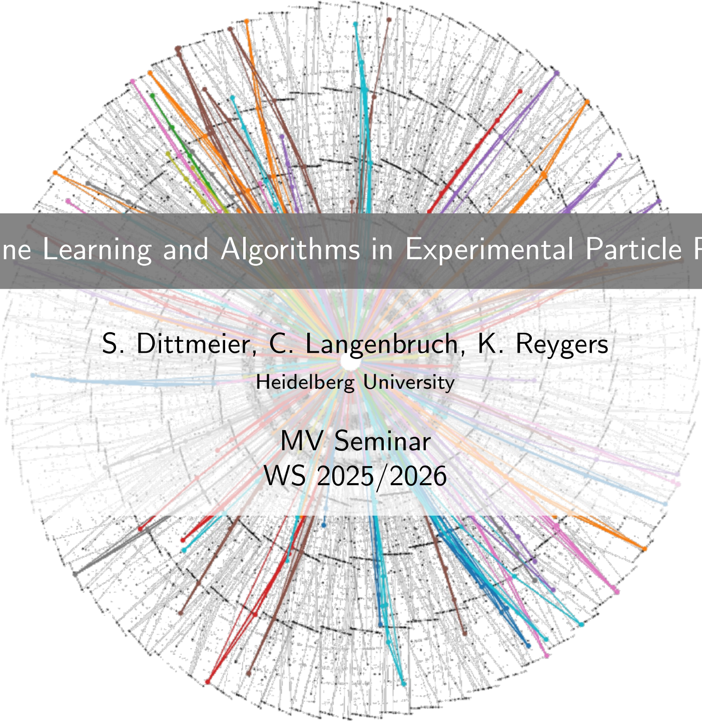


# Machine Learning and Algorithms in Experimental Particle Physics

S. Dittmeier, C. Langenbruch, K. Reygers
Heidelberg University

MV Seminar
WS 2025/2026

# Basic Coordinates

- Time: Friday 11:15-13:00
- Location: INF 226 1.106 (K4) Glassbox
- Contacts: Sebastian Dittmeier, Christoph Langenbruch, Klaus Reygers
- First date: Friday 17.10. 11:15: Introduction, discussion of topics
- [Seminar homepage]
- [HeiCO-Info]
- [Registration]

This seminar introduces machine learning techniques as well as classical algorithms, and explores their applications in contemporary particle physics experiments such as ATLAS, ALICE, CMS, and LHCb. Prior experience with machine learning is helpful but not required.

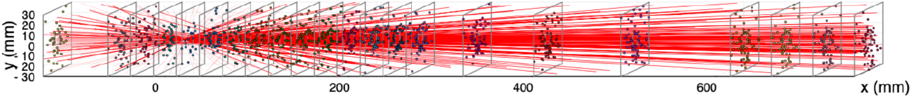
# Basic Coordinates II

- Explore specific application of modern machine learning methods and algorithms in particle physics
- Choose topic, starting point of relevant references will be provided
- Discussion with supervisor after first study of literature
- Prepare 1 hour presentation (45 minutes + 15 minutes discussion)
- Possible practice talk with supervisor
- Presentation in seminar
- Writeup (4–8 A4 pages) at end of semester

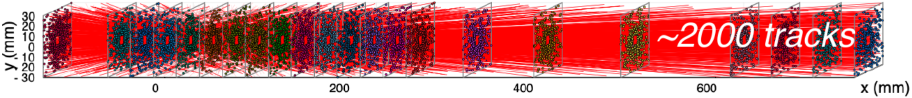
# Possible Topics

1. Bayesian Parameter Estimation
2. Graph Neural Networks for Track Reconstruction
3. Graph Neural Networks for Full Event Reconstruction
4. Particle Tracking with the Kalman Filter
5. Anomaly Detection
6. Fast Machine Learning for Triggering and Data Acquisition
7. Uncertainty Quantification in ML Predictions
8. Particle Identification with Neural Networks
9. Generative Models for Detector Simulation
10. Symbolic regression
11. Jet tagging with Transformers
12. Quark flavour tagging with deep NNs

