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Towards Fast, Machine-Learning-Based Calorimeter Simulations in the ALICE Experiment at CERN

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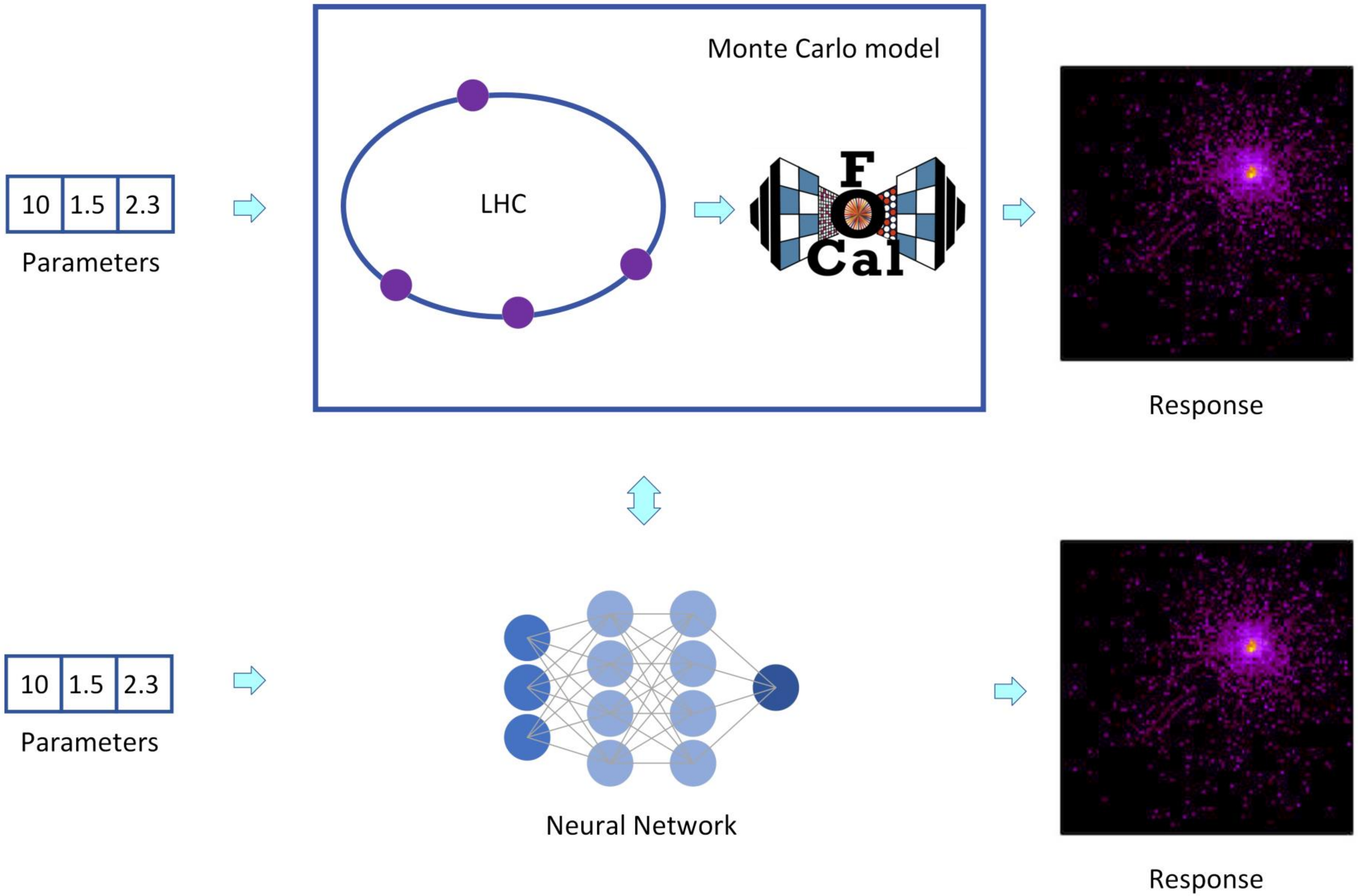
What do we do?


