Design of Experiments Using Machine Learning

FTCF Workshop Guangzhou (17-21 November 2024)

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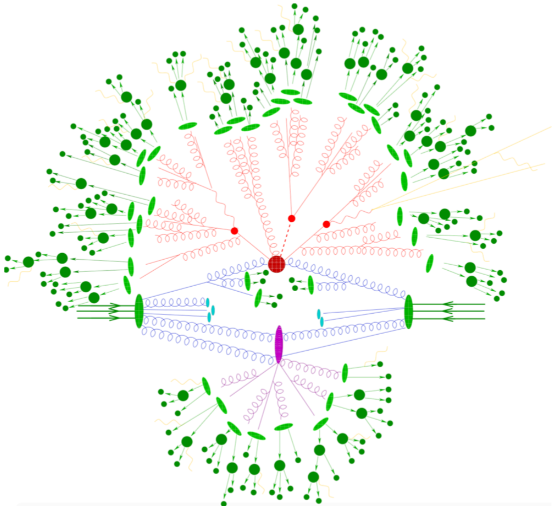
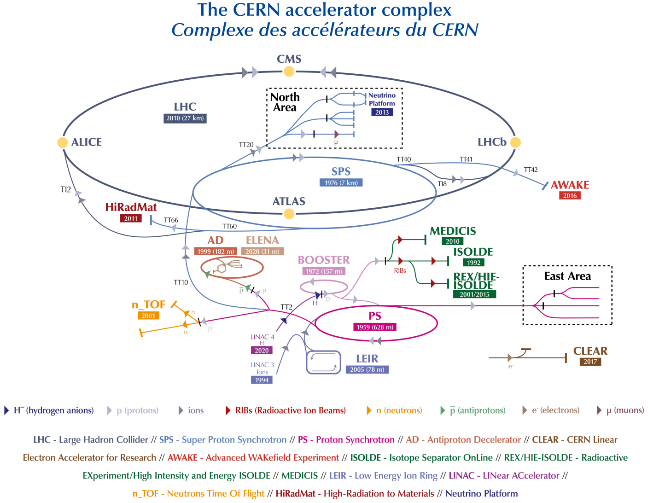
on behalf the MODE collaboration

