

GraphNeT Overview

GraphNeT Workshop / 2 May 2023

Andreas Søgaard

Niels Bohr Institute, University of Copenhagen



Danish
Data Science
Academy



This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 890778.

Outline

Background

Motivation for GraphNeT

Current status

First public release (v1.0)

Roadmap to v2.0

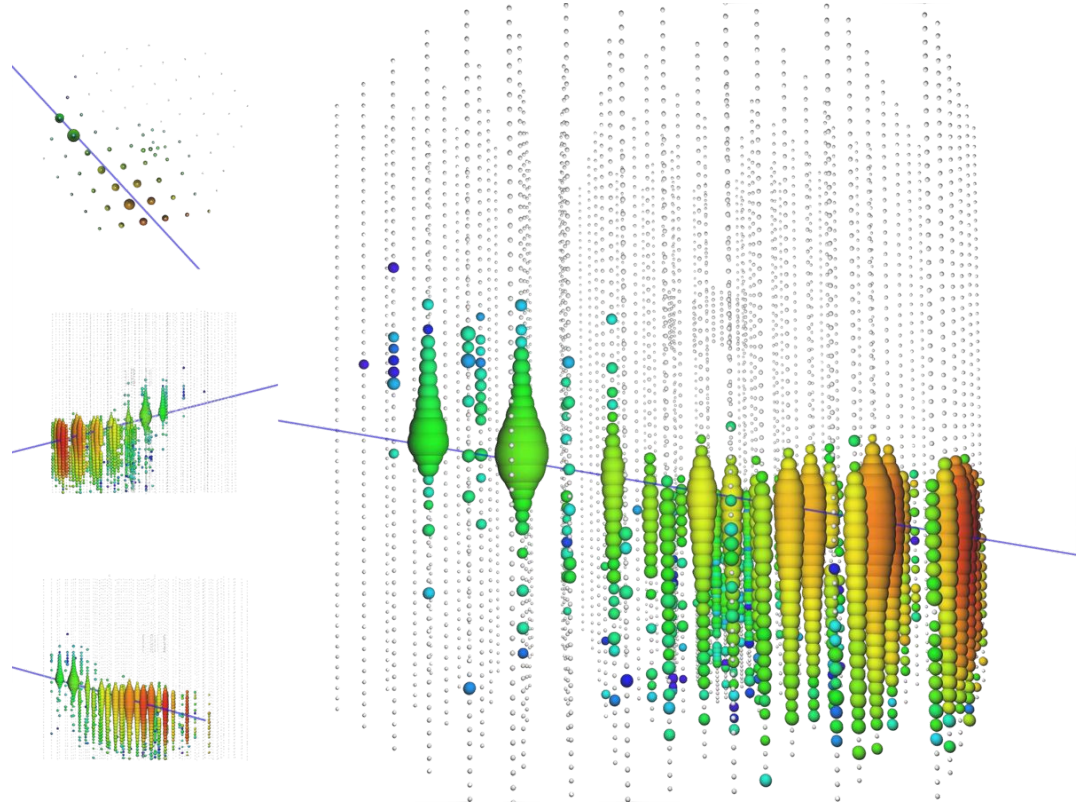


Background



Neutrino telescope data is unique

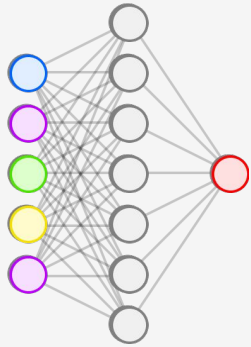
- High rates, $O(\text{kHz}) \times O(10 \text{ years})$
- Often sparse charge deposits
- Non-trivial geometry
- Geometrically heterogeneous, nested sub-detectors
- Similar detection method in all sub-detectors
- Very time-consuming for traditional optimisation-based reconstruction methods



Common types of neural networks

(Deep) Neural network – (D)NN

Occasionally: Multi-layer perceptron (MLP)



Structure

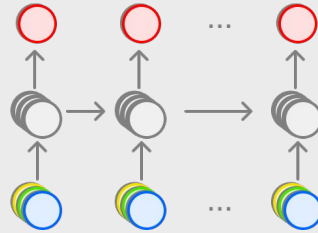
No inherent geometric structure

Example

Engineered, high-level event features

GraphNeT Overview

Recurrent neural network (RNN)



