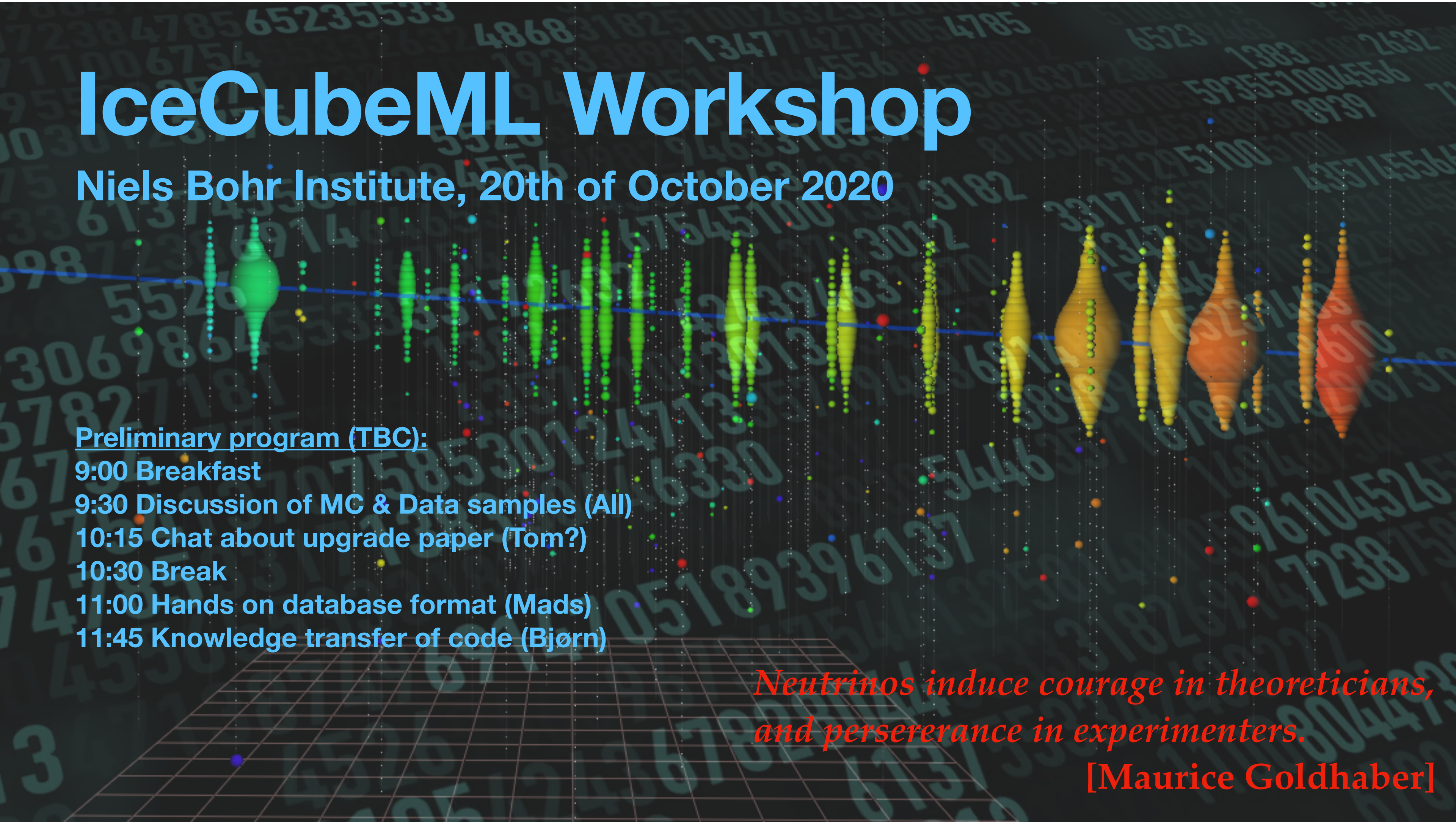
Welcome to the Fifth GraphNeT Workshop

Outline:

History of GraphNeT through Earlier Workshops
Example results with GraphNeT
Algorithm development
Explaining / visualising GNN output
User Experience
Time schedule & other plans
Next GraphNeT workshop

Initial Workshops

Initial Workshops



IceCubeML Workshop

Niels Bohr Institute, 20th of October 2020

<u>Preliminary program (TBC):</u>

9:00 Breakfast
9:30 Discussion of MC & Data samples (All)
10:15 Chat about upgrade paper (Tom?)
10:30 Break
11:00 Hands on database format (Mads)
11:45 Knowledge transfer of code (Bjørn)

Neutrinos induce courage in theoreticians,
and persererance in experimenters.
[Maurice Goldhaber]

GraphNeT

Graph Neural Networks for Neutrino Telescope Event Reconstruction

GraphNet is our attempt at putting GNN models for IceCube (and others) using the "DynEdge" architecture build in PyTorch Geometric into an easily available software package.

https://github.com/icecube/graphnet/

In the following, I will try to convince you, that GNNs "match" the IceCube data really well, and perhaps whet your appetite for using it.

Our results can be found in an IceCube paper, submitted to JINST in September.

GraphNeT Workshop II
Munich 2022

GraphNeT Workshop

from **Thursday, September 15, 2022 (9:00 AM)** to **Saturday, September 17, 2022 (5:00 PM)**
Garching (MDSI Meeting Room)

