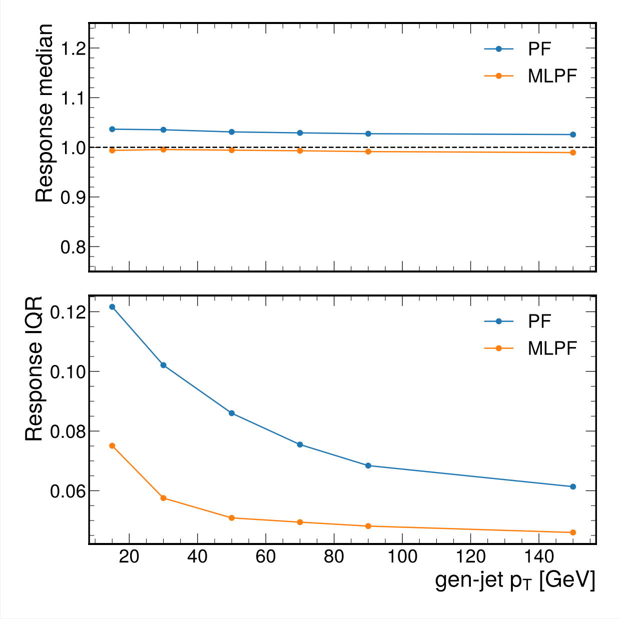


Jet and MET in ttbar + PU10 test data

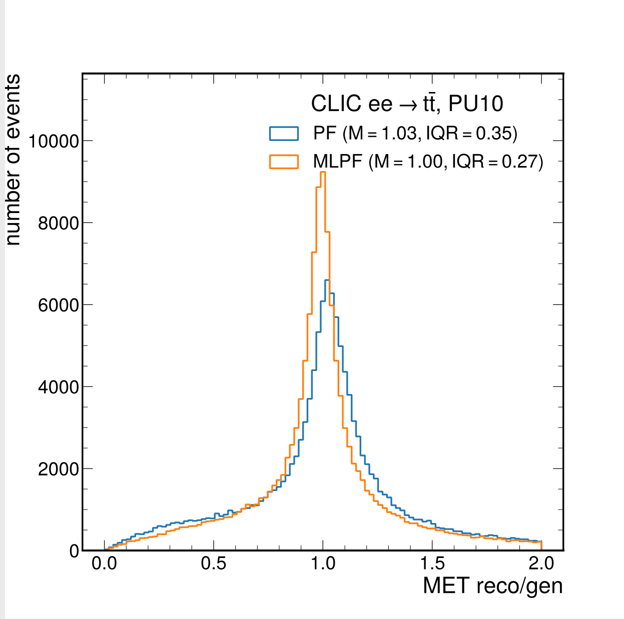
- For all test samples MLPF outperforms PF in Jet and MET reconstruction in terms of response width (quantified by median and interquartile range (IQR))
- MLPF also outperforms PF in terms of fraction of reconstructed jets $\left({}^{n_{reco\ jets}}/_{n_{ground-truth\ jets}}\right)$
- Very similar results are seen in ZH and WW events

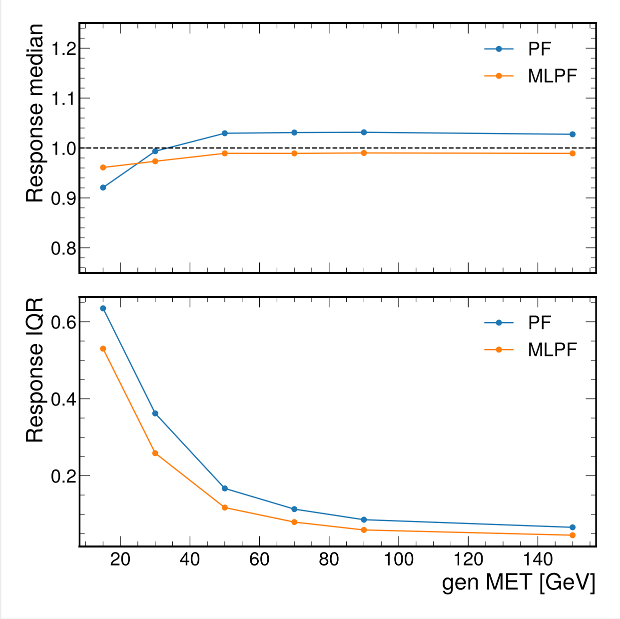
Jets resolution





MET resolution

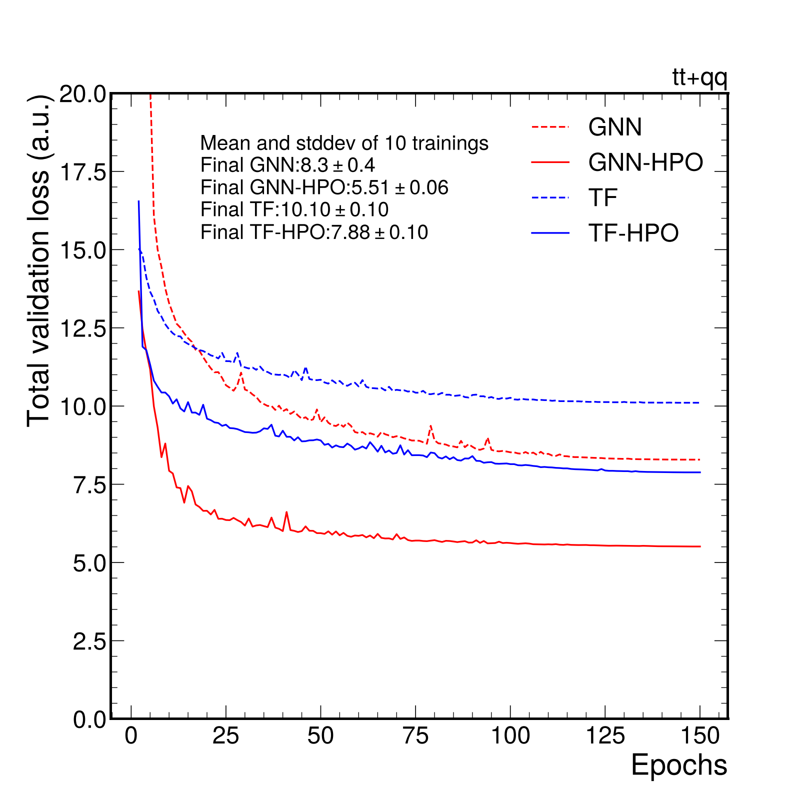




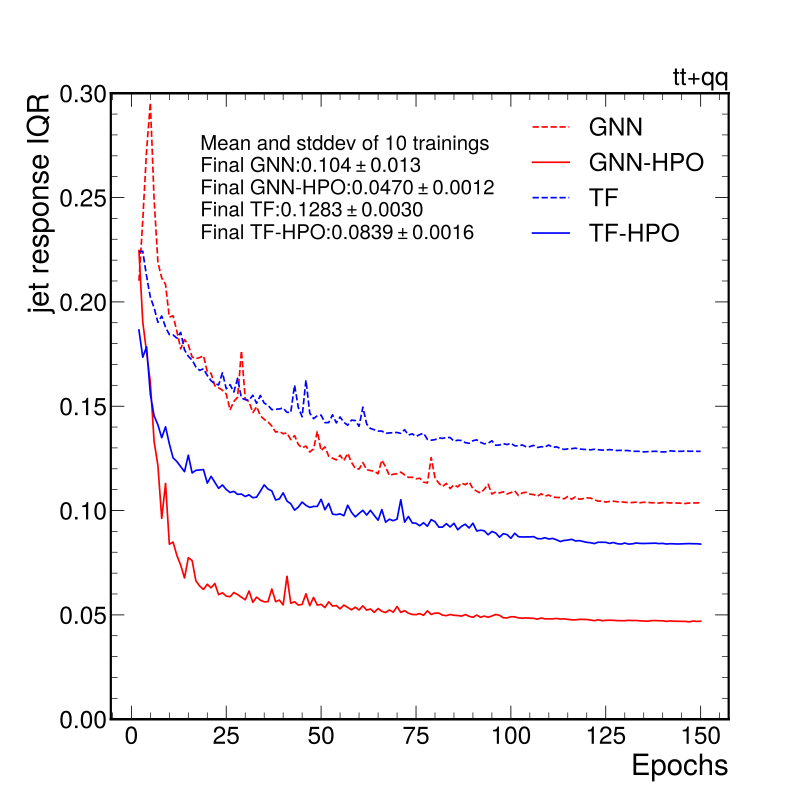
Improvement in training from HPO

- HPO significantly improved model performance for both the GNN-based and the transformer-based MLPF models
- GNN outperforms transformer

