PROCEEDINGS OF SCIENCE

Differentiable Physics Emulator for Water Cherenkov Detectors

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The water Cherenkov detector stands as a cornerstone in numerous physics programs such as precise neutrino measurements. In a conventional physics analysis pipeline, the understanding of detector responses often relies on empirically derived assumptions, leading to separate calibrations targeting various effects. The time-consuming nature of this approach can limit the timely analysis upgrades. Moreover, it lacks the adaptability to accommodate discrepancies arising from asymptotic inputs and factorized physics processes. Our work on the differentiable physics emulator enhances the estimations of systematic uncertainties and advances physics inference across all the aforementioned aspects. We construct a physics-based AI/ML model that is optimizable with data. We can infer convoluted detector effects using a single differentiable model, informed by robust physics knowledge inputs. Furthermore, our model is a robust solution for experiments employing similar detection principles.

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1. Introduction

Charged particles can traverse faster than photons in a medium due to the reduced speed of light by $1/n$—the medium's refractive index. Such a phenomenon is known as Cherenkov radiation [1]. The last few decades water Cherenkov detectors have been widely used in various particle physics experiments that achieved ground-breaking discoveries, including the atmospheric neutrino oscillation by Super-Kamiokande (Super-K) [2]. More water Cherenkov detectors, for example the Water Cherenkov Test Experiment (WCTE) [3], the Intermediate Water Cherenkov Detector (IWCD) [4], and Hyper-Kamiokande (Hyper-K) [5], are being prepared and constructed for the next generation experiments aiming at precise measurements of neutrino oscillation parameters.

In each of the aforementioned water Cherenkov detectors, an array of photo-multiplier tubes (PMTs) is mounted on the detector wall to detect the Cherenkov photons from the moving charged particles. These Cherenkov photons usually form unique ring-like hit patterns on the PMT array. Based on the topology of all the registered PMT hits and the signal charge and time of each hit, key features such as the particle type, kinetic energy, interaction position, and traverse direction of the particle can be inferred.

2. Challenges in Calibration and Reconstruction

The state-of-the-art event reconstruction tool in Super-K and T2K [6] is a maximum likelihood fitter: fiTQun [7]. The core of fiTQun is a likelihood function for particle hypotheses based on PMT hit information as written in eq. 1

$$L(\vec{x}) = \prod_{j}^{unhit} P_j(unhit|\vec{x}) \prod_{i}^{hit} \Big\{ [1 - P_i(unhit|\vec{x})] \, f_q(q_i|\vec{x}) f_t(t_i|\vec{x}) \Big\} \tag{1}$$

where $\vec{x}$ is a vector space for various particles including e, μ, γ, π^0, and $\pi^{\pm}$ and their kinematic information such as initial position and momentum. $P(unhit|\vec{x})$ represents the probability of a PMT that is not hit given particle state $\vec{x}$, while i and j iterate through the un-hit and hit PMTs respectively. f_q and f_t respectively represent the charge and time likelihood in a PMT given particle state $\vec{x}$.

To perform the fit on the free parameters in the particle vector space, one needs the detailed form of the terms to the right of eq. 1. Complex pre-tuning with calibration sources is needed for this purpose. In practice, $O(10^9)$ Monte-Carlo (MC) events are generated to achieve the likelihood functions f_q and f_t. Isotropic photon emitters are then used to calibrate the MC simulation and summarize the target likelihood functions into fixed look-up tables that depend on the quantities related to the relative spatial details of the photon emission point and every PMT. A few limitations exist in this pre-tuning and calibration process:

- Due to the use of look-up tables, the optimizability is broken between the MC simulation and the calibration. Therefore, even with a slight configuration change in the detector the whole tuning process needs to be redone.

