

Applications of GraphNeT

In IceCube Neutrino Observatory

3rd GraphNeT Workshop / 3rd of May, 2023

Rasmus Ørsøe

Technical University of Munich



In parallel to Development ...

Commits on Apr 19, 2023

- Merge pull request #485 from asogaard/labels Verified 62e86c <>
asogaard committed last week ✓
- Add more intuitive key for Direction label 59386cc <>
asogaard committed last week ✓
- Merge pull request #489 from JostMigenda/typos Verified b31367 <>
asogaard committed last week ✓

2000+ Commits in 240+ Pull Requests

Commits on Sep 22, 2021

- Addressed most of Andreas comments 2b28e95 <>
Rasmus OrsDe committed on Sep 22, 2021

Commits on Sep 21, 2021

- Added sqlite_converter that creates a database ala I3ToSQLite. Notice... c58573a <>
Rasmus OrsDe committed on Sep 21, 2021
- Added I3 extractor and general 06b3c11 <>
Rasmus OrsDe committed on Sep 21, 2021

Commits on Apr 12, 2021

- Initial commit Verified a243f7a <>
phlippeller committed on Apr 12, 2021

Today



First Commit



In parallel to **Development** ...

We've been investigating **Applications** in IceCube

Commits on Apr 19, 2023

- Merge pull request #485 from asogaard/labels
asogaard committed last week ✓
- Add more intuitive key for Direction label
asogaard committed last week ✓
- Merge pull request #489 from JostMigenda/typos
asogaard committed last week ✓

...

2000+ Commits in 240+ Pull Requests

...

Commits on Sep 22, 2021

- Addressed most of Andreas comments
Rasmus Orsteb committed on Sep 22, 2021

Commits on Sep 21, 2021

- Added sqlite_converter that creates a database ala I3ToSQLite. Notice...
Rasmus Orsteb committed on Sep 21, 2021
- Added I3 extractor and general
Rasmus Orsteb committed on Sep 21, 2021

Commits on Apr 12, 2021

- Initial commit
phlippeller committed on Apr 12, 2021

Today



First Commit



2 Papers,
4+ Posters,
~20 talks,

ML4Astro, A3D3, Neutrino22,
ML4LatticeQCD, NOW2022, ACAT,..

Applications in IceCube

Today



DynEdge Paper

Presents DynEdge and shows performance & robustness on oscillation dataset in IceCube

First Commit

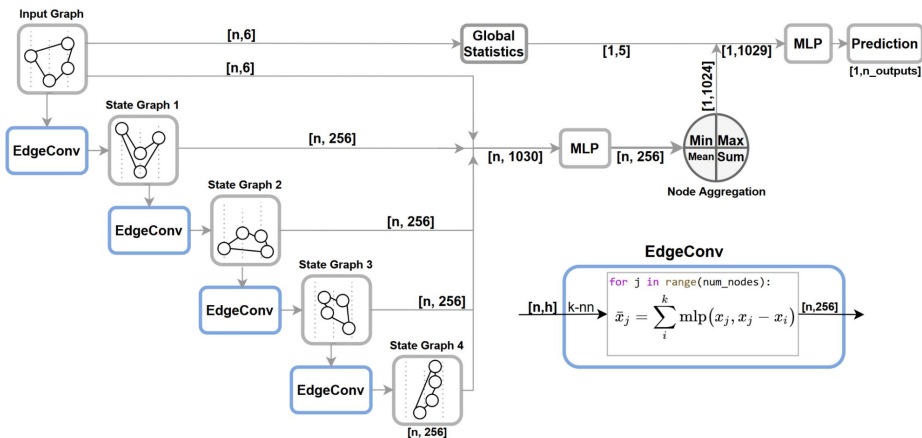


Diagram of DynEdge, from the paper.

Applications in IceCube

Today



JOSS Paper

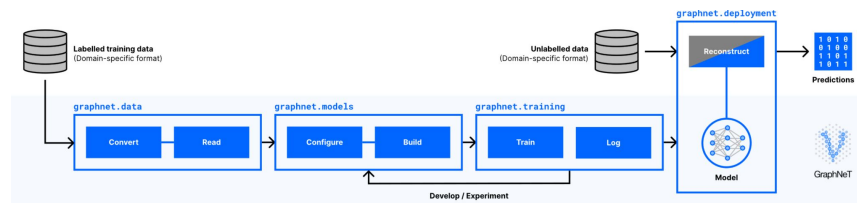
Presents GraphNeT, workflow and usage



DynEdge Paper

Presents DynEdge and shows performance & robustness on oscillation dataset in IceCube

First Commit



Overview of GraphNeT, from JOSS paper

Drop-in Replacement

In Existing Analyses





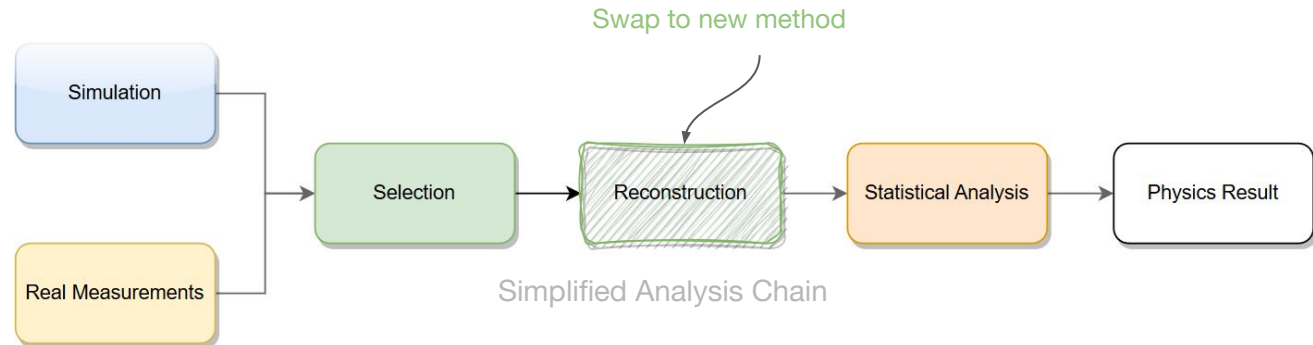
Drop-in replacement

(Low hanging fruits)

Physics results depend highly on the sensitivity, reliability and speed of reconstruction methods

Pro
Improved reconstructions likely to improve results in existing analyses.
Little overhead for analysis owners.

Con
The existing data selection is not always optimal for ML.
Potential improvement in selection not taken into account.