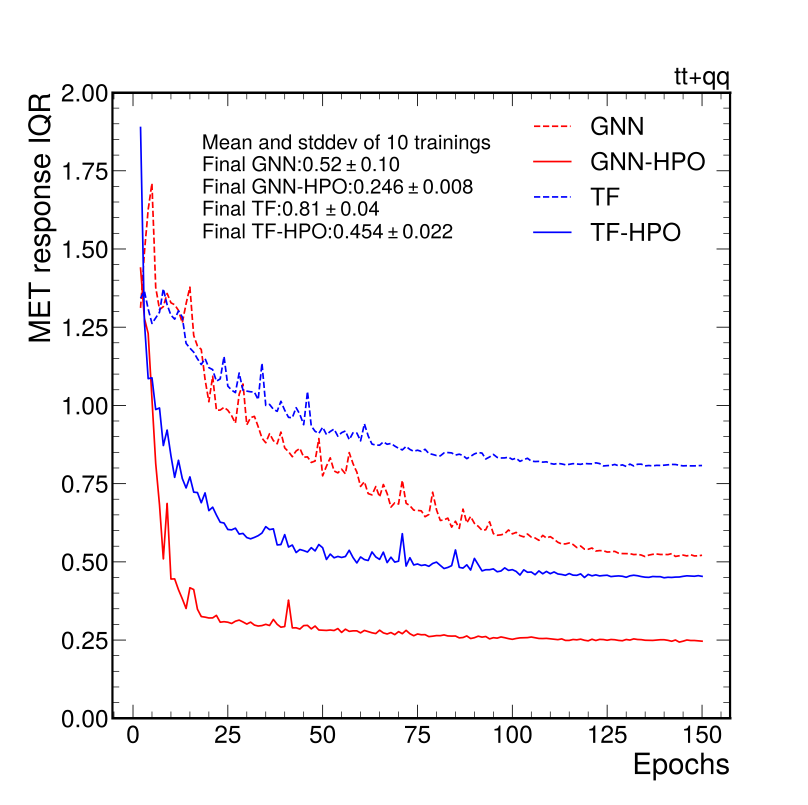
Validation loss



Jet resolution



MET resolution

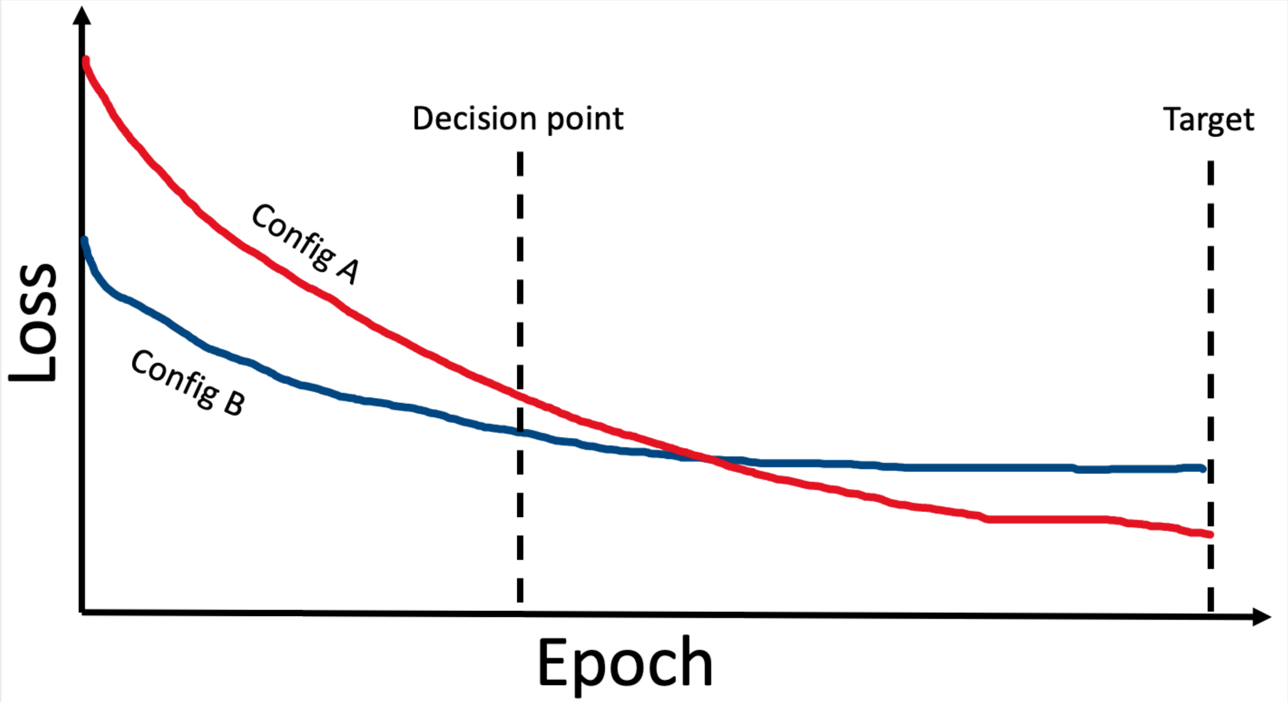


QSVR for model performance prediction

Hypertuning workflow

- Current STOTA hypertuning algorithms rely on early stopping
- Stopping criterion: ranking according to a single metric (e.g., validation loss)
- Potential problem: loss curves are not linear
- Idea 1: Use a non-linear stopping criterion
  - For instance, an SVR model, inspired by [1]
- Idea 2: Use quantum computing to fit Quantum-SVR (QSVR)

Sample random configs → Train n epochs → Terminate worst x% at last epoch



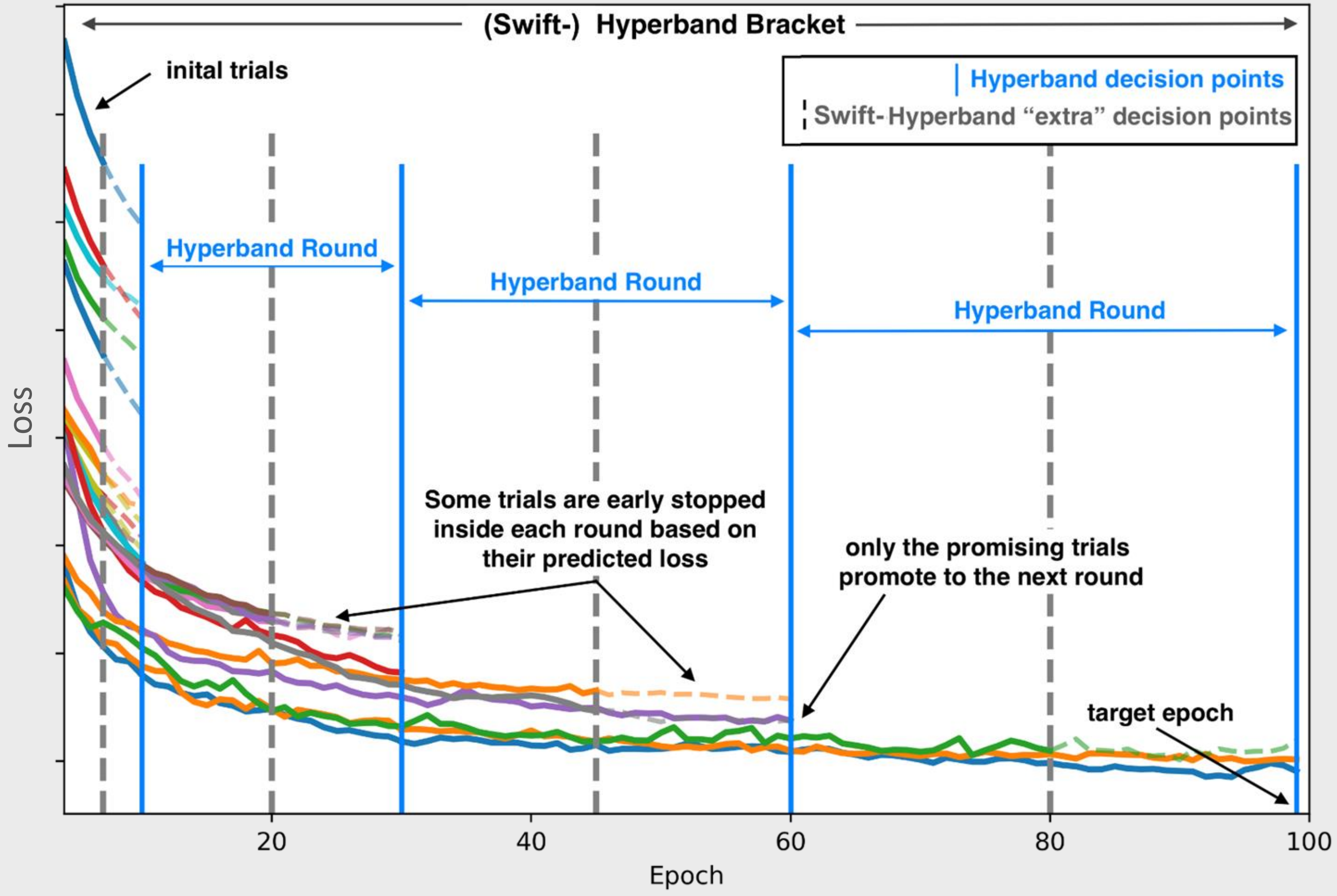
Swift-Hyperband

- Fast-Hyperband is not suitable for use with Quantum-SVRs
- Introducing: *Swift-Hyperband* – a new approach to combine performance prediction with Hyperband

Fast-Hyperband		Swift-Hyperband	
Multiple decision points inside each round	Trains **many** SVRs	Only 1 decision point inside each round	Trains **few** SVRs
Estimates σ for every SVR	↓	No need to estimate σ	↓
Sequential	**Not suitable for Q-SVRs**	**Easily parallelizable**	**Suitable for Q-SVRs**

Credit to Juan Pablo García Amboage, CERN Technical Student

Swift-Hyperband



- One extra decision in each round (dashed vertical lines)
- First, some trials are fully trained to define a threshold and to fit (Q)-SVR performance predictors
- Other trials are then partially trained
- If their predicted performance is worse than the threshold, they are stopped immediately

