Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

FY2025 NPP LDRD Type B Pre-Proposal

Risk Mitigation for DUNE AI/ML

Principal Investigator(s) Haiwang Yu (PI, PO), Yihui Ren (co-PI, CSI)

Date: Dec. 6, 2023

@BrookhavenLab

FY2025 NPP LDRD Type B Pre-Proposal

Proposal title: Risk Mitigation for DUNE AI/ML

Primary Investigator: Haiwang Yu (PI, PO), Yihui Ren (co-PI, CSI)

Other Investigators: Brett Viren (PO), Yi Huang (CSI)

Indicate if this is a cross-directorate proposal: Yes _X__ No___

If yes, identify other directorates/organizations: CSI

Proposal Term: From: Oct/24 To: Sep/26

Brookhaven National Laboratory

FY2025 NPP LDRD Type B Pre-Proposal

Proposal title and brief abstract:
Title: Risk Mitigation for DUNE AI/ML
Abstract: We propose an efficient, automated Human-Instructed-Machine-Learning method (InstructLArML) to reduce the algorithm systematic uncertainties originating from data-simulation discrepancies for DUNE.

Program: HEP

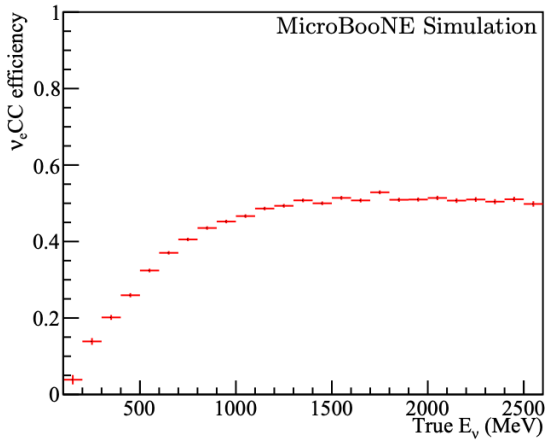
Return on Investment: Potential ECA of the PI

Broader impact on the activities at the laboratory: Explore responsible AI for HEP analysis with human knowledge embedding

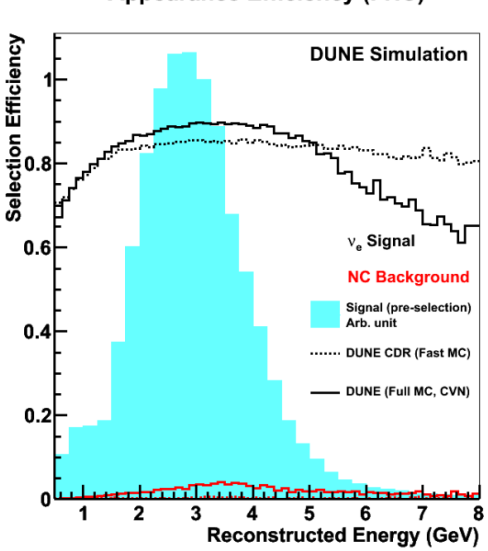
Total planned funding per year in FY25 and FY26: $250k/y

Motivation

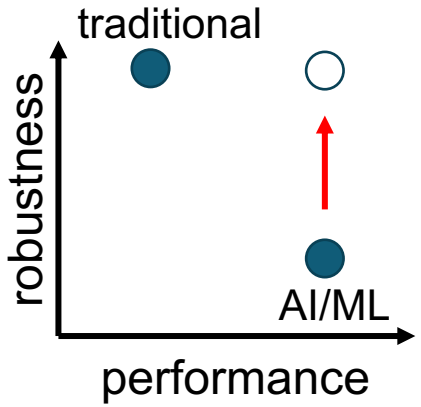
Phys.Rev. D 105 (2022) 11, 112005



Phys. Rev. D 102, 092003 (2020)