: Sessions / : Talks : Breaks

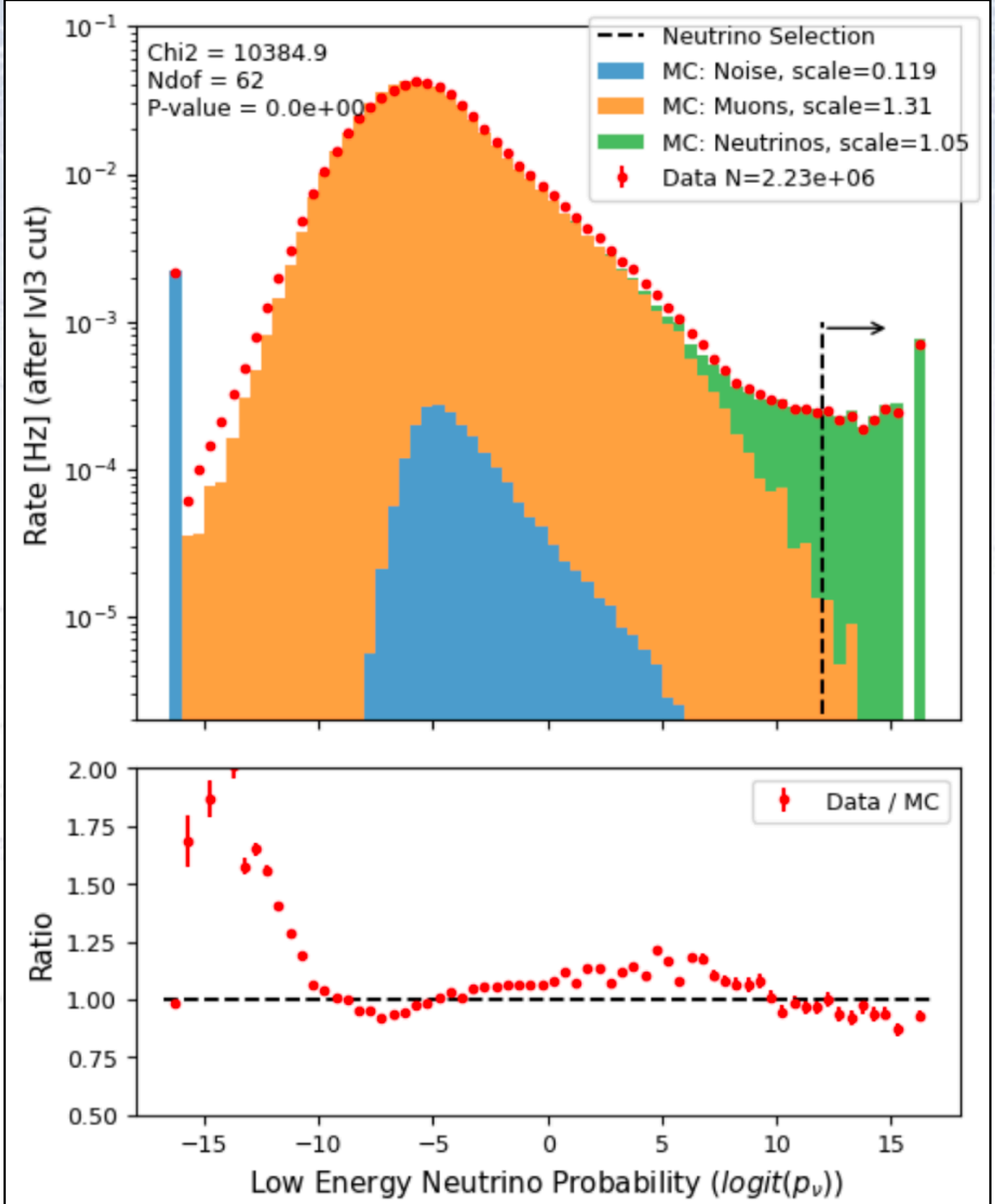
		Sep 15, 2022		Sep 16, 2022
AM	**9:00 AM**	**Check-in at venue** (until 9:45 AM) (MDSI Meeting Room)	9:45 AM	Impact So Far - Rasmus Ørsøe (TUM) (MDSI Meeting Room) GraphNeT Workshop @ Garching.pdf
	9:45 AM	GraphNeT Road Map - Mr Andreas Søgaard (MDSI Meeting Room) 220915_GraphNeT_Workshop_AndreasSogaard.pdf	10:30 AM	--- Coffee ---
	10:30 AM	--- Coffee ---	10:45 AM	Calibration & Other Ideas - Prof. Troels Petersen (MDSI Meeting Room) Munich_GraphNetWorkshop_AnalysisIdeas_16sep2022-1.pdf
	10:45 AM	Graphite & Bending Graphs - Mahdi Saleh (MDSI Meeting Room) GraphNet_talk_graphite.pdf	11:30 AM	GNNs in P-ONE - Arturo Anaya (MDSI Meeting Room) gnns-for-event-classification-at-p-one-detector.pdf
	11:30 AM	High Energy Update - Martin Ha Minh Martin Ha Minh (MDSI Meeting Room) 22_09_gnn_HE.pdf		
PM	12:00 PM	--- Lunch ---	12:00 PM	--- Lunch ---
	1:00 PM	**Hackathon** (until 3:00 PM) (MDSI Meeting Room)	**1:00 PM**	**Hackathon** (until 3:00 PM) (MDSI Meeting Room)
	3:00 PM	--- Coffee ---	3:00 PM	--- Coffee ---
	3:15 PM	**Hackathon** (until 5:00 PM) (MDSI Meeting Room)	**3:15 PM**	**Hackathon** (until 5:00 PM) (MDSI Meeting Room)
	6:30 PM	**Workshop Dinner** (until 8:30 PM) (MDSI Meeting Room)		

GraphNeT Workshop III Bornholm 2023

GraphNeT Workshop IV TUM 2024


GraphNeT Workshop V
The next steps for GraphNeT
Scientific advisory committee:
Rasmus Ørsøe (TUM)
Jorge Prado (IFIC)
Philipp Eller (TUM)
Aske Rosted (Chiba Univ.)
Ivan Mozun (LPC Caen)
Troels C. Petersen (NBI)
Local organising committee:
Troels C. Petersen (NBI)
Rasmus Ørsøe (TUM)
Johann Ioannou-Nikolaides (NBI)
Marc Jacquart (NBI)
Conference Link:
https://indico.nbi.ku.dk/event/2170/
Niels Bohr Institute 18th - 19th of August 2025

A highlight



Classification of neutrinos, muons, and noise interacting in DeepCore.

Not only was the performance increased, but the data/MC correspondence remained good.

We would like something similar for High Energy!

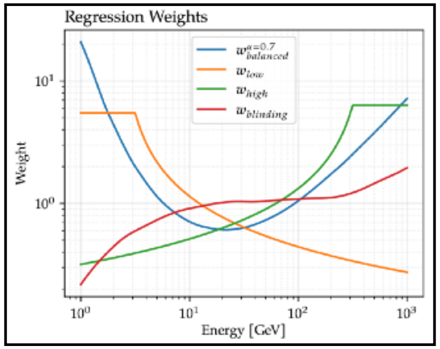
Algorithmic Developments

Algorithmic Developments

1. **GNN autoencoder (for general search)**
   If an AE learned to encode general IceCube events (say noise, muons, and neutrinos from simulation), it could be used to detect other objects.