Drop-in replacement

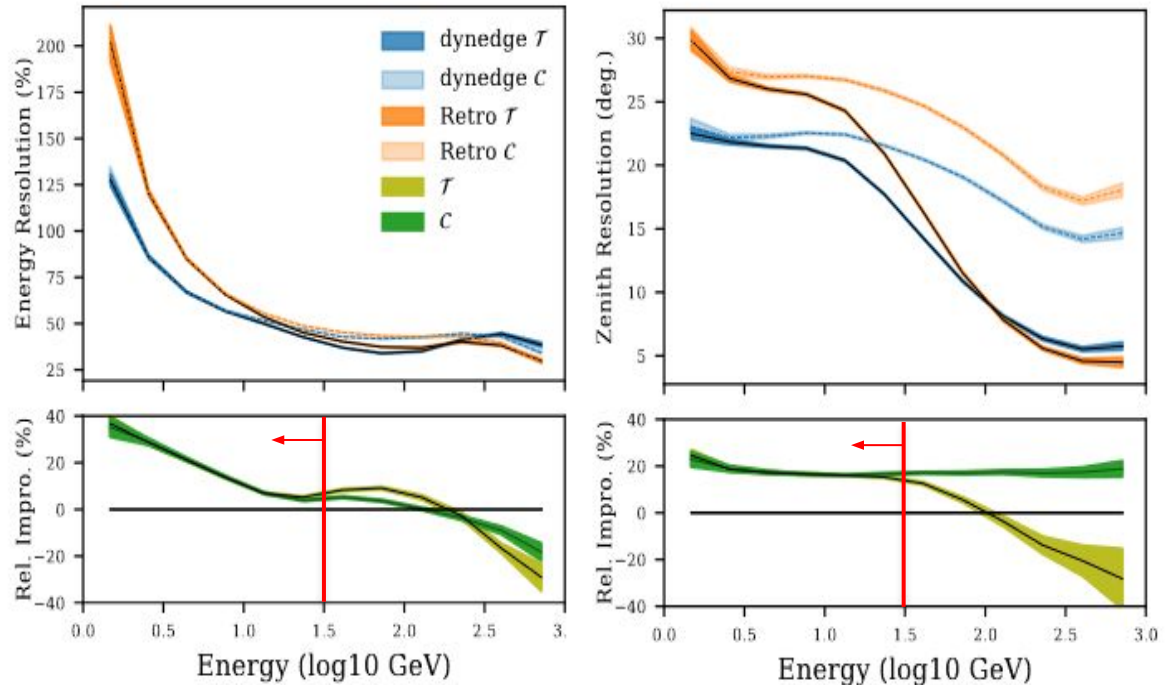
Oscillation Analysis in IceCube

Comparing current method with DynEdge:

Around 20% improvement in variables in relevant energy range used in the oscillation measurement

But what could that mean for the final result?

Resolution Performance

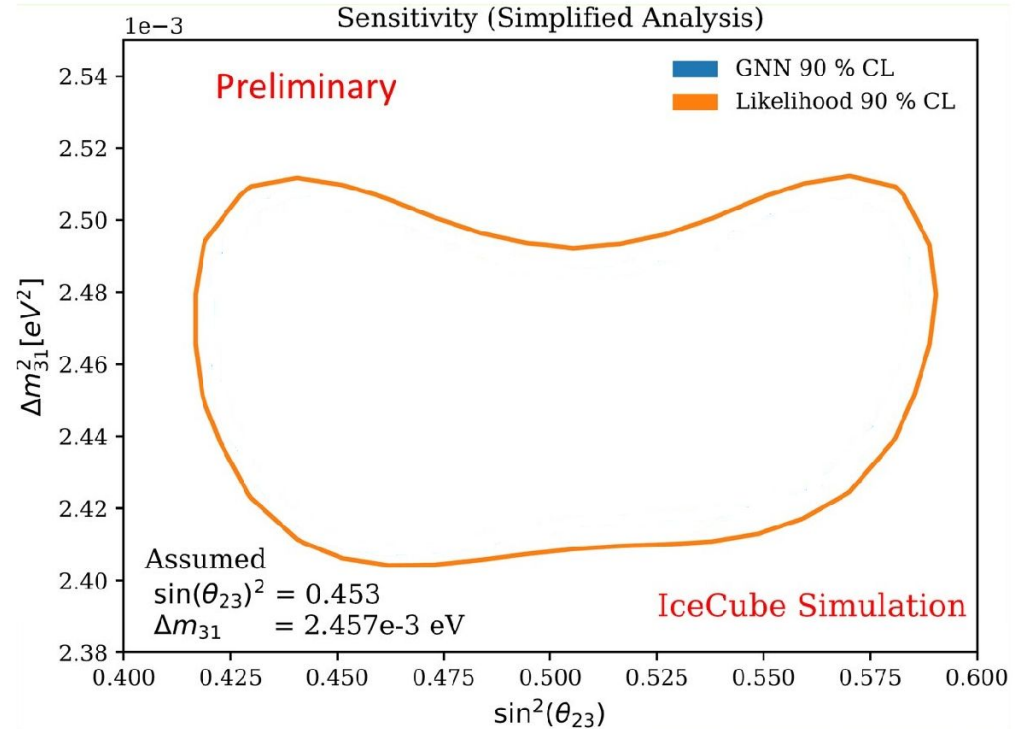




Drop-in replacement

Oscillation Analysis in IceCube

But what could that mean for the final result?



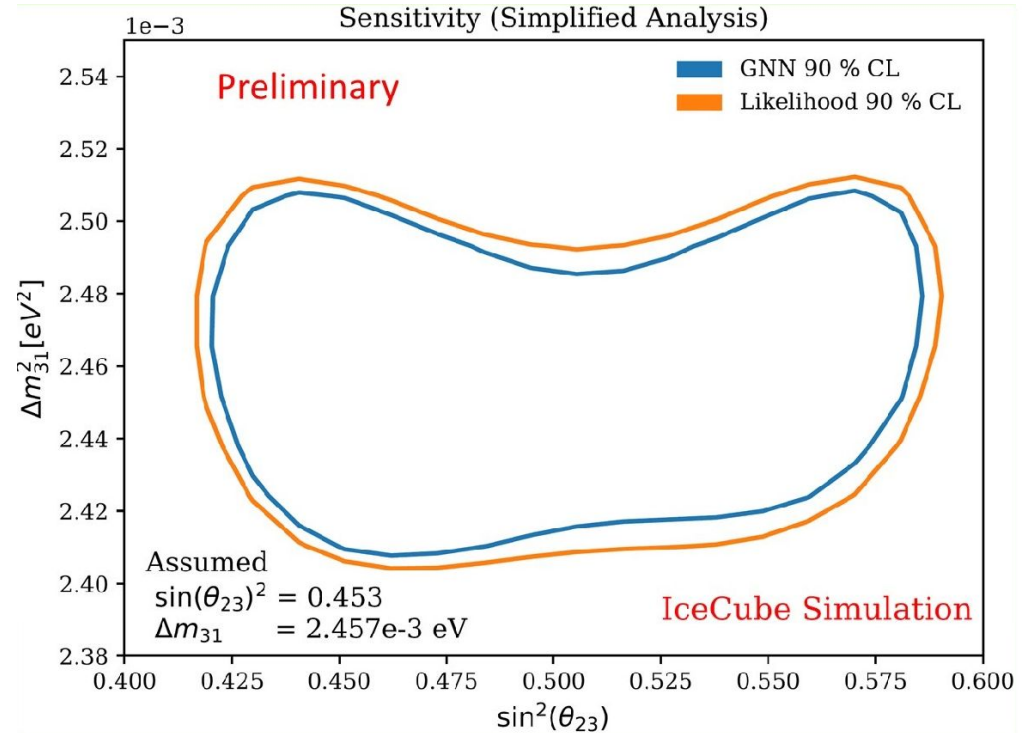


Drop-in replacement

Oscillation Analysis in IceCube

But what could that mean for the final result?

