# Differentiable Physics Modeling for the Data-Driven Optimization and Analysis of Long Baseline Neutrino Oscillation Experiments

US-JAPAN SCIENCE AND TECHNOLOGY COOPERATION PROGRAM COLLABORATION KICK-OFF MEETING, AUGUST 7/8<sup>TH</sup>, 2023

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WHEN WE SHOW AN IMAGE, APP SHOULD TELL US ELECTRON OR MUON NEUTRINO

SURE, CNN, EASY PEASY, 1 HOUR

OH AND ALSO TELL US THE LOCATION OF THE LEPTON WITH UNCERTAINTY

> ON IT. APPLYING FOR A 5-year research grant

#### (Physics) Model Optimization

#### Success of AI is through gradient-based optimization that works for millions, billions, or even trillions of parameters.

Journal of Machine Learning Research 23 (2022) 1-40

Submitted 8/21; Revised 3/22; Published 4/22

Switch Transformers: Scaling to Trillion Parameter Models with Simple and Efficient Sparsity

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#### Abstract

In deep learning, models typically reuse the same parameters for all inputs. Mixture of Experts (MoE) models devit this and instead select different parameters for each incoming example. The result is a sparsely-activated model—with an outrageous number of parameters—but a constant computational cost. However, chepite several notable successes of MoE, widespread adoption has been hindered by complexity, communication costs, and training instability, and training instability. And we show large parse models muy be trained, for the first time, with lower precision (blocat(b) to the disgn intuitive improved models with reduced communication (blocat(b) constant), with lower precision (blocat(b) contain up to 7x increases in per-training speed with the same computational resources. These improvements extend into multilingual settings where we measure gains over the mT5-Base version across all 101 languages. Finally, we advance the current scale of language models by metraining up to trillion parameter models on the "Colossal Clean Crawled Corp.", and achieve a 4x speedup over the mT5-Base version across the T5-T500 model. <sup>12</sup>

 $\label{eq:keywords:mixture-of-experts, natural language processing, sparsity, large-scale machine learning, distributed computing$ 



"To deal with hyper-planes in a 14-dimensional space, visualize a 3-D space and say "fourteen" to yourself very loudly. Everyone does it." - Geoffrey Hinton

#### Gradient-based Optimization







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### **Future Neutrino Oscillation Experiments**





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#### Machine Learning for Neutrino Oscillation Experiments

## **Unprecedented Statistical Precision**

• DUNE and Hyper-K aim to collect 1000s of  $v_e$  and  $\overline{v_e}$  appearance events

- Can measure CP
   violation (CPV) with
   ~3% statistical
   uncertainty!
- Controlling systematics becomes critical!



Event rates for different assumptions of true  $\delta_{CP}$ 



# **CP Violation Discovery Potential**

 Improved understanding of systematic errors is required for a robust and timely discovery of CPV

 Controlling systematics becomes critical!



## **Current Neutrino Oscillation Systematic Error Budget**

- Breakdown of current (T2K) state-of-the-art understanding
  - $\circ$   $\phi$ : Beam neutrino flux
  - $\circ$   $\sigma$ : Neutrino interaction cross-sections
  - ND: Near detector
  - SK (FD): Super-K (far detector)
  - NC: Neutral current
- Need reduction on all fronts

"T2K 2021 syst.": Phys. Rev. D 103, 112008

Error Source	% Error for CPV search
$\phi$ + $\sigma$ (ND constrained)	2.7
$\phi$ + $\sigma$ (ND unconstrained)	1.2
Nucleon removal energy	3.6
SK $\pi$ re-interactions	1.6
$\sigma(v_e), \sigma(v_e)$	3.0
NC $\gamma$ + other	1.5
SK detector (FD)	1.5
Total	6.0

Need to reduce to <3%

### Novel Beam-Spanning (PRISM) Near Detectors



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Error Source	% Error for CPV search	
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SK detector (FD)	1.5	
Total	6.0	
Need to reduce to <3%		

beam center

### **T2K-SK Water Cherenkov Detector Systematics**



assigned from data/MC

and atmospheric v data

discrepancies in cosmic ray

Nucleon removal energy3.6SK  $\pi$  re-interactions1.6 $\sigma(v_e), \sigma(\overline{v_e})$ 3.0NC  $\gamma$  + other1.5SK detector (FD)1.5Total6.0