2. **Hierarchical Graph Pooling**
   Would this work better? Or better only at high energies? Or…?

3. **GNN optimisation (architecture, training sample and reweighting, ensemble combination)**
   Much has been done, but we should push it to the limit :-)
   Perhaps put in 3D-PCA transformation to begin with?



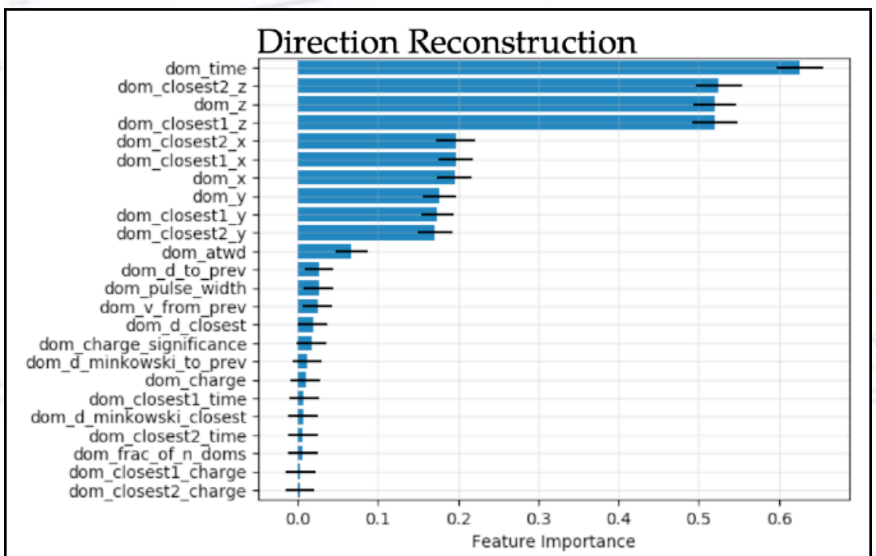
4. **Using "non-signal" DOMs as input**
   Do these contain information to be incorporated, or not?

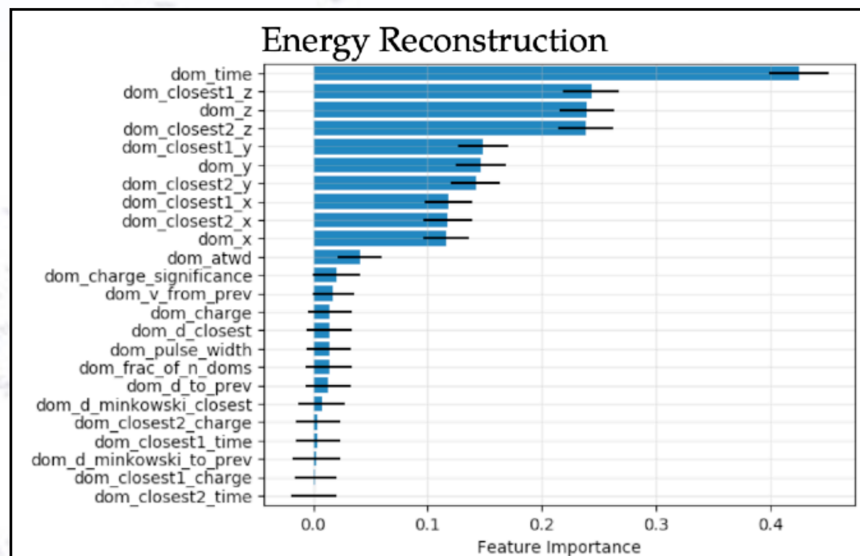
5. **Adversarial training for better performance in data**
   Do common data+MC training. But technically how?

Explaining/Visualising the GraphNeT answers

Explaining / Visualising GraphNeT output

1. **Overall feature ranking for each task**
   Which are the important features for energy regression and directional regression? Are they the same or do some cases stand out?





Results shown are for a GRU from 2021

User Experience

… or lack of the same!

Local information

Niels Bohr Institute
Locations for Workshop

Indico Timetable - Monday

09:00	**Beginning with Breakfast and Badges**		*Aud. B, Niels Bohr Institute*	09:00 - 09:30
	1 - Welcome and Framing of workshop	*Troels Petersen*		
	2 - GraphNeT: Status and Plans	*Rasmus Ørsøe*	*Aud. B, Niels Bohr Institute*	09:45 - 10:15
10:00	**3 - GraphNeT: Transformers and next steps**	*Iván Mozún Mateo*	*Aud. B, Niels Bohr Institute*	10:15 - 10:45
	Break		*Aud. B, Niels Bohr Institute*	10:45 - 11:15
11:00	**4 - Technical requirements to reconstruction software in IceCube**	*Philipp Soldin*	*Aud. B, Niels Bohr Institute*	11:15 - 11:45
	5 - GraphNeT as seen from a Magic point of view	*Jarred Green*	*Aud. B, Niels Bohr Institute*	11:45 - 12:15
12:00	**Lunch Break**		*Aud. B, Niels Bohr Institute*	12:15 - 13:15
13:00	**8 - Takeaways from training a foundation model for IceCube**	*Inar Timiryasov et al.*	*Aud. B, Niels Bohr Institute*	13:15 - 13:45
	9 - All the technicalities: Databases, MC labels, and such stuff	*Aske Rosted*	*Aud. B, Niels Bohr Institute*	13:45 - 14:15
14:00	**18 - Introduction to Hackathon & Implementation discussion**	*Troels Petersen*		
	Break		*Aud. B, Niels Bohr Institute*	14:30 - 15:00
15:00	**7 - Workshop Hackathon I**			

