Summary, next workshop, and goodbye

GraphNeT Workshop / 4 May 2023

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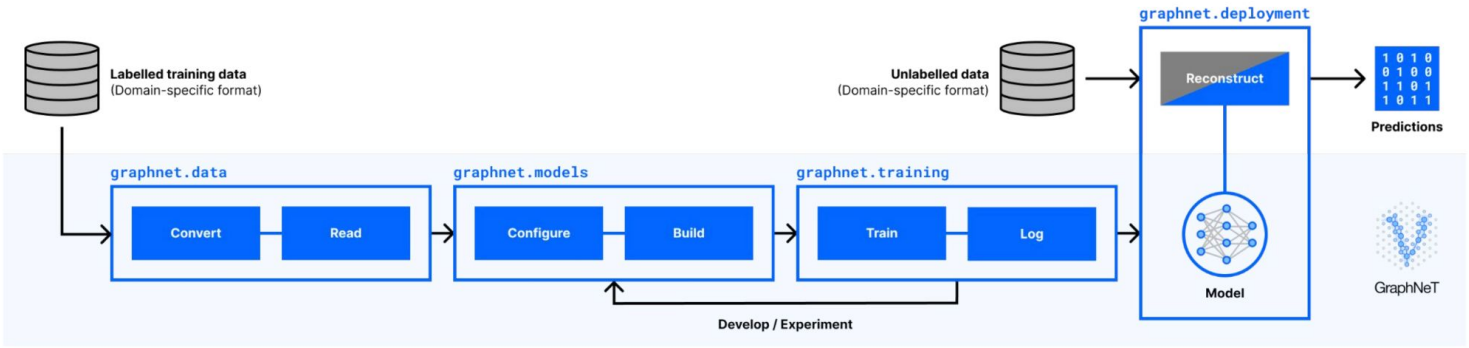
Trying to make GNNs (more) easily available to physicists

Factoring out ML from physics



GraphNeT Overview

Stack: PyTorch PyG PyTorch Lightning W&B docker

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Learning meaningful representations on graphs

UNIVERSITY OF COPENHAGEN

Meaningful interpolation in latent space

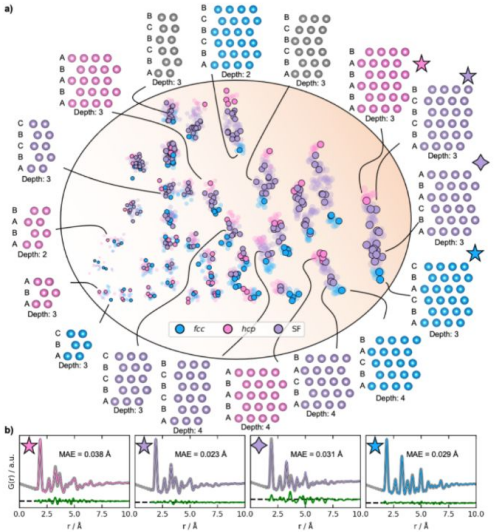

Fig. 6 | Latent space and reconstructions of stacking faulted nanoparticles. a) The latent space and reconstructed structures shown with their stacking sequence. The structures are shown in two dimensions, and

Anker .. Selvan et al. 2023, DeepStruc

Global reach, winning with transformers and ensembles

Stats

- 6,460 registrations
- 901 participants from 74 countries (!)
- 812 teams
- 11,206 submissions
- 220 Jupyter notebooks (https://www.kaggle.com/competitions/icecube-neutrinos-in-deep-ice/code)
- 194 Discussion threads (https://www.kaggle.com/competitions/icecube-neutrinos-in-deep-ice/discussion)

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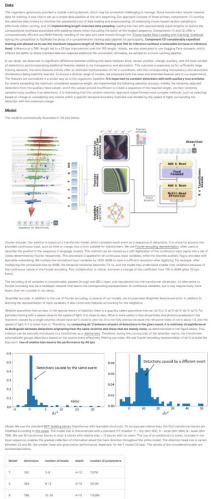
Top 3 Solutions