10
1.5
2.3
Parameters
Monte Carlo model
LHC
FOCal
Response
10
1.5
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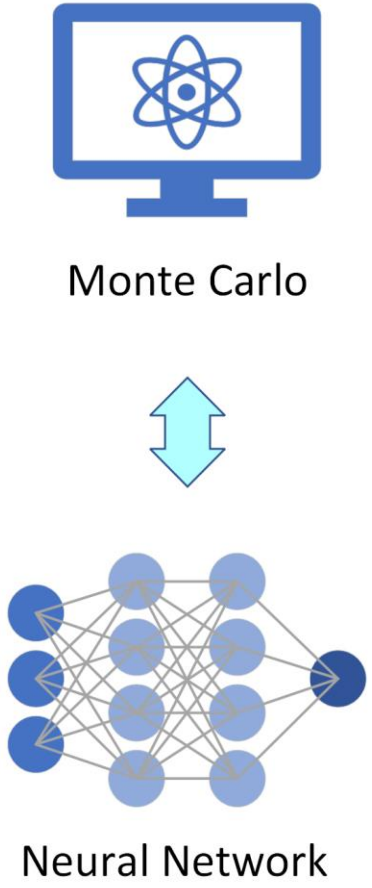
Parameters
Neural Network
Response

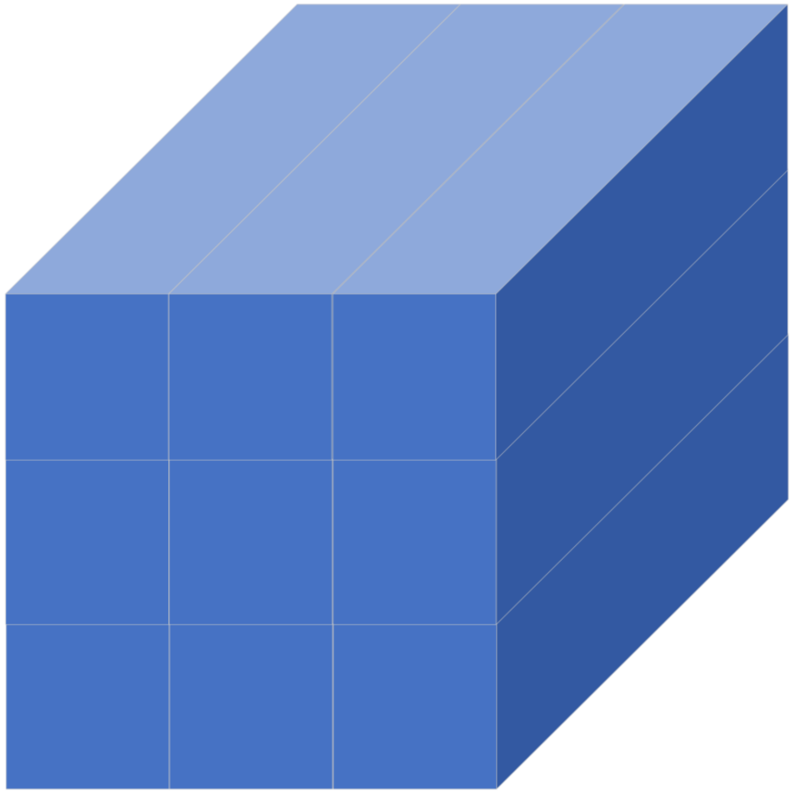
Fast simulations

- Using a surrogate of the whole mathematical model or its part.
  - The most computationally-intensive part → a faster surrogate.
- Fast simulations at CERN.
  - Existing approaches at different experiments.
  - DNN surrogates.
    - VAEs, GANs, NFs, Diffusion-based, Flow Matching.
- There's still a gap to fill!
  - Research done mostly on other experiments' calorimeters.
  - Physics-based machine learning.