# Graph Neural Networks for Track reconstruction



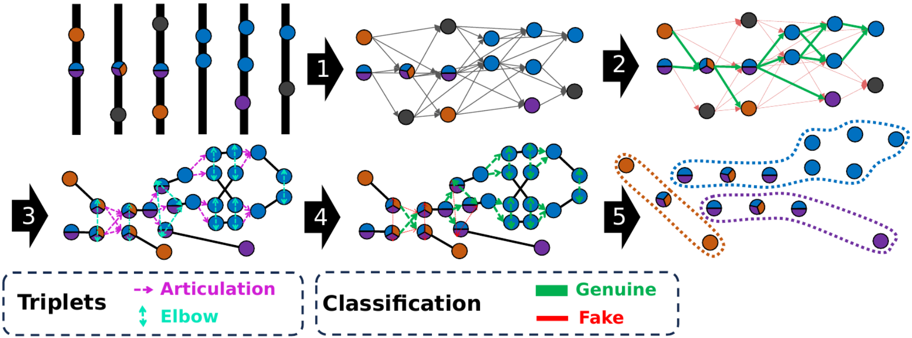

2024: $5\ pp$ collisions/event




Upgrade II: $\sim 40\ pp$ collisions/event

- Current tracking algorithms scale $\sim$ quadratically with # hits
- GNNs scale approx. linearly with # hits [EPJC 81 (2021) 876]
- Strong incentive to leverage ML algorithms for track reconstruction
- ETX4VELO [arXiv:2406.12869] uses Exa.TrkX approach to reconstruct tracks in LHCb Vertex Detector

# Graph Neural Networks for Track reconstruction

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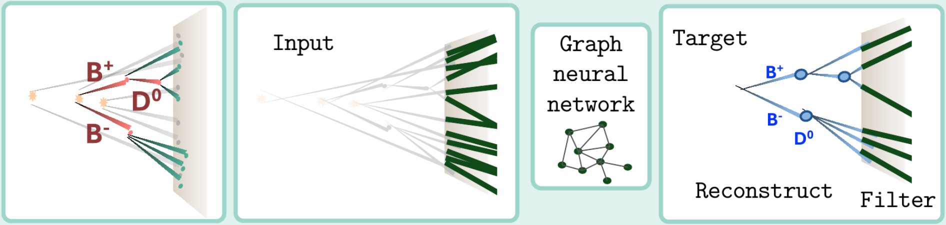
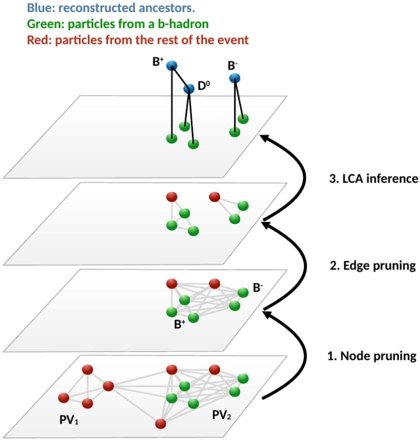
# Graph Neural Networks for Event reconstruction




- Deep-learning Full Event Interpretation (DFEI) [CSBS 7 (2023) 12] prototype to classify and reconstruct full heavy flavour decay chain
- Alternative to current approach of `OR` between trigger lines
- Could reduce event size in Upgrade II by only saving relevant particles
- Similar approach to FEI algorithm at Belle II which operates in cleaner environment [CSBS 3 (2019) 6]

# Graph Neural Networks for Event reconstruction

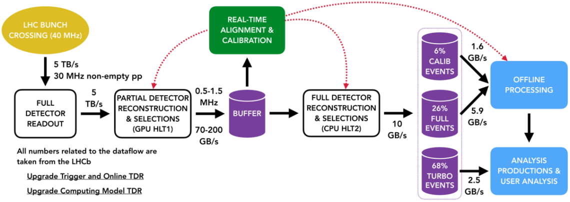


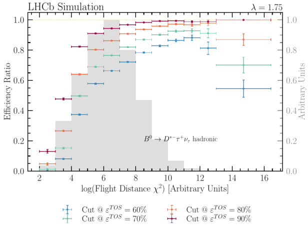

- Based on 3 sequential GNN modules
  1. Node pruning:
     Remove particles not from $b$-hadron
  2. Edge pruning:
     Remove edges between particles not from the same $b$-ancestor
  3. Lowest common ancestor inference:
     Reconstruct intermed. particles
- Trained on custom simplified simulation