- All sub-degree Track resolution!!
- All use transformer architecture (attention models)
- 1 & 2 use vMF loss, 3 uses also a cross-entropy classifier, and 1 a modification
- A lot of ensembling going on

- **1st Place uses GraphNeT!!!**

- More technical details in write-ups:
  → https://www.kaggle.com/competitions/icecube-neutrinos-in-deep-ice/leaderboard



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Encoding domain knowledges in NNs

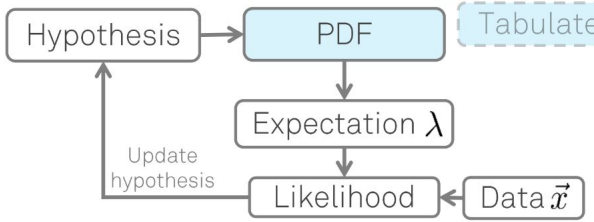
technische universität dortmund

IceCube South Pole Neutrino Observatory · SFB1491 · SFB 876 Providing Information by Resource-Constrained Data Analysis · DFG Deutsche Forschungsgemeinschaft German Research Foundation · Federal Ministry of Education and Research

Combining Deep Learning and Maximum-Likelihood Estimation

Reconstruct Events

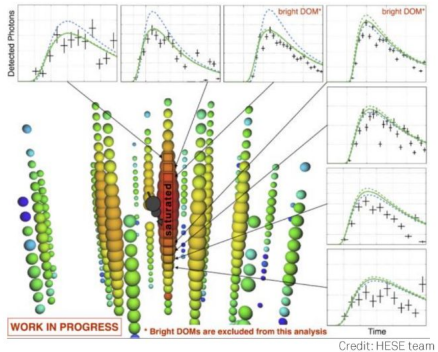
Re-Simulation
Analytic Approx.
Tabulated MC



Replace PDF with a NN ("Generator"):

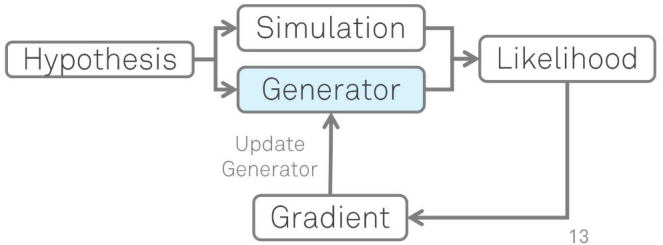
- Fast approximation of MC simulation
- Domain knowledge & symmetries can be easily incorporated into NN due to "forward" direction
- Exact detector geometry can be used
- Use in reverse mode for reconstruction