21 November 2024

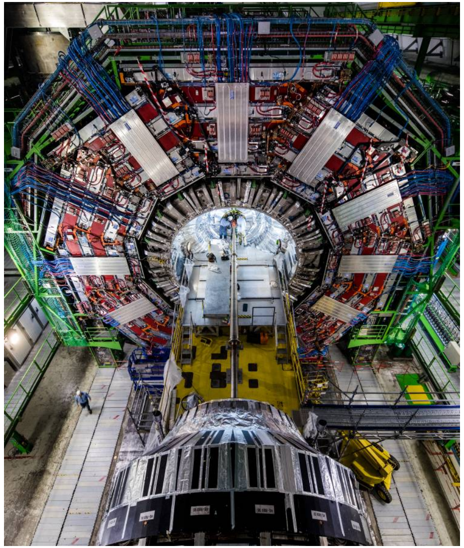
Complexity^3 of Modern HEP Experiments



Complex phenomena



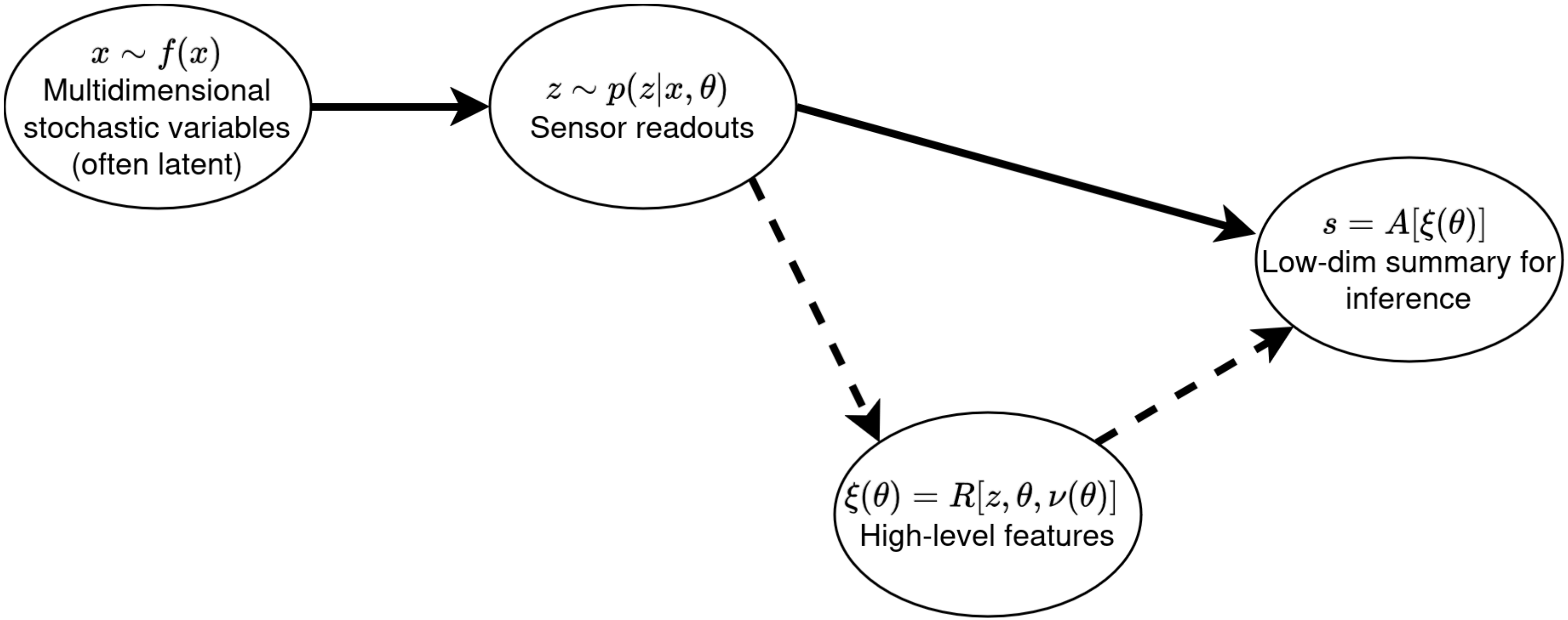
Complex machines



Complex detectors
and reconstruction

Stochastic processes → intractable likelihood (matrix element, parton shower, detector simulation... result in latent variables)

Typical Analysis Pipeline



The diagram is from Pietro Vischia's slides from ICHEP2024

Determining Multiple Parameters

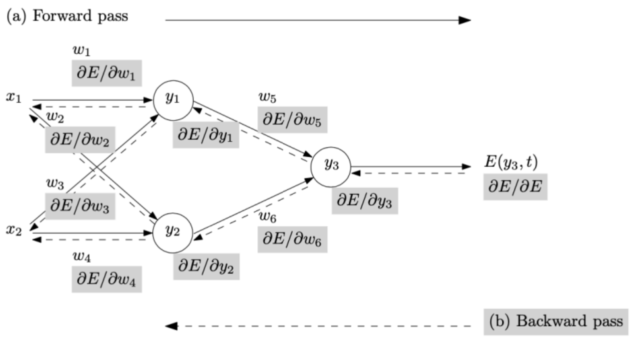
- Determining multiple parameters ~ fitting a function
- The optimisation of a detector or a reconstruction chain is conceptually the same thing
- To perform this optimisation we need to know $\frac{\partial \epsilon}{\partial \theta}$:

  how does our photon efficiency change w.r.t. the reconstruction parameters θ?