Algorithm Comparison

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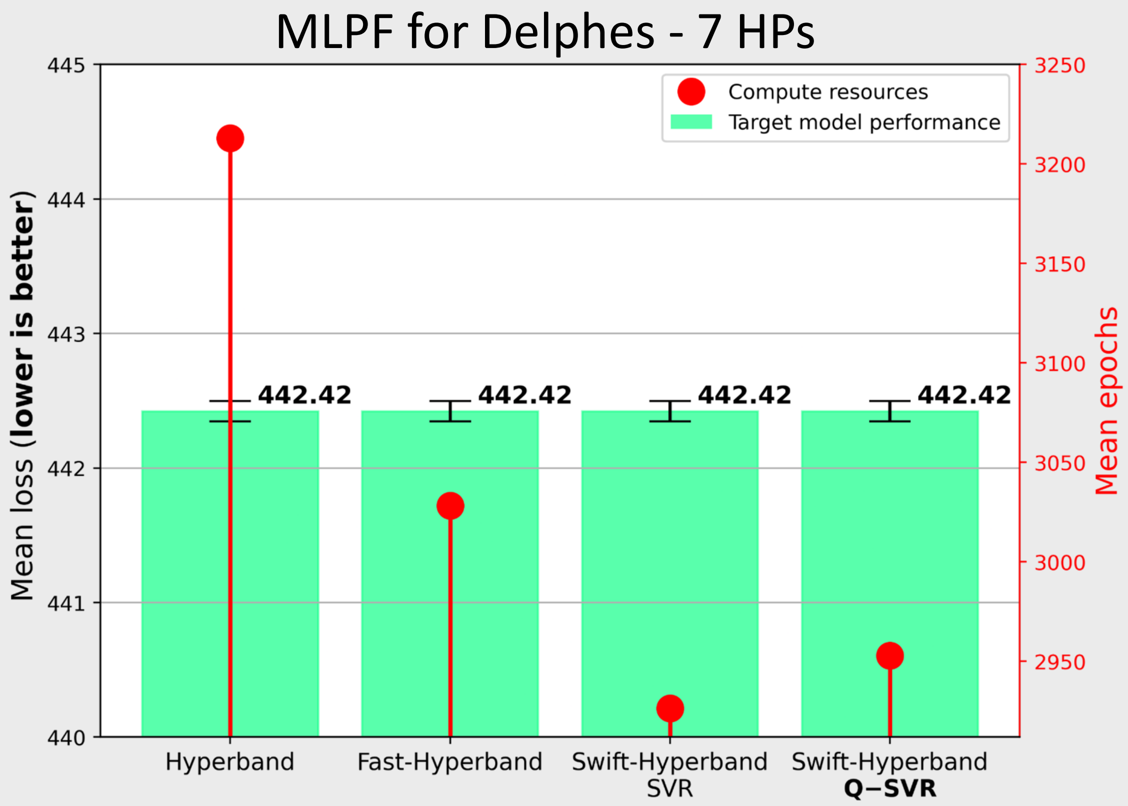
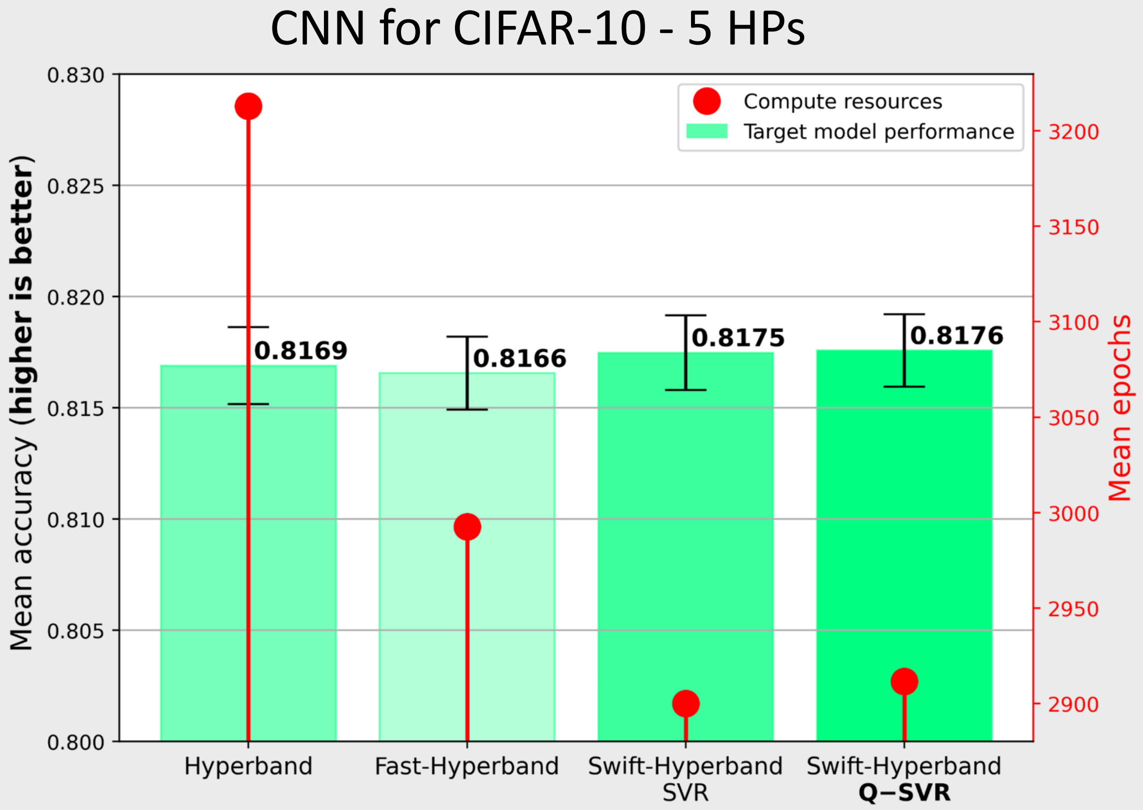
- Simulated results using datasets of existing learning curves

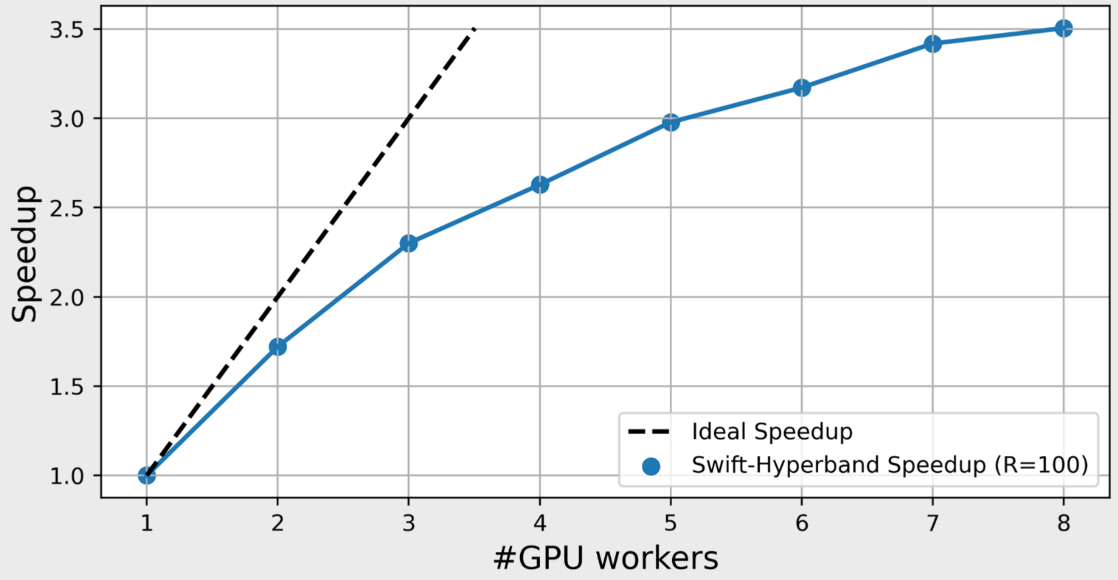




Credit to Juan Pablo García Amboage, CERN Technical Student

Distributed Swift-Hyperband

- Run on the DEEP-EST Extreme Scale Booster at FZJ
- Head node coordinates the workflow (1 CPU)
- Multiple GPU worker nodes for training trials
- Quantum Annealer for training the performance predictors
- Implemented using MPI and dwave-ocean-sdk



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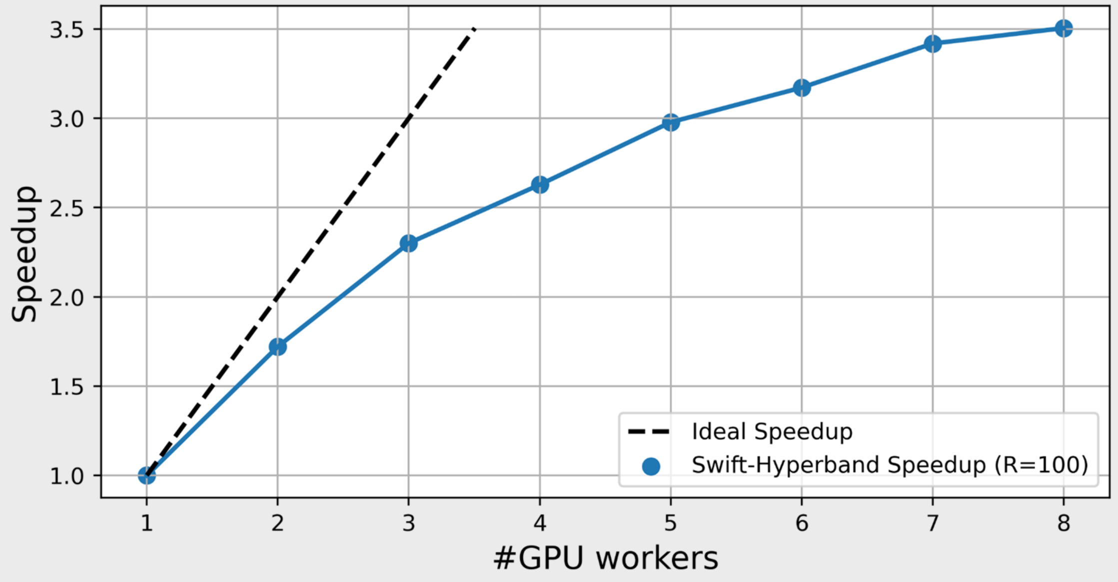