The comparison suggests improvements equivalent to an additional **25%** statistics.





Drop-in replacement

Oscillation Analysis in IceCube

These results were shown in a poster for **Neutrino2022**

Low Energy Neutrino Event Reconstruction using Graph Neural Networks

Rasmus Falck rasmus.orsoe@tum.de

IceCube is a gigaton Ice Cherenkov detector located at the South Pole that detects neutrinos from a few GeV to several PeV

5160 in-ice digital optical modules (DOMs) on measure pulses of Cherenkov radiation emitted during interactions.

Two things:

- Nodes**
Nodes are rows of data. For IceCube events, nodes represent pulses of measured Cherenkov radiation.
- Edges**
Edges represent the relationship between the nodes. For IceCube events, we connect each DOM with its 8 nearest DOMs in the ice.

It is the edges that allow us to describe the irregular geometry of IceCube directly. A convolution corresponds to a translation of the nodes and only the neighbors of a node contributes to the convolution. After a convolution, the neighbors of each nodes are re-calculated based on the new positions in a latent space. This feature lets the GNN learn the optimal connections.

Issues addressed in this poster:

- IceCube DeepCore:** low-energy events (5-100GeV) are crucial for atmospheric oscillation physics and have the largest opportunity for improvement through ML-based reconstruction techniques
- IceCube Upgrade:** future low-energy array (1-100GeV) will feature IceCube's first multi-PMT modules for which noise mitigation will be essential, laying the foundation for developing the Upgrade's first event selection

New DOM Types
mDOM dtgg

Graph Neural Networks (GNNs)
GNNs are neural networks that accepts graphs as input. A graph is a collection of

Impact on Oscillation Sensitivities

Our GNN-based reconstruction method ([preprint](#)) leads to about 20% improvement in resolutions of energy and zenith and offers a clearer separation of track/cascade events in the oscillation relevant energy range as compared to the current state-of-the-art ([preprint](#)). These variables are the key reconstruction targets for oscillation studies in IceCube.

Using 10 years' worth of simulated neutrino events, the improvement to the contour is demonstrated by implementing our GNN corresponds to the equivalent gains achieved with 25% more statistics.

Conclusion
We have developed a general GNN-based reconstruction method and applied it to the low energy range of IceCube (0 – 3 log 10 GeV) as a proof-of-concept. The improvement in reconstruction resolutions for key oscillation variables lead to improved oscillation sensitivities as compared to the currently in-use method. In addition, we show that, when trained on upgrade simulation, the GNN effectively identifies noise hits in new module types and provides reasonable event quality indicators based on reconstruction error estimates.

Noise Classification and Event Selection in Upgrade

The GNN also provides uncertainty estimates (σ_{Zenith}) for reconstructed variables, which can be used as an event quality indicator. The ZENITH uncertainty as Event Quality Indicator

The GNN can remove noise hits from upgrade events with very good separation.

Example Cut Chain:
10% better estimated σ_{μ} leads to 10.5% and 20.7% resolution improvements for zenith and energy reconstructions w.r.t. events with worst estimated σ_{Zenith} .

mDOM Noise Classification:
95.0% Efficiency → 96.5% Purity
95.0% Efficiency → 99.0% Purity

At 95% of physical pulses kept, the sample is 96.9% pure for modules with 24 PMTs (mDOMs)

"[Low Energy Neutrino Event Reconstruction using Graph neural Networks](#)", Neutrino2022




Drop-in replacement

Oscillation Analysis in IceCube

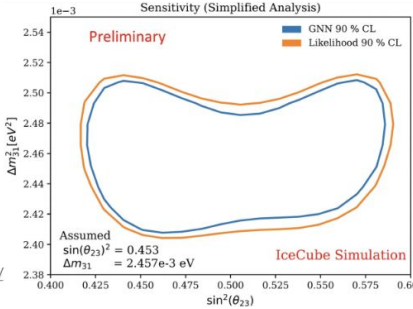
.. and they were mentioned at **NOW2022**

in a talk given by Fernanda Psihas



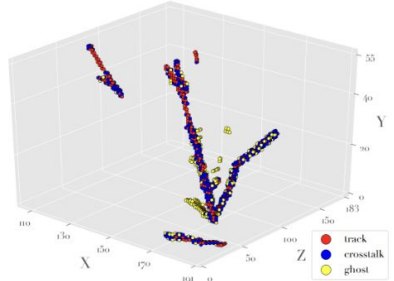
Graph NNs are natural for clustering PMT signals. GNN based reco. Yields 20% + resolution in energy & zenith.
Expected sensitivity equivalent to 25% more statistics.

GNNs Neutrino Event Reconstruction. Neutrino 2022 poster. Rasmus Orsøe. <https://indico.kps.or.kr/event/30/contributions/785/>



Sensitivity (Simplified Analysis)

Assumed $\sin^2(\theta_{23}) = 0.453$
 $\Delta m_{31}^2 = 2.457e-3 \text{ eV}^2$



(a) Prediction: voxels are colored based on the GNN predictions.

T2K is also using GNNs for removing crosstalk & ghost hits from tracks in preparation for The SuperFGD near detector for improvements with respect to charge cuts.

	GNN		Charge Cut	
	Track	Other	Track	Other
Efficiency	94%	96%	93%	80%
Purity	96%	95%	80%	91%

Graph neural network for 3D classification of ambiguities and optical crosstalk in scintillator-based neutrino detectors Sa'ul Alonso-Monsalve, et.al. <https://arxiv.org/pdf/2009.00688.pdf>

Fernanda Psihas

THIS SLIDE: NOT YET IMPLEMENTED FOR OSCILLATIONS 10

"The Role of Machine Learning in Neutrino Physics", NOW2022

Unlocking New Physics Analyses



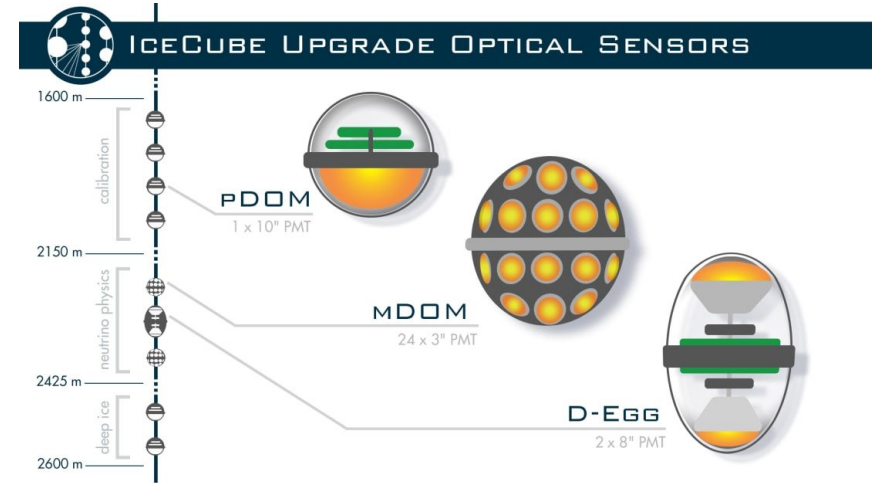


Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

“The goal of IceCube Upgrade is to provide world-leading sensitivity to neutrino oscillations and to take unique measurements of tau neutrino appearance with high precision. It also serves as a R&D platform for the future IceCube-Gen2 experiment.”