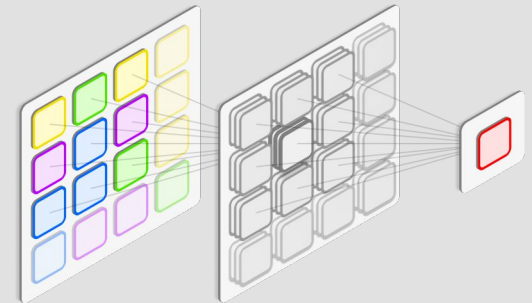
Structure

Sequential

Example

Time-series

Convolutional neural network (CNN)



Structure

Orthogonal data, translation invariance

Example

Images

Unifying “zoo” of architectures

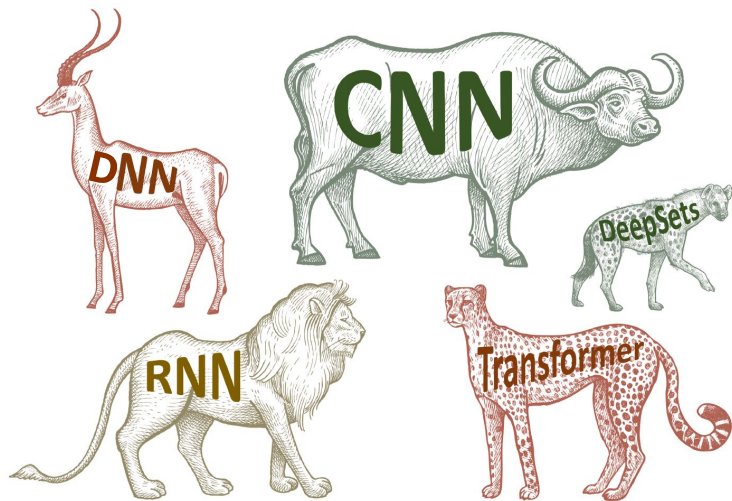


Image adapted from:
Bronstein, Geometric foundations of deep learning (2021)

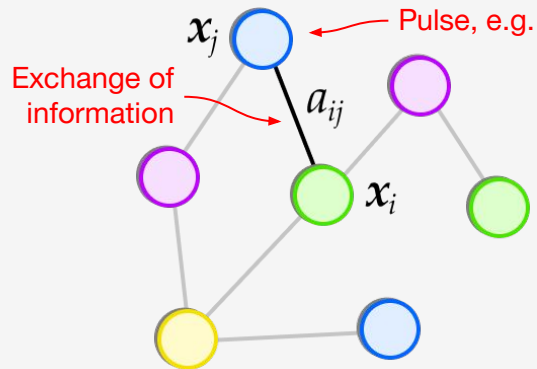
Graph neural network — GNN

Representation

Data x_i on nodes a graph; nodes connected by edges a_{ij}

Structure

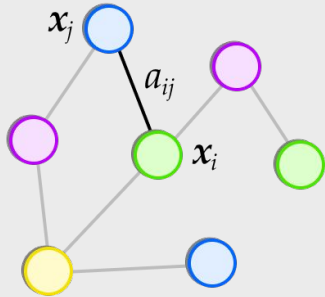
Any that can be encoded through *adjacency* of nodes



Most neural network architectures can be seen as special cases of the GNN with added structure

(Bronstein et al., 2021)

Why GNNs are a natural choice in neutrino telescopes



Challenge

- 🏔 Sparse charge deposits
- 🏔 Non-trivial geometry
- 🏔 Nested sub-detectors

Addressed

- ✅ Only ingest hit PMTs in each event
- ✅ No requirements on structure
- ✅ Information transfer among all nodes

Plus:

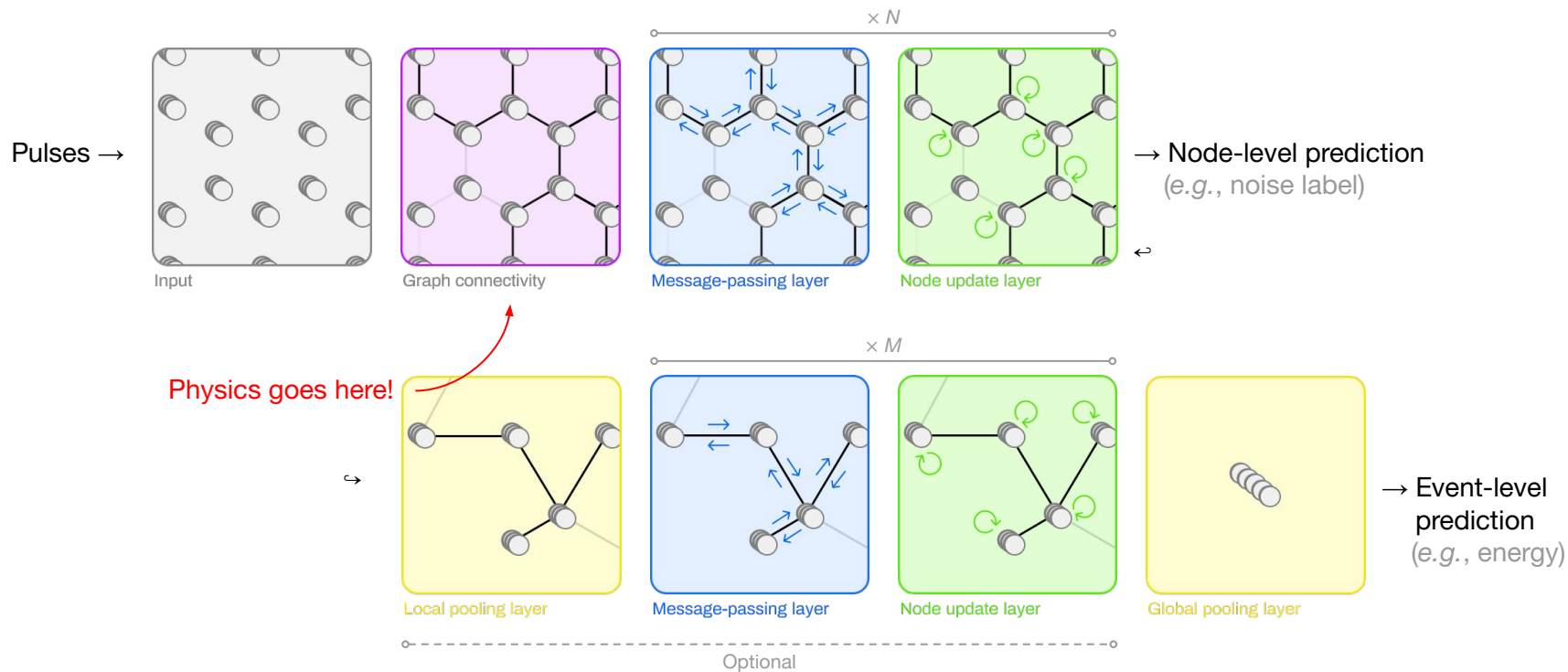
- ✅ No need to “summarise” pulses to DOM-level
- ✅ No need for specialised kernels
- ✅ Ability to *encode* physics, material properties, etc. into structure, e.g.,

... with the regular DL benefit:

- ✅ Fast inference

$$a_{ij} \sim \frac{\text{sign}(\Delta t_{ij})}{1 + \|x_i^t - x_j^t\|^2}$$

Anatomy of a graph neural network



The challenge with machine learning in physics

Challenge

- 🏔 Developers may have little ML experience
- 🏔 Siloed development, often from scratch

