NuGraph2

A Graph Neural Network for 3D Reconstruction in Liquid Argon Time Projection Chambers

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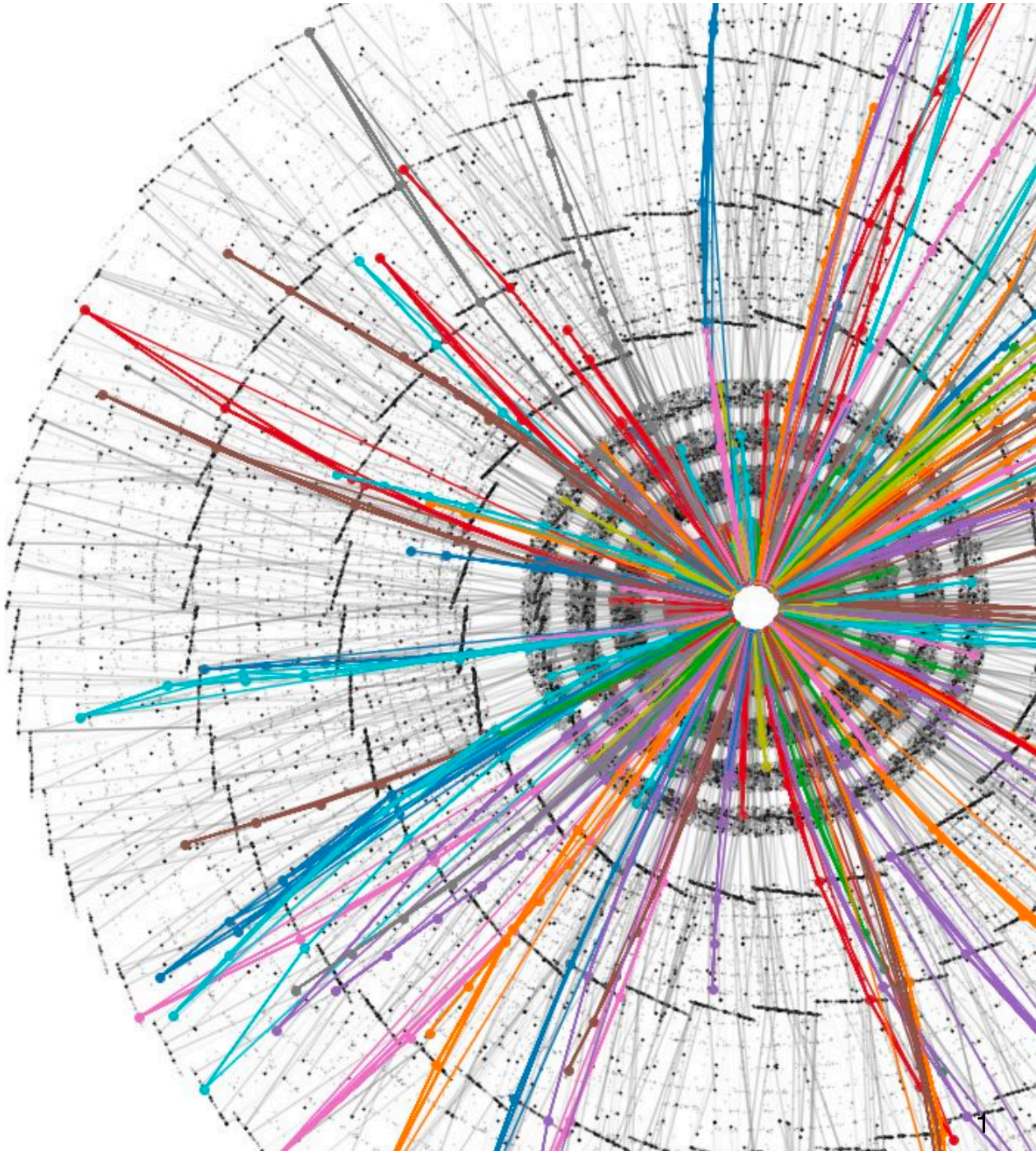
V Hewes

9th May 2022

26th International Conference on Computing in High Energy & Nuclear Physics (CHEP23)

Exa.TrkX

- Exa.TrkX is a collaboration developing next-generation Graph Neural Network (GNN) reconstruction for HEP:



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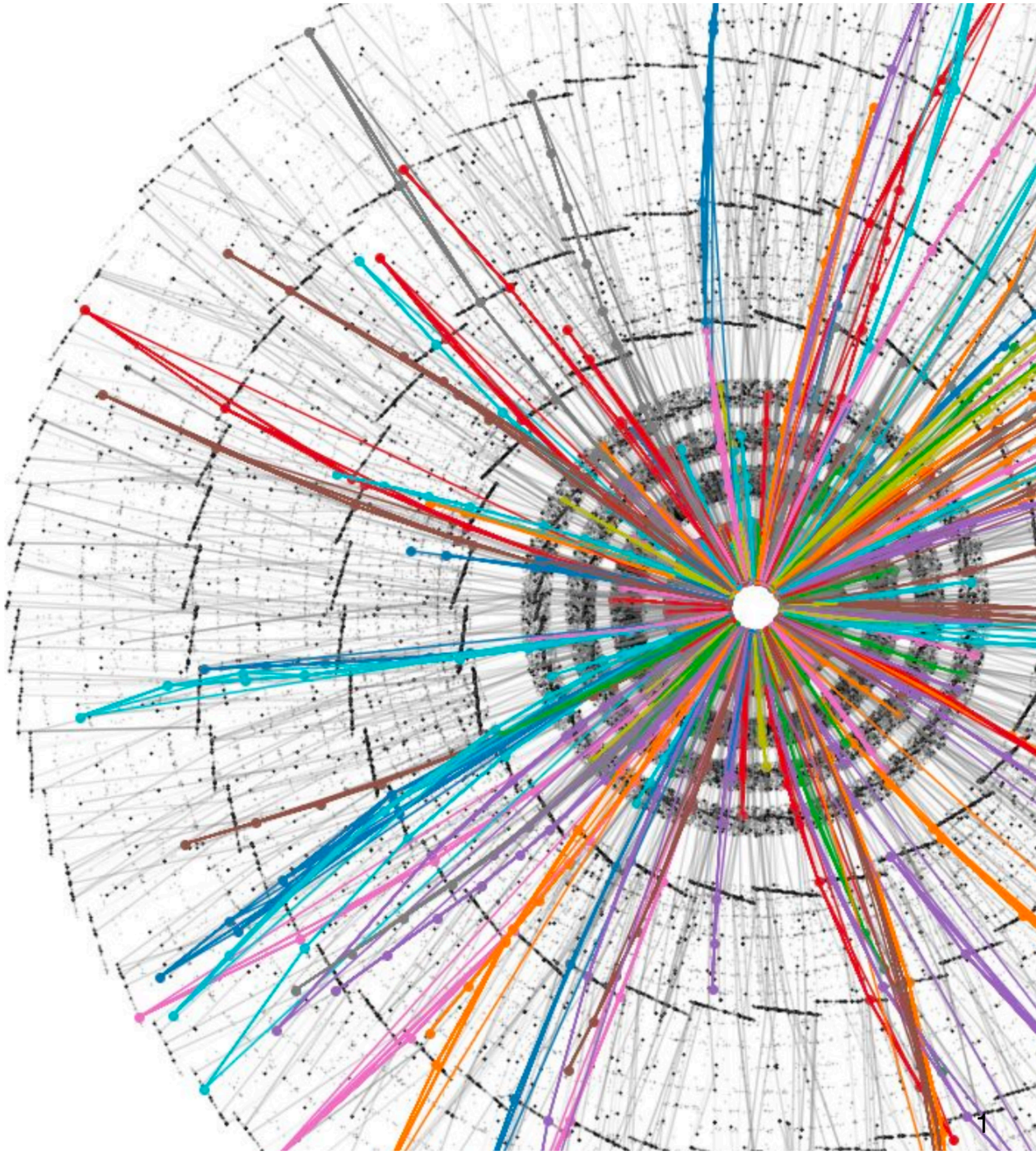
    - Expand on HEP.TrkX's prototype GNN for HL-LHC.
    - Incorporate into ATLAS's simulation and validation chain.