- The observables from calibration represent a combined result of various detector effects, for example water quality, reflection and scatter, and so on. One thus has to rely on other calibration constants that represent a factorized likelihood space in the detector domain to avoid biasing the likelihood functions (f_q and f_t) designed for optical responses. Moreover, given the limited number of calibration sources and observables, it is impractical to completely disentangle the degenerate detector effects.

3. ML-based Approach

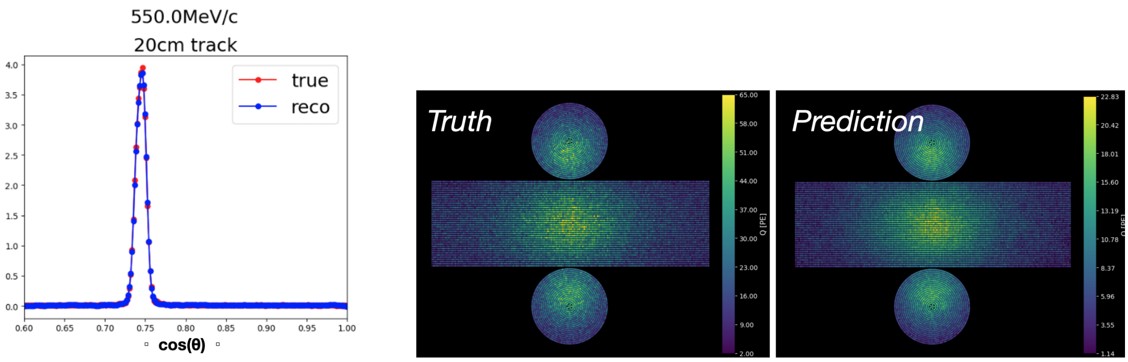
A machine-learning based calibration and reconstruction algorithm (differentiable physics emulator) is designed in this work to improve the limitations mentioned in Sec. 2. Such a differentiable algorithm represents the whole phasespace of the transformation from physics domain to detector domain, and thus remove the need of factorized detector response likelihood functions. Unlike the fixed look-up tables, the algorithm itself can be optimized by the gradient of target-prediction discrepancy, thanks to the existence of *autograd* [8] that is commonly used in the training of neural networks (NNs). The NN in this work is inspired by the architecture in [9], in which the authors claimed that the use of sinusoidal activation functions help achieve better image resolution.

This work treats the calibration and reconstruction pipeline as a two-fold process with 2 sequential NNs and is demonstrated in fig. 1:

$\boxed{\text{Particle physics: } p, s \text{ (track length), PID}} \longrightarrow \boxed{\text{Cherenkov radiation: } N\gamma, (x,y,z), (\theta,\phi)} \longrightarrow \boxed{\text{Detector domain: } Q, T}$

Figure 1: Schematic view of the differentiable physics emulator in this work. The inputs in the first step are particle type (PID), momentum (p), and the track length. The first NN yield the Cherenkov photon emision position (x, y, z) and direction (θ, ϕ) with these inputs. This 5D vector is input to the second NN along with a normalization factor representing the number of emitted Cherenkov photons. The charge (Q) and timing (T) responses of every PMT are the final outputs of the full pipeline.

The preliminary results in fig. 2 show great potential of this work. At the current stage without any fine-tuning, the sequential NNs are able to produce Cherenkov photons given particle kinematics and detector charge responses given photon sources.



(a) Production of Cherenkov photons

(b) PMT charge responses to an isotropic photon emitter.

Figure 2: Panel (a) shows the Cherenkov photon emission angle with respect to a muon of p = 550 MeV/c at track length of 20 cm. The red and blue curves are the MC input and NN prediction respectively. Panel (b) shows the PMT charge responses to an isotropic optic photon source in the center of a toy water Cherenkov detector, with the MC input shown in the left and NN prediction the right.

4. Conclusion

This work presents the concept of a differentiable physics emulator as to realize a optimizable detector simulation and calibration pipeline and some preliminary results. The first milestone is expected to be a demonstration with the WCTE calibration data that is expected around 2024 to 2025.

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