**Error Source** 

 $\varphi + \sigma$  (ND constrained)

 $\varphi + \sigma$  (ND unconstrained)

"T2K 2021 syst.": Phys. Rev. D 103, 112008

Need to reduce to <3%

% Error for

**CPV** search

2.7

1.2

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#### Machine Learning for Neutrino Oscillation Experiments

## **Traditional Paradigm of Detector Physics Modeling**



#### Limitations

- $\circ$  Lack of "end-to-end" optimization
- $\circ$  Some models are not even optimizable (e.g. look-up tables)
- $\circ$  Same physics, two separate software (i.e. simulation & calibration)
- Goals toward "detector systematics @ <1% level"</li>
   Automation + fast compute that can scale for HK/DUNE
  - $\circ$  Accurate model optimized directly to minimize data/MC disagreement



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## **Automation of Physics Model Tuning**

#### **Research Proposal: differentiable detector physics simulator (DDSim)**

- "End-to-end": gradient-based optimization using control (calibration) dataset
- Interpretable: analytical physics models for well understood physics
- Flexible: neural representation to incorporate complex features in real data
- Fast: utilization of modern computing accelerators (e.g. GPUs)



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- LAr "Visibility Map" (or light scattering table for WC) derived from massive photon MC, encoded in a multi-dimensional table ... but static & not scalable
- Candidate: "SIREN"
  - Implicitly represents a continuous function in space
  - Designed to learn the gradient surface = enables applications using gradient-based optimization



Probability of detecting photon produced at given position (2D slice of 3D voxelized volume)



### **Detector Inverse Solver (DIS) using a differentiable simulator**

A novel application enabled with a DDSim



 $\mathbf{X} \in \mathcal{D}_I$ Input domain of detector simulator (inaccessible)

 $G(X|Y, \theta_G)$ **Inverse Image Solver (DIS)** 

$$\mathcal{L}_{\rm inv} = \left| G(\mathbf{Y}) - \mathbf{X} \right|^2$$

and / or 
$$| T(C(X)) \rangle = X$$

$$\mathcal{L}_{\rm cc} = |F(G(\mathbf{Y})) - \mathbf{Y}|^2$$



 $\mathbf{Y} \in \mathcal{D}_O$ Output domain of detector simulator (e.g. real data) Differentiable Detector Simulator (DDSim)

Enables near-far comparison of neutrino events at the event-by-event level for the first time

 $F(Y|X, \theta_F)$ 

## The Water Cherenkov Test Experiment (WCTE)

- Prototype for IWCD at CERN in 2024
- Well-understood p, e,  $\pi^{\pm}$ ,  $\mu^{\pm}$  particle beam from 140-1200 MeV/c
  - Control samples to constrain neutrino experiment modeling:
    - Detector response: Cherenkov light emission;  $\pi^{\pm}$  interactions
    - Neutrino flux & interactions: lepton scattering and hadron production
  - Immediate impact to existing experiments (T2K, Super-K)
- Demonstration of these new ML simulation and calibration techniques for WC, and optimization towards Hyper-K/IWCD





~102 mPMT modules x19, 3" PMTs each

### ArgonCube 2x2

- Prototype for ND-LAr (LArTPC component of DUNE Near Detector) at Fermilab
  - 2x2 array of 0.7x0.7x1.2 m<sup>3</sup> modules deployed in NuMI beam with elements of MINERvA
  - Installation and operation in NuMI anticipated in summer 2023
- NuMI provides an intense source of neutrinos & muons
- Demonstration of these new ML simulation and calibration techniques for LArTPCs, and optimization towards DUNE
  - AI/ML reconstruction already under development
  - SIREN optical model developed



1st module testing at Bern

Module at Fermilab





#### **Research Schedule**



## **In-person Workshop at SLAC**

- Japan-side budget allows e.g. 4 people travel for 2 weeks, this fiscal year (FY)
  - Project will be reviewed then budget decided for the following 2 FYs
- Hack-a-thon-like format with code sprints
  - Tasks to be defined as we ramp up these coming months
- Candidate dates to be decided this meeting, then poll will follow
  - Sep. 25 Oct. 6 (too soon?)
  - Not Oct. 9 13 (JPS-APS Hawaii)
  - Not Oct. 23 27 (HK CM)
  - Not Nov. 6 10 (T2K CM)
  - Not Nov. 27 Dec. 1 (SK CM)
  - Dec. 4 15?
  - Early next year?