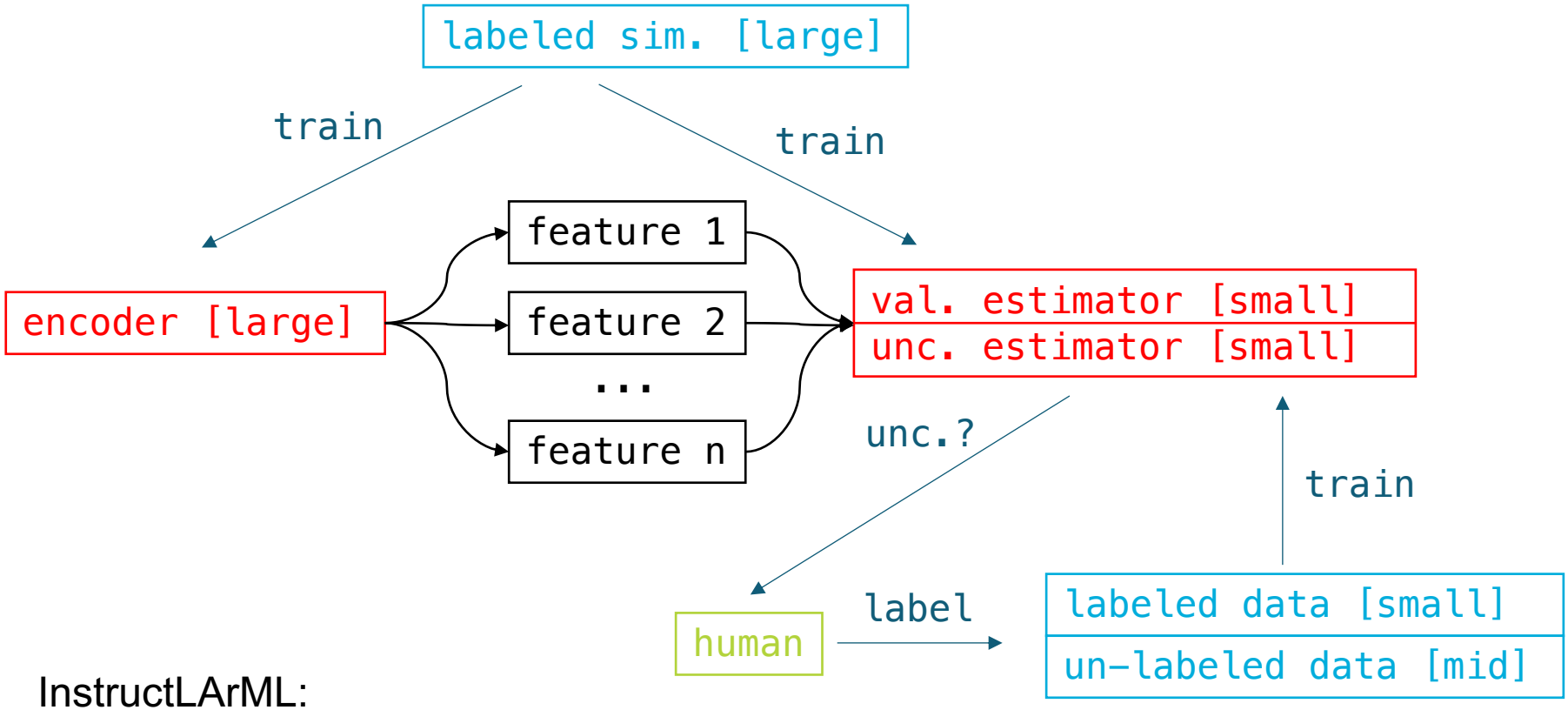


- To improve the AI/ML robustness against data-simulation discrepancies for DUNE
- E.g., ν_e selection efficiency differences in MicroBooNE and DUNE:
  - DUNE task is different from MicroBooNE
  - Simulation is still different from data



Brookhaven National Laboratory

Approach: InstructLArML



InstructLArML:

1, large labeled sim. to train large encoder

2, hybrid human labeled and un-labeled real data to train small val./unc. estimators

3, un-labeled data is useful to strengthen the model when unc. is small

4, human only labels data with large unc.