Physics Potential of the IceCube Upgrade



IceCube Press Release

Around 700 new modules



Unlocking New Physics Analyses:

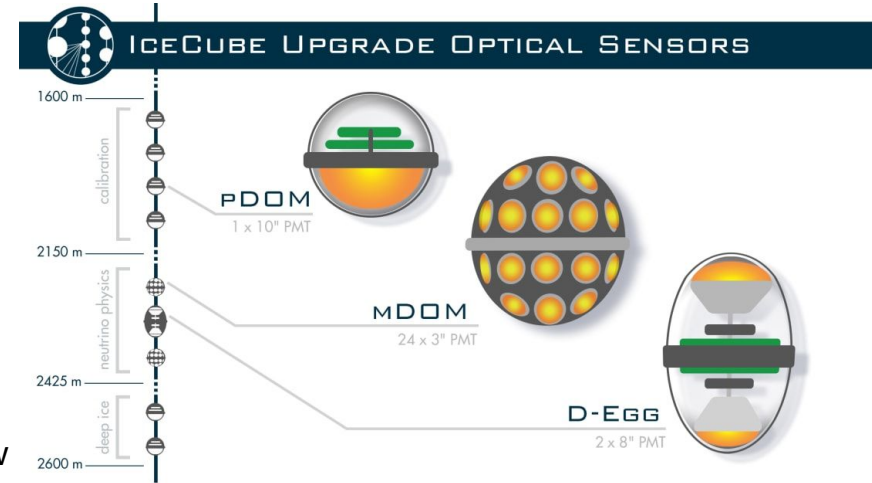
IceCube Upgrade Oscillation Sensitivity Projections

“The goal of IceCube Upgrade is to provide world-leading sensitivity to neutrino oscillations and to take unique measurements of tau neutrino appearance with high precision. It also serves as a R&D platform for the future IceCube-Gen2 experiment.”

Physics Potential of the IceCube Upgrade

Challenges (From a Data Science Perspective)

- 1) Current reconstruction methods not compatible with new modules
- 2) Cleaning algorithms doesn't work on new modules



IceCube Press Release

Around 700 new modules

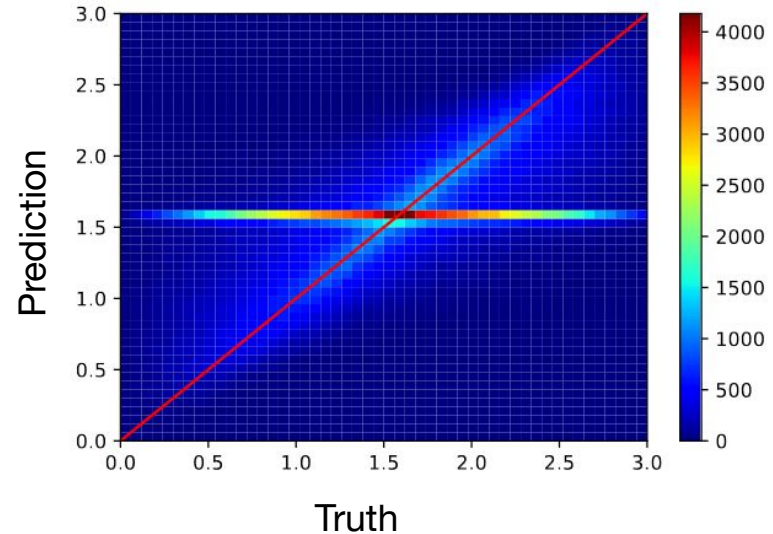


Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

Challenges (From a Data Science Perspective)

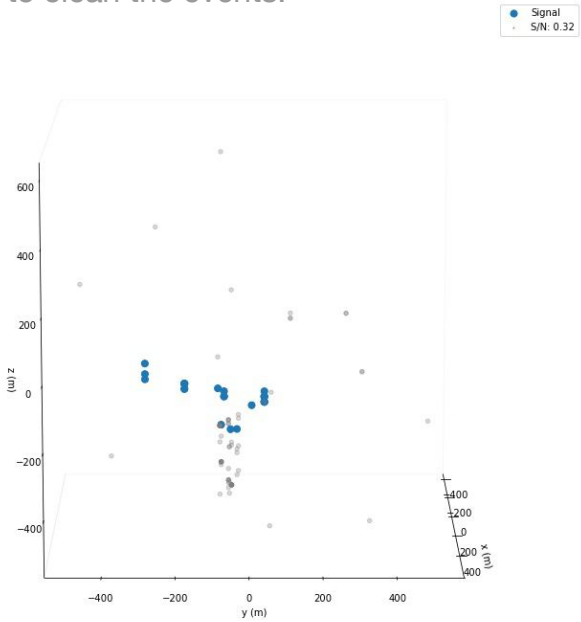
- 1) Current reconstruction methods not compatible with new modules, [but DynEdge is!](#)
- 2) **Cleaning algorithms doesn't work on new modules**



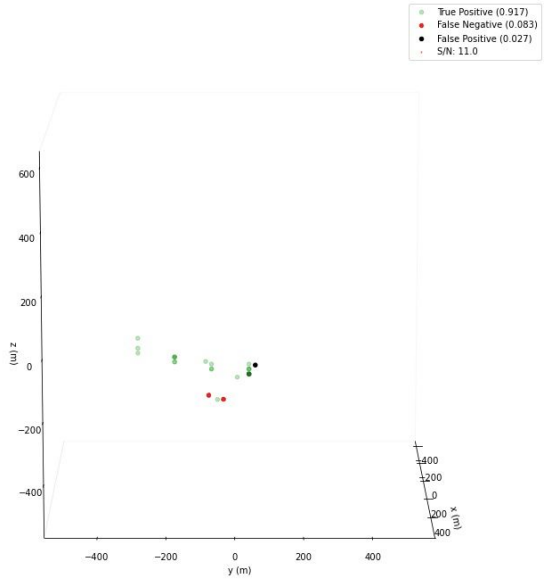


Unlocking New Physics Analyses: IceCube Upgrade Oscillation Sensitivity Projections

We phrased noise cleaning as a node classification problem, and used DynEdge to clean the events.