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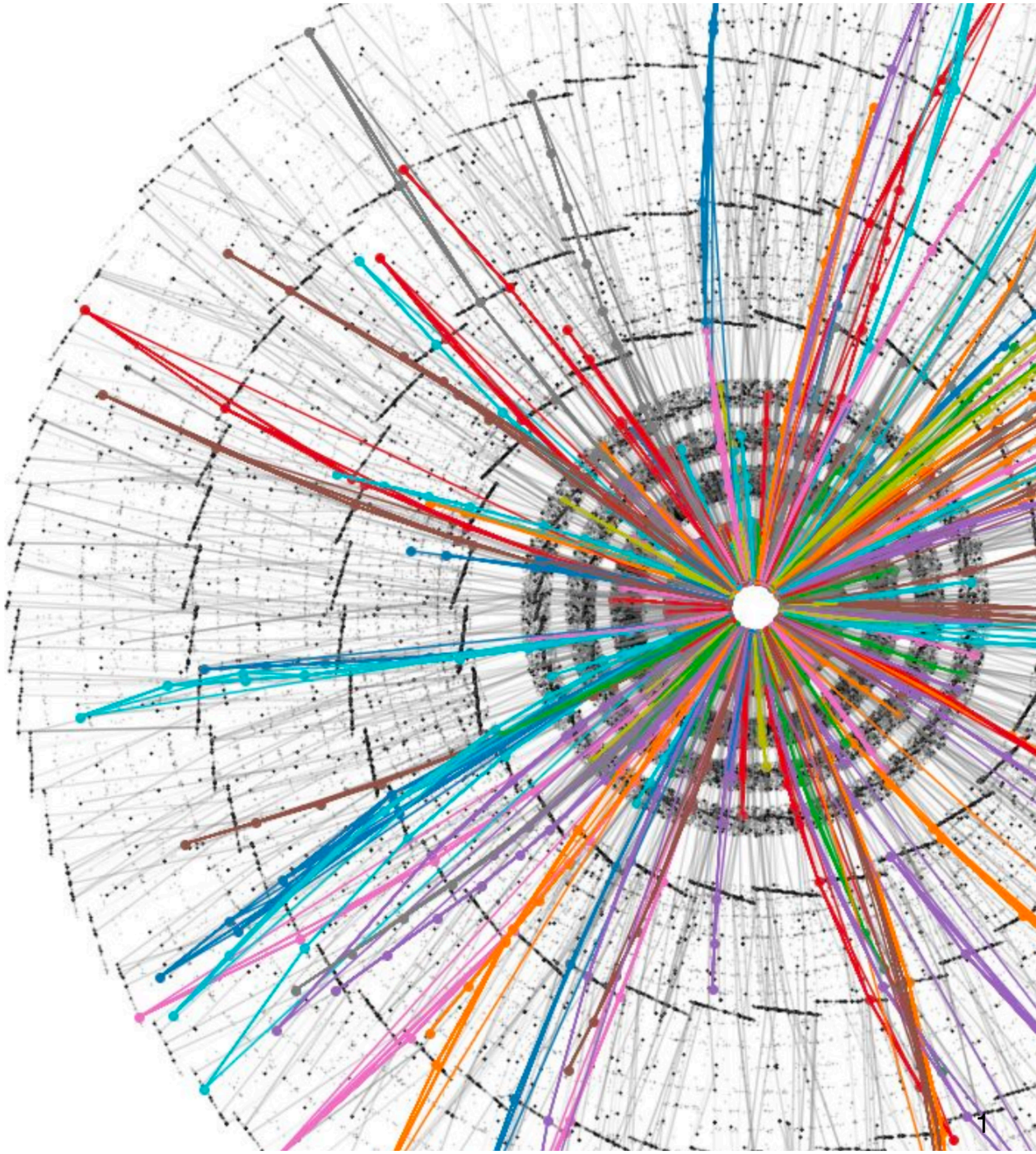
    - Explore viability of HEP.TrkX network for neutrino physics.
    - Develop GNN-based reconstruction for Liquid Argon TPCs.



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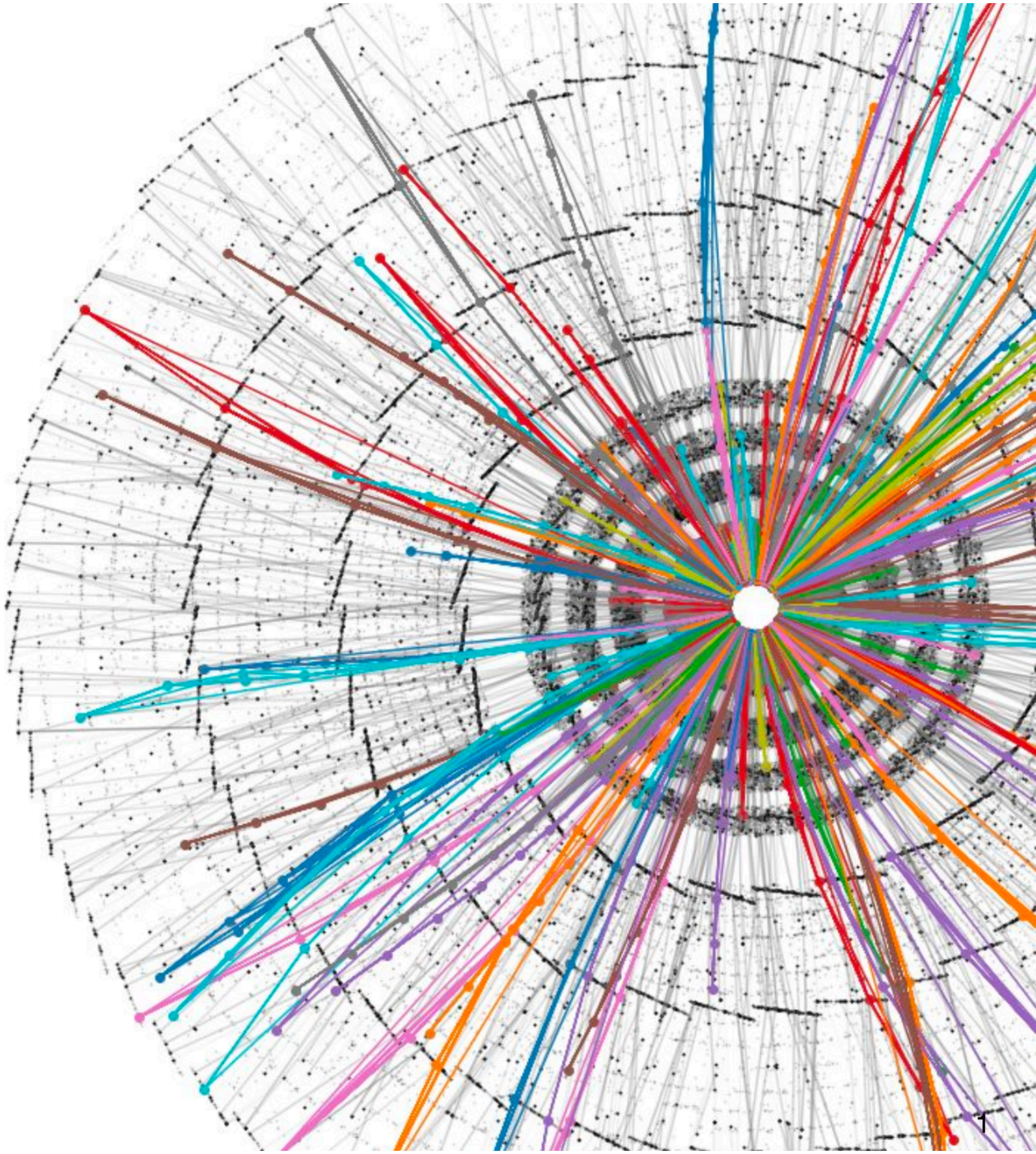
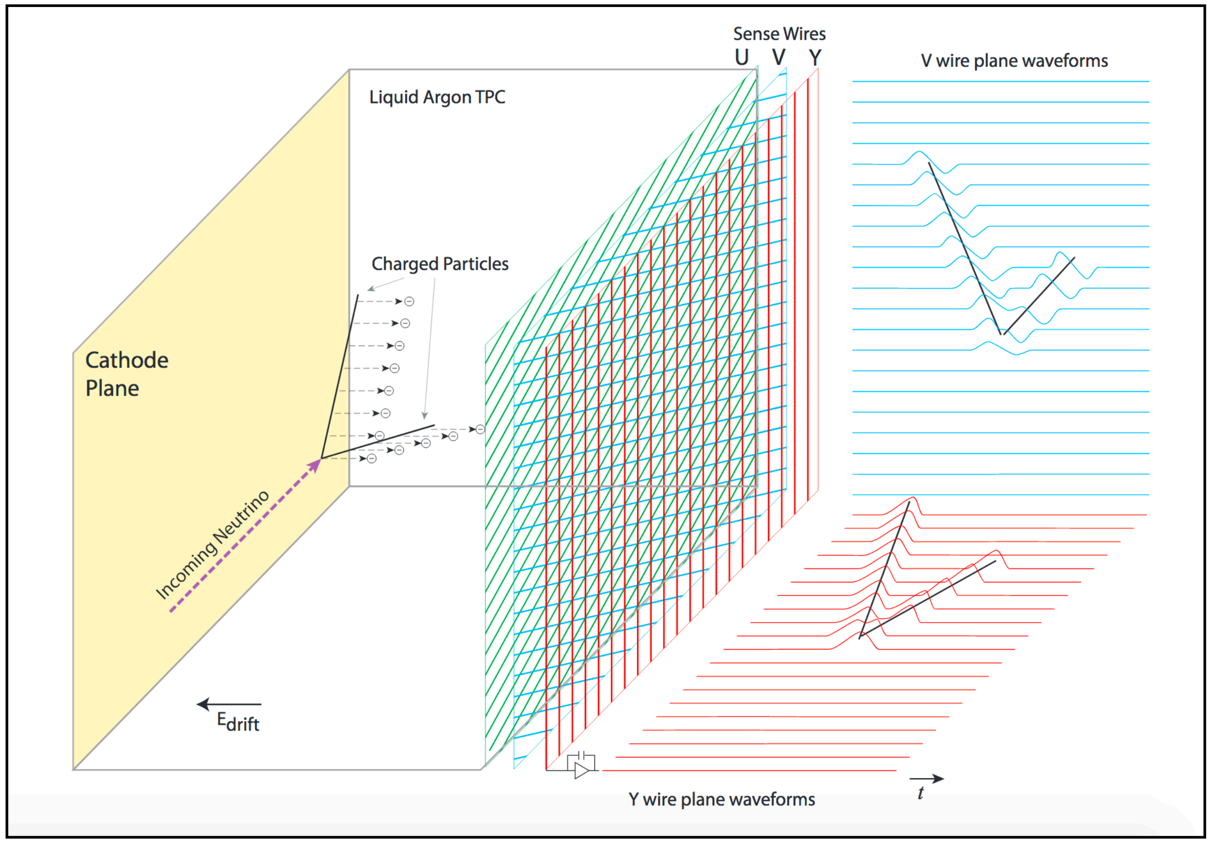
    - Develop GNN-based reconstruction for Liquid Argon TPCs.
- **See <u>Paulo Calafiura's overview talk</u>!**



Liquid Argon TPCs

- Liquid Argon Time Projection Chambers (LArTPCs) currently a heavily utilised detector technology in neutrino physics.
  - At FNAL: MicroBooNE, Icarus, SBND.
  - Future: DUNE (70kT LArTPC deep underground, plus near detector).