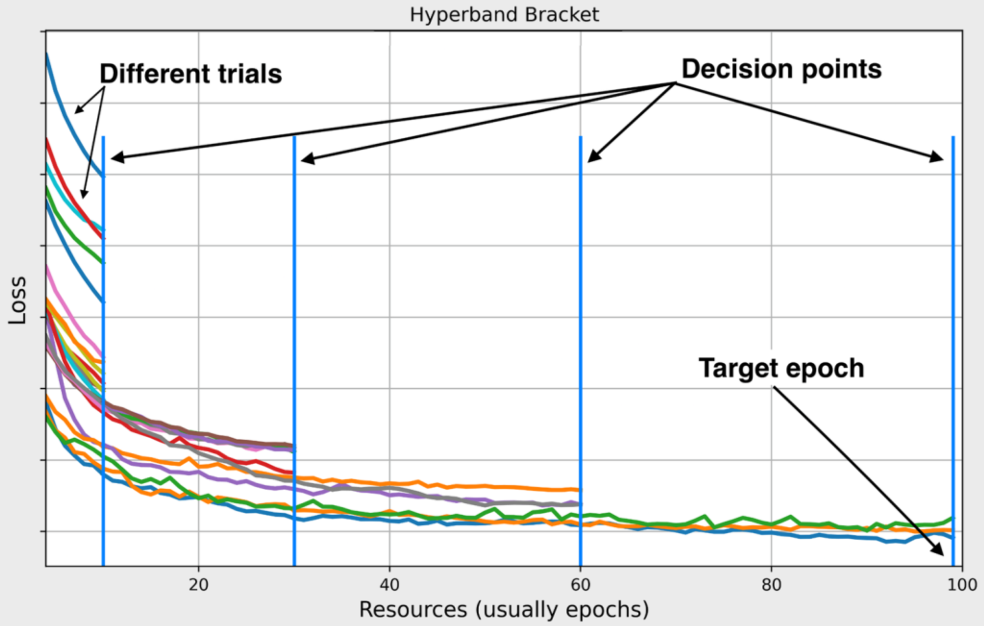

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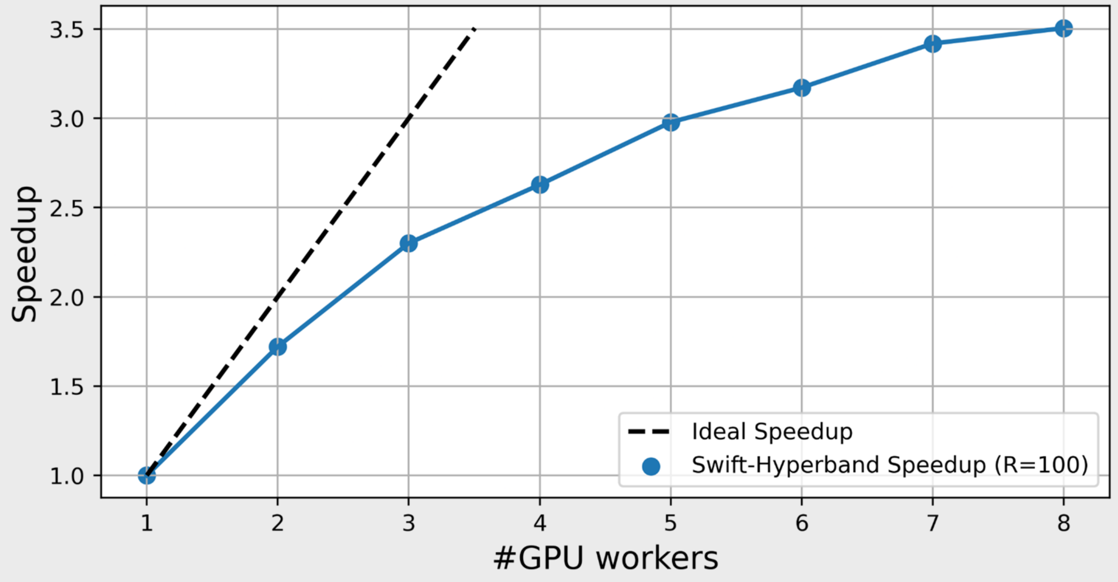

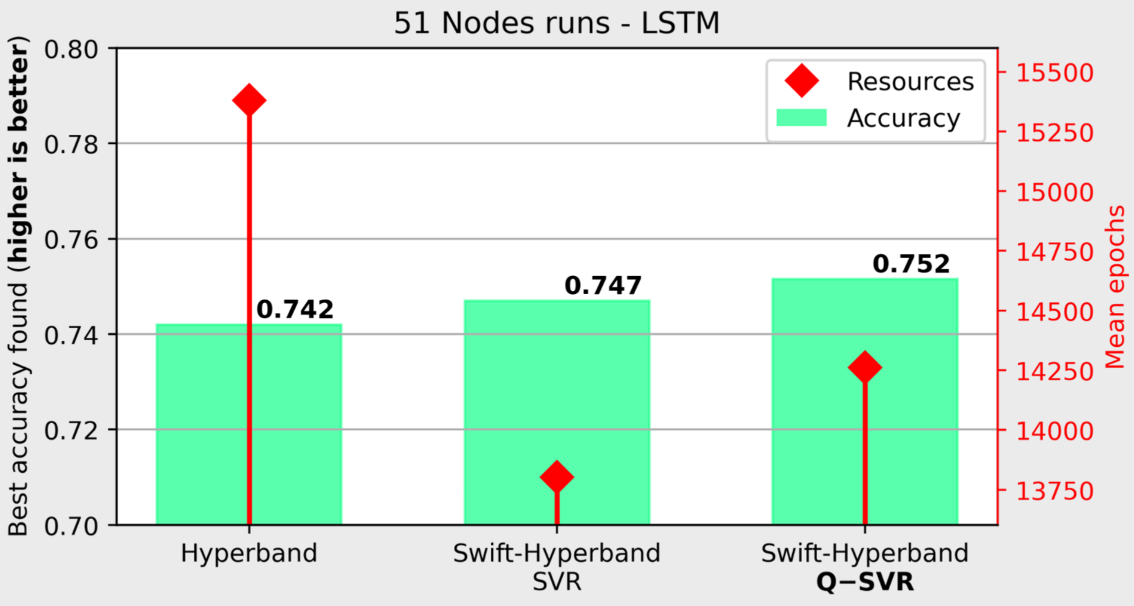

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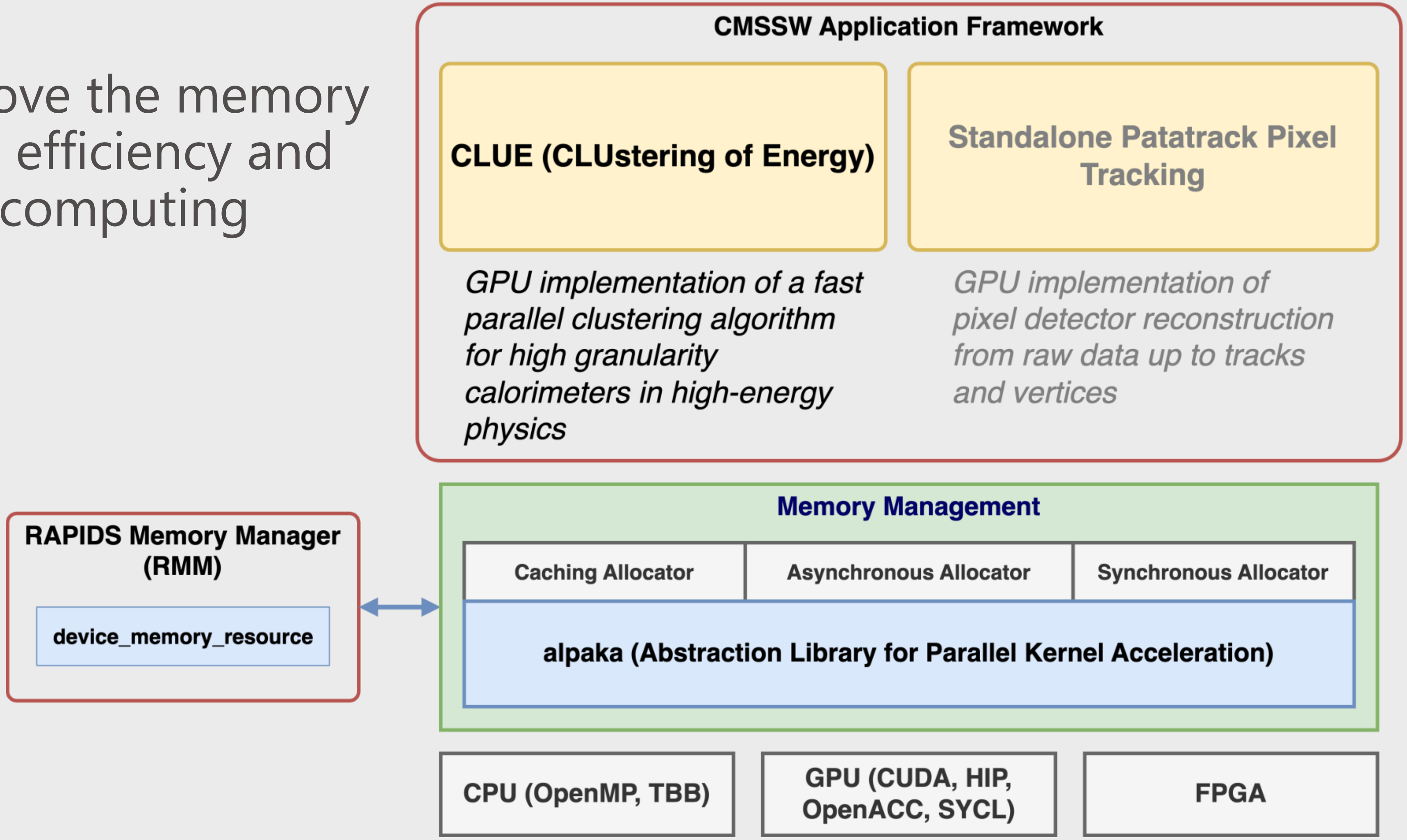
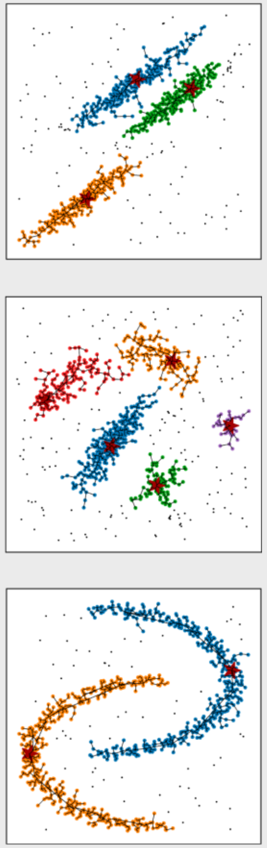
Performance tuning and generalization of CLUE