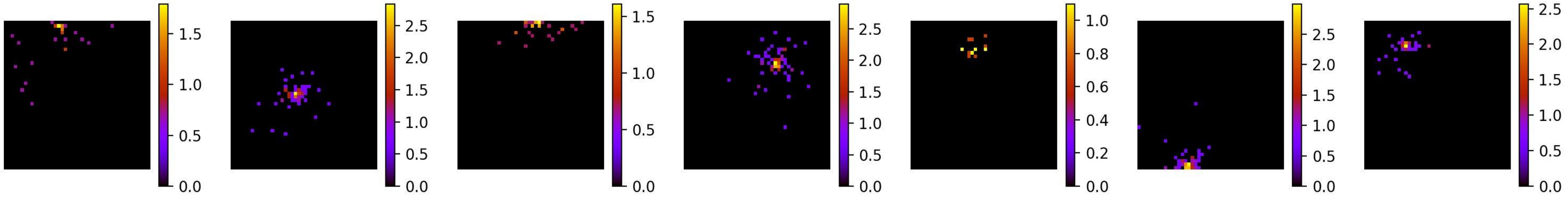
Detectors

- Two calorimeters: Zero Degree Calorimeter (ZDC) and the hadronic section of the Forward Calorimeter (FoCal-H).
- Both detect energy deposited by passing particles as light output.
- Material: ZDC – quartz fibres, FoCal-H – copper tubes.

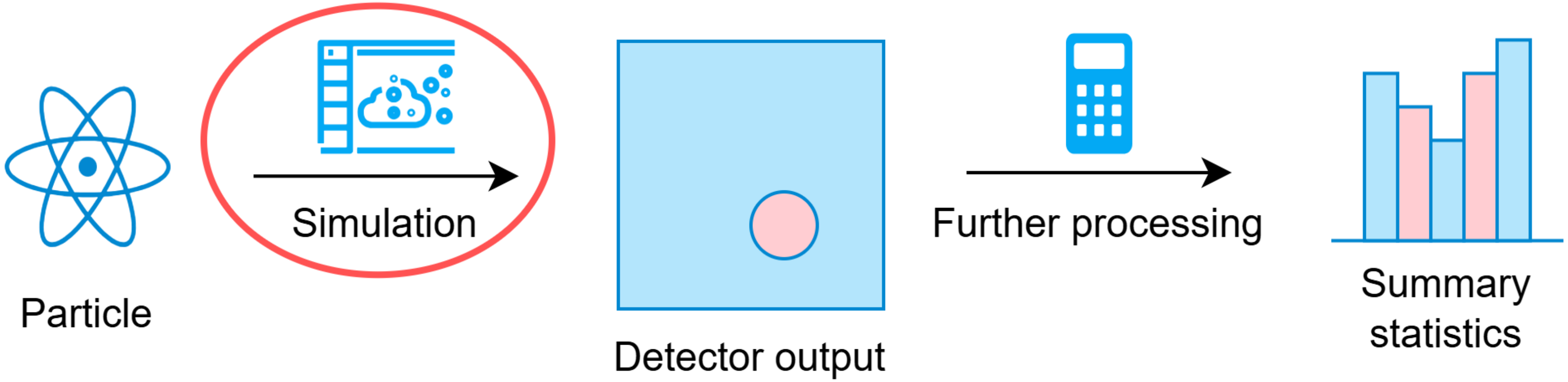


Detector simulation

- Simulated using Monte Carlo approach.
  - Computationally expensive method!
- Each simulation begins with a primary particle with known features.
- We work with 2-D representations of detector outputs.
- Simulation of such structure is a perfect task for generative neural networks.