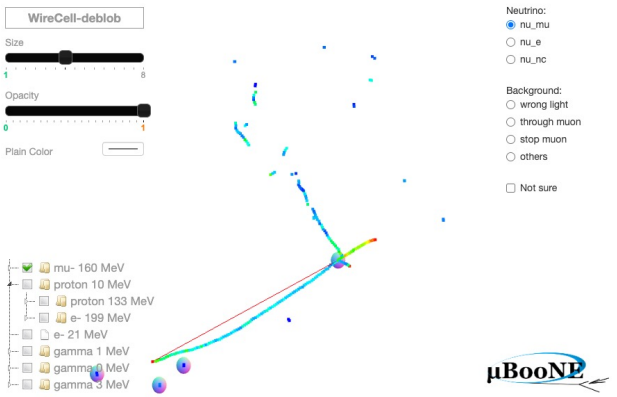
Assumptions:

1, sim. and data have enough common features

2, Human labeling is reliable in all/part of the scenarios

Related works

JINST 17 P01037

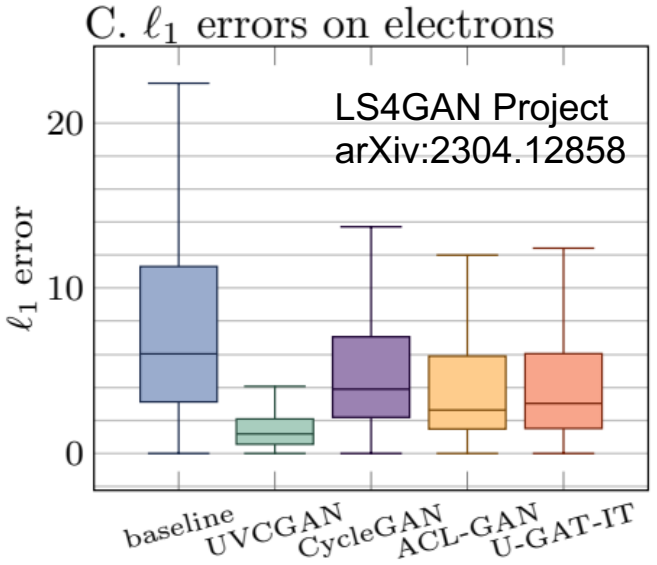


This human helped AI/ML is inspired by:

1. The hand-scan approach used to develop current Wire-Cell LArTPC reconstruction
2. InstructGPT [arXiv:2203.02155] which uses human input to align human preference and LLM output

LD4GAN: pilot studies on AI/ML technologies to translated samples between domains

- Estimate systematic unc. from data-sim. discrepancies
- Improve simulation



Summary I

Proposed work in this LDRD

- Implement an InstructLArML system for ν flavor tagging
- Generate multiple sim. dataset with variations (flux, generator, detector effect, etc.). One with large statistics servers as “sim.” Others with smaller statistics as “data”
- Study various uncertainty estimators (e.g., ensemble, Bayesian NN)
- Study the fine-tuning mechanism (e.g., Latent Representation Learning)

Estimated total effort

- Post-doc: 0.5-1.0 FTE
- Scientific staff (EDG, CSI): 0.5 FTE
- GPU resources

Summary II

- Intellectual merit
  - Develop a human instructed AI/ML model that is more robust to data-sim. discrepancies for DUNE
    - Combine AI/ML and human knowledge
  - Use AI/ML techniques to boost the labeling/training efficiency
    - Active Learning, Latent Representation Learning, Uncertainty Quantification

- Return on Investment
  - The PI is eligible for ECA application until 2029.
  - The PI intends to submit an ECA related to “Responsible AI for DUNE”; this LDRD provides a key step towards that goal.

- Broader impacts
  - This proposal targets to solve a critical question that whether human inputs can help AI/ML in HEP.
  - A positive answer could establish a new direction for AI/ML applications in HEP/physics.

backup

Responsible AI for DUNE

To fully address these concerns and to maximize DUNE's physics potential, we plan to build a system on three foundational blocks,

(1) a method to estimate DSD related systematic uncertainties (Risk Estimation);

(2) a method to build AI/ML algorithms with reduced DSD related systematic uncertainties (Risk Mitigation);

(3) a method to understand and reduce DSD (Simulation Augmentation).

A pilot study on (1) was conducted in another LDRD project and can be adopted for DUNE.

We plan to study (2) in this proposal.

So that a potential follow-up ECA can study (3) and then build a Responsible AI System for DUNE based on them.