Heterogeneous CLUE Algorithm

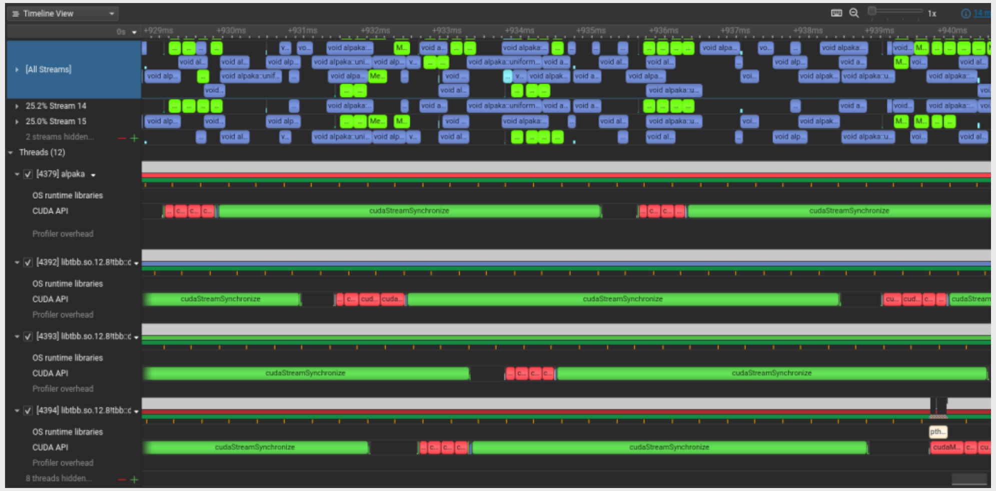
- Task: to improve the memory management efficiency and multi-thread computing performance

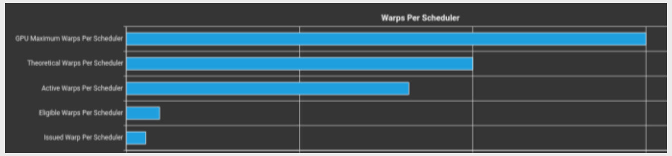




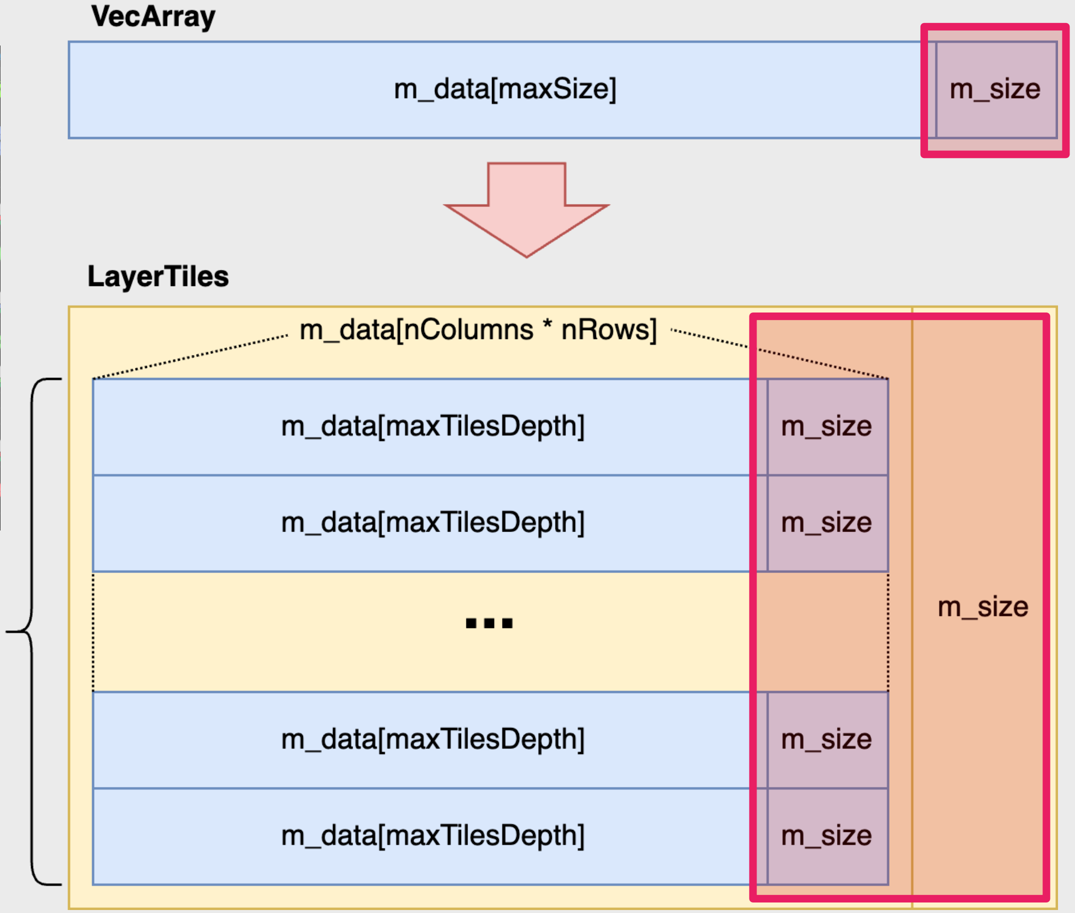
CLUE Performance Optimization

Application profiling with *Nsight Compute*





CLUE Data Structures

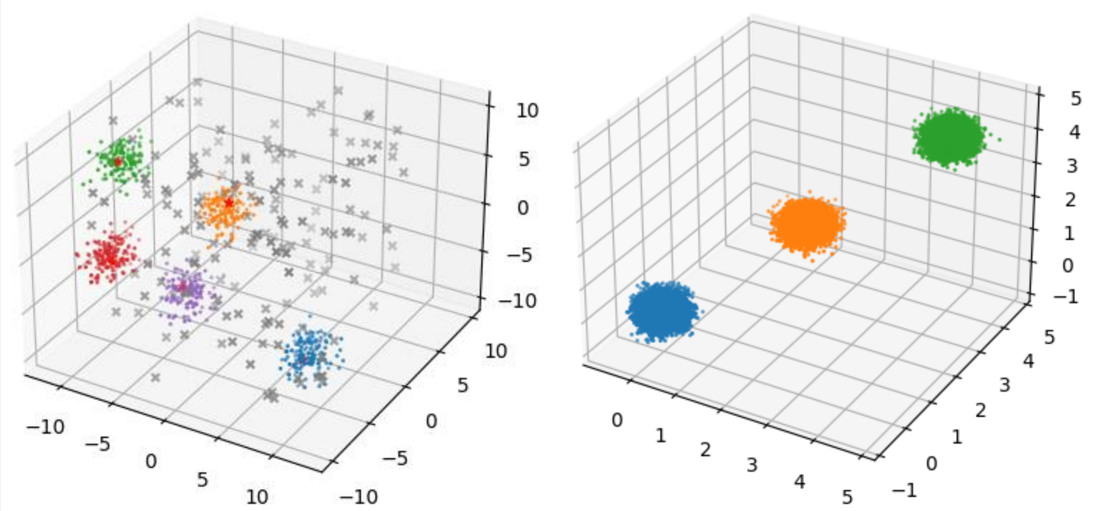


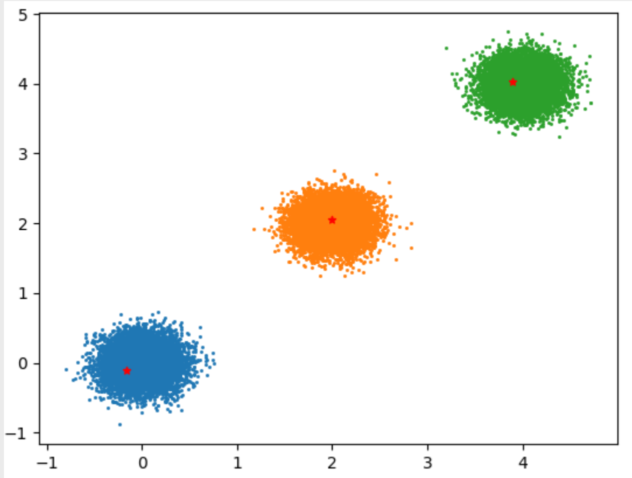
Memory coalescing and threadlocking issues

Solution: use <u>Structure of Arrays (SoA)</u> instead of *Array of Structures* (AoS)

N-Dimensional CLUE

- Generalization of the original algorithm, making it N-dimensional
  - The original algorithm was designed to work in 2 dimensions, with the data distributed in parallel layers
  - CLUE takes the coordinates of the points and their weight, which represents their energy, and calculates the energy density of each point
- Development of Python API





Summary

Conclusions and future work

- An extensive open dataset of physics events has been released on the CoE RAISE Open Data website
- MLPF outperforms PF in both particle level and event-level physics performance metrics
- Swift-Hyperband is a new HPO algorithm that integrates performance prediction with Hyperband
- Swift-Hyperband can run in a hybrid Quantum-Classical workflow manner
- Next steps:
  - Focus MLPF efforts on CMS datasets again
  - Together with WP2, submitted abstract to the *Quantum Technologies in Machine Learning* conference (QTML) which will take place at CERN 19th to 24th of November
  - Implement a Swift-ASHA with the aim of solving the straggler issues inherent to Hyperband