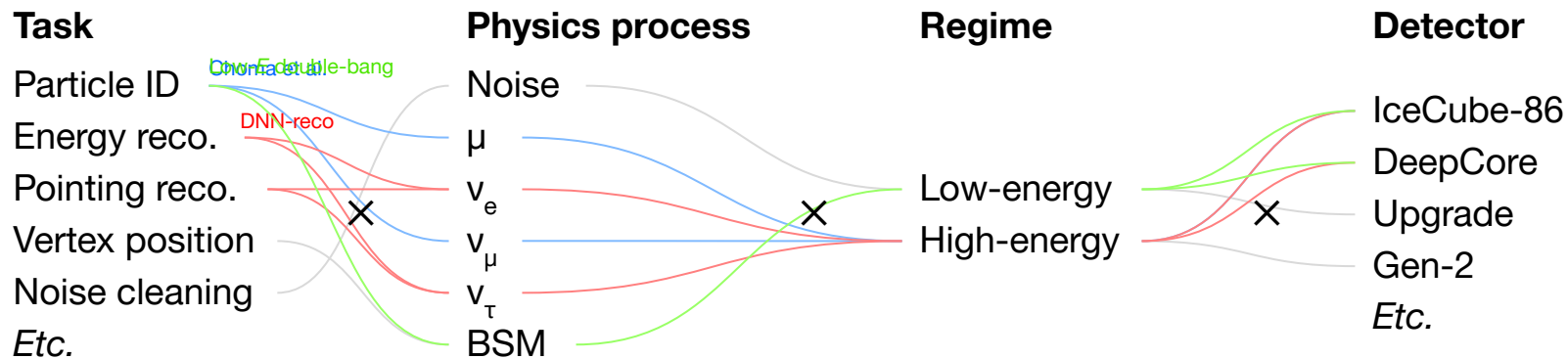
Risk

- ✗ Brittle, suboptimal solutions
- ✗ Time spent on “boilerplate” instead of physics

```
from tensorflow.keras import *
```

We're working on very related problems

Similar detectors, data, physics processes, deployment setting, end-users, etc.



“Zoo” of use cases not solved holistically

Potential for new ways of working with ML in physics

Potential

- Address “zoo” of ML use cases holistically
- Using validated, best-practices code
- Efficient software/ML development workflows

Outcome

- More time for physics
- Better, more reliable results
- Contributions of individual ML developers has a broader, lasting impact in the collaboration

Proposition

A framework for developing GNN-based tools for neutrino telescopes (and beyond!)

One-stop-shop for **model development** to **deployment**:

- **ML developers**
 - Everything needed to build, train, and validate GNNs for physics
- **Physics end-users**
 - Can choose from a library of pre-trained models and apply them, e.g., as IceTray modules



GraphNeT

Graph Neural Networks for
Neutrino Telescope Event Reconstruction



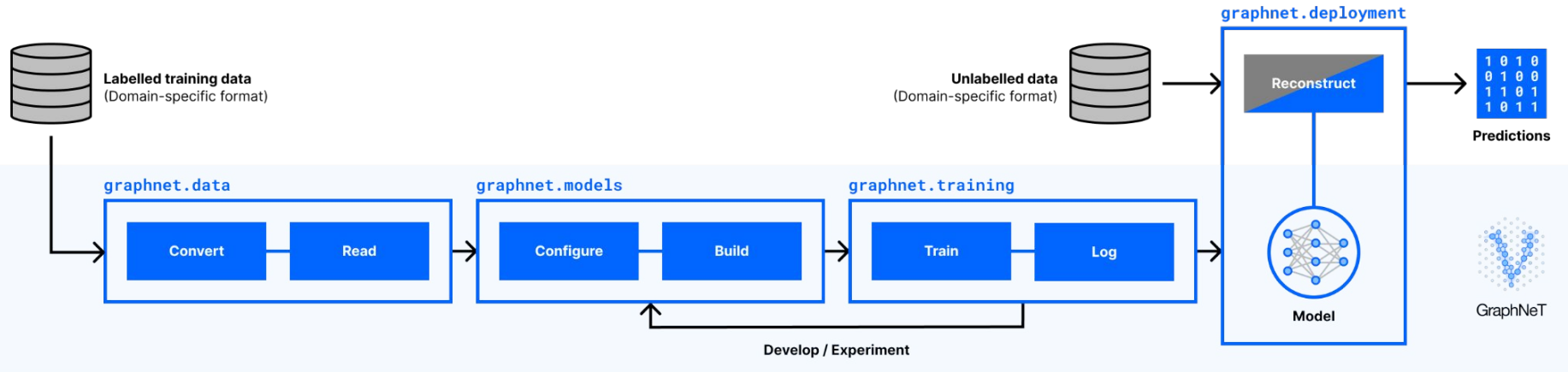
[graphnet-team/graphnet](https://github.com/graphnet-team/graphnet)



[graphnet-team](https://github.com/graphnet-team)