Indico Timetable - Tuesday

09:00	**Breakfast**		*Aud. B, Niels Bohr Institute*	09:00 - 09:30
	10 - State of the Art in AstroPhysics research	*Markus Ahlers*	*Aud. B, Niels Bohr Institute*	09:30 - 10:00
10:00	**12 - GraphNeT as seen from an analyser and software perspective**	*Tom Stuttard*	*Aud. B, Niels Bohr Institute*	10:00 - 10:30
	Break		*Aud. B, Niels Bohr Institute*	10:30 - 11:00
11:00	**13 - GraphNeT from a student user point of view**	*Cyan Yong Ho Jo*	*Aud. B, Niels Bohr Institute*	11:00 - 11:30
	14 - GraphNeT from an experienced outsider view	*Antonin Vacheret*	*Aud. B, Niels Bohr Institute*	11:30 - 12:00
12:00	**Lunch Break**		*Aud. B, Niels Bohr Institute*	12:00 - 13:00
13:00	**19 - GraphNeT Issues and Wishes**	*Jorge Prado González*	*Aud. B, Niels Bohr Institute*	13:00 - 13:30
	20 - GraphNeT Community Discussion	*Iván Mozún Mateo et al.*	*Aud. B, Niels Bohr Institute*	13:30 - 14:30
14:00				
	Break		*Aud. B, Niels Bohr Institute*	14:30 - 15:00
15:00	**15 - Workshop Hackathon II**		*Aud. B, Niels Bohr Institute*	15:00 - 15:45
	16 - Summary and Organisation of Plans		*Aud. B, Niels Bohr Institute*	15:45 - 16:15
16:00				

Directions to Troels' place

Troels' place
for dinner!

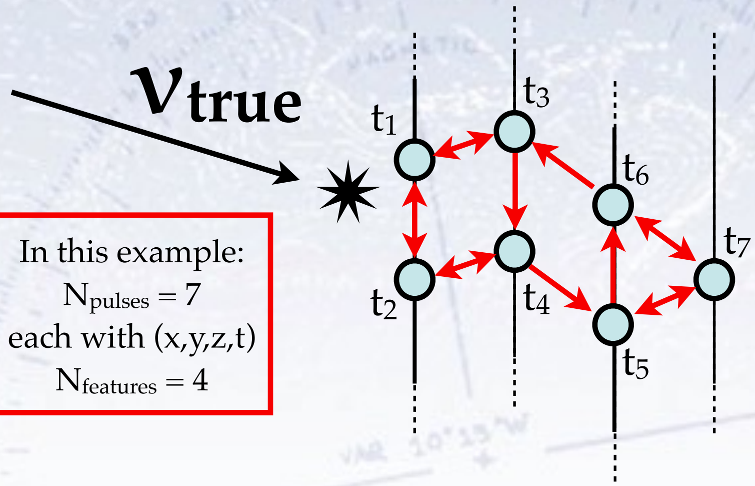
GraphNeT workshop

Addresse: Willemoesgade 54, 3.th.
Probably enter the door at 56!
Nearest station: Østerport (0.8km)
Problems: +45 26 28 37 39 (Troels)


GraphNet Workshop VI
Germany/Denmark/???
Xth to Yth of Z 2026?

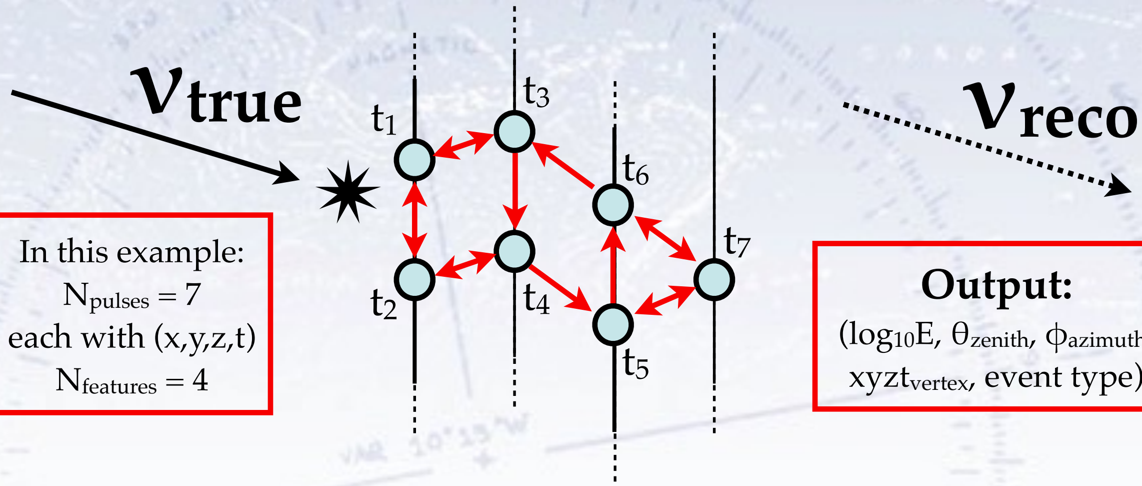
Bonus slides

Details of GNN reconstruction



In this example:
$N_{pulses} = 7$
each with (x,y,z,t)
$N_{features} = 4$

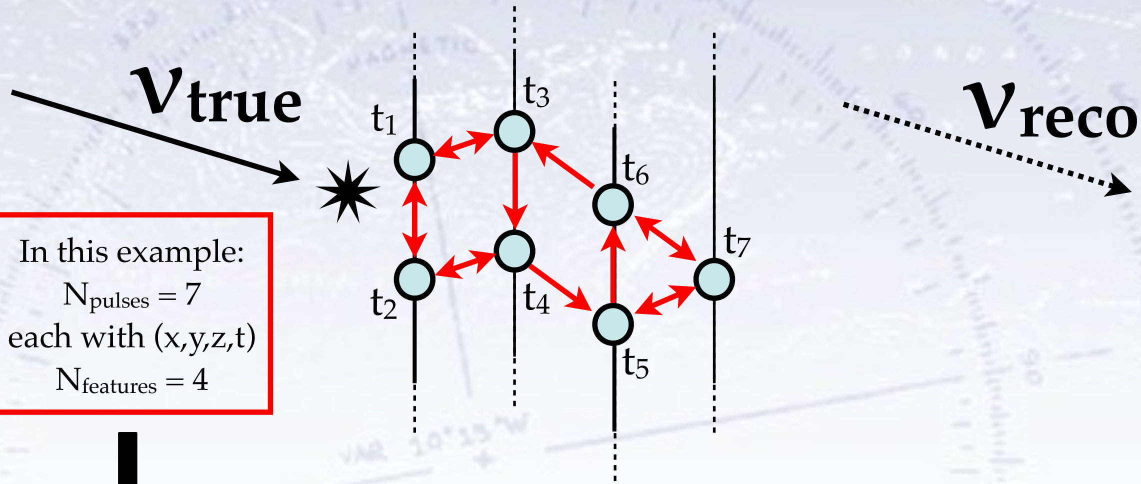
Details of GNN reconstruction



In this example:
$N_{pulses} = 7$
each with (x,y,z,t)
$N_{features} = 4$

Output:
($\log_{10}E$, θ_{zenith}, $\phi_{azimuth}$, $xyzt_{vertex}$, event type)