- Gradients can be calculated
  - Numerically: unfeasible for many parameters
  - Algorithmically: requires unbroken gradients throughout the whole chain: every step needs to be differentiable
  - **Differentiable programming**

Differentiable Programming

- Differentiable programming is used by, but is independent of ML
- At its core: in any operation, include a way to access its gradient w.r.t. all parameters (if it exists): auto differentiation
- Auto-differentiation is neither pure numeric nor pure symbolic differentiation
  - Numerical differentiation is not feasible for large optimisation problems
  - Fully symbolic differentiation can easily become not feasible from computational point of view
- In most cases, back propagation is used ($A \to X \to L$)
  - Calculate the numerical values of $b = dL/dx$ using the analytic gradient of the operation
  - Calculate the numerical values of $b \cdot dx/dA$ in the same way



What is MODE about?

Use differentiable programming to optimise particle physics detectors given a quantification of the physics target(s) and the detector cost

Machine-Learning Optimized Design of Experiments

MODE Collaboration

https://mode-collaboration.github.io

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27 NISER, India
28 HEPHY OeAW, Austria

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The MODE Goals

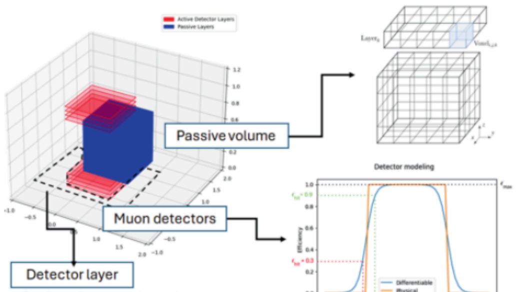
- "We aim to create a versatile, scalable, customizable infrastructure, where a generic detector design task can be encoded, along with all the players (pattern reco, nuisances, cost constraints, a well constructed objective function)"
  - Then **automatic scanning** of the space of design solutions becomes possible!
- This doesn't replace the work of the physicist! We aim at **extending the physicist's abilities** by producing **design assistance tools**, focusing on diagnostic tools and visualizations for **interpretability**
- We don't propose the one *optimal solution* to a given problem, we aim at proposing a **distribution of solutions** in a region of optimality, to assist design choices!
- Optimization targets are not only strictly physics-related (e.g. significances): we consider also **financial cost** and other constraints in the optimization

The MODE Goals

- We identified and started studying some **relatively simple use cases**: muon tomography detector optimization, calorimeter optimization
- Plan to proceed to other simple use cases (e.g. small detectors for HL-LHC), providing **proofs of concept of increasing complexity**
  - "*Every problem is difficult if you want to solve it well and make an impact*"

TomOpt: Muon Scattering Tomography Optimization

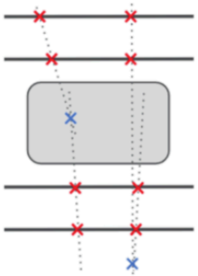
Volume modelling



- Region of space where detectors can move

Muon propagation

- Muons: (p,x,y,z,θ,φ)
- Hits are generated in the detector panels.
- Trajectories reconstructed
- The scattering points are found using the POCA (Point of Closest Approach) method.

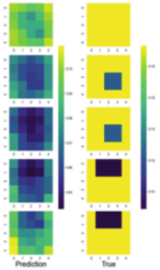


Passive volume mapping

POCA points let us pinpoint the area of the volume in which the muon has scattered.

Averaging the scattering angles and momenta of the muons one can estimate the value of the radiation length in that area.

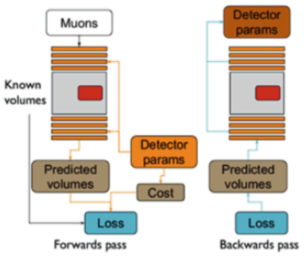
The precision of this computation is subject to the spatial resolution of the detectors and the number of voxels of the passive volume.



$$X_0 = \left(\frac{0.0136\ GeV}{p^{rms}}\right)^2 \frac{\delta z}{\cos(\hat{\theta}^{rms})} \frac{2}{\theta_{tot}^{rms}} \quad (2)$$