- Charged particles ionize liquid argon as they travel.
- Ionisation electrons drift due to HV electrode field, and are collected by anode wires.
- Wire spacing ~3mm – **high-resolution detector**.



NuGraph2

- NuGraph2 is Exa.TrkX's second-generation GNN architecture for **semantically labelling LArTPC detector hits according to particle type**.
  - Utilise a **multi-head attention message-passing mechanism** within each detector plane.
  - Incorporate a number of improvements over first-generation proof-of-concept model (arxiv:2103.06233).
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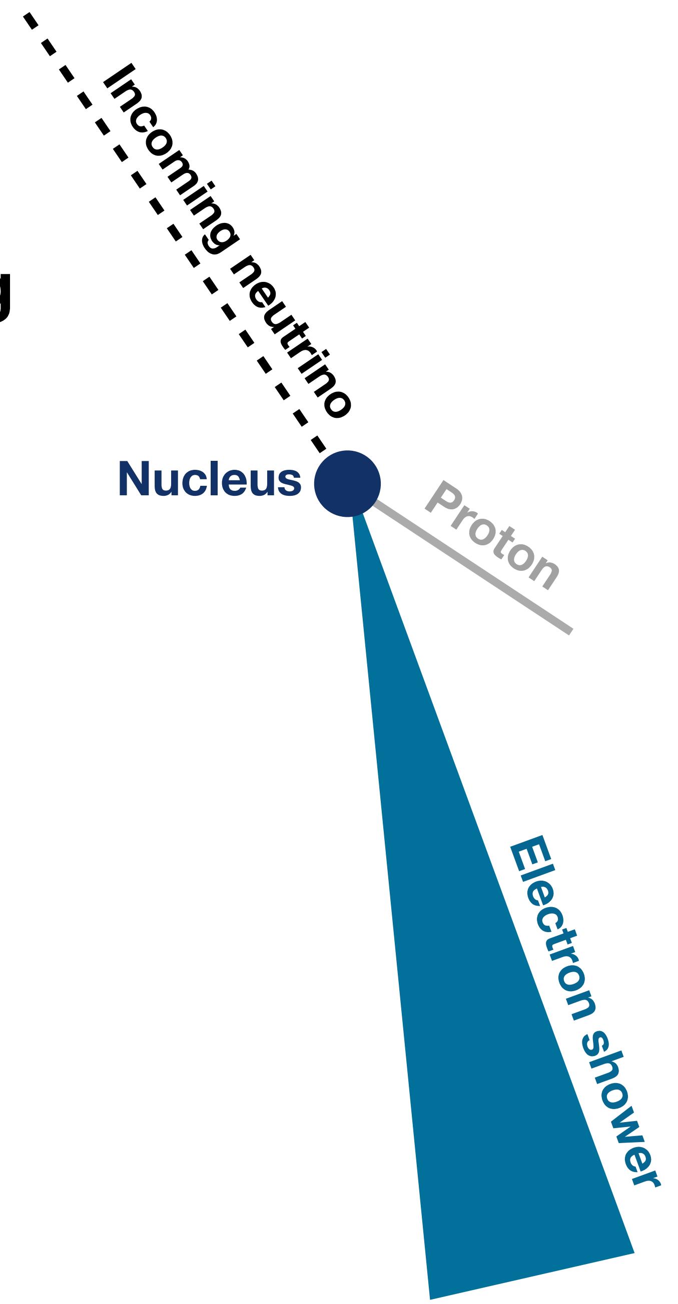
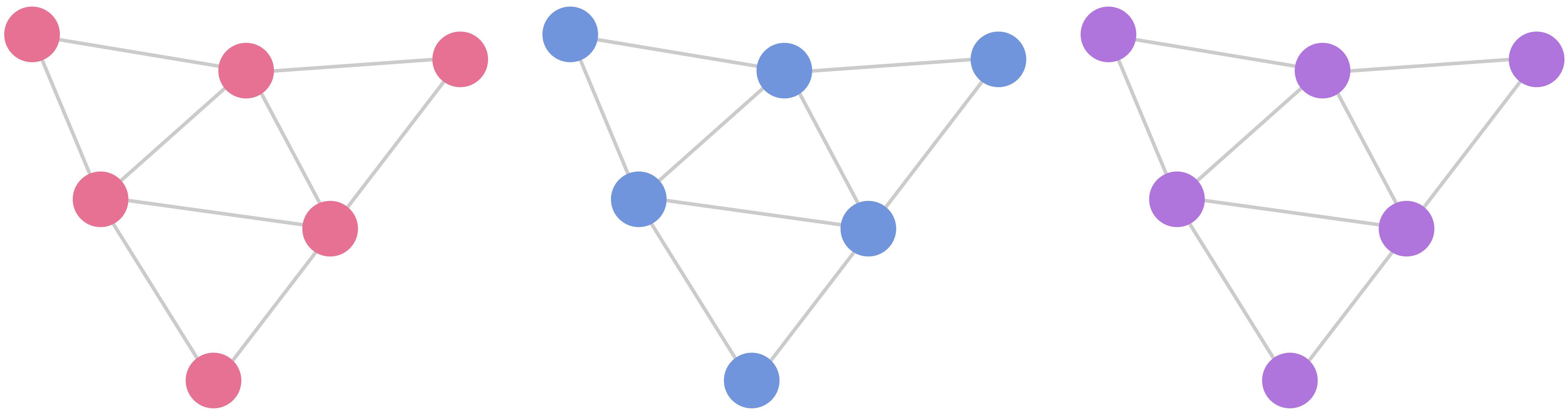
- Network trained on **simulated neutrinos** from **MicroBooNE's Open Data Release**.
  - **See talk by Giuseppe Cerati this afternoon!**



3D Nexus convolutions

- Perform message-passing independently in each detector view.



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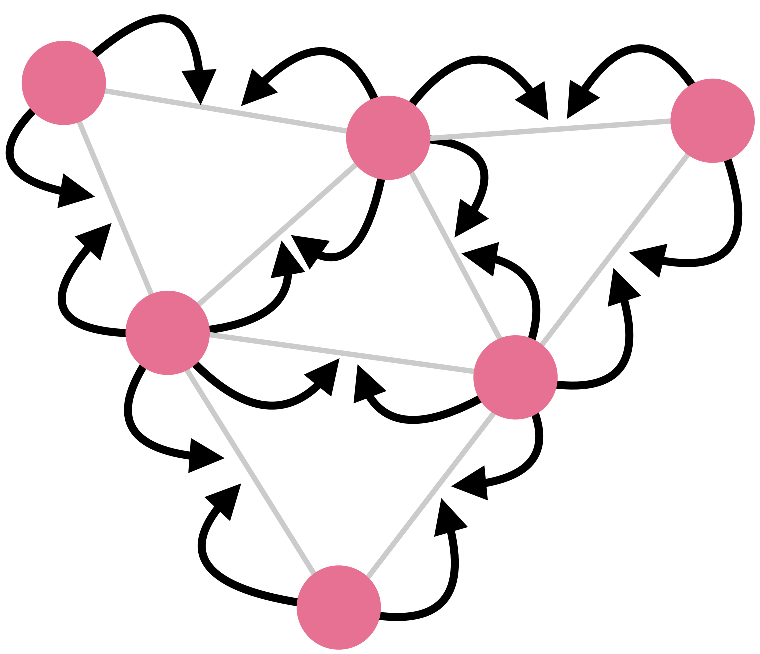

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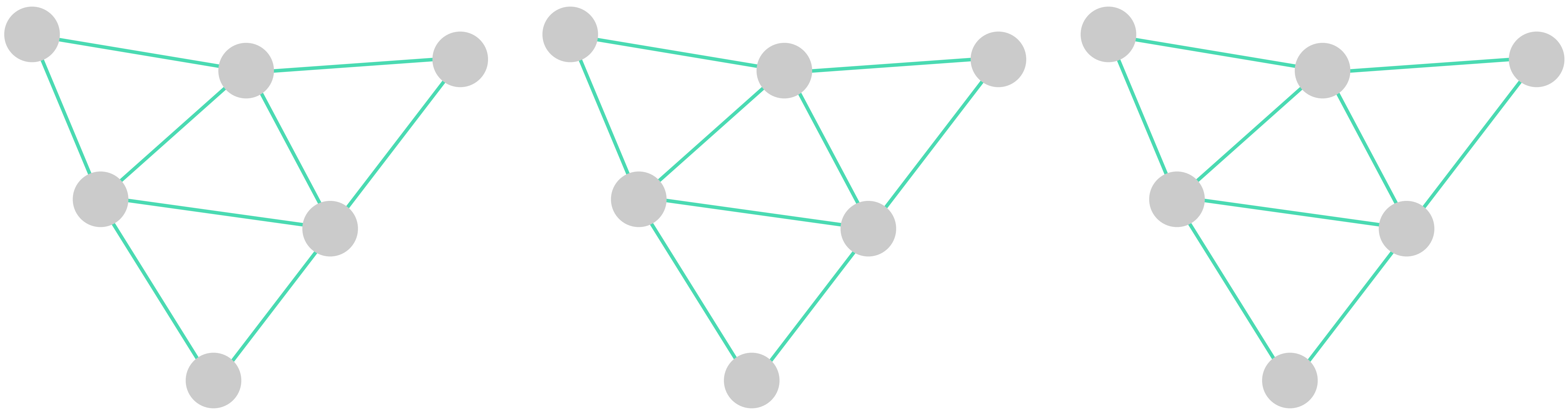