Details of GNN reconstruction



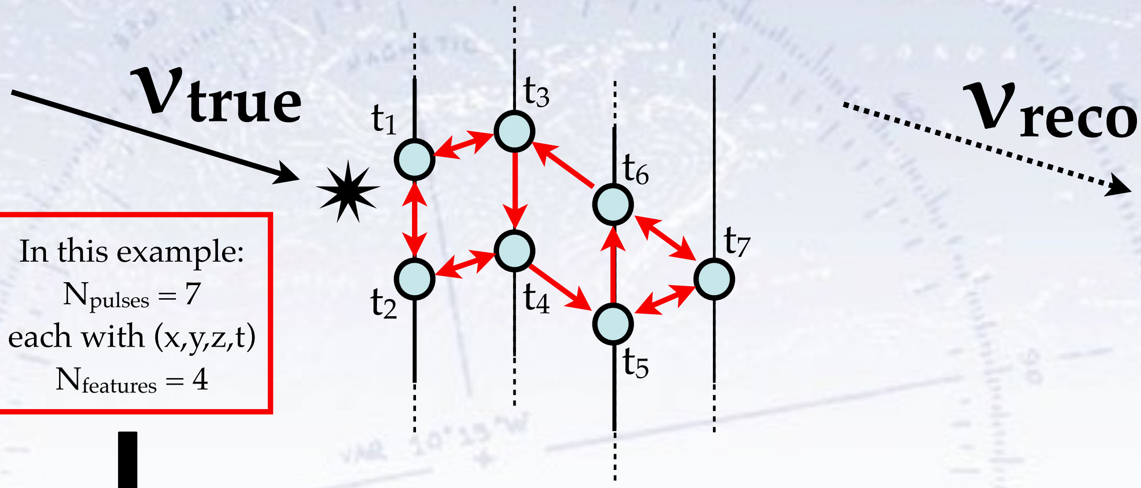
In this example:
$N_{pulses} = 7$
each with (x,y,z,t)
$N_{features} = 4$

$$\vec{v}_1 = [x_1\, y_1\, z_1\, t_1]$$
$$\vec{v}_2 = [x_2\, y_2\, z_2\, t_2]$$
$$\vdots$$
$$\vec{v}_7 = [x_7\, y_7\, z_7\, t_7]$$

Input:
$N = N_{pulses} \times N_{features}$

The input features of a node are combined with that of N (=2) nearby nodes

Details of GNN reconstruction



In this example:
$N_{pulses} = 7$
each with (x,y,z,t)
$N_{features} = 4$

$$\vec{v}_1 = [x_1\, y_1\, z_1\, t_1] \xrightarrow{EC(\vec{v}_1, \vec{v}_2, \vec{v}_3)} [g_{11} \dots g_{1N_1}]$$

$$\vec{v}_2 = [x_2\, y_2\, z_2\, t_2] \qquad [g_{21} \dots g_{2N_1}]$$

$$\vdots \xrightarrow{EC(\vec{v}_4, \vec{v}_5, \vec{v}_6)} \vdots$$

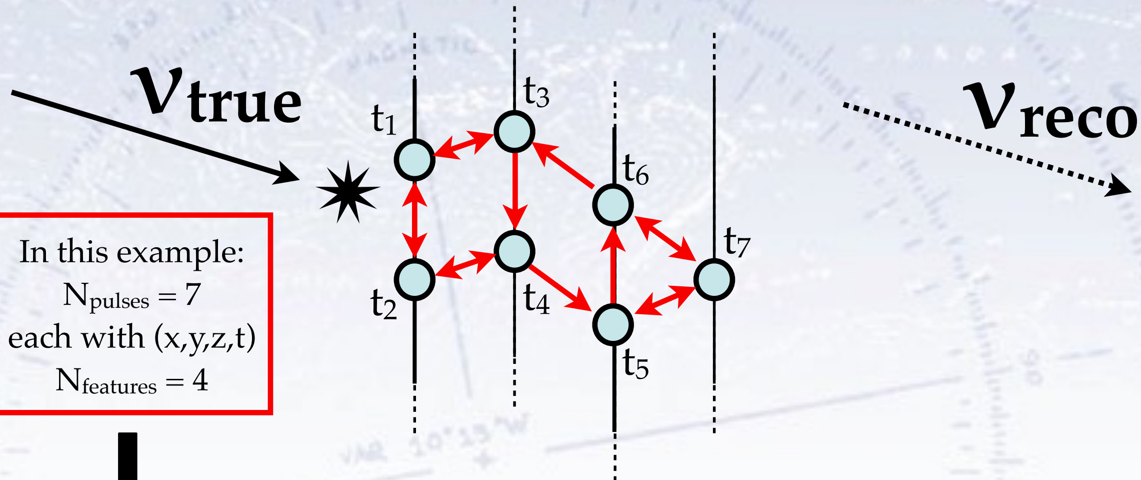
$$\vec{v}_7 = [x_7\, y_7\, z_7\, t_7] \qquad [g_{71} \dots g_{7N_1}]$$

Input:
$N = N_{pulses} \times N_{features}$

Convolution(s):
$N = N_{pulses} \times N_1$

The input features of a node are combined with that of N (=2) nearby nodes through an NN (MLP0) function, yielding an (abstract) vector for each node. This can be repeated (not shown).