→ Fully differentiable: Gradient based minimizer



Credit: HESE team

Train Generator via MC simulation



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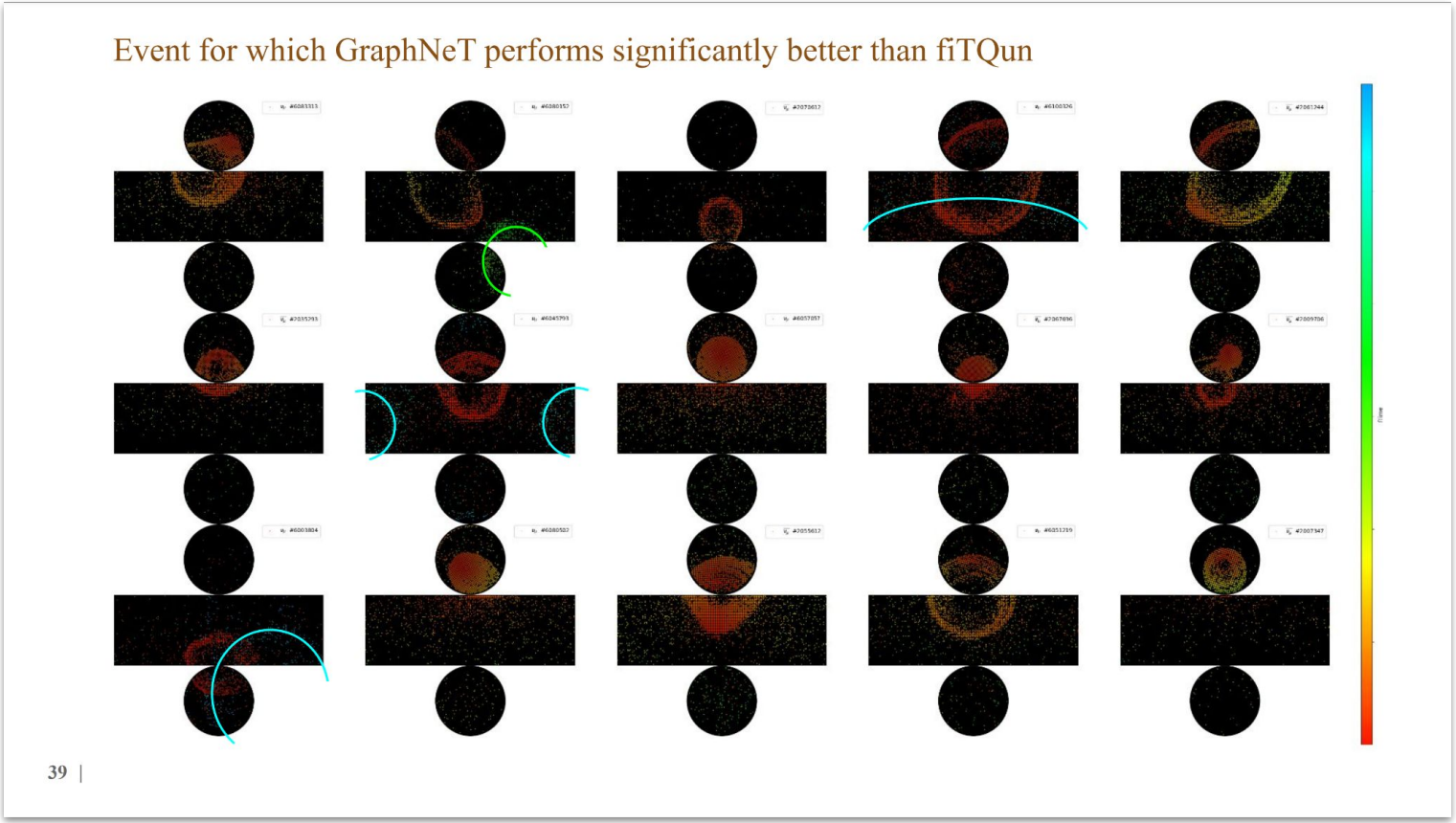
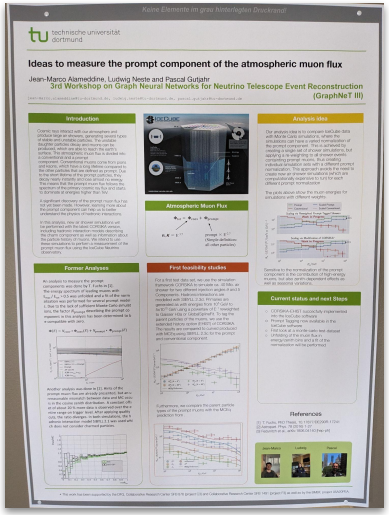
Mirco Hünnefeld

Using GraphNeT outside “NeT”

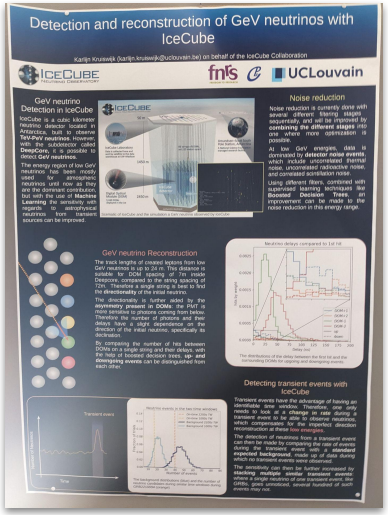


Posters!