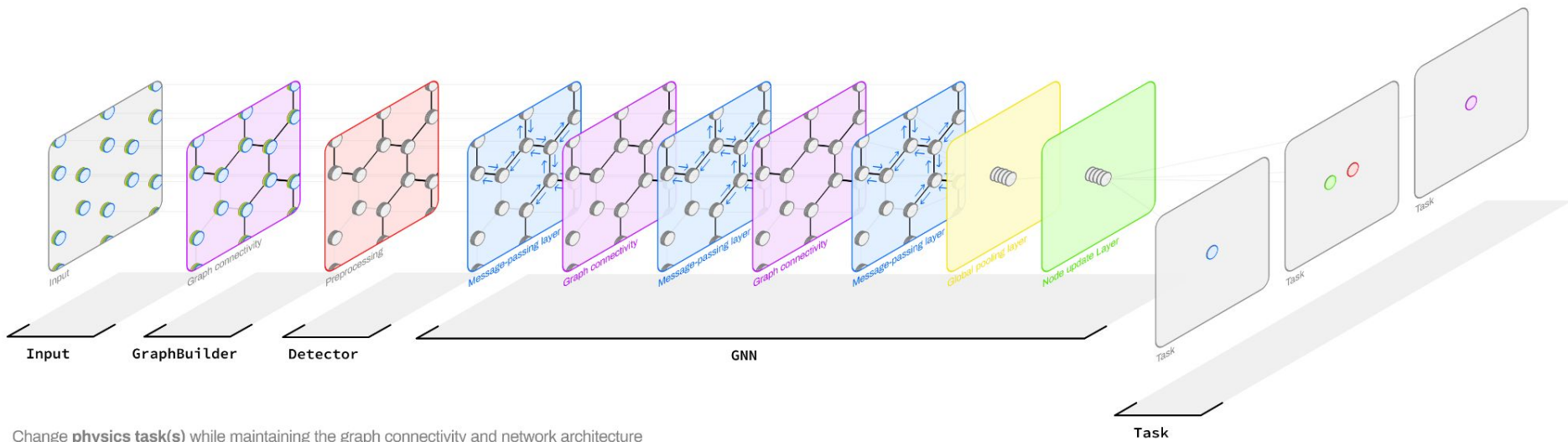
- Reusable GNN components for plug-and-play ML
- All components for end-to-end ML pipeline (data → prod.)
- Validated code, following best practices
- Applicable across all of IceCube + **other experiments**

Factoring out ML from physics



GraphNeT in a nutshell

Modularised, plug-and-play ML components for any use case.



GraphNeT in a nutshell

```
● ● ●  
  
from graphnet import (  
    EuclideanGraphBuilder as GraphBuilder,  
    IceCubeUpgrade as Detector,  
    DynEdge_V2 as GNN,  
    EnergyReconstruction as Task,  
)  
  
# Go do physics!
```


...ideally

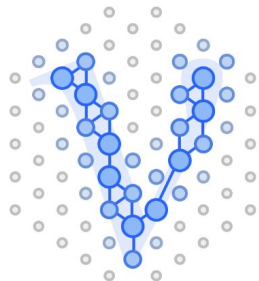
```
from graphnet import Model

model = Model.from_pretrained(
    "icecube-low-energy-neutrino-v2"
)

# Go do physics!
```

Current status





GraphNeT

Graph Neural Networks for
Neutrino Telescope Event Reconstruction

Usage	Development
slack	Build passing
DOI 10.5281/zenodo.6720188	Code quality passing
License Apache 2.0	code style black
python 3.7 3.8 3.9 3.10	maintainability B
version v0.2.3	test coverage 56%

About

GraphNeT is an open-source Python framework aimed at providing high quality, user friendly, end-to-end functionality to perform reconstruction tasks at neutrino telescopes using graph neural networks (GNNs). GraphNeT makes it fast and easy to train complex models that can provide event reconstruction with state-of-the-art performance, for arbitrary detector configurations, with inference times that are orders of magnitude faster than traditional reconstruction techniques.

Pulse
Contributors
Community
Community Standards
Traffic
Commits
Code frequency
Dependency graph
Network
Forks

People

Forks







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About


Graph neural networks for neutrino telescope event reconstruction

[graphnet-team.github.io/graphnet/](https://github.com/graphnet-team/graphnet)


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- [Create a new release](#)

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 [graphnet](#)

Contributors 13



+ 2 contributors

Environments 1

 [github-pages](#) Active

20

Code quality



Review required Add your review

At least 1 approving review is required by reviewers with write access. [Learn more.](#)

Some checks were not successful Hide all checks

11 successful, 1 in progress, and 1 failing checks

✓		Build / Unit tests - Python versions (3.8) (pull_request)	Successful in 1m	Details
✓		Build / Unit tests - Python versions (3.9) (pull_request)	Successful in 2m	Details
✓		Build / Unit tests - Python versions (3.10) (pull_request)	Successful in 2m	Details
🟡		Build / Unit tests - macOS (pull_request)	In progress — This check has started...	Details
✗		Build / Unit tests - IceTray (pull_request)	Failing after 4m	Details
✓		codeclimate	All good!	Details