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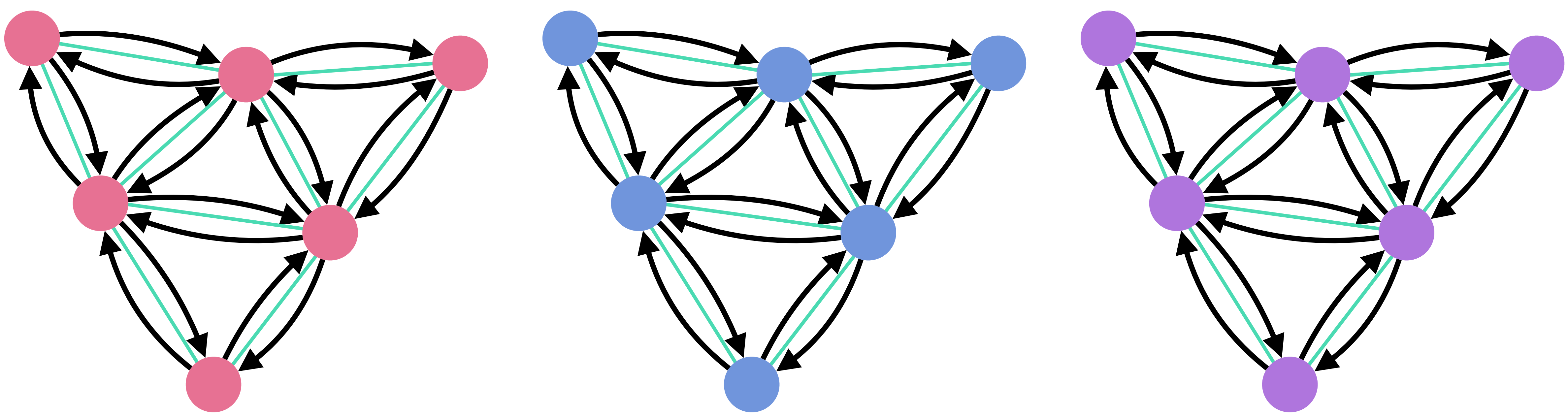
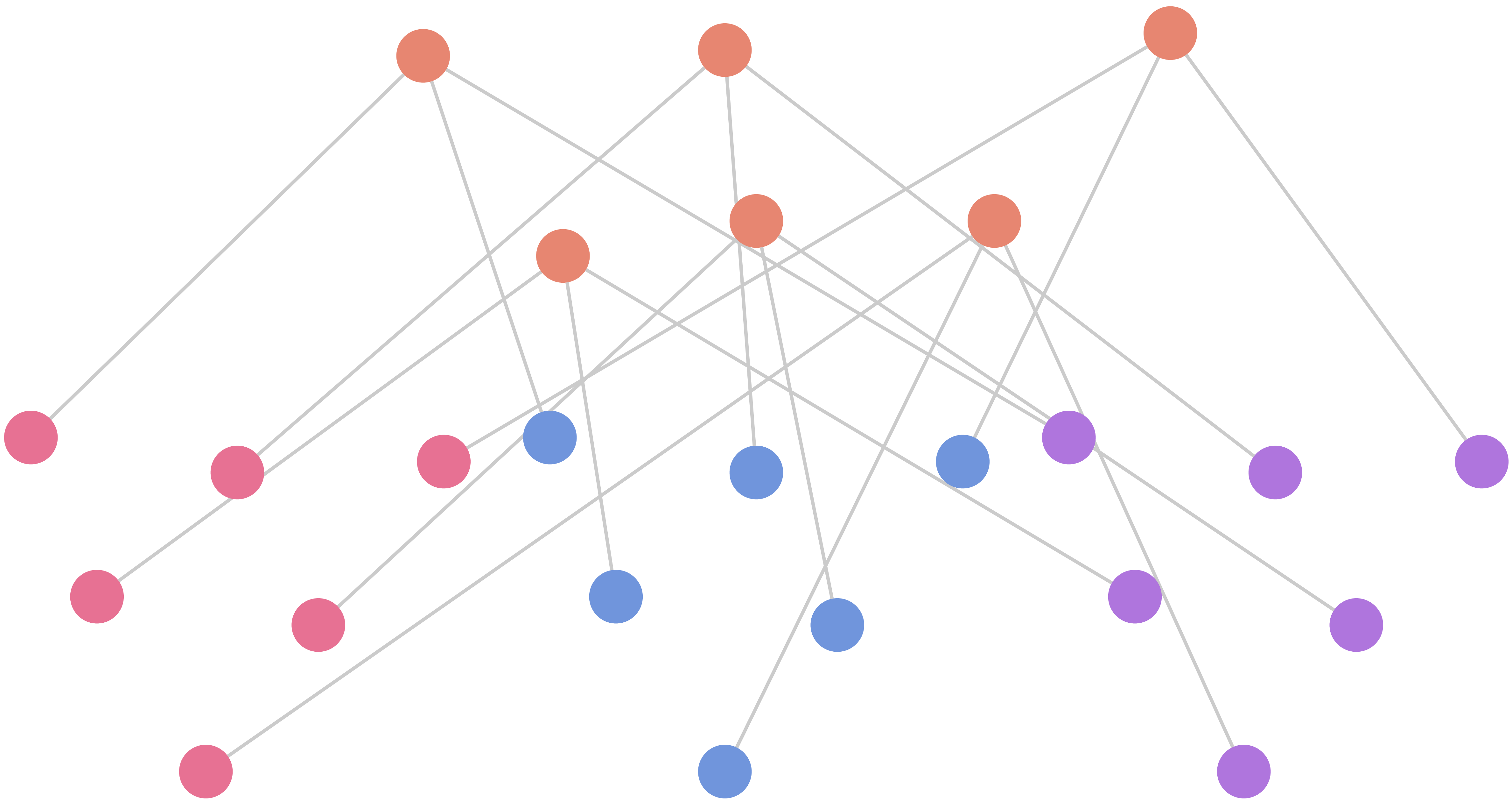


3D Nexus convolutions

- Add additional 3D step to the standard message-passing loop.



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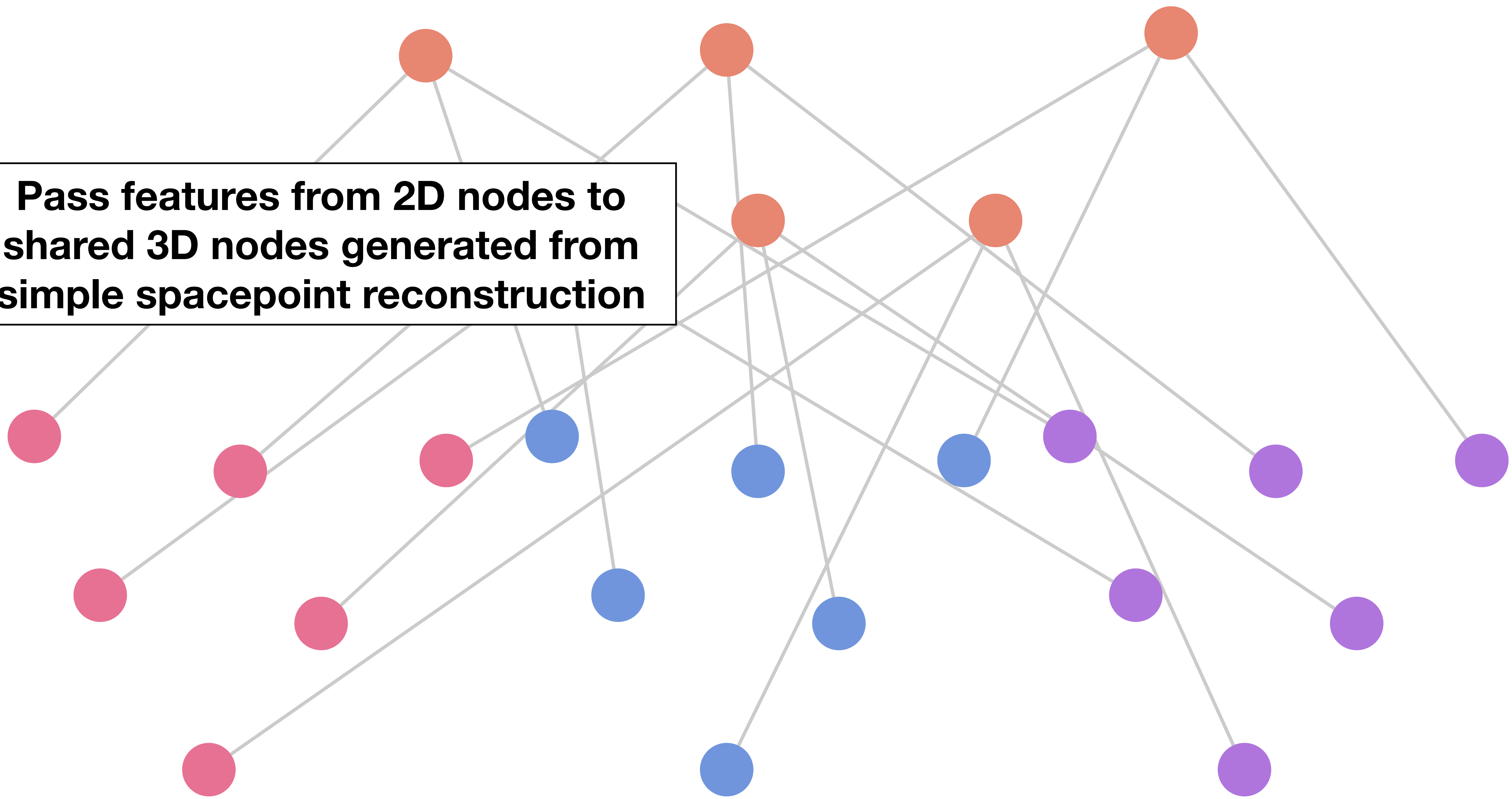
Pass features from 2D nodes to shared 3D nodes generated from simple spacepoint reconstruction