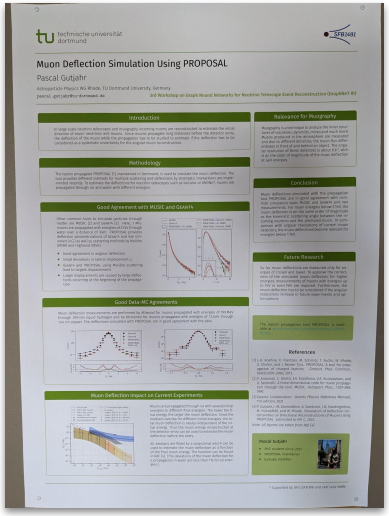
Ludwig



Karlijn

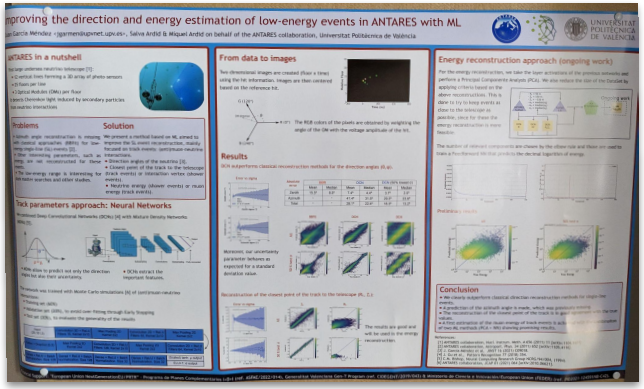


Pascal



Jonathan

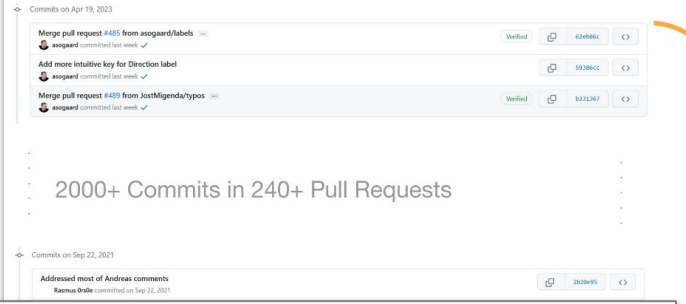
Juan



Using one framework to solve several physics problems

In parallel to Development …

We've been investigating Applications in IceCube