# Anomaly detection

- Anomaly detection spots outliers in a given collection of data
- No NP signal at LHC so far, maybe not looking at right places?
- Design searches with minimal assumptions (model-independent) for anomalous events
- Several ML-based approaches:
  - Classification w/o labels [JHEP 10 (2017) 174] + Bump hunting [PRD 99, 014038]
  - Autoencoders [SciPost Phys. 6, 030 (2019), . . .
- LHC Olympics 2020: Challenge for Anomaly detection [arXiv:2101.08320]

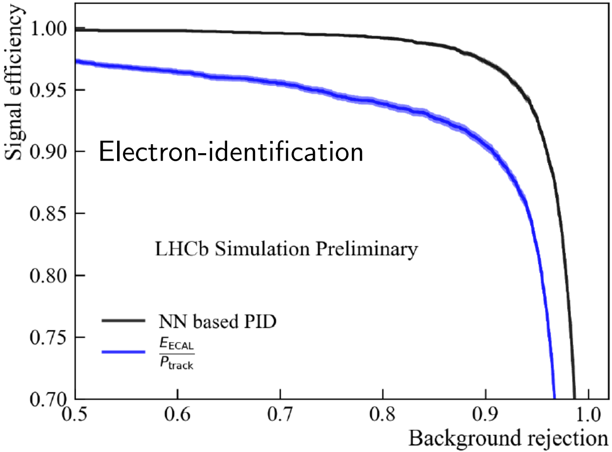
# Fast Machine Learning for Triggering



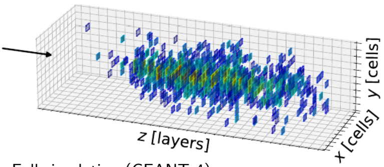

- Enormous challenge to fit inside the bandwith constraint
- ML techniques can identify potential signal events with high efficiency
  [JINST 8 P02013] [JPCS 664 082025] [JINST 14 (2019) P04013]
- Need to be efficient, fast, robust
- Monotonic Lipschitz NNs can address these requirements
  [ML:ST 4 035020] [arXiv:2312.14265]

# Particle Identification with Neural Networks

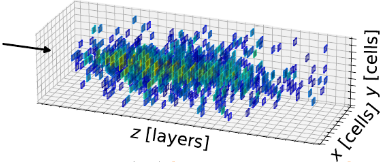



- Lipschitz-constrained NNs also used in particle identification in the HLT1
- Large improvement compared to conventional algo. [LHCB-FIGURE-2024-003]

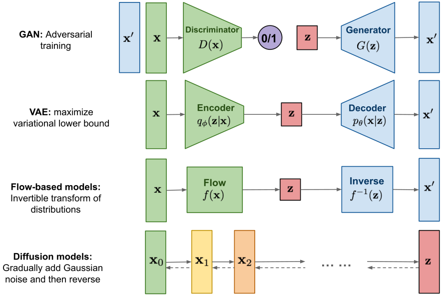
# Generative Models for Detector Simulation



Full simulation (GEANT 4)



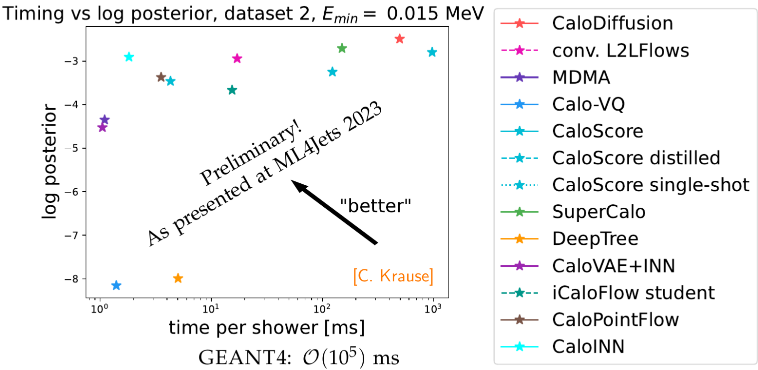
Fast simulation (NF) [2023 JINST 18 P10017]



[L. Weng]

- MC simulation can be extremely expensive, in particular shower simulation *e.g.* repeated $\gamma$ emission (Bremsstrahlung) and $\gamma \rightarrow e^+e^-$ pair production
- Employ generative models for fast simulation of particle showers
- [CaloChallenge] to trigger development and evaluate performance
- Some tradeoff between accuracy and timing