### **Collaboration Name?**

- Urgent in case we want to include in mailing list name, GitHub name, etc.
- Any ideas?
  - Differentiable Signal Propagation Project (DSPP)

o ...

	Monday, 7 August			
18:00 → 20:00 Day 1: ht	tps://ipmu.zoom.us/j/94250009765			
18:00	Project overview: Differentiable physics modeling Speakers: Kazuhiro Terao (SLAC) , Patrick de Perio (Kavli IPMU)		Tuesday, 8 August	
18:30	Questions/Discussion	<b>17:00</b> → 19:00 Day 2: ht	ttps://ipmu.zoom.us/j/97884442440	
18:40	LArTPC: differentiable neural implicit representation for physics modeling Speaker: Patrick Tsang (SLAC)	17:00	Alternative methods for signal propagation	
	2023-08-07 SIREN U	17:30	Questions/Discussion	
19:10	Questions/discussion	17:40	Brainstorming Session Speakers: Kazuhiro Terao (SLAC) , Patrick de Perio (Kavii IPMU)	
19:20	Water Cherenkov applications/challenges Speaker: Ka Ming Tsui (Kavli IPMU)			
19:50	Questions/			

## Summary

- Next generation long-baseline neutrino oscillation experiments will require unprecedented precision understanding of their detectors
- Existing simulation, calibration, and reconstruction analysis pipelines are becoming a limiting factor in this endeavor
- Proposed novel machine learning algorithms to solve these modeling and computational issues
  - Common tools to be shared between US-Japan
  - Seed for community-wide effort
- <u>Meeting notes</u> (feel free to contribute):

https://docs.google.com/document/d/1aw6Yv7exMGs7tk4SyKdBMq-r3j7zVS58mY JjLiUT3hw/edit?usp=sharing

#### References

- Project Abstract
- Project Proposal
- Project Plan (for KEK)

#### Appendix

### How: Differentiable Detector Physics Simulator (DDSim)

#### **Gradient-based optimization**



### Neural differentiable surrogate for optical detectors

#### **Differentiable Neural Scene Representation**



$$(x, y, z, \theta, \phi) \rightarrow \square \rightarrow (RGB\sigma)$$
$$F_{\Theta}$$

**NeRF**: breakthrough on high resolution image representation by a very simple neural network





ACORN: scalable version of SIREN by adding spatial feature compression (essentially a learnable kd-tree)

### ... only a few examples

**<u>SIREN</u>**: success of learning the 1st and 2nd order derivatives

## **AD-Enabled Detector Physics Simulator**

- Enable Automatic Differentiation (AD):
  - Same physics formula, now differentiable
  - Backed-up by a large AI/ML research community
  - Speed up by enabling co-processors (GPUs/TPUs)



- Successful demonstration for LArTPC imaging detector
  - End-to-end: simultaneous optimization of multiple detector physics parameters
  - On-going study: the robustness of the fits, modeling of poorly understood physics (e.g. electric field)



#### Machine Learning for Neutrino Oscillation Experiments

#### Data Reconstruction in Experimental Particle Physics Cross-domain HEP AI ecosystem

**ML is a "solution pattern"** v.s. a domain-specific "hard-coded" solution. It's **naturally reusable across domains including software tools** supported by a large community of researchers.



HEP Ecosystem for AI research

- Accessible **education and training** at all levels
- **Reusable software tools** to unlock modern compute accelerators and networking (distributed ML)
- **Public datasets** with documentation and performance metrics for transparent, reproducible science
- Artificial Intelligence and Technology Office (AITO)
  - $\circ~$  Federated, equitable, responsible, trustworthy AI
  - AI is an accelerator. It is coming. Don't avoid. Participate to make sure the use is good.