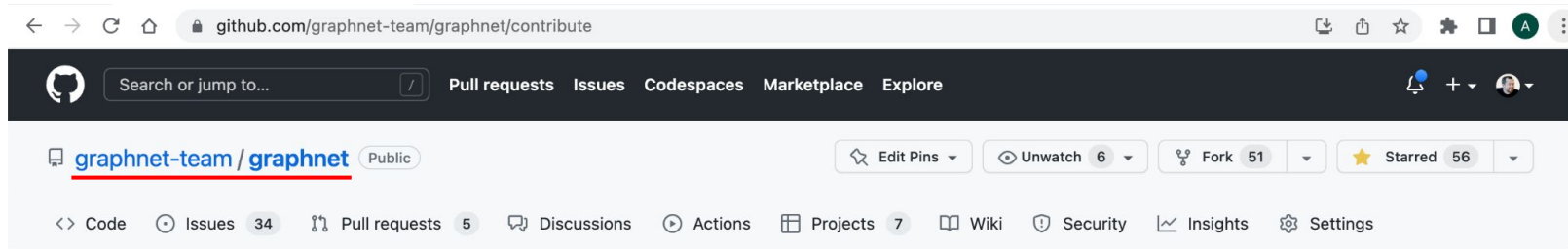
Merging is blocked

Merging can be performed automatically with 1 approving review.

Merge without waiting for requirements to be met (bypass branch protections)

[Merge pull request](#) ▼ You can also [open this in GitHub Desktop](#) or view [command line instructions](#).

How to start contributing



Contribute to graphnet-team/graphnet

Make your first contribution to this repository by tackling one of the issues listed below.

Each issue displayed here is a "good first issue," selected for its relative approachability for first-time contributors.

[Read the contributing guidelines](#)

graphnet / CONTRIBUTING.md

Good first issues

- [Profiling existing code modules and examples](#) feature good first issue 1
#275 opened on Aug 31, 2022 by MortenHolmRep
- [make an interactive event viewer](#) feature good first issue 1
#263 opened on Aug 23, 2022 by RasmusOrsoe
- [Model and data config files](#) good first issue
#226 opened on Jun 28, 2022 by asogaard

[See all issues](#)

First public release (v1.0)



Graph Neural Networks for Low-Energy Event Classification & Reconstruction in IceCube