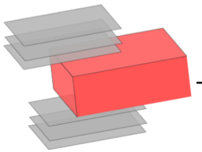
Detector optimisation

Learnable parameters (x, y, z, dx, dy)

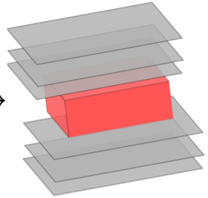


Reproduced from [1]

- Differential optimization = minimisation of loss function $\mathcal{L}(a_n)$
  - where a_n are detector parameters
- $\mathcal{L}(a_n)$ = inference error + constraints
- Gradient descent : $a_{n+1} = a_n - \gamma \nabla \mathcal{L}(a_n)$

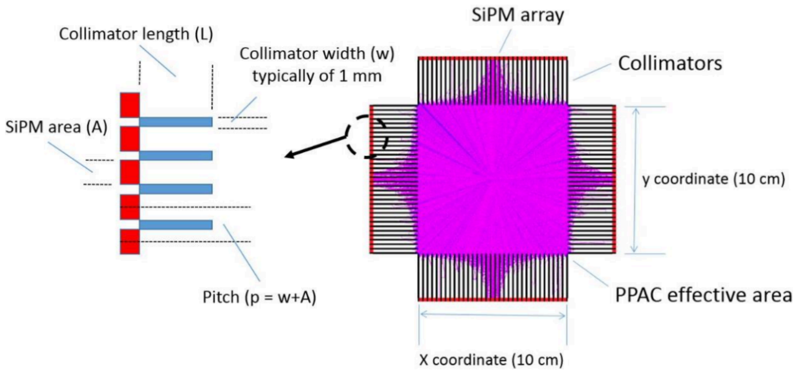


Repeat optimisation loop until $\nabla \mathcal{L}(a_n) = 0$



Automatic Optimization of O-PPAC

(Parallel-Plate Avalanche Counter with Optical Readout)
33 SiPMs per array



1. Define parameters of interest:

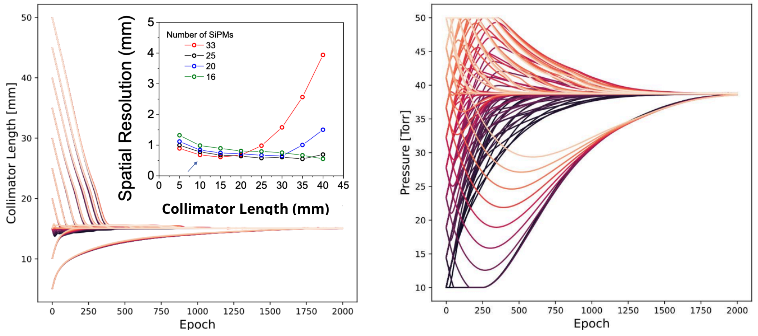
- Collimator Length (L)
- Pressure of the scintillating gas (p)

2. Set loss function:

$$\mathcal{L}(p, L, x, y) = \frac{1}{2}\left[\left(x - \hat{x}(p, L, x, y)\right)^2 + \left(y - \hat{y}(p, L, x, y)\right)^2\right]$$

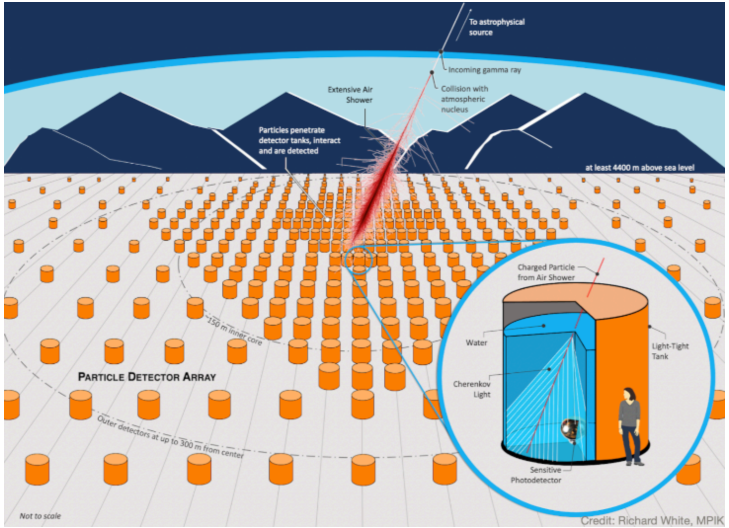
3. Use AD to find the minimum of $\mathcal{L}$ w.r.t. p and L:

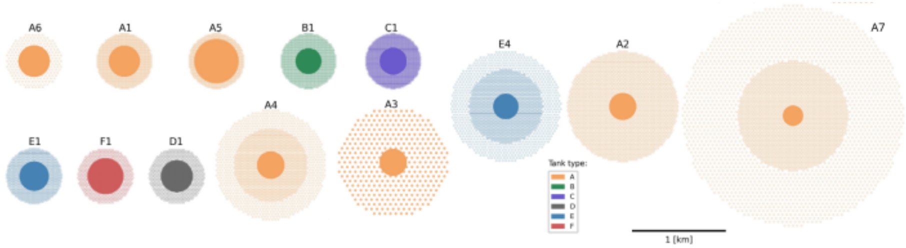
- Fully-Connected NN with 3 layers
- 64 neurons per layer



L matches the traditional approach (superimposed)

Optimizing SWGO Array Layout

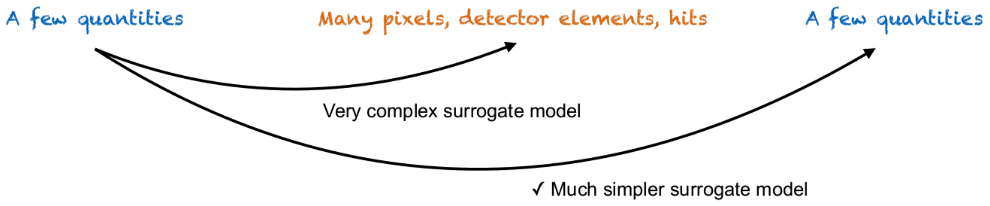


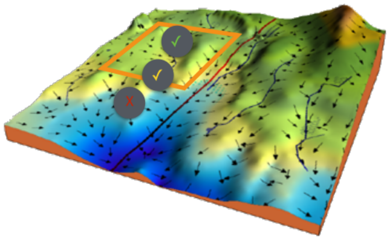


(13 configurations are provided by SWGO collaboration)

- The Southern Wide-Field Gamma Observatory (SWGO) is planned to be built at high altitude in south America.
- The optimization goal is to arrange $N = \mathcal{O}(6000)$ tanks of Cherenkov detectors that SWGO plans to deploy
  - Full configuration space is highly-dimensional: $\mathbb{R}^{2\times N-3}$

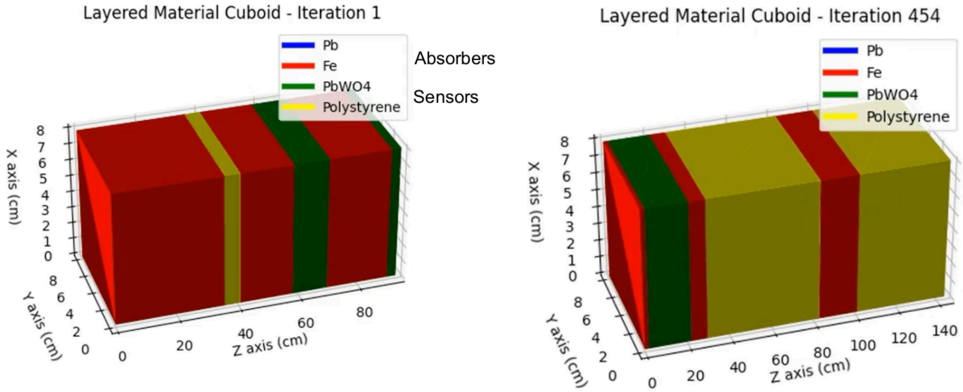
Calorimeters Optimization





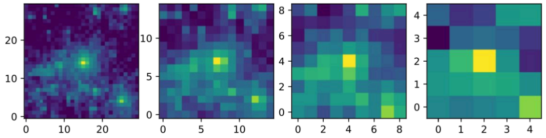
Calorimeters:

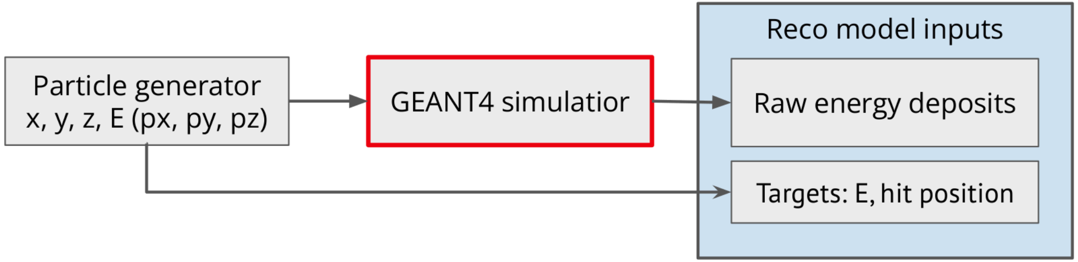
- Complex showers
- So far designs relatively simple
- Good place to invest in systematic gradient-based optimization
- Requirements:
  - Length < 180 cm



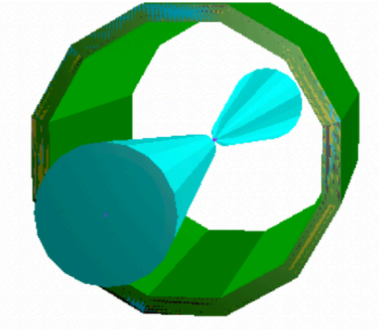
Robust Reconstruction Models for ECal Optimization

Module granularity from
15×15 to 255×255 cells^2



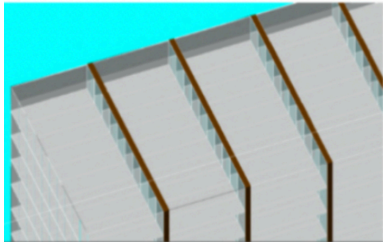


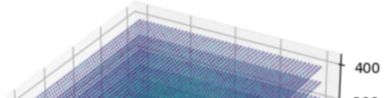
Future Muon Collider Calorimeter Optimization

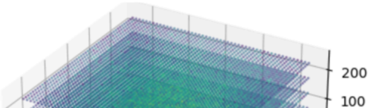


Beam Induced Background (BIB) problem for TeV-scale muon collider

- BIB simulation at 1.5 TeV center-of-mass energy
  - Energy deposits in ECal
- Reference design is CRILIN for ECal
  - Array of $1 \times 1 \times 4.5\text{cm}^3$ PbF_2 voxels arranged in a dodecahedron
  - 5 layers per wedge
  - Modular design
- Optimizing photon reconstruction efficiency and material cost