#### **Evolution of the Universe**



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- Example: "Visibility Map" (or light scattering table for WC) derived from massive photon simulations, encoded in a multi-dimensional table
- **Issues**: "static" and not scalable
  - SIREN is an implicit representation of a continuous function
    - Can be seen as a trade-off between an analytical function and a table



- SIREN is designed to represent (learn) the gradient surface hence "differentiable"
- Can be optimized directly by minimizing "a data/MC discrepancy" with control samples
- SIREN is an implicit
   representation of a continuous function
   in space
  - Can be seen as a trade-off between an analytical function and a table



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- Preliminary demonstration on real DUNE ND prototype data strongly promising
- Optimized as a simulator + applied in reconstruction (inverse solver)



#### **ML for Detector Physics Modeling SIREN** as a differentiable surrogate for optical detectors

#### **Differentiable Neural Scene Representation**

#### **SIREN** for LArTPC detectors

- Designed as an implicit representation of a continuous function in space (suited to "visibility", "E-field", etc.)
   Can be seen as a trade-off between an analytical function and a table
- "Differentiable" implies we can directly optimize against "data v.s. simulation discrepancy" given control samples

SIREN trained on "Toy + Noise" successfully learned the underlying analytical function shape (simulation)



### The NuPRISM Concept

Neutrino energy spectrum depends on off-axis angle to the neutrino beam source

Moving IWCD vertically  $\rightarrow$  varying off-axis angle  $\rightarrow$  measurements with differing energy spectra

Linear combinations of measurements at off-axis angles can mimic a monochromatic beam, or the far-detector spectrum







near and far detectors



Large energy reconstruction errors

T2K: Phys. Rev. D 103, 112008 (2021)

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SK detector	1.5	
Total	6.0	

Need to reduce to <3% for Hyper-K



Need to reduce to <3% for Hyper-K

# IWCD Measurement of $v_e$ ( $\overline{v_e}$ )

Constrain  $\frac{\sigma(\mathbf{v}_{e})/\sigma(\mathbf{v}_{\mu})}{\sigma(\bar{\mathbf{v}_{e}})/\sigma(\bar{\mathbf{v}_{\mu}})}$  using **1%**  $\mathbf{v}_{e}$  ( $\overline{\mathbf{v}_{e}}$ ) contamination in beam

y background mostly mitigated by water Cherenkov active shielding





 $^{
u}e/\mu$  $\nu_{e/\mu}$ Snn ' N N Neutral current backgrounds lacking data driven constraints

#### T2K: Phys. Rev. D 103, 112008 (2021)

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SK detector	1.5		
Total	6.0		

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## e I µ Classification in IWCD



- Constrain  $\frac{\sigma(\mathbf{v}_e)/\sigma(\mathbf{v}_{\mu})}{\sigma(\bar{\mathbf{v}}_e)/\sigma(\bar{\mathbf{v}}_{\mu})}$  using 1% intrinsic  $\mathbf{v}_e(\bar{\mathbf{v}}_e)$  in beam
- Need >~1000 in  $\mu$  rejection (>99.9%)
- Can be achieved in IWCD with ML
- Factor 10<sup>5</sup> speedup





## Gamma (y) Identification



• Need data driven constraints on γ backgrounds



- $\gamma$  and *e* almost indistinguishable in water Cherenkov detectors
  - Potential discrimination shown for the first time
- ML shows promise with at least statistical separation



# **Detector Modeling Uncertainties**

- The fundamental v–Ar interaction is the same in the ND and FD, so some detector error cancelation is possible
  - lonization, recombination, drift velocity may be similar provided that the detector conditions are similar (e.g. E-field, Ar purity, etc.)
- However, there are several important differences
  - ND pixel readout vs FD wire or strip readout -
  - Large pileup at ND (10's of events per spill)
  - Geometry: ND has smaller active volume, dead regions within the active volume, shorter drifts (less diffusion)
  - Different calibration strategies (e.g. ND has plentiful muons; FD has ~5,000/day and will rely more on calibration systems)
- Currently, a conservative assumption of uncorrelated ND/FD • energy response uncertainties for each particle type is assumed
  - Estimated from calorimetric approaches (Minerva + NOvA) and LAr-TPCs (LArIAT, MicroBooNE, ArgoNeuT)
- Other uncertainties include fiducial volume size and energy ٠ resolution(s), and selection uncertainties on the muon identification and hadronic energy containment

$$E_{rec}' = E_{rec} \times \left(p_0 + p_1 \sqrt{E_{rec}} + \frac{p_2}{\sqrt{E_{rec}}}\right)$$