Bonus slide

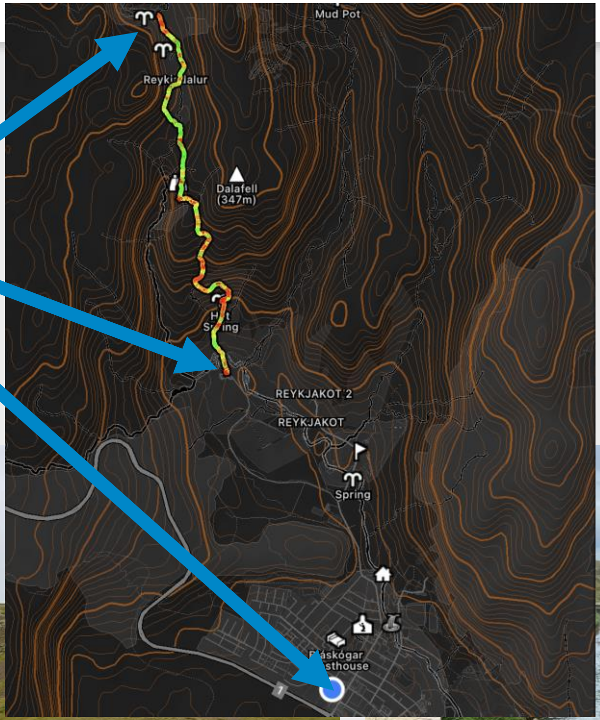
Hot spring hike

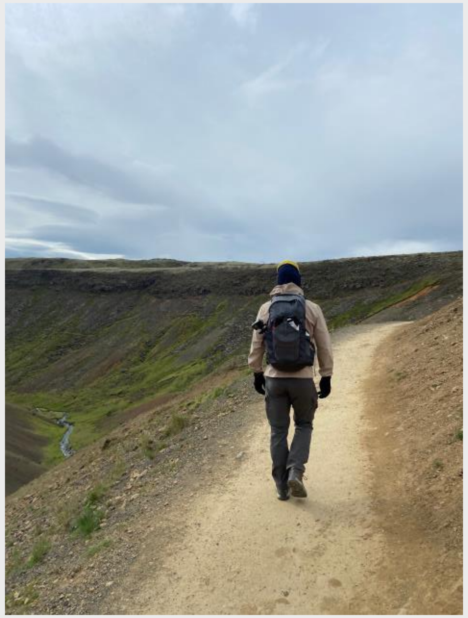
- https://www.alltrails.com/trail/iceland/southern/reykjadalur-hot-spring-thermal-river
- A car would be nice to get to the start of the hike
- Hike took ~2h15m for me, including a ~20 minutes bath in the river and stopping to take photos on the way

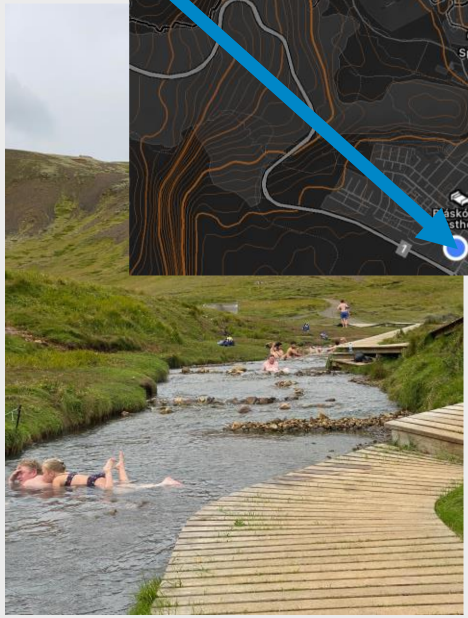
Hot spring

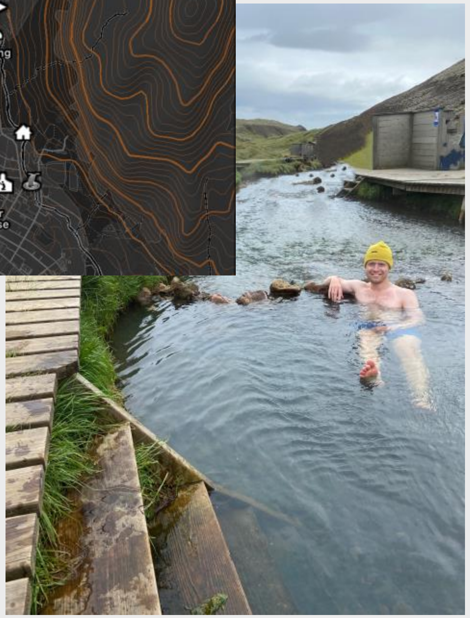
Start of hike

Hotel Örk









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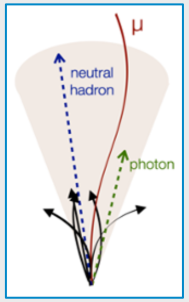
Deep Learning for particle flow reconstruction

Physics simulation

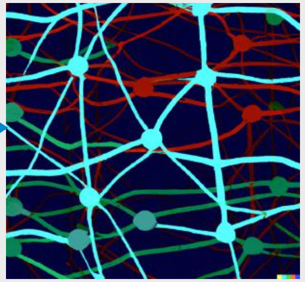


Data selection

Dataset creation

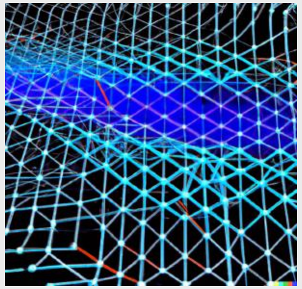
Data pre-processing

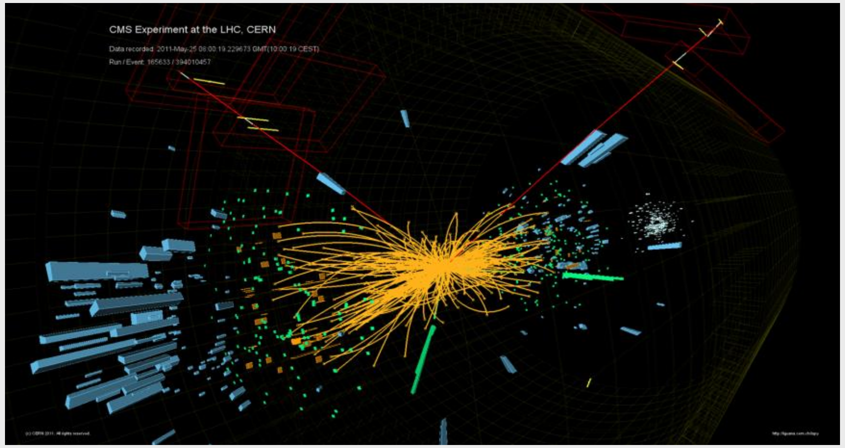
AI training



Model export

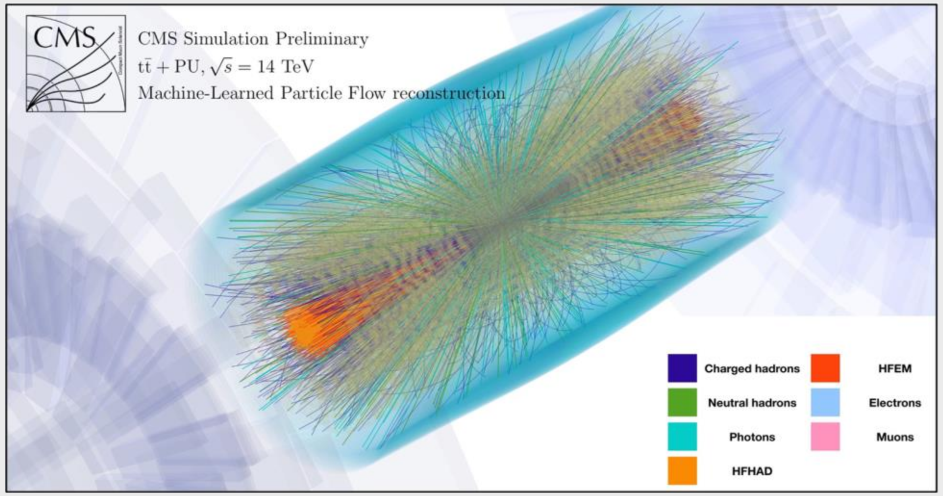
Trained model





CMS Collision event

Event reconstruction



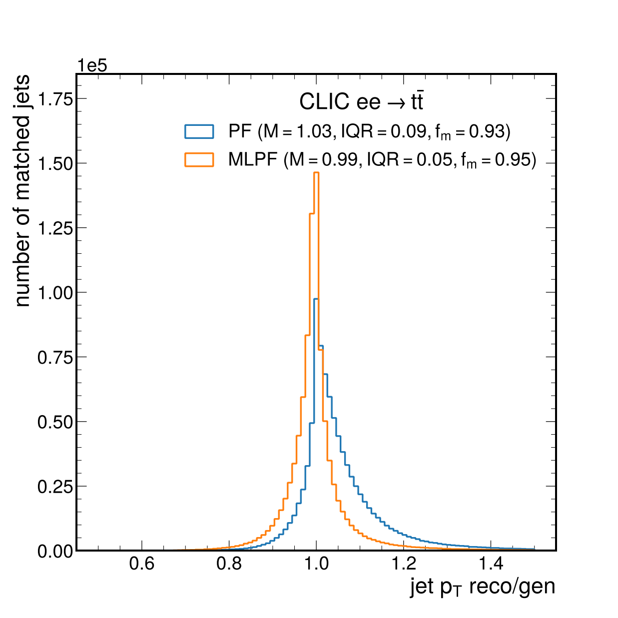
MLPF event reconstruction [1]

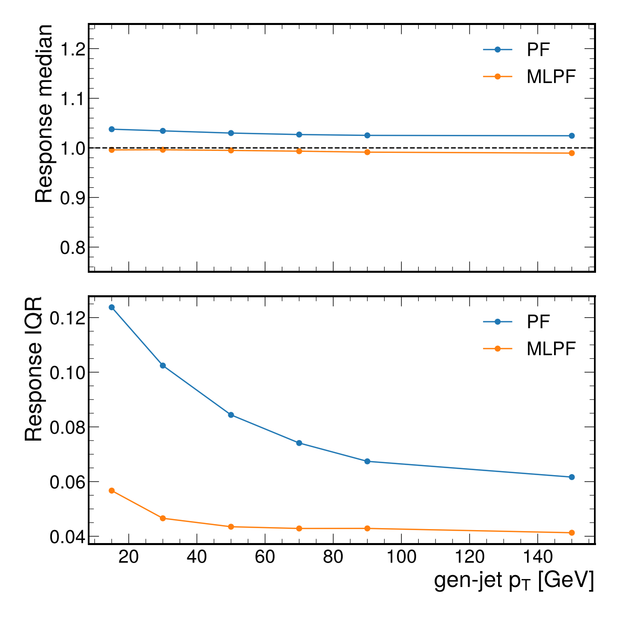
[1] Pata, J., Duarte, J., Mokhtar, F., Wulff, E., Yoo, J., Vlimant, J.-R., Pierini, M., Girone, M. (2022). *Machine Learning for Particle Flow Reconstruction at CMS*. Retrieved from http://arxiv.org/abs/2203.00330