Details of GNN reconstruction



In this example:
$N_{pulses} = 7$
each with (x,y,z,t)
$N_{features} = 4$

$$N_{all} = N_{features} + N_1$$

$$\vec{v}_1 = [x_1\, y_1\, z_1\, t_1] \xrightarrow{EC(\vec{v}_1, \vec{v}_2, \vec{v}_3)} [g_{11} \dots g_{1N_1}] \qquad [x_1\, y_1\, z_1\, t_1\;\; g_{11} \dots g_{1N_1}]$$

$$\vec{v}_2 = [x_2\, y_2\, z_2\, t_2] \qquad [g_{21} \dots g_{2N_1}] \qquad [x_2\, y_2\, z_2\, t_2\;\; g_{21} \dots g_{2N_1}]$$

$$\vdots \xrightarrow{EC(\vec{v}_4, \vec{v}_5, \vec{v}_6)} \vdots \qquad \vdots$$

$$\vec{v}_7 = [x_7\, y_7\, z_7\, t_7] \qquad [g_{71} \dots g_{7N_1}] \qquad [x_7\, y_7\, z_7\, t_7\;\; g_{71} \dots g_{7N_1}]$$

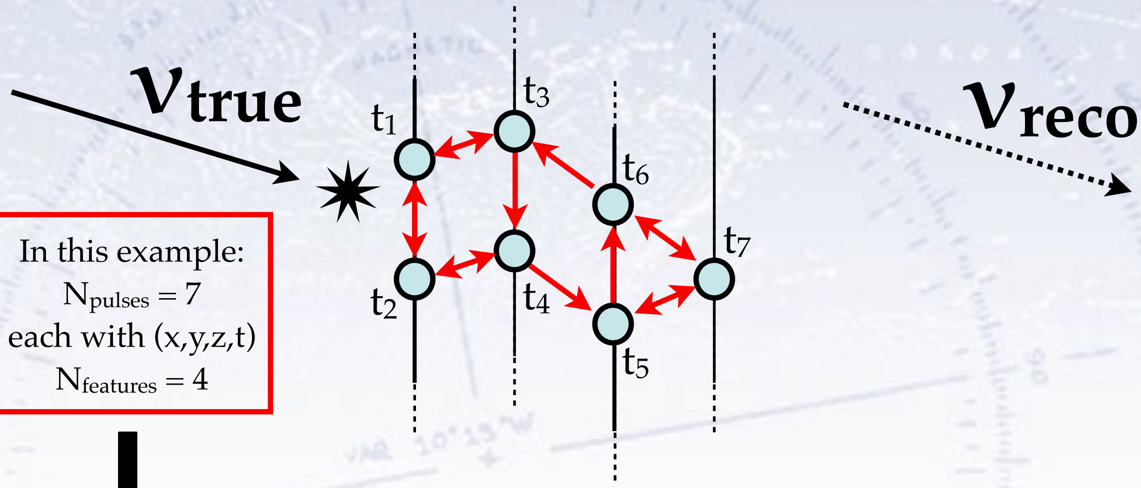
Input:
$N = N_{pulses} \times N_{features}$

Convolution(s):
$N = N_{pulses} \times N_1$

Concatenation:
$N = N_{pulses} \times N_{all}$

The input features of a node are combined with that of N (=2) nearby nodes through an NN (MLP0) function, yielding an (abstract) vector for each node. This can be repeated (not shown). All the features are then combined (concatenated) into long vectors,

Details of GNN reconstruction



In this example:
$N_{pulses} = 7$
each with (x,y,z,t)
$N_{features} = 4$

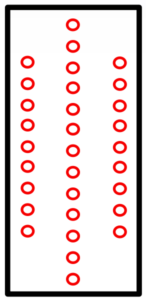
$N_{all} = N_{features} + N_1$

$$\vec{v}_1 = [x_1\, y_1\, z_1\, t_1] \xrightarrow{EC(\vec{v}_1, \vec{v}_2, \vec{v}_3)} [g_{11} \dots g_{1N_1}] \qquad [x_1\, y_1\, z_1\, t_1\;\; g_{11} \dots g_{1N_1}] \rightarrow \quad \rightarrow [h_{11} \dots h_{1N_{all}}]$$

$$\vec{v}_2 = [x_2\, y_2\, z_2\, t_2] \qquad [g_{21} \dots g_{2N_1}] \qquad [x_2\, y_2\, z_2\, t_2\;\; g_{21} \dots g_{2N_1}] \rightarrow \quad \rightarrow [h_{21} \dots h_{2N_{all}}]$$

$$\vdots \xrightarrow{EC(\vec{v}_4, \vec{v}_5, \vec{v}_6)} \vdots \qquad \vdots \qquad \vdots$$

$$\vec{v}_7 = [x_7\, y_7\, z_7\, t_7] \qquad [g_{71} \dots g_{7N_1}] \qquad [x_7\, y_7\, z_7\, t_7\;\; g_{71} \dots g_{7N_1}] \rightarrow \quad \rightarrow [h_{71} \dots h_{7N_{all}}]$$