Particle type	Allowed variation		
	$p_0$	$p_1$	$p_2$
all (except muons)	2%	1%	2%
$\mu ~({ m range})$	2%	2%	2%
$\mu$ (curvature)	1%	1%	1%
p, $\pi^{\pm}$	5%	5%	5%
e, $\gamma$ , $\pi^0$	2.5%	2.5%	2.5%
n	20%	30%	30%

Eur. Phys. J. C 80, 978 (2020)



# **Constrained Modeling of the Experiment**

- A coherent method exists for constraining (degenerate) fundamental physics parameters of the neutrino flux and interactions with measurements
- This still needs to be developed for detector physics parameters



## **IWCD & Hyper-K Photosensor Development**

- Multi-PMT (mPMT): 19 x 3" diameter
   PMTs in a watertight vessel with
   HV and electronics
- Pulsed and continuous LEDs for calibration:
  - PMT timing
  - Water properties
  - Detector geometry
- Sensors for magnetic field monitoring







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#### Machine Learning for Neutrino Oscillation Experiments

## **Overview: Next Generation Experiment**







- Bigger and more sensitive than ever
  - Fiducial mass 8x Super-K
  - J-PARC beam 2.5x more powerful
    - $\rightarrow$  Neutrino rates 20x T2K
- Precise systematic understanding becomes critical to the % level
  - New near detectors and photon detectors
  - New calibration and event reconstruction techniques
  - New supporting external data from auxiliary experiments

# T2K-SK Multi-Ring Datasets for Future Analyses

- Second dominant interaction channel: resonant 1π production
- Expected to improve oscillation parameter measurements
  - E.g. ~12% increase in  $v_e$  signal statistics
- New BDT pushing the limits of traditional likelihood reconstruction algorithm







# **Multi-Ring Reconstruction in the Further Future**

- More machine learning: panoptic segmentation
- Towards improving multi-ring & multi-GeV event classification and reconstruction
  - $\circ$  v mass ordering, v<sub>t</sub> appearance,  $\delta_{CP}$





#### Modeling Detector Physics



**Example**: Liquid Argon TPC **Objective**: given a calibration dataset (i.e. images of particle trajectories with approximated dE/dX values), "fit" the detector physics parameters





#### **Example**: Liquid Argon TPC

- Charged particle ionize electrons
- Electrons drifts under E-field
- Signal diffuse and attenuated

Detector Simulation  

$$\mathcal{R}_{\text{ICARUS}} = \frac{A_B}{1 + k_B \cdot (dE/dx)/\mathscr{E}}$$

$$Q = Q_0 \exp(-v_{\text{drift}} t/\tau)$$

$$\sigma_t^2(t) \simeq \sigma_t^2(0) + \left(\frac{2D_L}{v_d^2}\right)t$$



Optimizing the "lifetime" physics parameter directly from calibration dataset

#### **Example**: Liquid Argon TPC

- Charged particle ionize electrons
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Detector Simulation  

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$$\sigma_t^2(t) \simeq \sigma_t^2(0) + \left(\frac{2D_L}{v_d^2}\right)t$$





Work credit due (from left): ML/Math: Youssef N., Sean G., Daniel R. neutrino: Yifan C., Roberto S.

#### Lots of applications

- Simultaneous multi-parameter fit
- Inter-parameter dependency study
- Automation of calibration workflow
- Inverse imaging (i.e. reconstruction)

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#### The Core Idea: Differentiable Physics Modeling And Applications in DUNE/HK

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Machine Learning for Neutrino Oscillation Experiments