Uncleaned Event



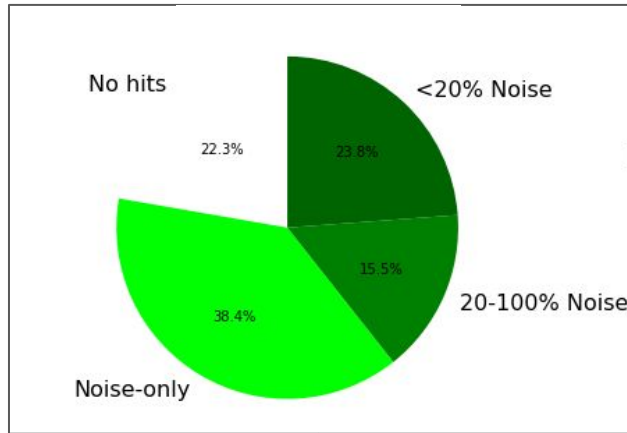
Cleaned by DynEdge



Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

“Classical” Cleaning algorithm



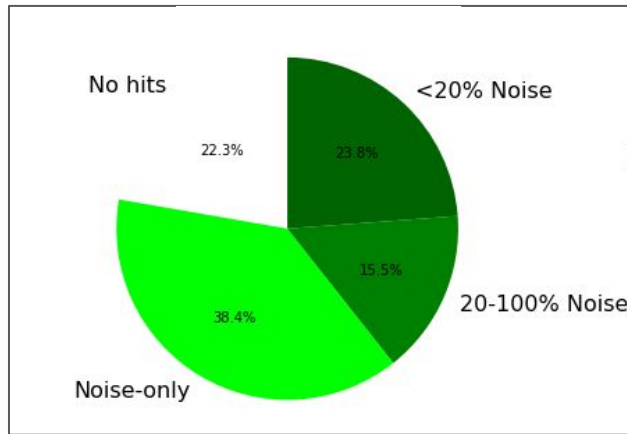
Only 24% of examples have reasonable noise pollution after cleaning



Unlocking New Physics Analyses:

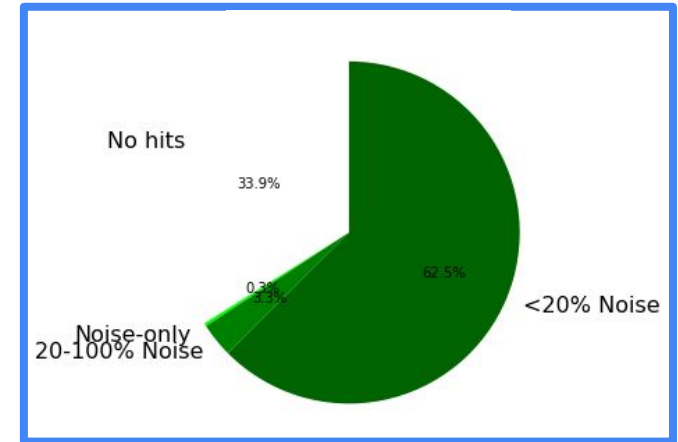
IceCube Upgrade Oscillation Sensitivity Projections

“Classical” Cleaning algorithm



Only 24% of examples have reasonable noise pollution after cleaning

GraphNeT: DynEdge



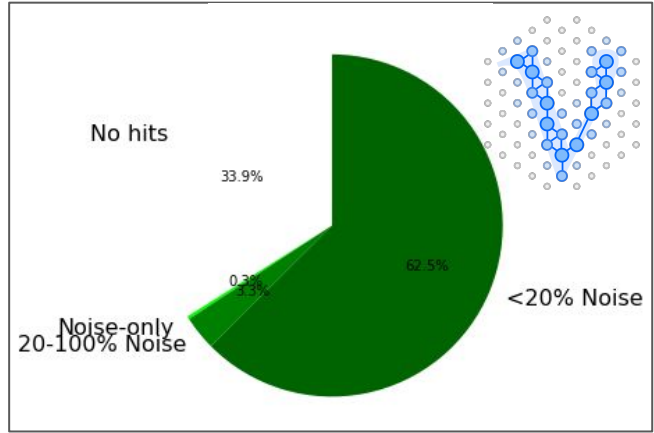
63% of examples have reasonable noise pollution after cleaning



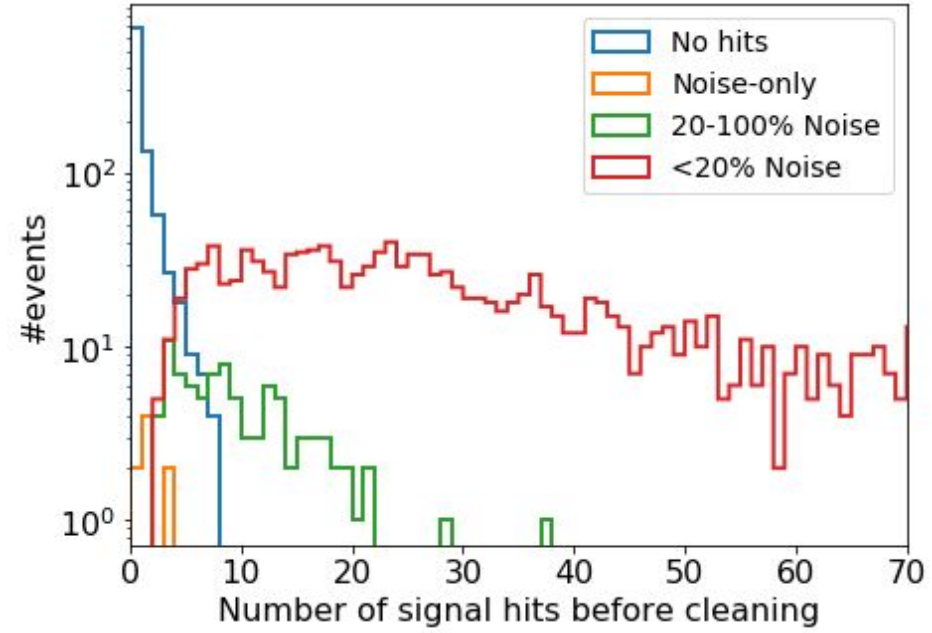
Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

GraphNeT: DynEdge



Distribution of signal hits before cleaning
(in categories from pie-chart)



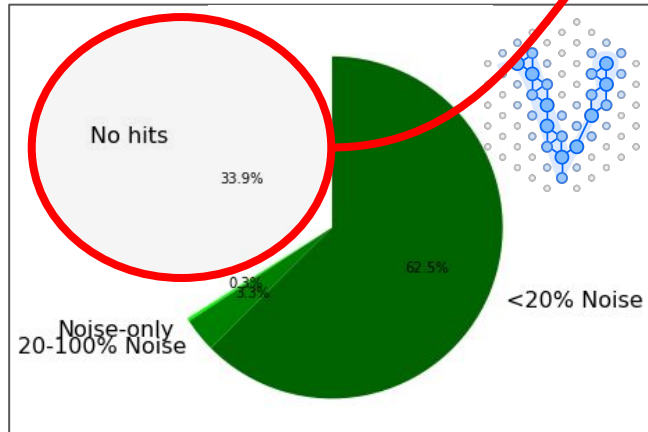
(Plot made by Jan Weldert)