Input: $N = N_{pulses} \times N_{features}$

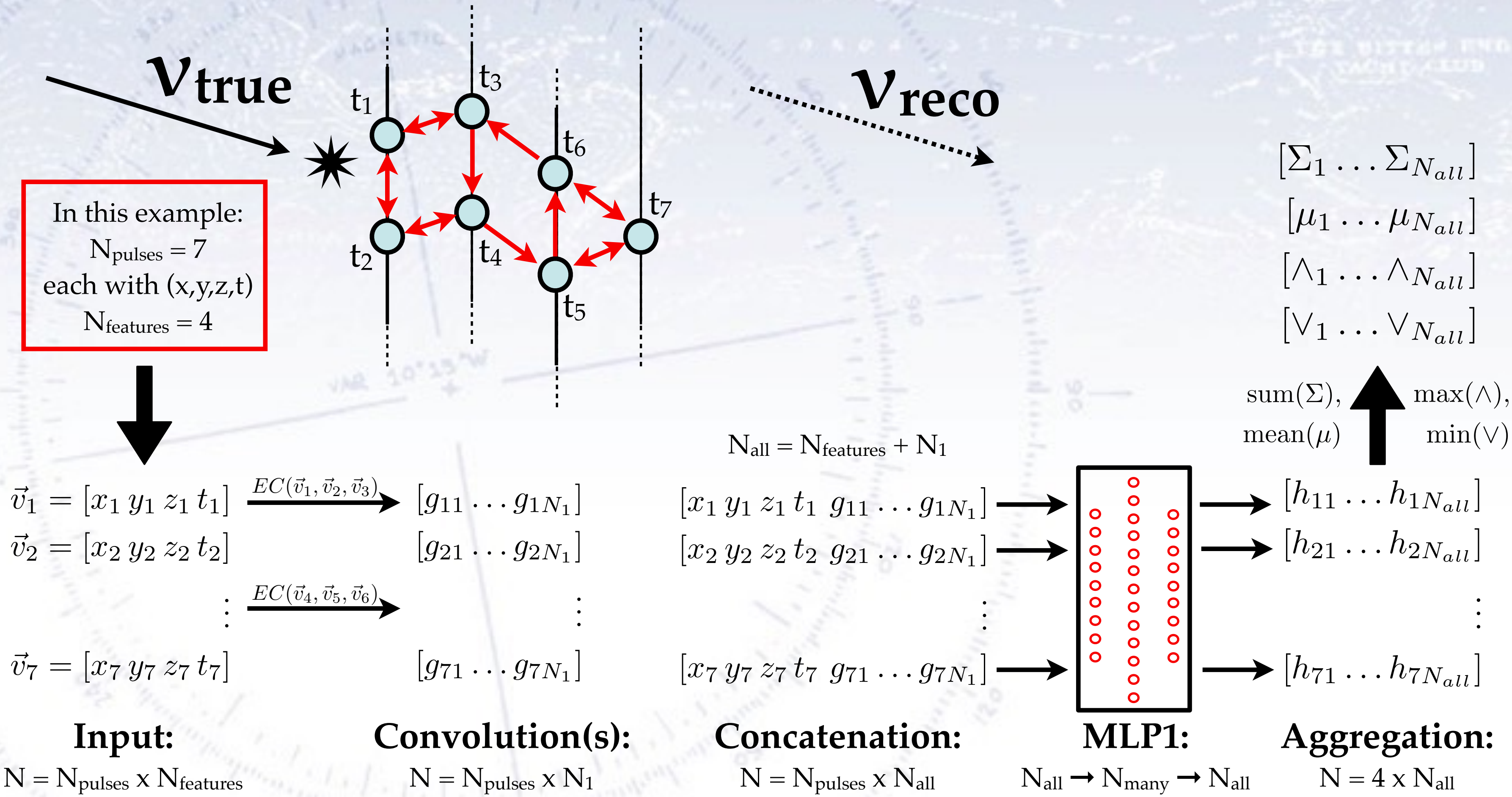
Convolution(s): $N = N_{pulses} \times N_1$

Concatenation: $N = N_{pulses} \times N_{all}$

MLP1: $N_{all} \rightarrow N_{many} \rightarrow N_{all}$

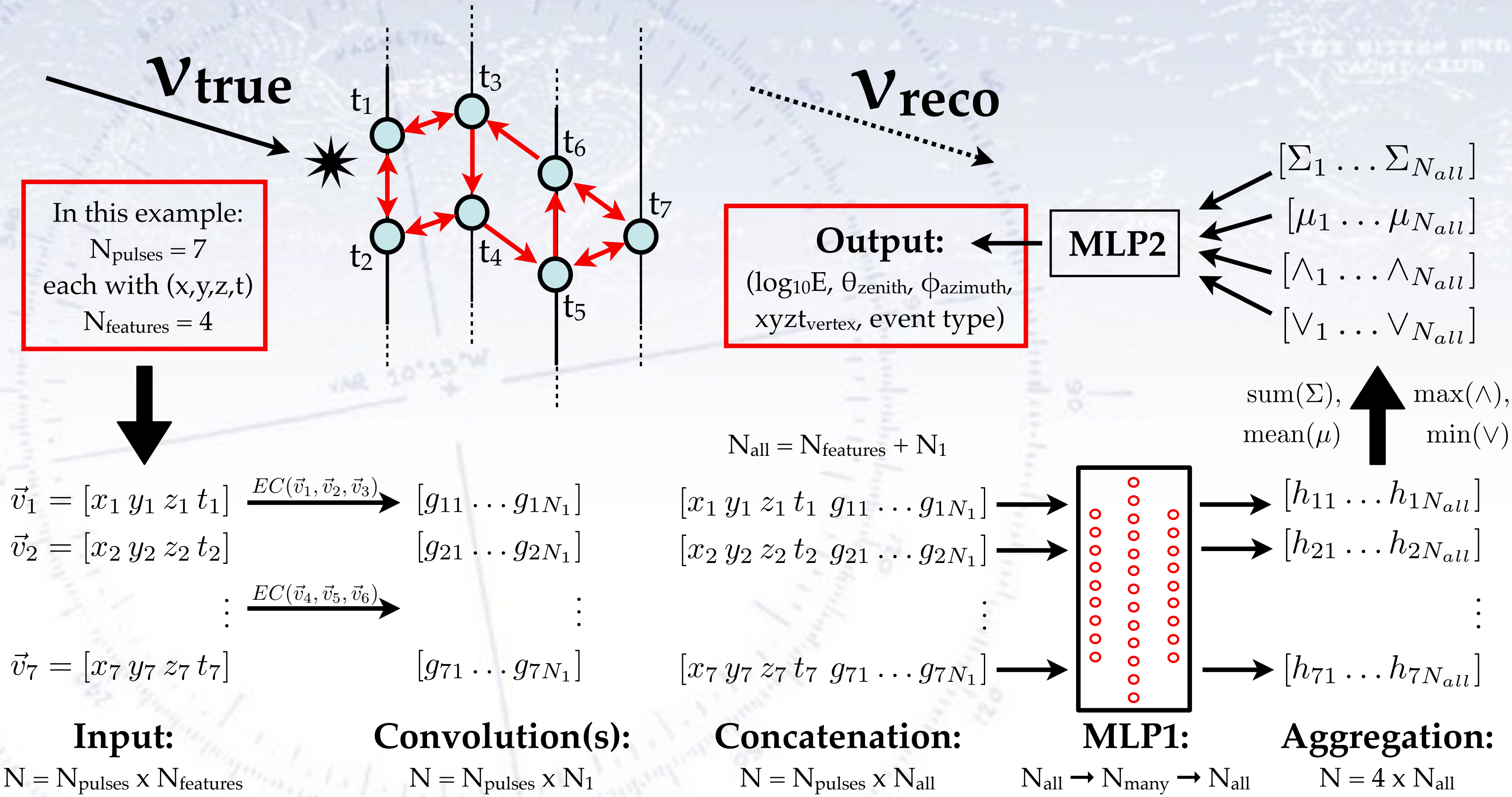
The input features of a node are combined with that of N (=2) nearby nodes through an NN (MLP0) function, yielding an (abstract) vector for each node. This can be repeated (not shown). All the features are then combined (concatenated) into long vectors, which are again put through an NN (MLP1) function with a large hidden layer.