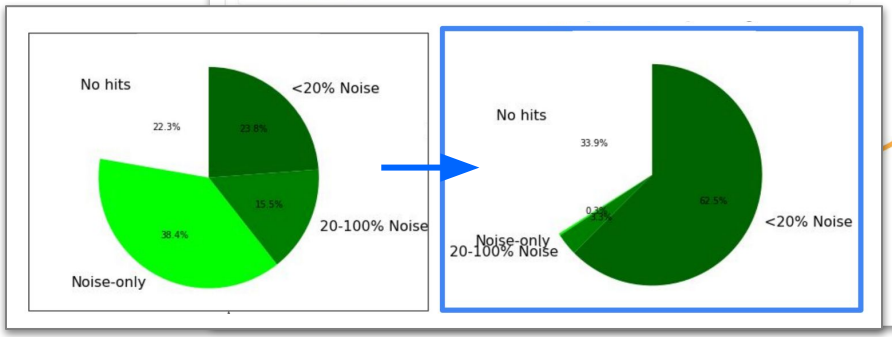


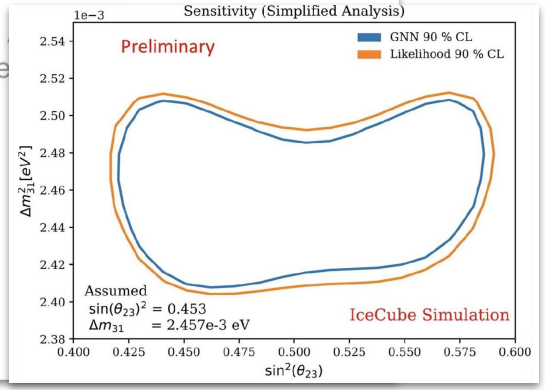
Today

First Commit

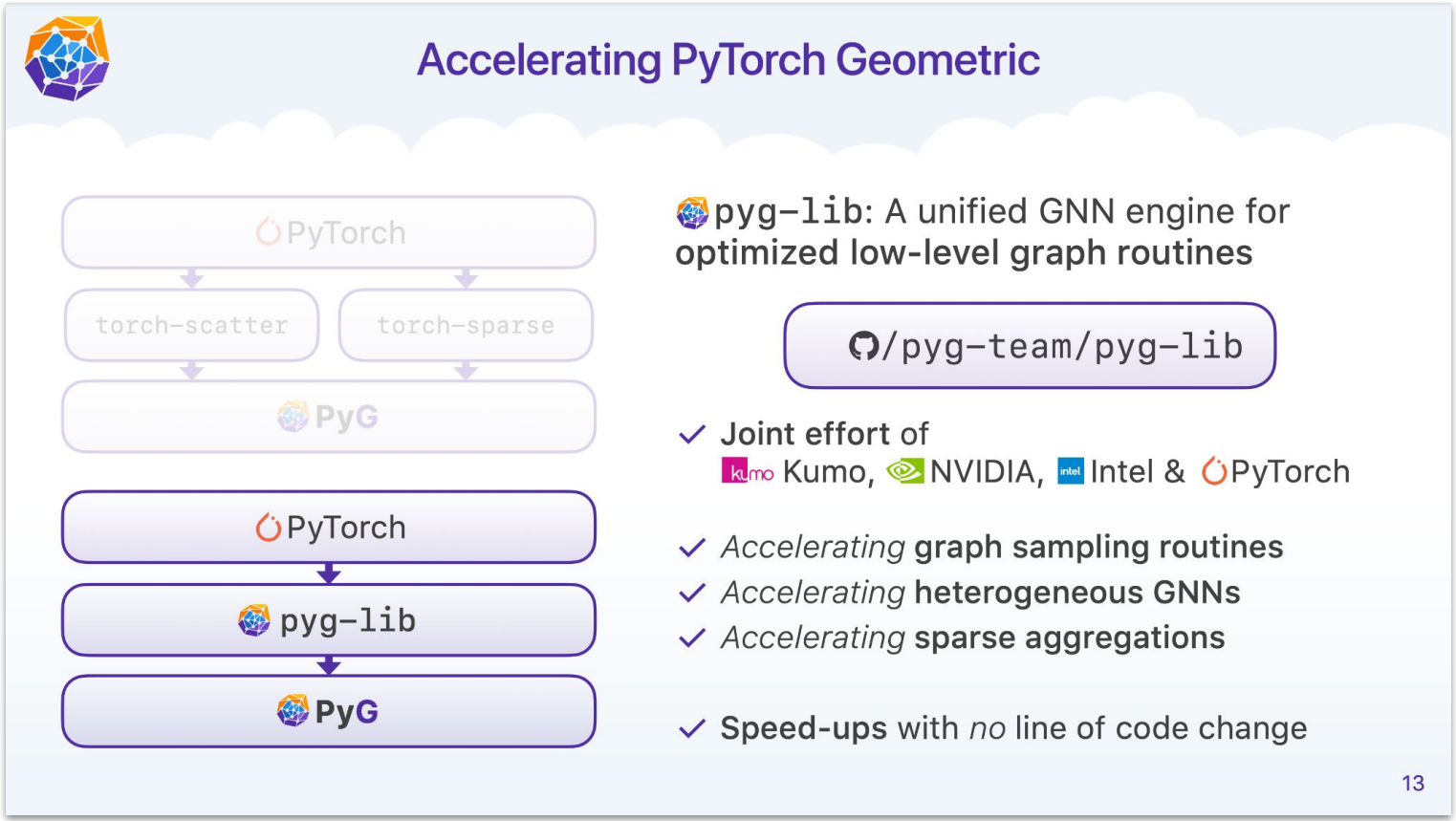
2 Papers,
4+ Posters,
~20 talks,

ML4Astro,
ML4Lattice





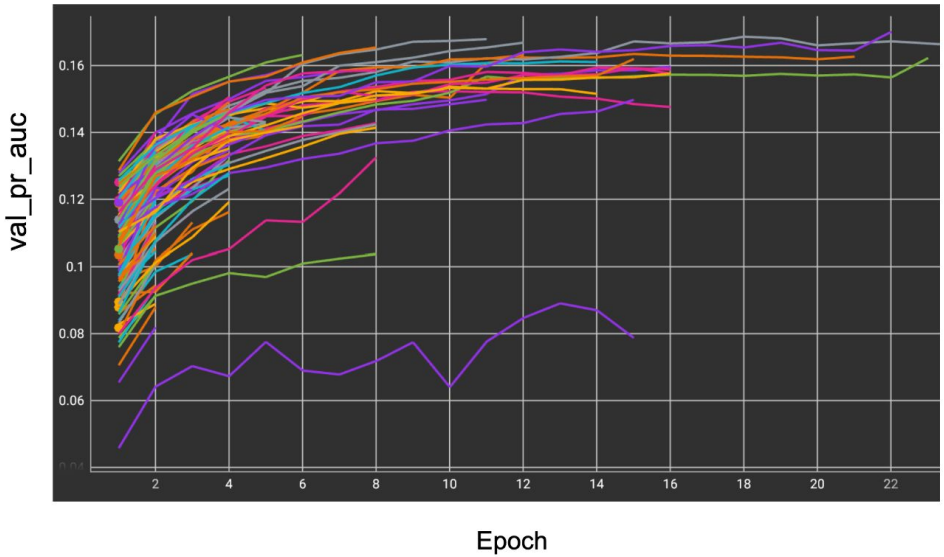
Accelerating GNNs, and their use, with every release