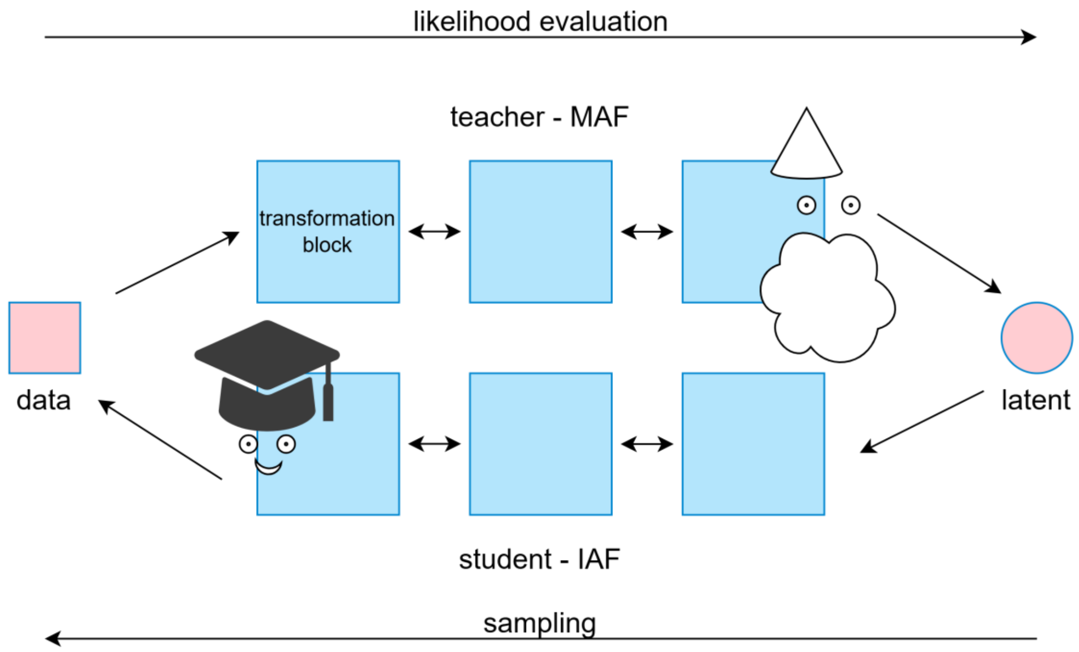
Physics-based ZDC simulation



We combine physics-based learning and data-driven optimisation to make outputs of generative models more consistent with physics principles.

Normalizing flows approach

- We leverage the teacher-student Normalizing Flow framework with a physics-based approach:
  - Train a Masked Autoregressive Flow (MAF) teacher - slow to sample, fast to evaluate likelihoods.
  - Train an Inverse Autoregressive Flow (IAF) student - fast to sample, mimicking the teacher's behaviour.
  - The transformations are invertible, so we can closely match student to the teacher.



Physics-based enhancements

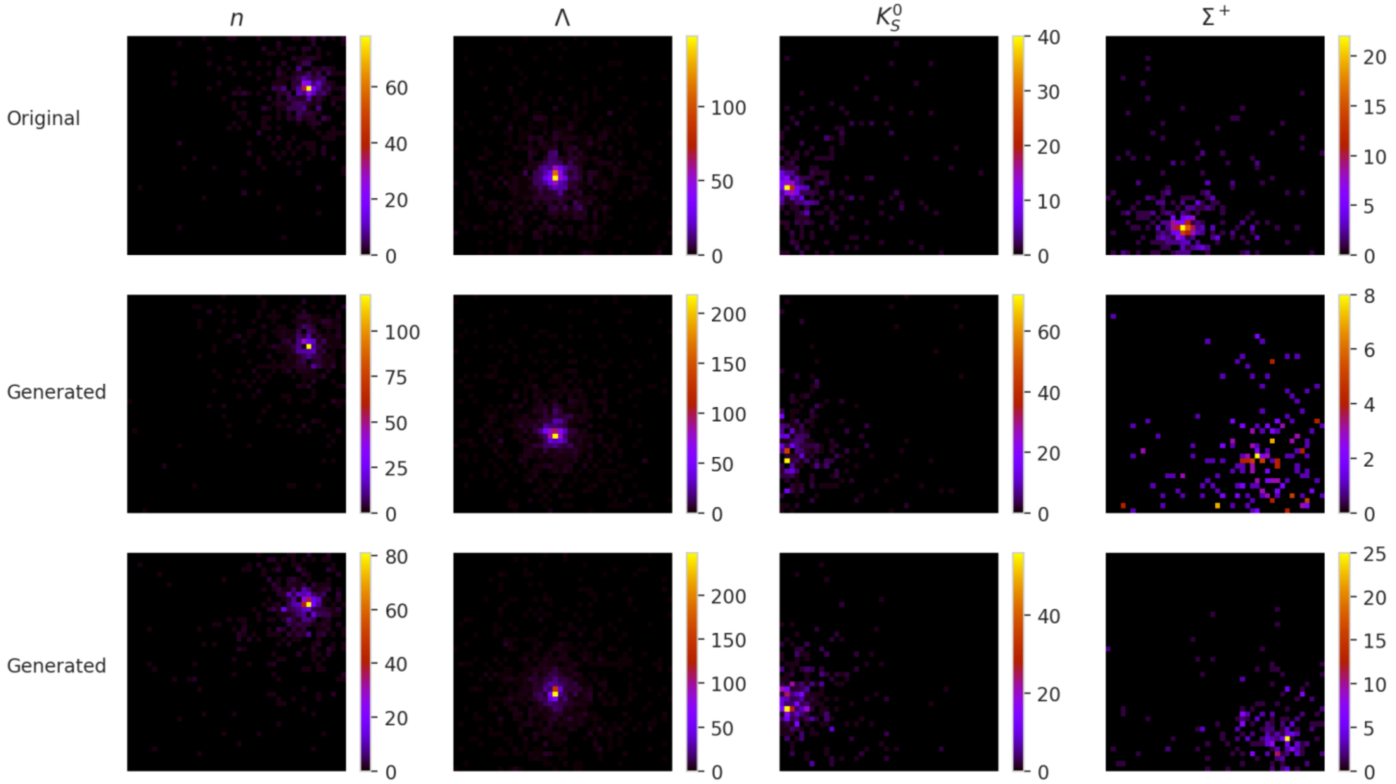
- The baseline - MSE-driven optimisation between respective outputs of transformations and in-transformation networks.
- Physics-based loss function to help with spatial features modelling.
- Physics-based loss scaler to mitigate the influence of rare artefacts on the training.