Details of GNN reconstruction



The input features of a node are combined with that of N (=2) nearby nodes through an NN (MLP0) function, yielding an (abstract) vector for each node. This can be repeated (not shown). All the features are then combined (concatenated) into long vectors, which are again put through an NN (MLP1) function with a large hidden layer. The outputs are aggregated in four ways: Min, Max, Sum & Mean, breaking the variation with number of nodes.

Details of GNN reconstruction



The input features of a node are combined with that of N (=2) nearby nodes through an NN (MLP0) function, yielding an (abstract) vector for each node. This can be repeated (not shown). All the features from all the convolutions are then combined (concatenated) into long vectors, which are again put through an NN (MLP1) function with a large hidden layer. The outputs are aggregated in four ways: Min, Max, Sum & Mean, breaking the variation with number of nodes. These are then fed into a final NN (MLP2), which outputs the estimated type(s) and parameters of the event.

Further specifics of DynEdge

In DynEdge, there are several "enlargements" compared to the previous illustration of the GNN architecture. These are essentially:

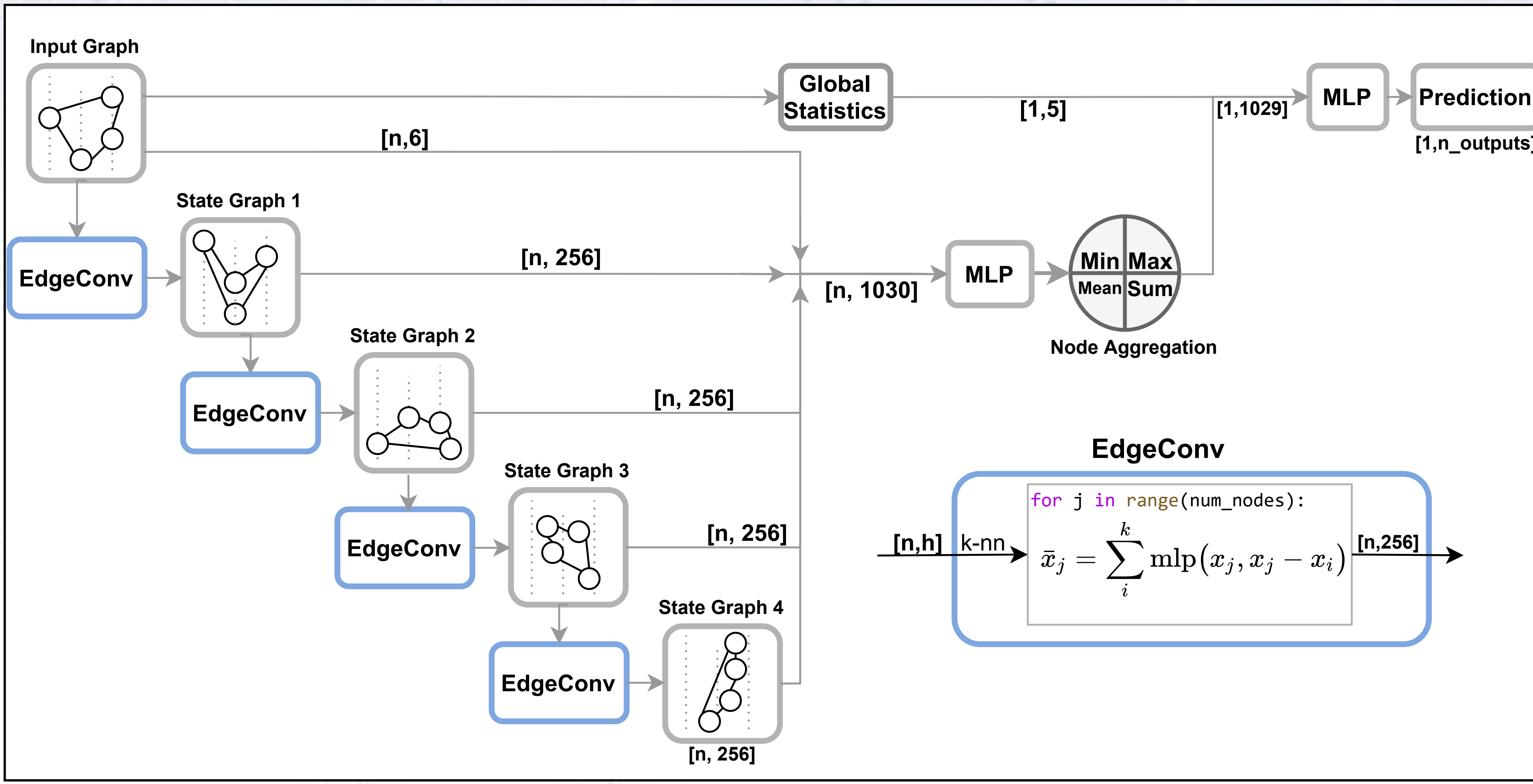
- We use 6 input features: x, y, z, t, charge, and Quantum Efficiency.
- We convolute each node with the nearest 8 nodes (not two).
- We do 4 (not 1) convolutions, each with 192 inputs and outputs.
- The concatenation is of all convolution layers and the original input.
- In the results to be shown, we have trained separate GNNs for each output.

The repeated convolutions allows all signal parts to be connected.
The EdgeConv convolution operator ensures permutation invariance.

The number of model parameters is about 750.000 for the angular regressions, while the energy only requires 150.000. In principle one can go down to 70.000 parameters, but there is no reason for this - it is already a "small" ML model.

GraphNet

The GNN model is outlined more simply below, which is also the (current) figure for the GNN paper in process.




SCIENCE
Hard Rock