R. Abbasi,¹⁶ M. Ackermann,⁶² J. Adams,¹⁷ N. Aggarwal,²⁴ J. A. Aguilar,¹¹ M. Ahlers,²¹ M. Ahrens,⁵² J.M. Alameddine,²² A. A. Alves Jr.,³⁰ N. M. Amin,⁴² K. Andeen,⁴⁰ T. Anderson,^{58,59} G. Anton,²⁵ C. Argüelles,¹³ Y. Ashida,³⁸ S. Athanasiadou,⁶² S. Axani,¹⁴ X. Bai,⁴⁸ A. Balagopal V.,³⁸ M. Baricevic,³⁸ S. W. Barwick,²⁹ V. Basu,³⁸ R. Bay,⁷ J. J. Beatty,^{19,20} K.-H. Becker,⁶¹ J. Becker Tjus,¹⁰ J. Beise,⁶⁰ C. Bellenghi,²⁶ S. Benda,³⁸ S. BenZvi,⁵⁰ D. Berley,¹⁸ E. Bernardini,⁴⁶ D. Z. Besson,³³ G. Binder,^{7,8} D. Bindig,⁶¹ E. Blaufuss,¹⁸ S. Blot,⁶² F. Bontempo,³⁰ J. Y. Book,¹³ J. Borowka,⁰ C. Boscolo Meneguolo,⁴⁶ S. Böser,³⁹ O. Botner,⁶⁰ J. Böttcher,⁰ E. Bourbeau,²¹ J. Braun,³⁸ B. Brinson,⁵ J. Brostean-Kaiser,⁶² R. T. Burley,¹ R. S. Busse,⁴¹ M. A. Campana,⁴⁷ E. G. Carnie-Bronca,¹ C. Chen,⁵ Z. Chen,⁵³ D. Chirkin,³⁸ K. Choi,⁵⁴ B. A. Clark,²³ L. Classen,⁴¹ A. Coleman,⁴² G. H. Collin,¹⁴ A. Connolly,^{19,20} J. M. Conrad,¹⁴ P. Coppin,¹² P. Correa,¹² S. Countryman,⁴⁴ D. F. Cowen,^{58,59} R. Cross,⁵⁰ C. Dappen,⁰ P. Dave,⁵ C. De Clercq,¹² J. J. DeLaunay,⁵⁷ D. Delgado López,¹³ H. Dembinski,⁴² K. Deoskar,⁵² A. Desai,³⁸ P. Desiati,³⁸ K. D. de Vries,¹² G. de Wasseige,³⁵ T. DeYoung,²³ A. Diaz,¹⁴ J. C. Díaz-Vélez,³⁸ M. Dittmer,⁴¹ H. Dujmovic,³⁰ M. A. DuVernois,³⁸ T. Ehrhardt,³⁹ P. Eller,²⁶ R. Engel,^{30,31} H. Erpenbeck,⁰ J. Evans,¹⁸ P. A. Evenson,⁴² K. L. Fan,¹⁸ A. R. Fazely,⁶ A. Fedynitch,⁵⁶ N. Feigl,⁹ S. Fiedlschuster,²⁵ A. T. Fienberg,⁵⁹ C. Finley,⁵² L. Fischer,⁶² D. Fox,⁵⁸ A. Franckowiak,¹⁰ E. Friedman,¹⁸ A. Fritz,³⁹ P. Fürst,⁰ T. K. Gaisser,⁴² J. Gallagher,³⁷ E. Ganster,⁰ A. Garcia,¹³ S. Garrappa,⁶² L. Gerhardt,⁸ A. Ghadimi,⁵⁷ C. Glaser,⁶⁰ T. Glauch,²⁶ T. Glüsenkamp,²⁵ N. Goehlike,³¹ J. G. Gonzalez,⁴² S. Goswami,⁵⁷ D. Grant,²³ S. J. Gray,¹⁸ T. Grégoire,⁵⁹ S. Griswold,⁵⁰ C. Günther,⁰ P. Gutjahr,²² C. Haack,²⁶ A. Hallgren,⁶⁰ R. Halliday,²³ L. Halve,⁰ F. Halzen,³⁸ H. Hamdaoui,⁵³ M. Ha Minh,²⁶ K. Hanson,³⁸ J. Hardin,^{14,38} A. A. Harnisch,²³ P. Hatch,³² A. Haungs,³⁰ K. Helbing,⁶¹ J. Hellrung,⁰ F. Henningsen,²⁶ L. Heuermann,⁰ S. Hickford,⁶¹ C. Hill,¹⁵ G. C. Hill,¹ K. D. Hoffman,¹⁸ K. Hoshina,^{38,a} W. Hou,³⁰ T. Huber,³⁰ K. Hultqvist,⁵² M. Hünnefeld,²² P. Hussain,³⁸ K. Hymon,²² S. In,⁵⁴ N. Jain,¹¹ A.

arXiv:2209.03042v3 [hep-ex] 11 Oct 2022

[2209.03042]

1 GraphNeT: Graph neural networks for neutrino 2 telescope event reconstruction

3 **Andreas Sjøgaard** ¹✉, **Rasmus F. Ørsøe** ², **Leon Bozianu**¹, **Morten Holm**¹,
4 **Kaare Endrup Iversen**¹, **Tim Guggenmos**², **Martin Ha Minh** ², **Philipp**
5 **Eller** ², and **Troels C. Petersen** ¹

6 ¹ Niels Bohr Institute, University of Copenhagen, Denmark ² Technical University of Munich, Germany
7 ✉ Corresponding author

DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

Software

- [Review](#) 
- [Repository](#) 
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Editor: [Dan Foreman-Mackey](#) 

Reviewers:

- [@JostMigenda](#)
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Submitted: 06 October 2022

Published: unpublished

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8 Summary

9 Neutrino telescopes, such as ANTARES ([ANTARES Collaboration, 2011b](#)), IceCube ([IceCube
10 Collaboration, 2012, 2017](#)), KM3NeT ([KM3NeT Collaboration, 2016](#)), and Baikal-GVD ([Baikal-
11 GVD Collaboration, 2018](#)) have the science goal of detecting neutrinos and measuring their
12 properties and origins. Reconstruction at these experiments is concerned with classifying the
13 type of event or estimating properties of the interaction.