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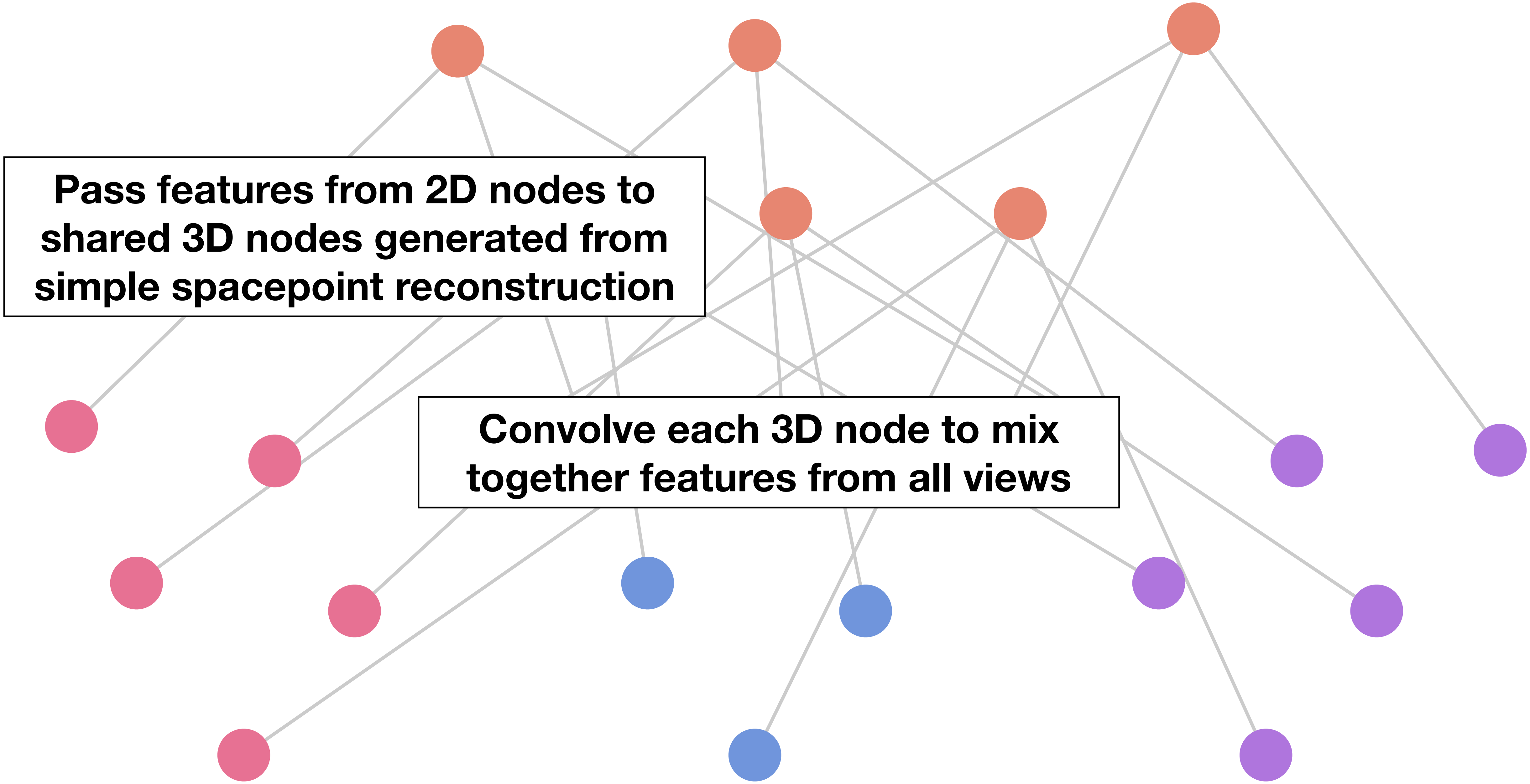

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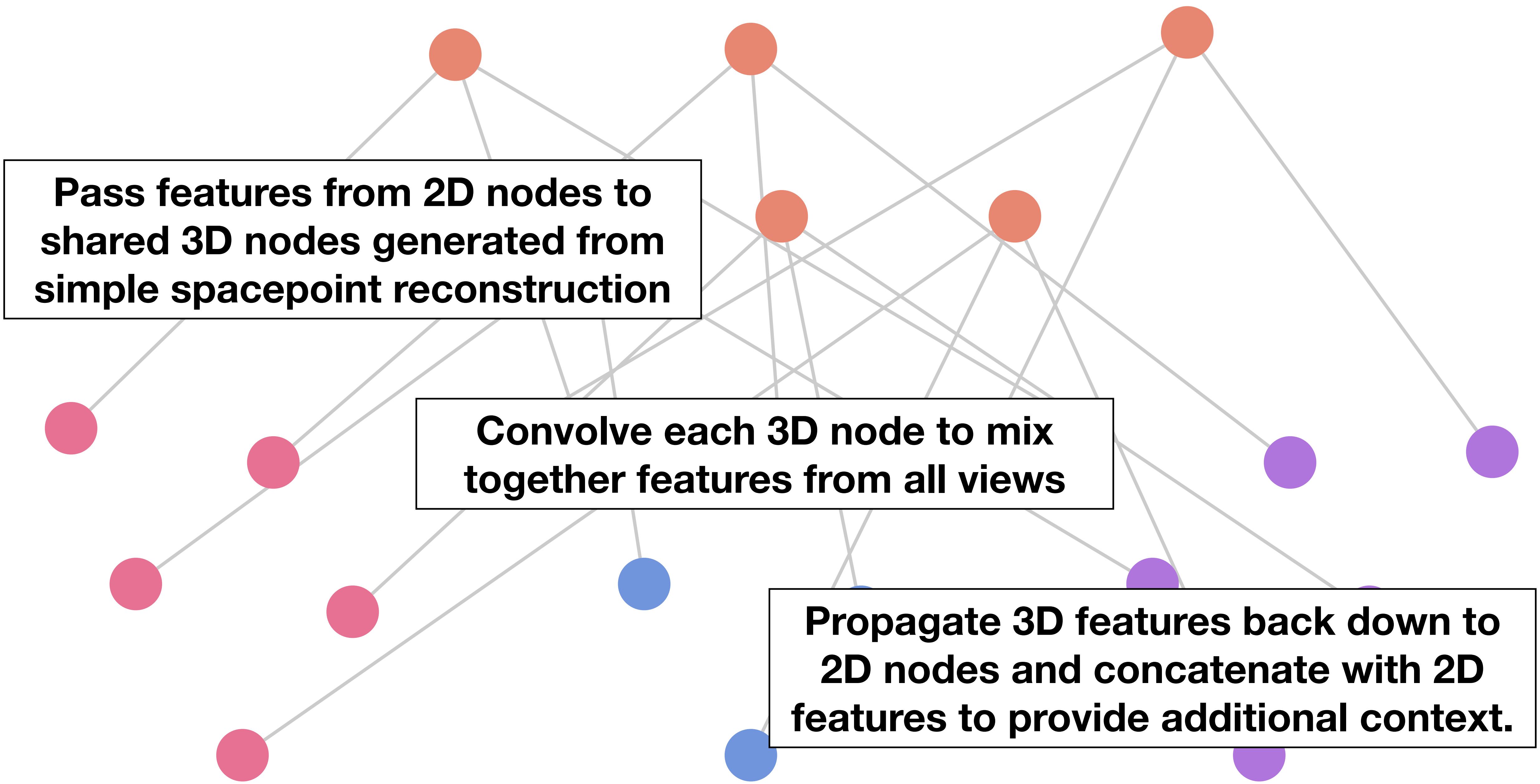

NuGraph2

- Network achieves **~86%** overall hit classification accuracy.
- With 3D connections, consistency of representations between views is now around **98%**, compared to ~70% without.