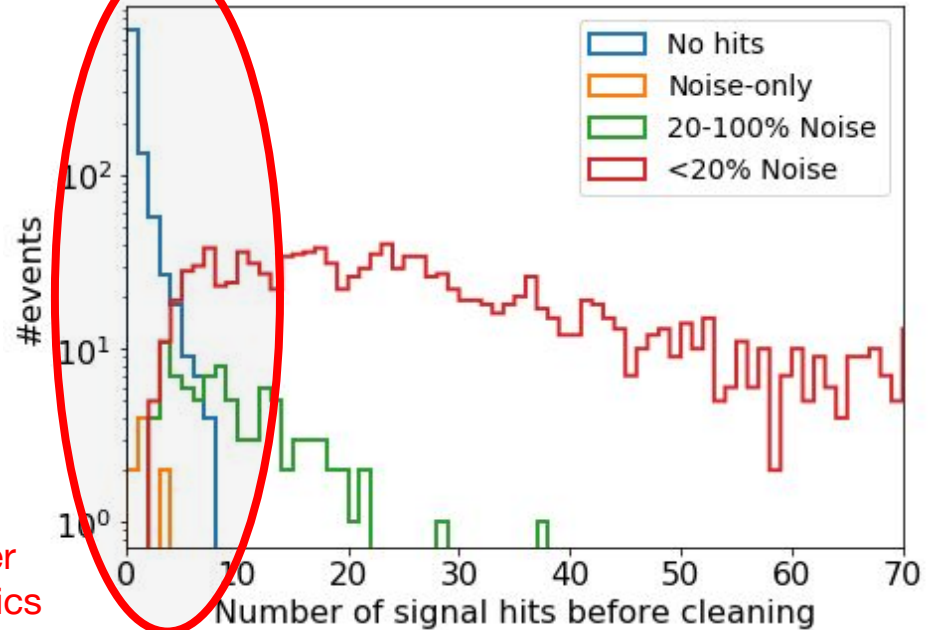
Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

GraphNeT: DynEdge



Distribution of signal hits before cleaning
(in categories from pie-chart)



All events with 0 pulses after cleaning had 9 or less physics pulses; most have 0 (log-scale)

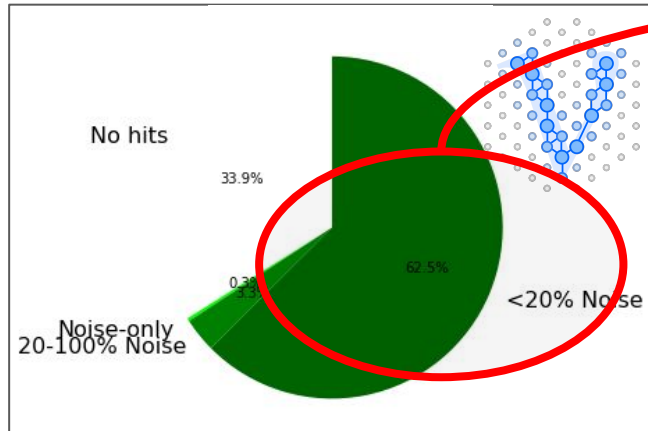
(Plot made by Jan Weldert)



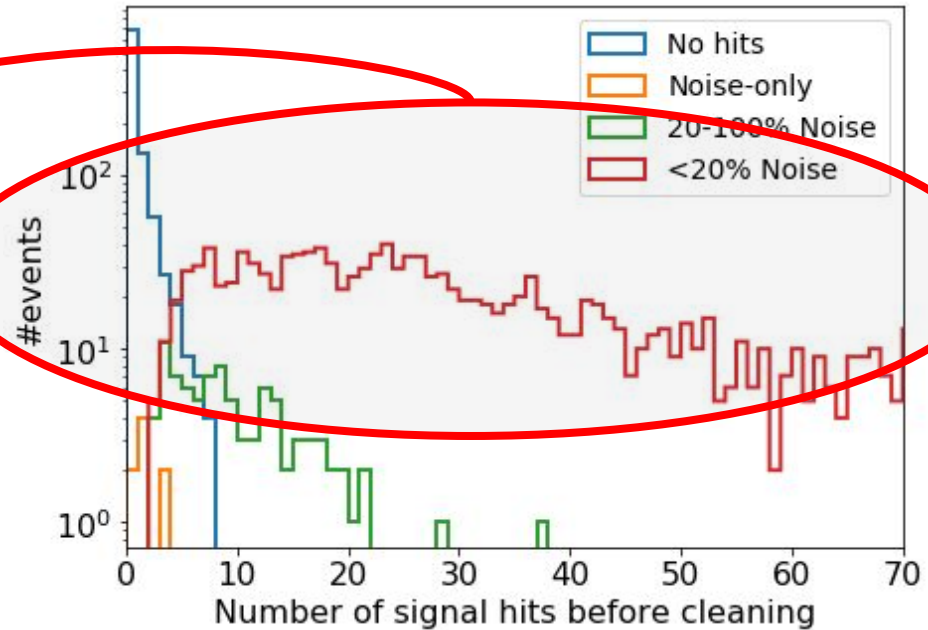
Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

GraphNeT: DynEdge



Distribution of signal hits before cleaning
(in categories from pie-chart)

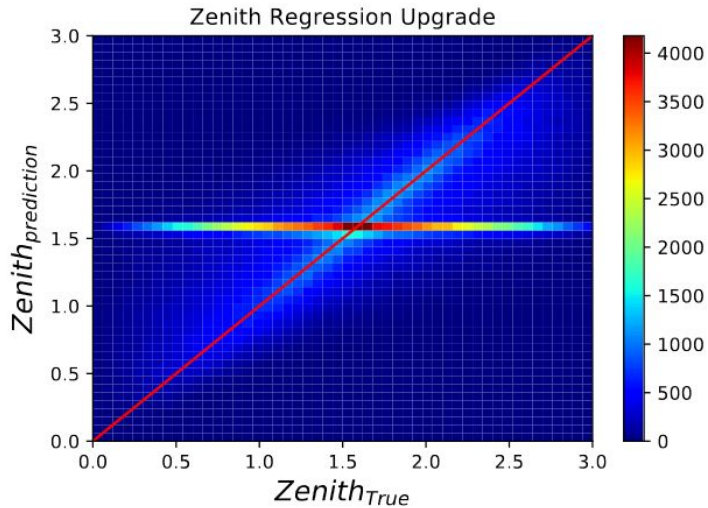


(Plot made by Jan Weldert)

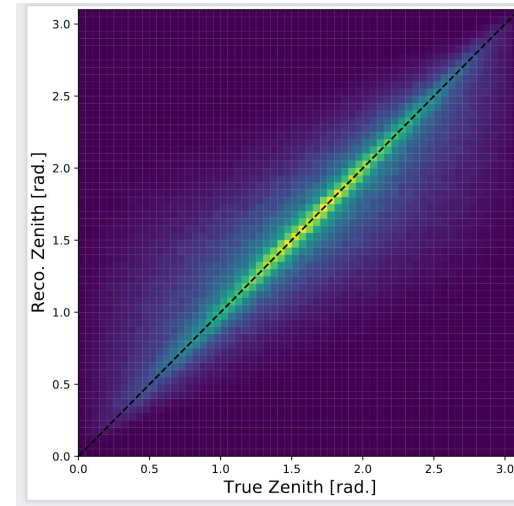


Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections



“Classically” cleaned events



GNN cleaned events



Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

Deploy pre-trained models with a minimal technical threshold:

```
from graphnet.deployment.i3modules import GraphNeTI3Deployer
```

```
# Construct I3 deployer
deployer = GraphNeTI3Deployer(
    graphnet_modules=[deployment_module],
    n_workers=1,
    gcd_file=gcd_file,
)

# Start deployment - files will be written to output_folder
deployer.run(
    input_files=input_files,
    output_folder=output_folder,
)
```




Unlocking New Physics Analyses:

IceCube Upgrade Oscillation Sensitivity Projections

Conclusion:

The pulse cleaning & reconstruction paved the way for Kayla and Jan to project sensitivities for multiple oscillation measurements, and the results will be shown at ICRC2023 this summer, and likely followed up by an IceCube paper.