14 GraphNeT ([Sjøgaard et al., 2022](#)) is an open-source Python framework aimed at providing high
15 quality, user friendly, end-to-end functionality to perform reconstruction tasks at neutrino
16 telescopes using graph neural networks (GNNs). GraphNeT makes it fast and easy to train
17 complex models that can provide event reconstruction with state-of-the-art performance, for
18 arbitrary detector configurations, with inference times that are orders of magnitude faster than
19 traditional reconstruction techniques ([IceCube Collaboration, 2022a](#)).

20 GNNs from GraphNeT are flexible enough to be applied to data from all neutrino telescopes,
21 including future projects such as IceCube extensions ([IceCube-Gen2 Collaboration, 2017, 2021](#);
22 [IceCube-PINGU Collaboration, 2014](#)) or P-ONE ([P-ONE Collaboration, 2020](#)). This means
23 that GNN-based reconstruction can be used to provide state-of-the-art performance on most
24 reconstruction tasks in neutrino telescopes, at real-time event rates, across experiments and
25 physics analyses, with vast potential impact for neutrino and astro-particle physics.

🏠 4 Open ✓ 2 Closed		Sort ▾
<h3>v1.0.0 / Documentation</h3> <p>📅 Due by May 01, 2023 ⌚ Last updated 10 days ago</p> <p>This milestone collects issues related to the documentation of the project, i.e. docstrings, API documentation, READMEs, infographics, wikis, etc.</p>	 <p>100% complete 0 open 16 closed</p> <p>Edit Close Delete</p>	
<h3>v1.0.0 / Features</h3> <p>📅 Due by May 01, 2023 ⌚ Last updated 13 days ago</p> <p>This milestone collects issues related to data, model building, tra...(more)</p>	 <p>88% complete 2 open 15 closed</p> <p>Edit Close Delete</p>	
<h3>v1.0.0 / Quality</h3> <p>📅 Due by May 01, 2023 ⌚ Last updated about 1 month ago</p> <p>This milestone collects issues related to the tools/tech stack used...(more)</p>	 <p>94% complete 1 open 16 closed</p> <p>Edit Close Delete</p>	
<h3>v1.0.0 / Physics</h3> <p>📅 Due by May 01, 2023 ⌚ Last updated about 1 month ago</p> <p>This milestone collects all issues related to the application of Gr...(more)</p>	 <p>75% complete 1 open 3 closed</p> <p>Edit Close Delete</p>	

We aim to release GraphNeT v1.0 during this week

Roadmap to v2.0



You can help decide!

indico.nbi.ku.dk/event/1885/timetable/#20230504.detailed

1-4 May 2023
Strandhotellet, Sandvig
Europe/Copenhagen timezone

Enter your search term

Overview
Timetable
Contribution List
My Conference
My Contributions
Application
Participant List
Workshop activities
Hackathon
Poster session
Practical information
Travel and accommodation
Venue and local information
Contact
andreas.sogaard@nbi.k...

Timetable

Mon 01/05 Tue 02/05 Wed 03/05 **Thu 04/05** All days

Print PDF Full screen Detailed view Filter
Session legend

Hackathons Presentations Social

08:00

Check-out and coffee
Strandhotellet, Sandvig 08:30 - 09:00

09:00 **Hackathons: Presentation of results**
Strandhotellet, Sandvig 09:00 - 10:00

10:00 **Roadmap towards v2.0 - mini-workshop introduction** *Andreas Søgaard*
Strandhotellet, Sandvig 10:00 - 10:30

Coffee
Strandhotellet, Sandvig 10:30 - 11:00

11:00 **Roadmap towards v2.0 - mini-workshop** *Andreas Søgaard*
Strandhotellet, Sandvig 11:00 - 12:10

12:00 **Summary, next workshop, and goodbye** *Andreas Søgaard*
Strandhotellet, Sandvig 12:10 - 12:30






Lunch

28



GraphNeT

Graph Neural Networks for
Neutrino Telescope Event Reconstruction

Usage	Development
 slack	 Build passing
DOI 10.5281/zenodo.6720188	 Code quality passing
License Apache 2.0	code style black
python 3.7 3.8 3.9 3.10	 maintainability B
 version v0.2.3	 test coverage 56%