Confusion matrix weighted by
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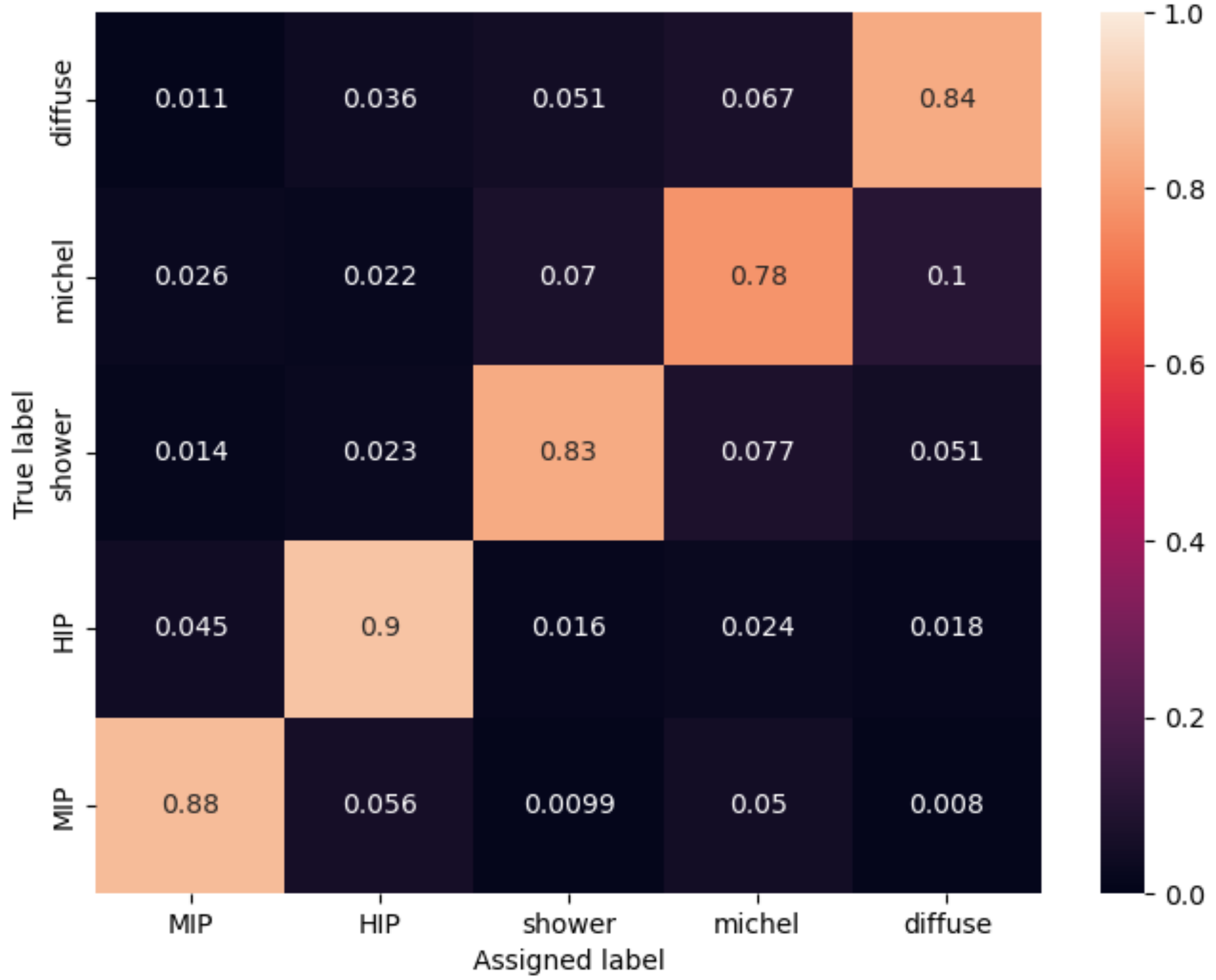
to show **efficiency**.



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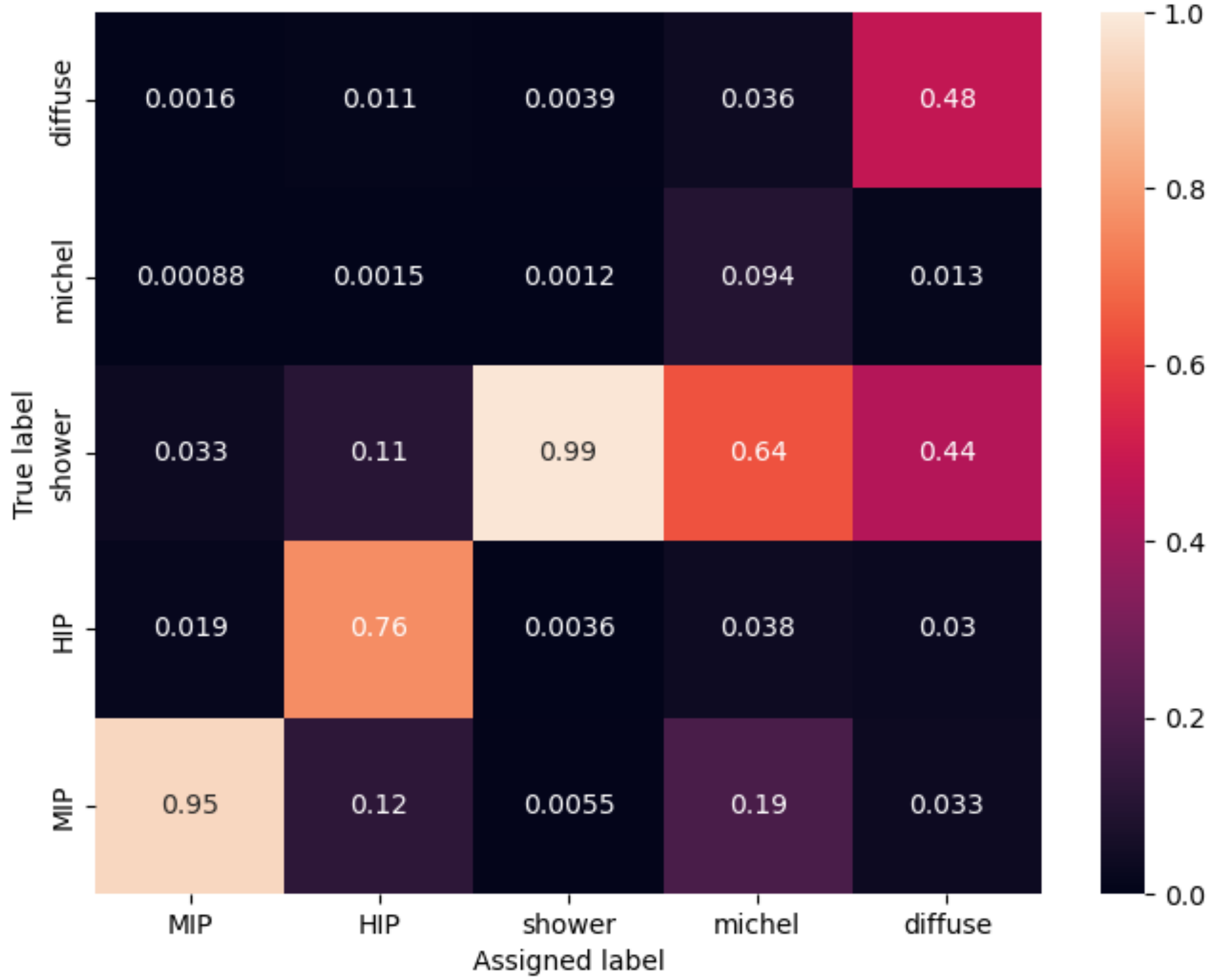
Confusion matrix weighted by **predicted semantic label**. to show **purity**.



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- Network achieves **~86%** overall hit classification accuracy.
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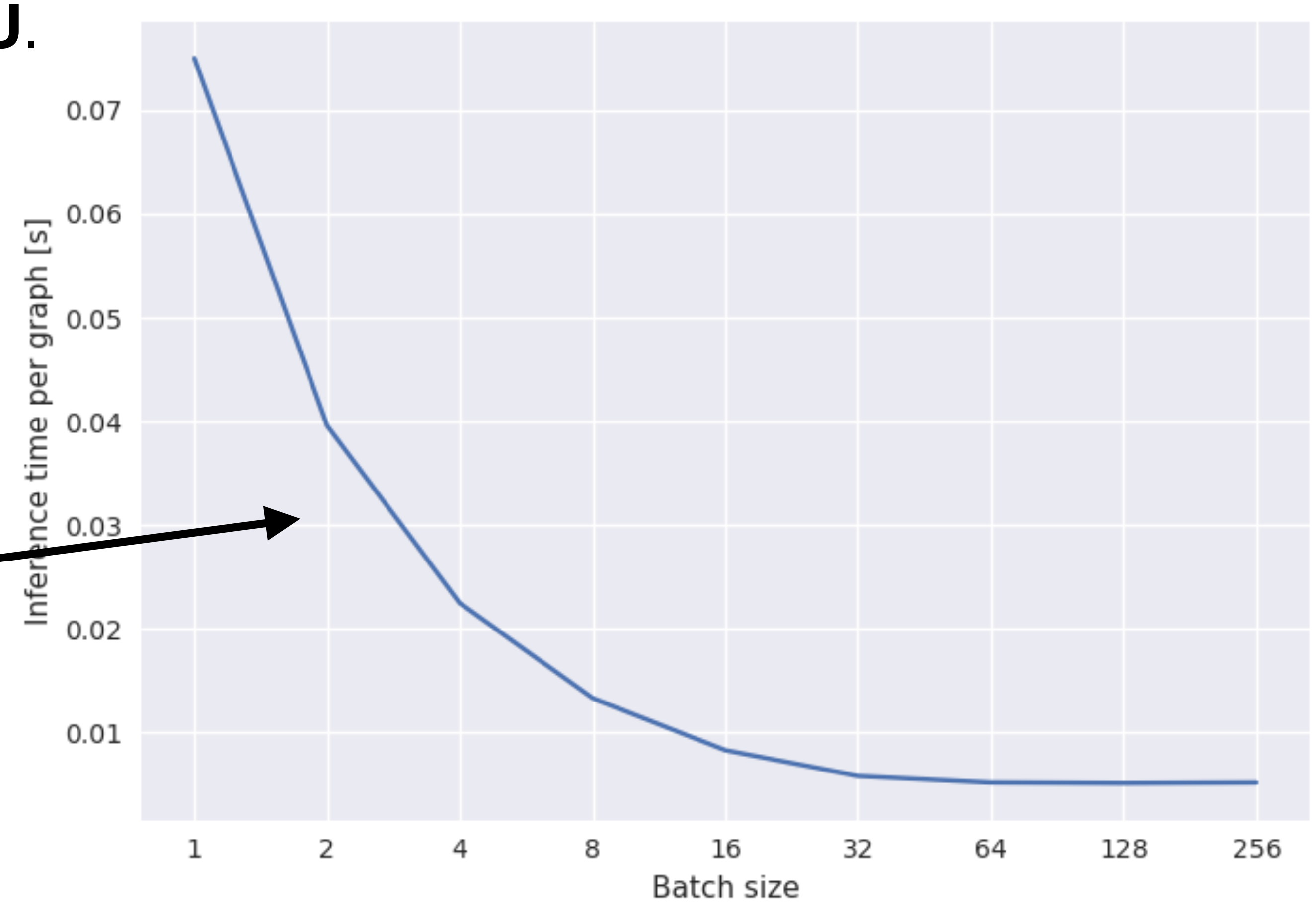
- Inference takes **0.12 s / event on CPU**.