Results

	n	Λ	K_S^0	Σ^+	all
teacher WS	3.56 ± 0.07	16.00 ± 0.26	10.94 ± 0.23	31.52 ± 0.64	1.74 ± 0.02
teacher MAE_w	6.11 ± 0.06	9.39 ± 0.15	11.41 ± 0.20	23.83 ± 0.55	5.17 ± 0.03
bs WS	$\mathbf{3.37 \pm 0.08}$	16.42 ± 0.42	10.55 ± 0.18	33.53 ± 0.31	1.73 ± 0.02
bs MAE_w	6.45 ± 0.08	11.00 ± 0.17	11.87 ± 0.16	25.38 ± 0.34	5.57 ± 0.03
bs+div WS	3.45 ± 0.05	$\mathbf{16.32 \pm 0.14}$	11.02 ± 0.25	33.60 ± 0.16	$\mathbf{1.62 \pm 0.02}$
bs+div MAE_w	6.40 ± 0.05	10.56 ± 0.24	12.29 ± 0.13	25.75 ± 0.33	5.40 ± 0.04
bs+ch WS	4.24 ± 0.05	16.61 ± 0.12	10.86 ± 0.21	$\mathbf{31.25 \pm 0.49}$	2.00 ± 0.02
bs+ch MAE_w	6.32 ± 0.07	9.22 ± 0.20	11.24 ± 0.25	$\mathbf{18.47 \pm 0.66}$	5.17 ± 0.02
bs+ch+div WS	4.19 ± 0.07	16.49 ± 0.38	$\mathbf{10.49 \pm 0.16}$	31.64 ± 0.32	1.71 ± 0.02
bs+ch+div MAE_w	$\mathbf{6.20 \pm 0.04}$	$\mathbf{8.88 \pm 0.10}$	$\mathbf{10.75 \pm 0.20}$	19.14 ± 0.84	$\mathbf{5.00 \pm 0.02}$

bs - baseline, ch - with physics-based loss, div - with physics-based loss scaler

Example simulations



ZDC study conclusions

- Physics-based modelling enhances generative frameworks by better capturing underlying physical dependencies.
  - Physics-based models can even outperform their purely data-driven teachers!
- Relying on distribution metrics is insufficient for assessing calorimeter fast simulation performance.

Theory-inspired approach for FoCal

- Additional loss: distance between the simulated and expected shower center positions.
- Calculated using azimuthal angle and pseudorapidity:

$$x = z \cdot \tan\left(2\arctan\left(e^{-\eta}\right)\right) \cdot \cos\phi$$

$$y = z \cdot \tan\left(2\arctan\left(e^{-\eta}\right)\right) \cdot \sin\phi$$

- Currently under development.
  - Primary experiments showed encouraging results for some generative architectures, while not helping in other cases.

Technological stack & hardware

- Python.
- TensorFlow, PyTorch, NumPy, scikit-learn and Uproot libraries.
- Weights & Biases platform.
- NVIDIA A100 GPU available on the Athena cluster and NVIDIA Tesla V100 on Ares.

Conclusions and next steps

- Promising results with physics-based approach for ZDC.
- Further development of theory-inspired approach for FoCal-H.
- Other ML tasks in ALICE: exploring contrastive, multi-layer, and generative approaches for muon track matching in reconstruction.

Acknowledgements

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