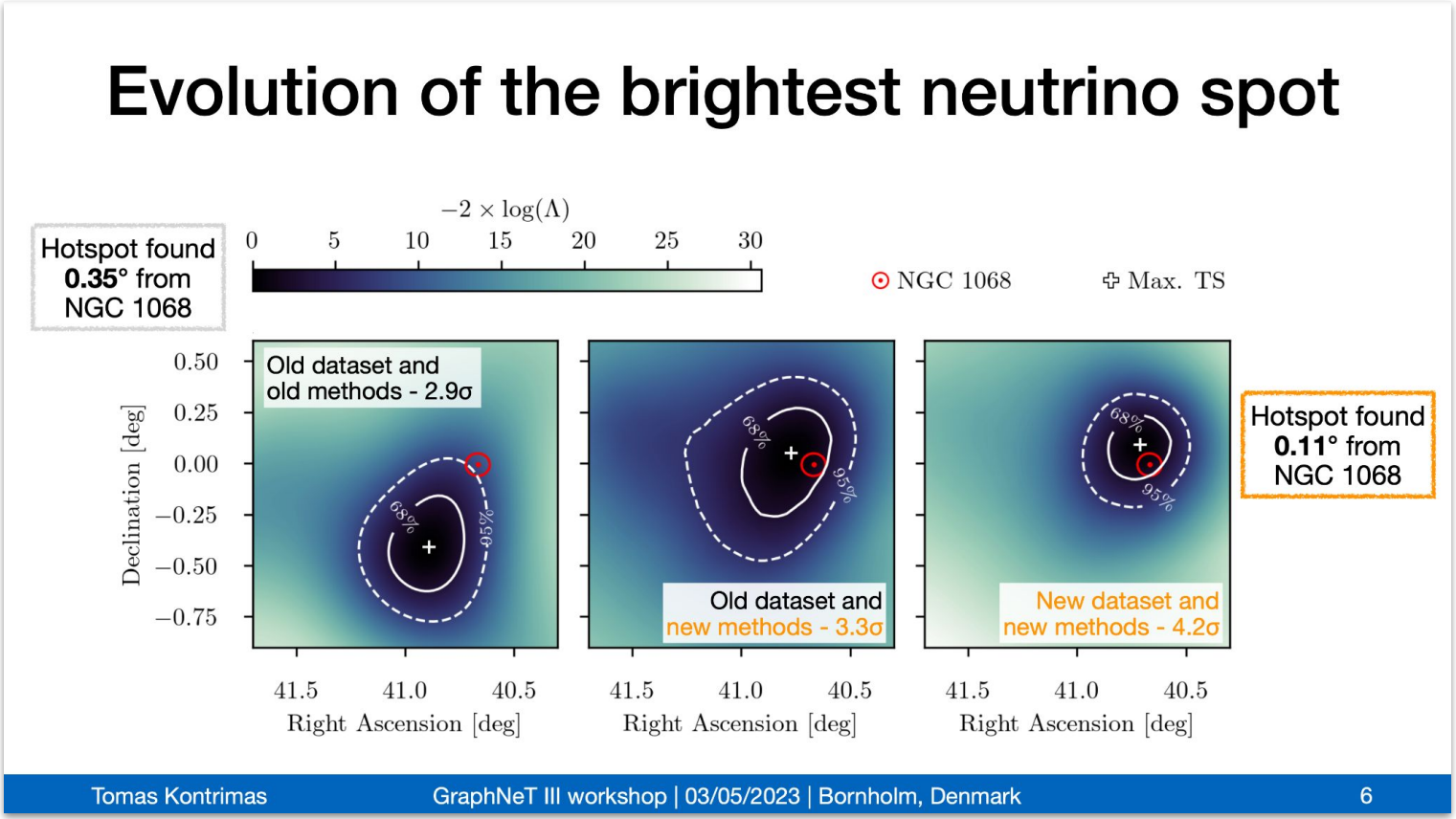
Optimising GNN hyperparameters with/-out automation

Second AHPO

- Second AHPO is currently running
- Results look much more promising
- Analysis of the relevance of different hyperparameters is in preparation
- In total, I got granted 50k GPU hours from the NHR@FAU in Erlangen
- About 1/3 of that is used so far



Aiming for discoveries using better reconstruction