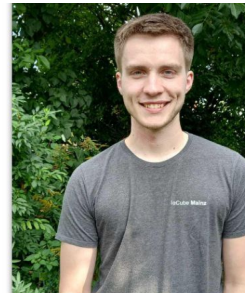
Other groups within IceCube studying different physics will use their work as a stepping stone for new analyses.

Steps are being taken to compare the GNN cleaning with methods on other datasets..

Penn State University



Kayla DeHolton



Jan Weldert

On-Going Studies





On-Going Studies:

Simulation / Data Disagreement at Low Energies

Because of its speed and similar response to systematic uncertainties, **DynEdge** has been used frequently to help **probe causes of MC/Data disagreement** in the low energy range of IceCube.

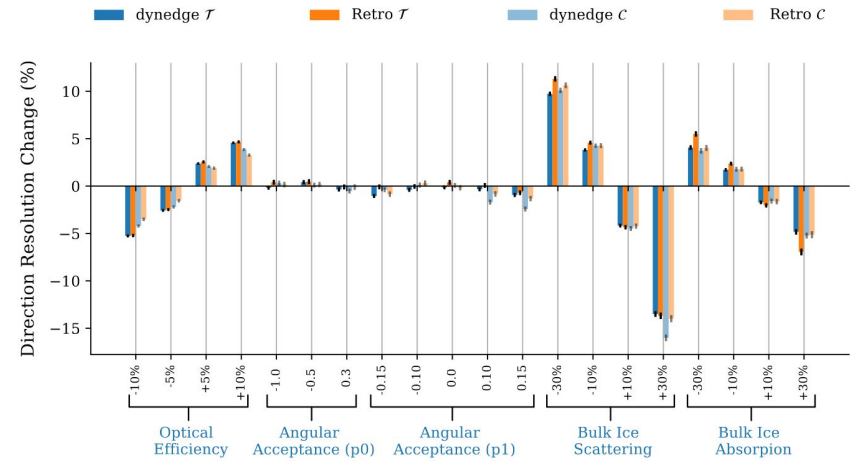


Figure 10. The variation in resolution for **DYNEDGE** and **RETRO** on the 20 different systematic sets for reconstruction targets energy, zenith, and direction.

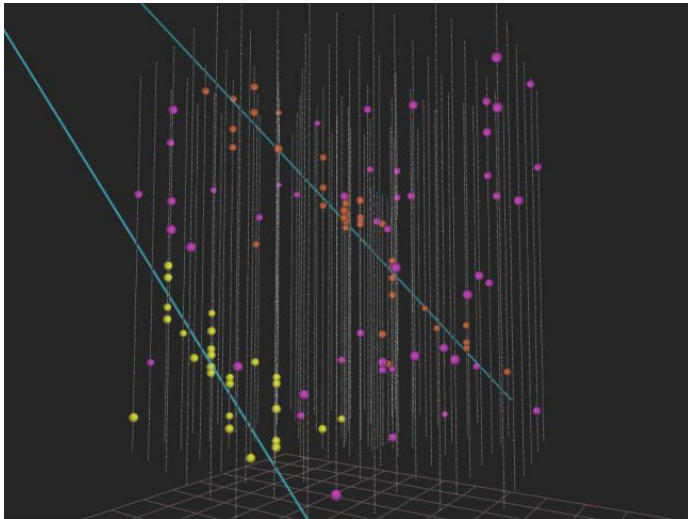
([DynEdge paper](#))



On-Going Studies:

Event Splitting

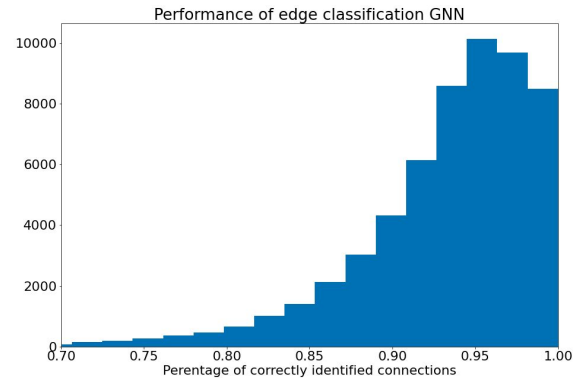
Patrick Hatch, PhD Student at Queen's University is phrasing the splitting of coincidental events as an *edge classification* problem in [GraphNeT](#).



Example of coincidental event



Patrick Hatch



Early results from Patrick, suggesting that the method is working. Further studies in progress.



On-Going Studies:

Event Selection for Low Energy Range

Morten, Peter & Andreas, MSc Students at Niels Bohr Institute
Are working on an **event selection** using **GraphNeT** at the energy range typically used for neutrino oscillations in IceCube.

Early results suggest that a significant improvement in signal retention is possible, which is likely to improve the contours shown at Neutrino2022 even further.



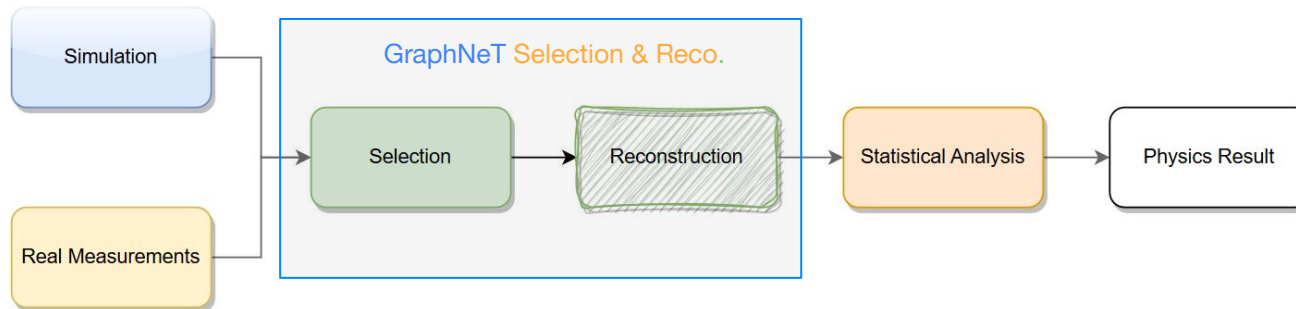
Morten Holm



Peter Andresen



Andreas Mogensen





On-Going Studies:

Neutrino Emissions from NGC1068 - Extended Analysis

IceCube telescope: High-energy neutrinos discovered in galaxy NGC 1068

First neutrino image of an active galaxy

For over ten years the IceCube Observatory in the Antarctic has been monitoring the light traces of extragalactic neutrinos. While evaluating the observatory's data, an international research team led by the Technical University of Munich (TUM) discovered a high-energy neutrino radiation source in the active galaxy NGC 1068, also known as Messier 77.