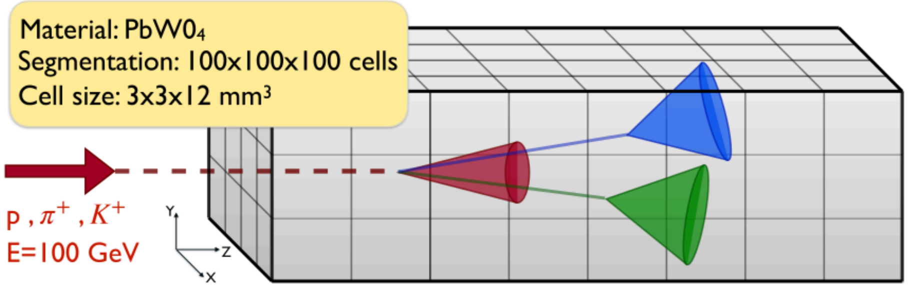


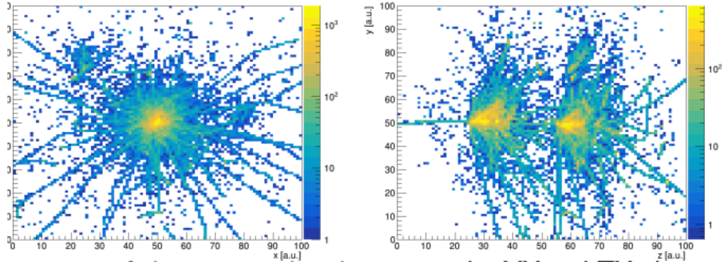




Hadron Calorimeters

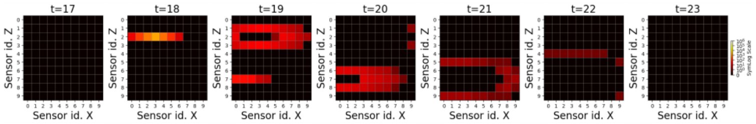
1. Toward Particle ID in Granular HCal: XGBoost-based reco provides 64% accuracy in p/π PID





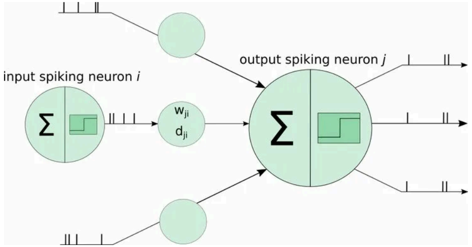
Projection of the energy distribution in the XY and ZY planes.

2. Neuromorphic Readout for Homogeneous HCal



- First ever attempt to use neuromorphic solutions for calorimetry readout
- Development of multi-nanowire photodetector for physical readout
- Employ Spiking Neural Network for precise energy measurement and for particle identification

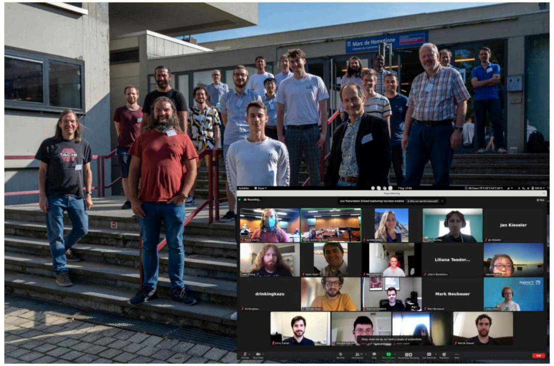
Neuromorphic Computing



"Computing approach that mimics the structure and function of the human brain using artificial neurons and synapses"
C. Mead. “Neuromorphic electronic systems” (1990)

Approach is applied to develop hardware trigger for UHE neutrino detection

Previous MODE Workshops



2021: In Louvain-la-Neuve (Belgium)

2022: In Kolymbari, Crete (Greece)

2023: In Princeton University (USA)

2024: In Valencia (Spain)

We’re Waiting You at Fifth MODE Workshop in 2025

Want to Join MODE Collaboration?

- According to the collaboration Statute, you need to:
  - be interested in our research plan, and to produce research in that area
  - bring competence of relevance, or vow to acquire it
  - aim to contribute to it within your (time and resource) possibilities
- If you are interested, send the MODE Steering board (Dorigo, Donini, Giammanco, Ratnikov, Vischia) an email with confirmation of the above and a short bio/CV: chances are we'll get you in!

https://mode-collaboration.github.io

Conclusions

- Maximum extraction of scientific value
- Challenge current design concepts
- Assist with a landscape of solutions
- Modular pipelines powered by autodiff
- Make generators differentiable where possible
- Create and guide a multidisciplinary community

[redacted]