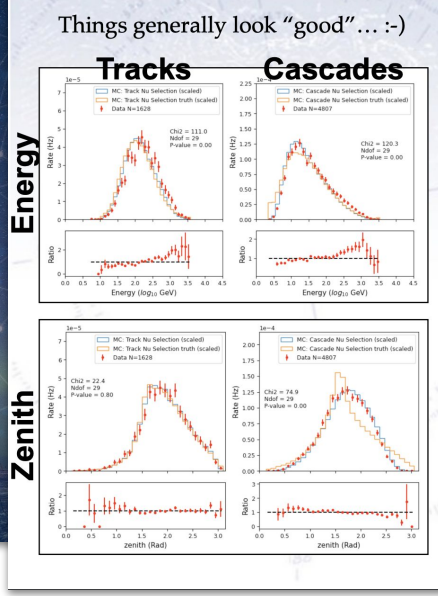
Pondering the myriad more ways to use GNNs for physics

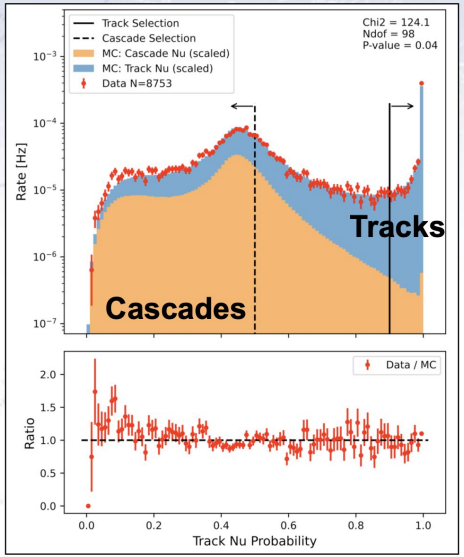
Overview

Tasks using Monte Carlo only
Large scale neutrino selection in data
An AtmosphericEvent tagger (trained in data?)
Real-time analysis/alerts
Algorithm development
Explaining / visualising GNN output
Thoughts on where to begin