GPU inference time as a function of batch size



Discussion

- Network performance on the Michel class primarily driven by **class imbalance in training dataset**.
  - **EM showers** have large hit multiplicity, and make up **> 50% of hits** in training dataset.
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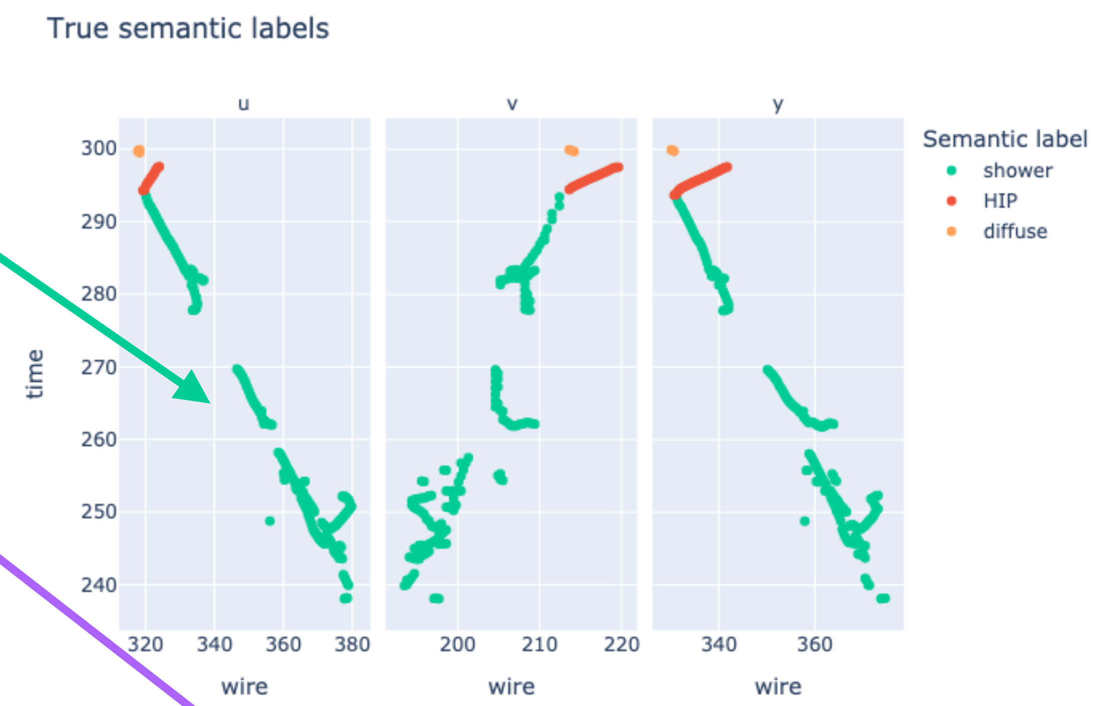

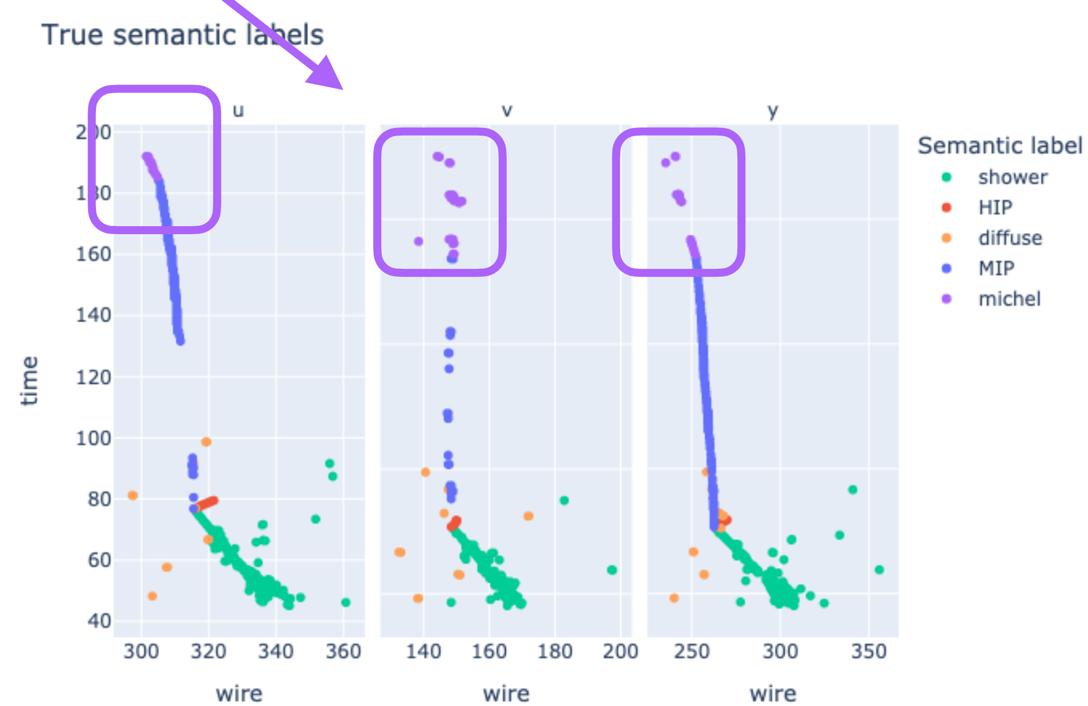

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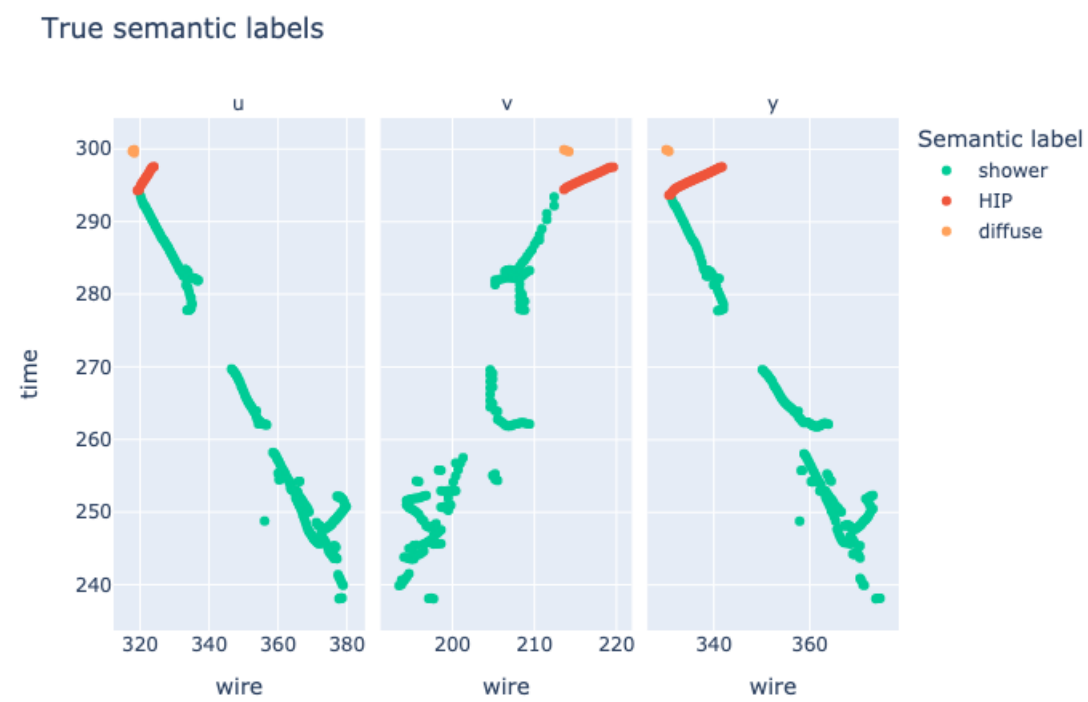