# Generative Models for Detector Simulation




GEANT4: $\mathcal{O}(10^5)$ ms

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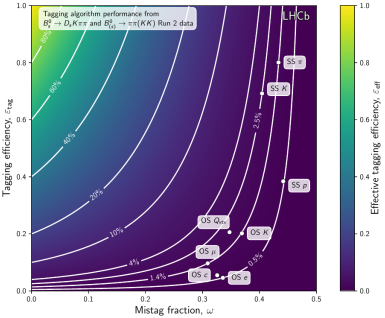
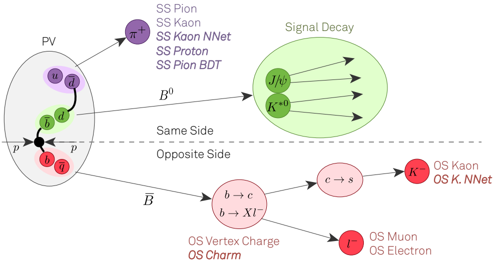
# Quark Flavour Tagging

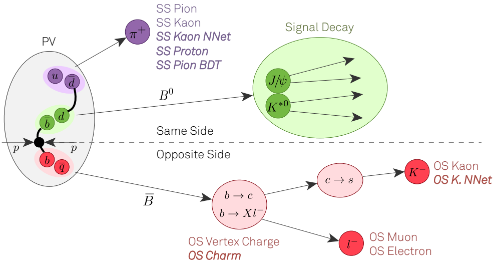



- Classically: Identify one specific tagging particle, use BDT to predict mistag
- Inclusive Tagger: DeepSet NN considering the full event [arXiv:2404.14145]
- Tagging power higher than combination of exclusive taggers on simulation
- Promising performance, but needs to be validated/calibrated on data

# Quark Flavour Tagging

| | $\epsilon_{\text{tag}}[\%]$ | $\epsilon_{\text{eff}}[\%]$ |
|---|---|---|
| $\boldsymbol{B^0 \to J/\psi\, K^{*0}}$ | | |
| OS Combination | 38.5 | 3.81 |
| SS Combination | 80.1 | 1.71 |
| **Classical Taggers Combination** | 87.0 | 5.39 |
| **DeetSet NN** | 100 | 6.38 |
| $\boldsymbol{B^+ \to J/\psi\, K^+}$ | | |
| OS Combination | 38.2 | 3.94 |
| SS Kaon | 67.7 | 1.22 |
| SS Pion | 69.9 | 3.94 |
| **Classical Taggers Combination** | 92.0 | 6.39 |
| **DeepSet NN** | 100 | 8.0 |
| $\boldsymbol{B_s^0 \to D_s^+ \pi^-}$ | | |
| **DeepSet NN** | 100 | 8.7 |

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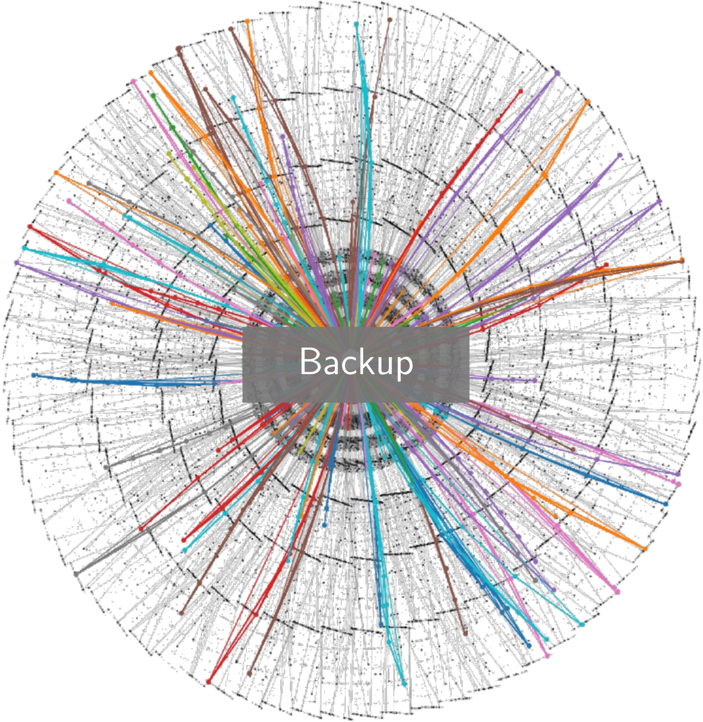
Backup