Jet and MET in ttbar test data

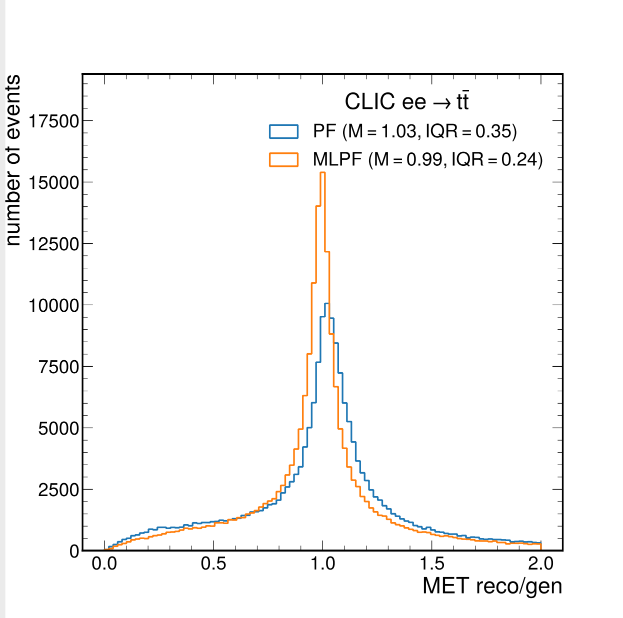
- For all test samples MLPF outperforms PF in Jet and MET reconstruction in terms of response width (quantified by median and interquartile range IQR)
- MLPF also outperforms PF in terms of fraction of reconstructed jets $\left({}^{n_{reco\ jets}}/_{n_{ground-truth\ jets}}\right)$

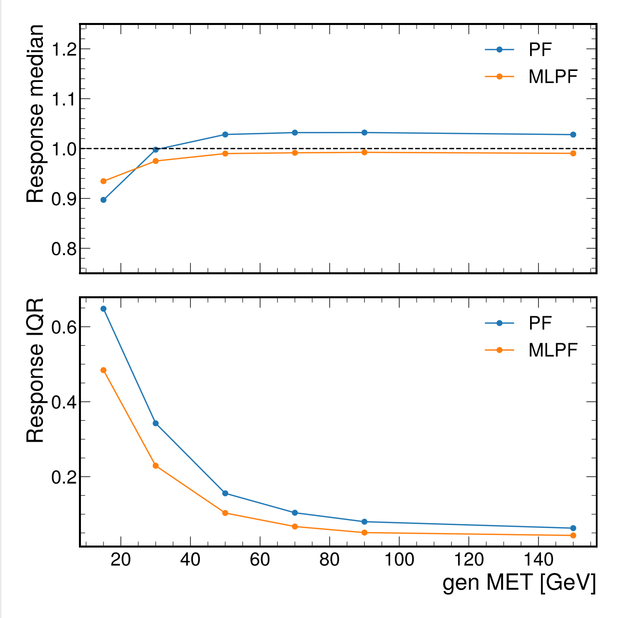
Jets resolution





MET resolution

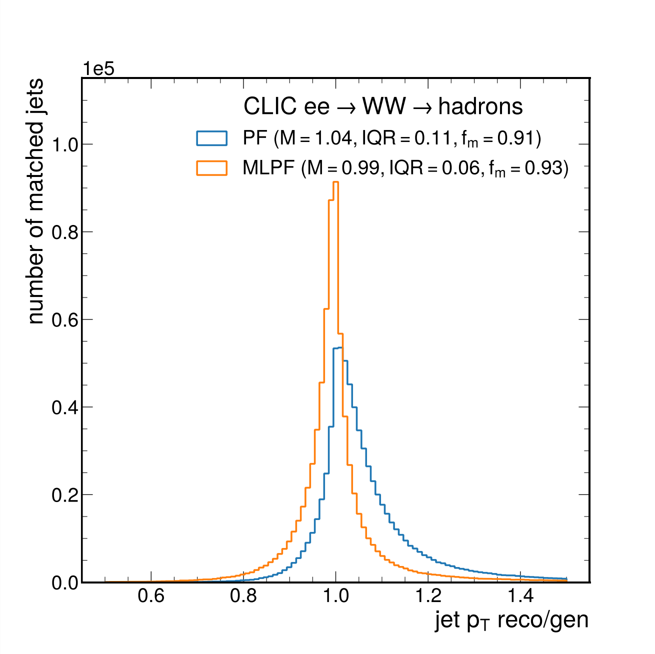




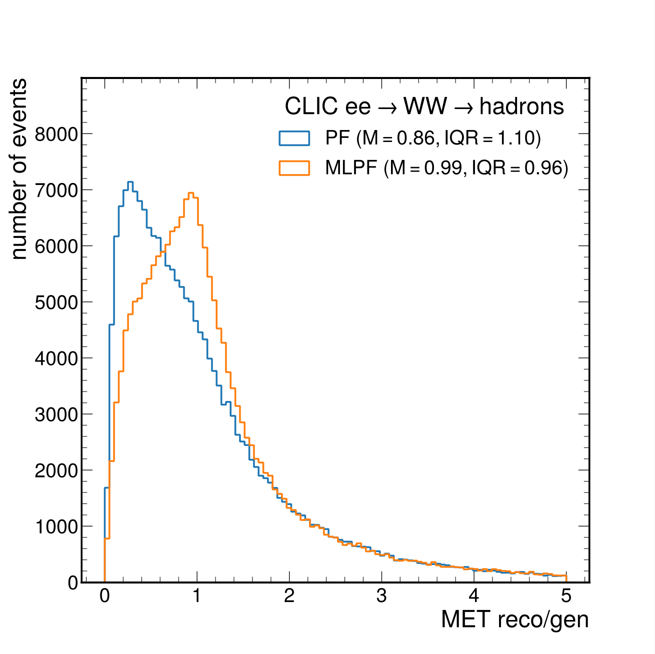
Jet and MET in WW test data

- For all test samples MLPF outperforms PF in Jet and MET reconstruction in terms of response width (quantified by median and interquartile range IQR)
- MLPF also outperforms PF in terms of fraction of reconstructed jets $\left({}^{n_{reco\ jets}}/_{n_{ground-truth\ jets}}\right)$

Jets resolution



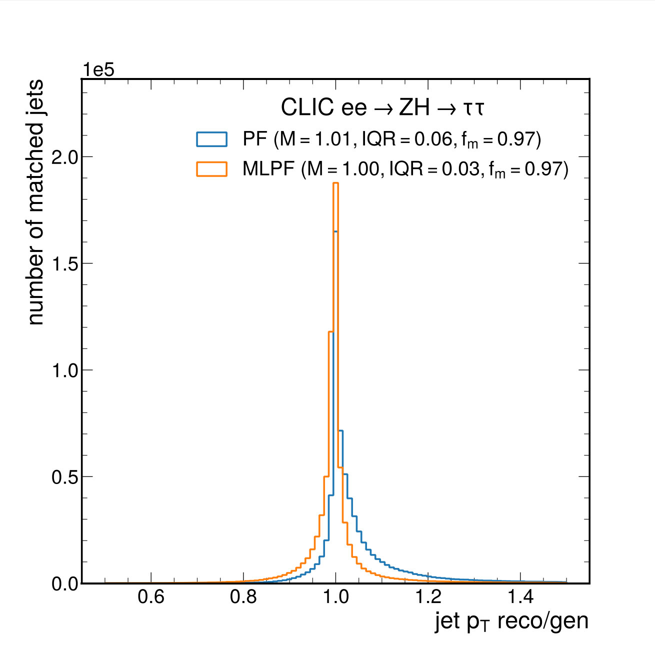
MET resolution



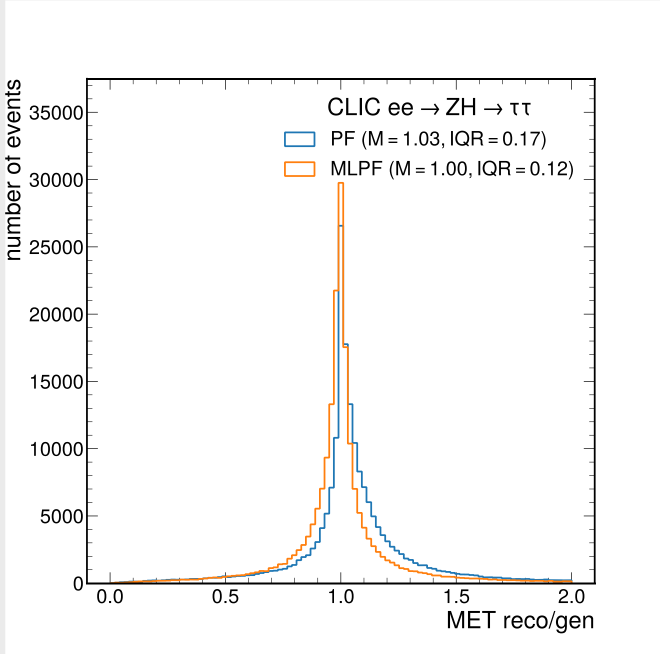
Jet and MET in ZH test data

- For all test samples MLPF outperforms PF in Jet and MET reconstruction in terms of response width (quantified by median and interquartile range IQR)
- MLPF also outperforms PF in terms of fraction of reconstructed jets ($^{n_{reco\ jets}}/_{n_{ground-truth\ jets}}$)