Low Energy Selection/Reco status

Things generally look "good"… :-)





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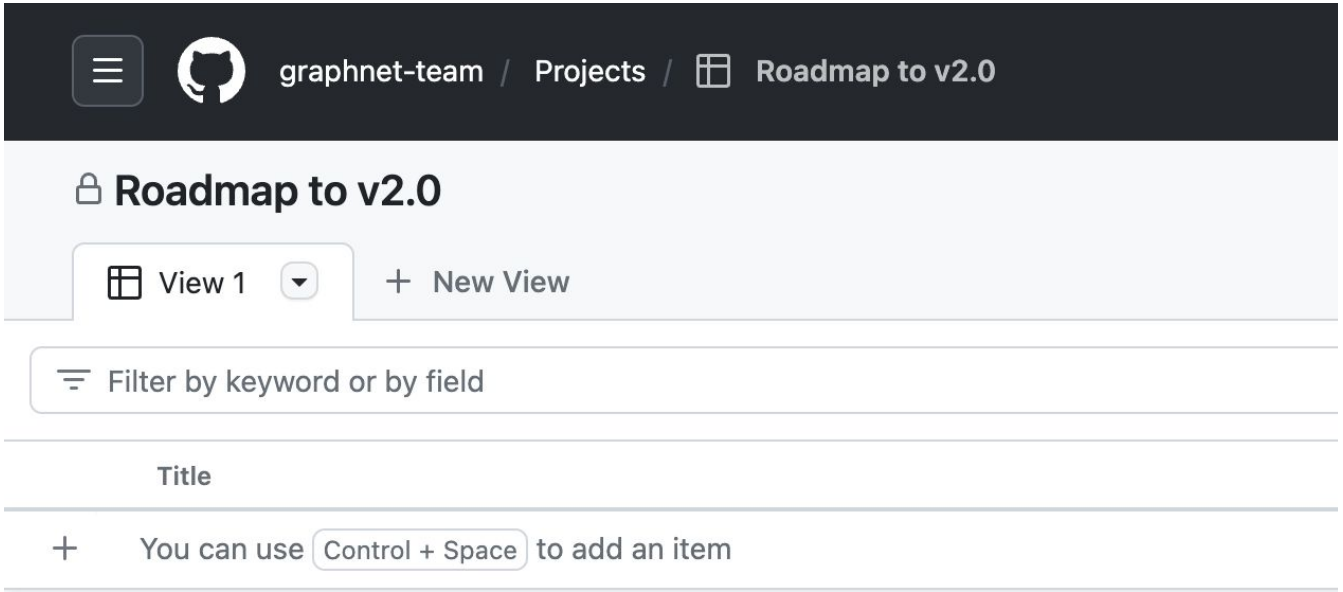
What’s next?


graphnet-team / Projects / Roadmap to v2.0
Roadmap to v2.0
View 1
New View
Filter by keyword or by field
Title
You can use Control + Space to add an item

Where to go from here

- Feedback form, please complete by **Friday 12 May.**
- Stay in touch through the GraphNeT Slack group.
- Weekly GraphNeT developer meetings on Zoom (Tuesdays, alternating weekly between 9:00 or 15:00 CEST) — announced in the Slack group.
- If you want a **certificate of attendance,** please let me know.

Those who have a bit of time before leaving: Hammeren natural area and trail (1 hr 20 mins)


Strandpromenaden
STRANDHOTELLET
GraphNeT III


See you at the next GraphNeT workshop!
Tentatively autumn 2023 in Munich