(NGC1068 by Hubble Space Telescope)

Published in [Science](#) - at 4.2 sigma - teasingly close to discovery

Extended analysis underway with more statistics



On-Going Studies:

Neutrino Emissions from NGC1068 - Extended Analysis

Include data taken while IceCube was still under construction

Datasets with a different number of deployed strings:

- Requires retraining of existing energy reconstruction (CNN)
- Will introduce multiple estimators instead of a single

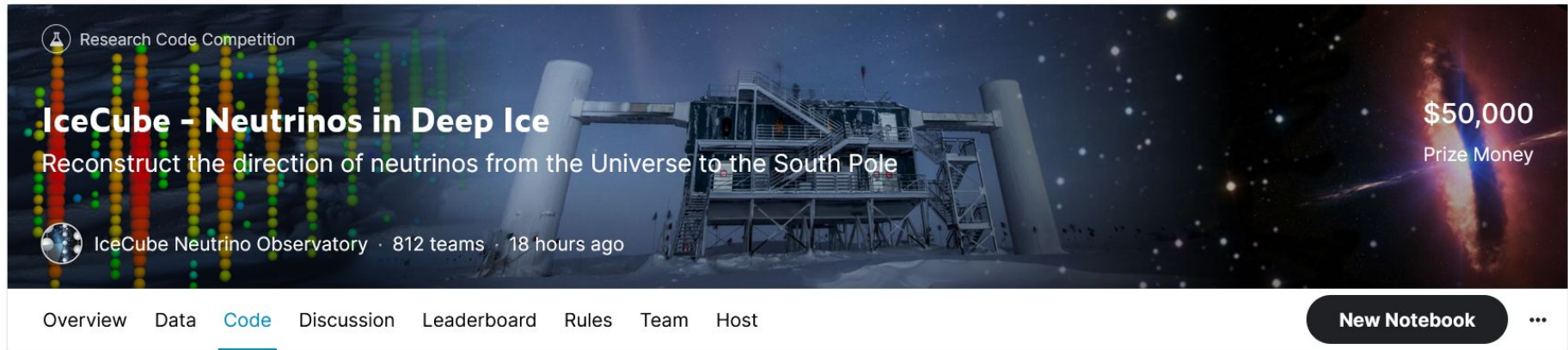
Early results suggests **20 - 40% improvement** in reco. energy.

Will be part of ICRC2023 proceeding



(NGC1068 by Hubble Space Telescope)

Lessons from



Research Code Competition

IceCube - Neutrinos in Deep Ice

Reconstruct the direction of neutrinos from the Universe to the South Pole

\$50,000
Prize Money

IceCube Neutrino Observatory · 812 teams · 18 hours ago

Overview Data Code Discussion Leaderboard Rules Team Host

New Notebook ...

For the past months, an IceCube reconstruction challenge has been ongoing, and yesterday it was concluded!

Lessons from



Early on we shared a pre-trained DynEdge with the competitors, along with an example notebook introducing GraphNeT.

Many have played around with GraphNeT, made their own GNNs or modified DynEdge.

Solutions in the top 30 is still being shared, but a general picture is emerging

Graph Neural Networks on Competition Data

Graph Neural Networks (GNNs) are a class of neural networks that work on graph representation of data. In recent years, development and application of GNNs have been of high interest in the machine learning community, and includes areas of research

such as protein folding, computer vision and knowledge graphs. Part of the appeal of GNNs is the data representation itself - the graphs - as they provide an abstract and flexible format to represent a wide range of issues as GNN problems. Specifically for IceCube, GNNs are interesting because graphs allow us to naturally represent the irregular geometry.



GraphNeT

Graph Neural Networks for
Neutrino Telescope Event Reconstruction

(Snapshot of example notebook)



My model has a simple structure with EdgeConv and Transformer connected.

in several of our models, we incorporated GraphNet feature extractor.

combining GraphNet and Transformer

GNN and Transformer part

I used VonMisesFisher3DLoss

I focused on fine-tuning the baseline GraphNet solution

GNNs Ensemble

I used the `DirectionReconstructionWithKappa` task directly from GraphNet

Lessons from kaggle



8 solutions in the top 10 has been made public:

Ensembling	7/8
GNN + Transformer	6/8 (4/6 is DynEdge)
VonMisesFisherLoss	6/8 (2/8 is cross entropy)
Pure Transformer	1/8
Pure GNN	1/8

Most solutions used functionality from GraphNeT.

One solution ensemble many RNN-based models, where one of the ensemble members used 1D CNN layers.



The internet has spoken

GNN + Transformer trained w. VonMisesFisher3DLoss in ensemble

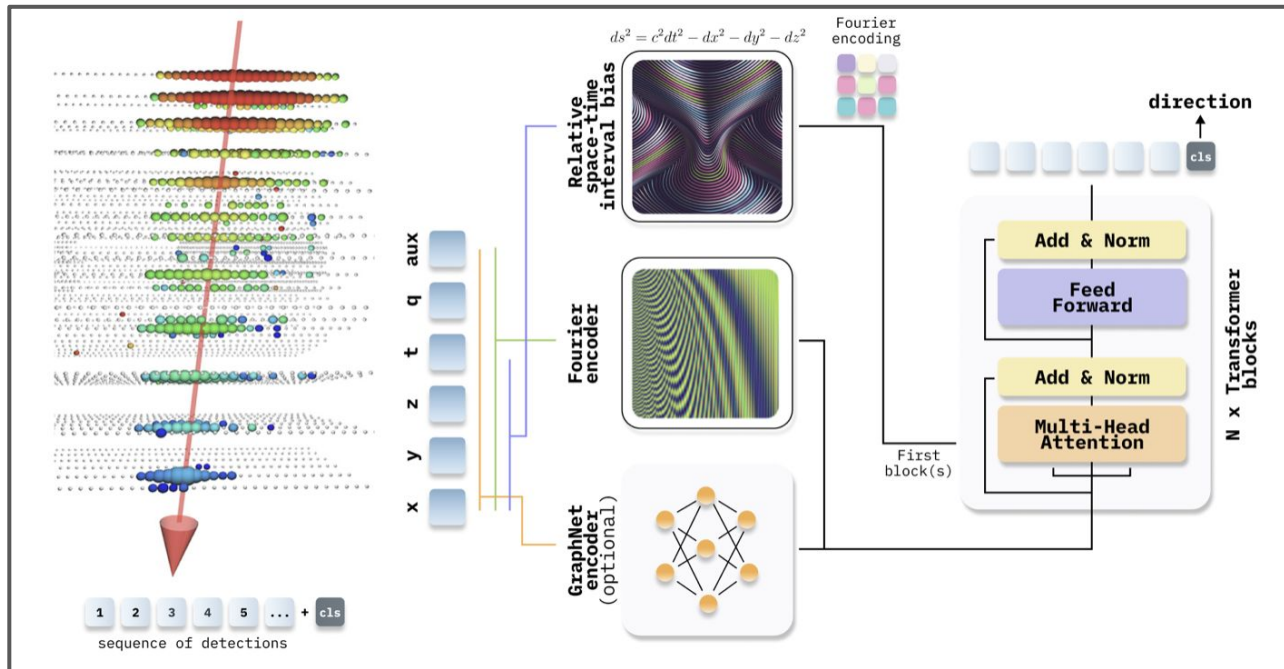
But how?

Lessons from kaggle



(2nd place architecture)

(1st place architecture)



Thank you for listening!



GraphNeT

Graph Neural Networks for
Neutrino Telescope Event Reconstruction



[icecube/graphnet](https://github.com/icecube/graphnet)