Jets resolution



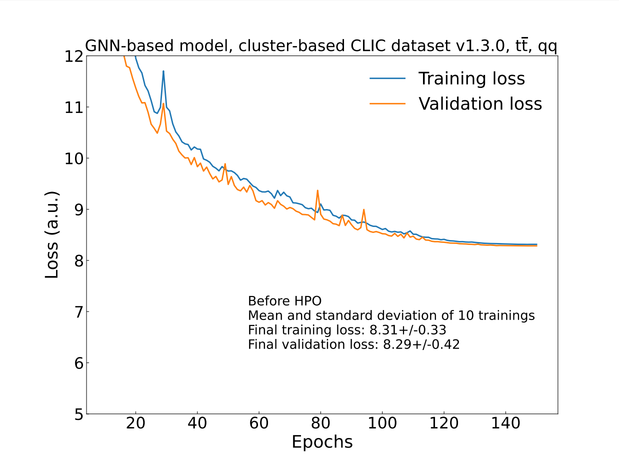
MET resolution

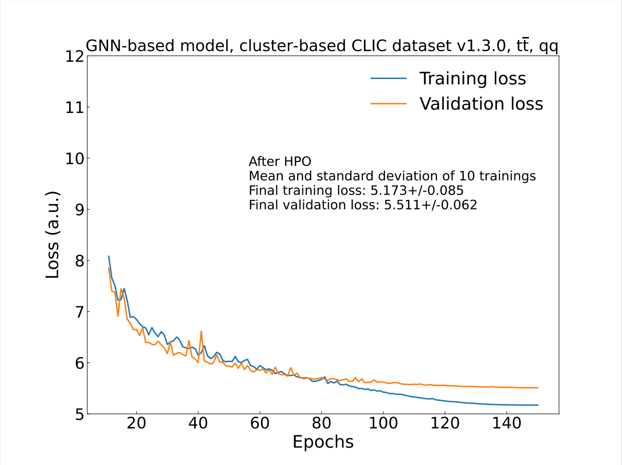


Improvement in training from HPO

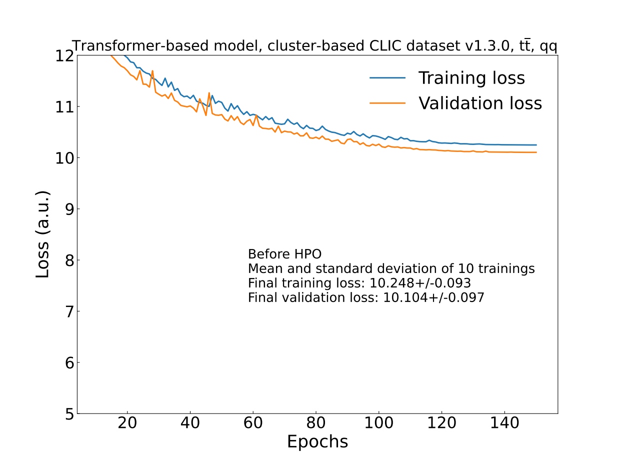
- Same learning curves as in the previous slide but separated into one plot per model and HP-set

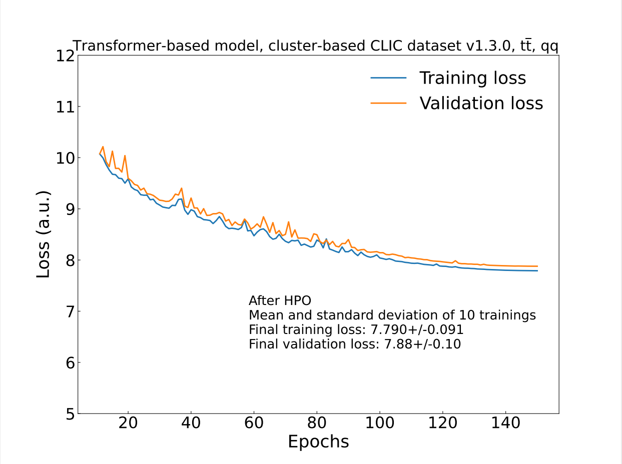
GNN





Transformer



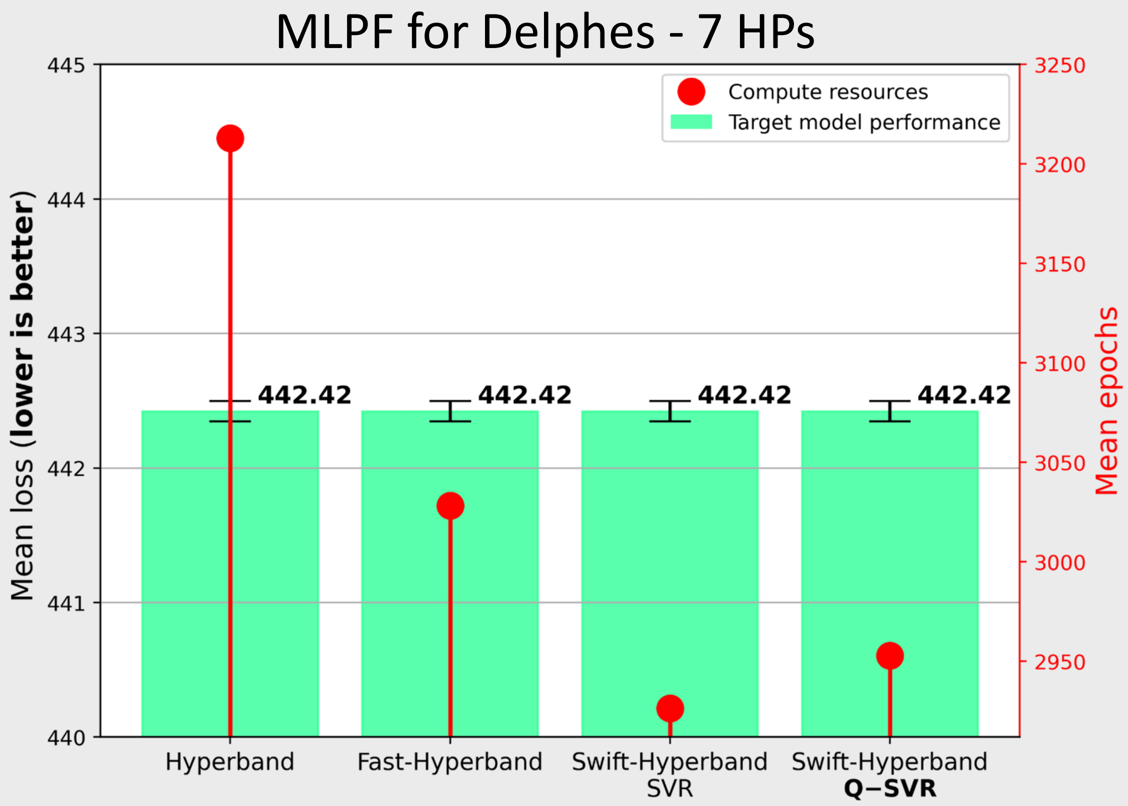


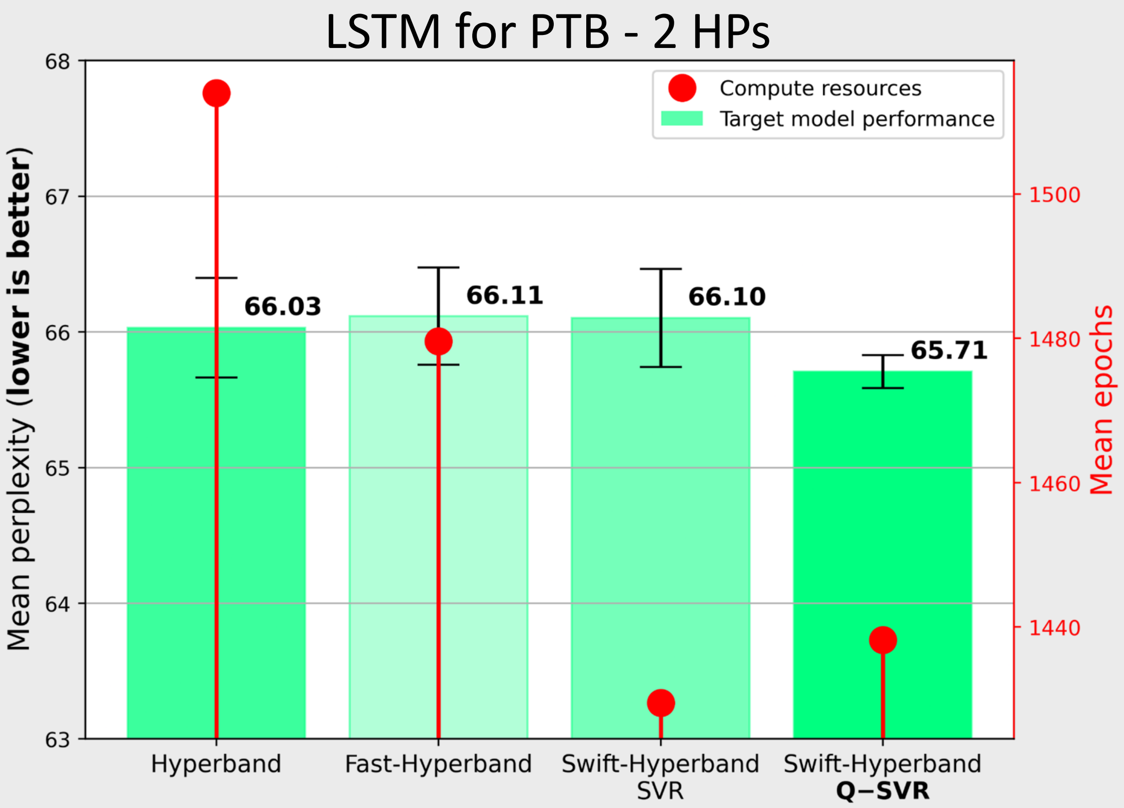
Before HPO

After HPO

Algorithm Comparison

- Simulated results using datasets of existing learning curves





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