University of CINCINNATI

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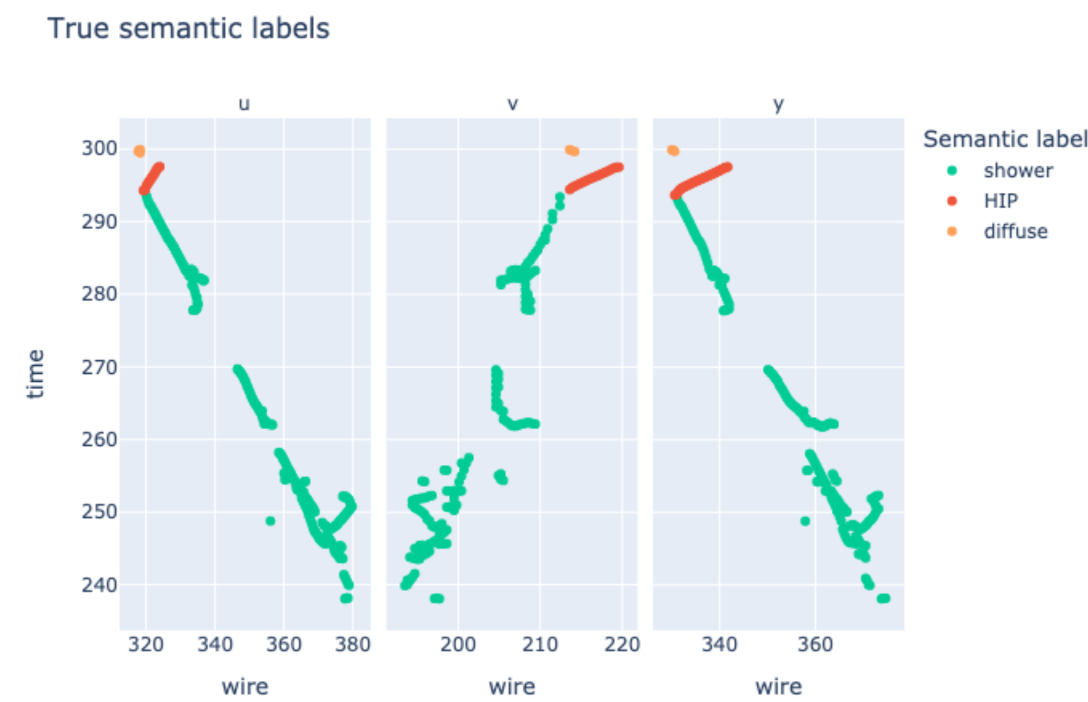

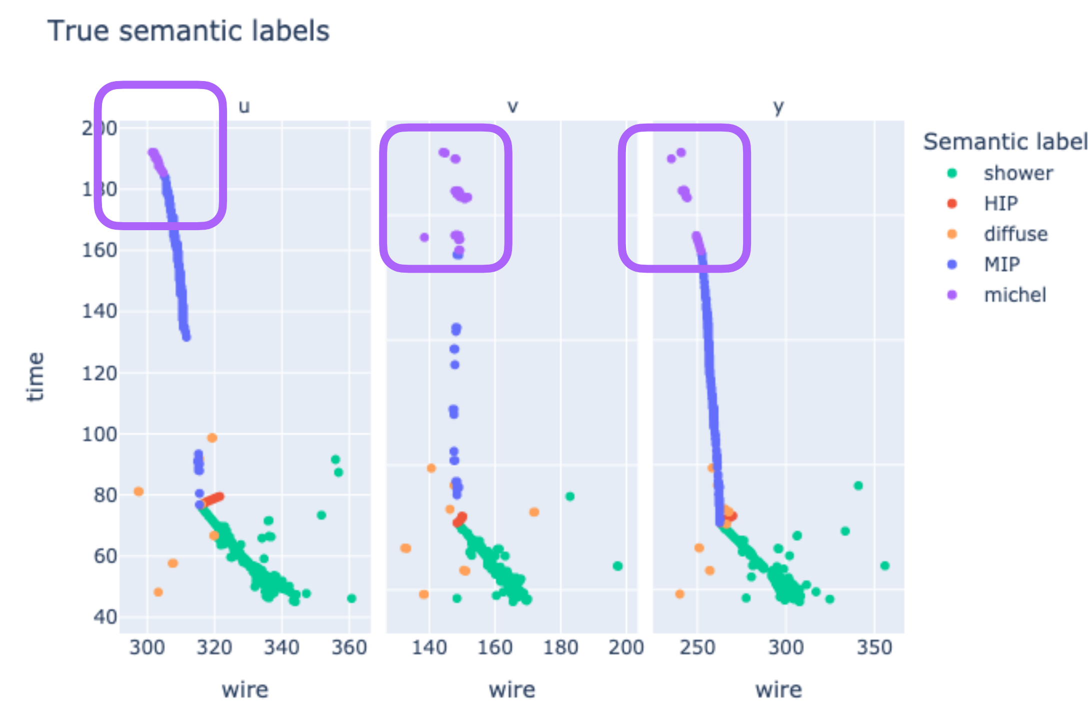

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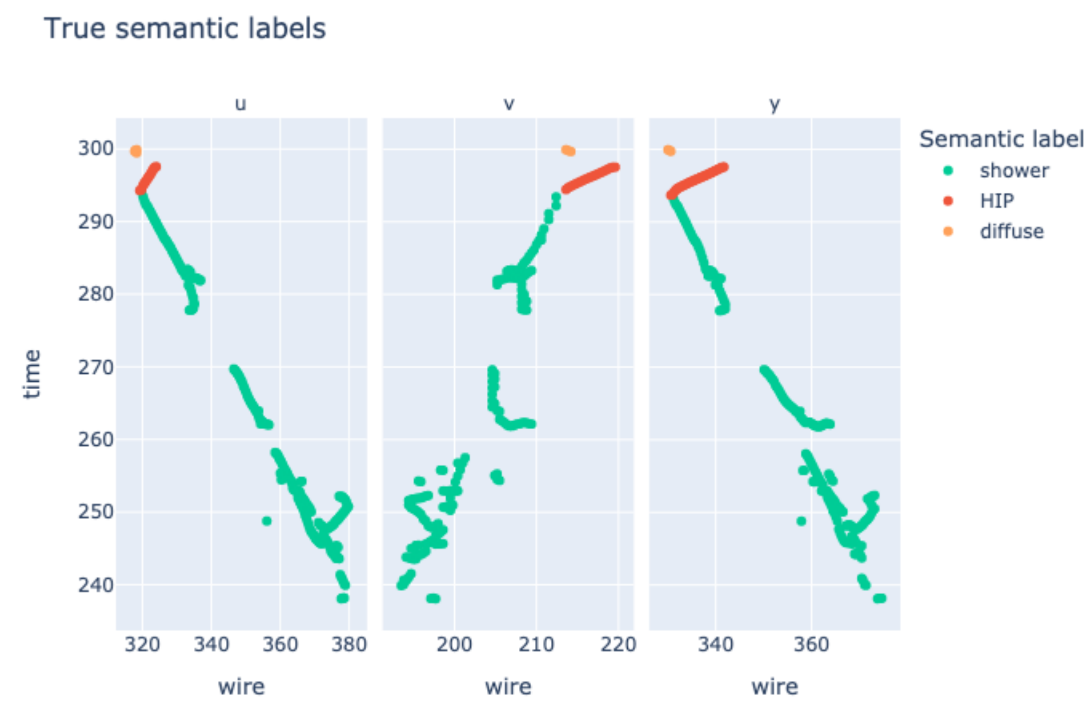

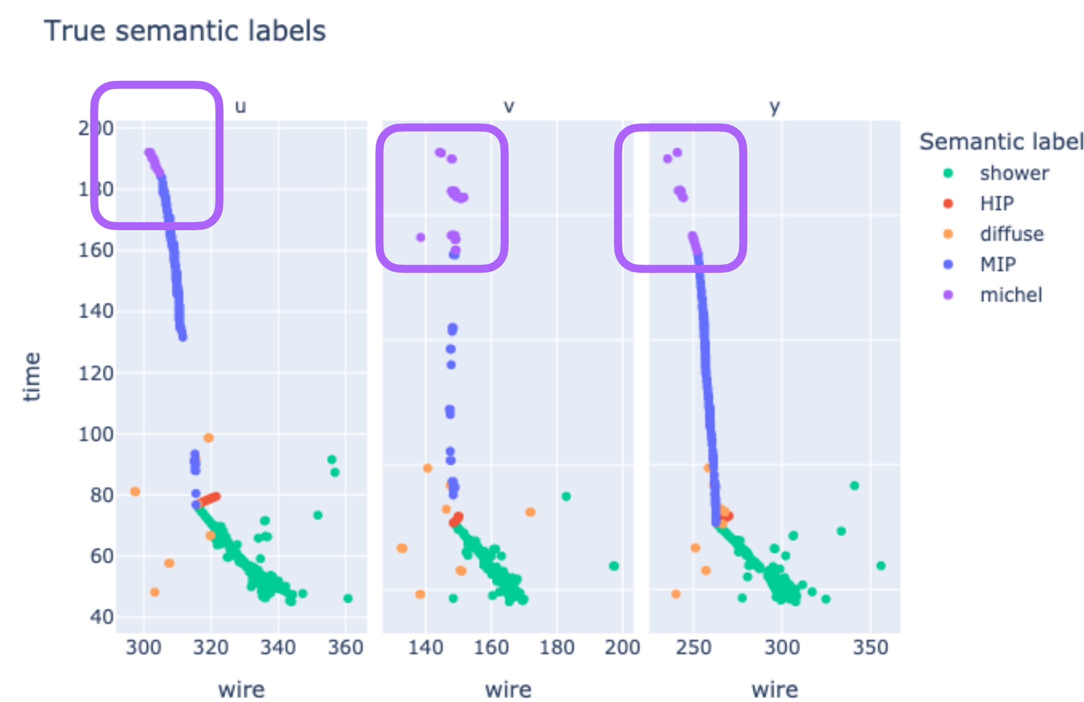

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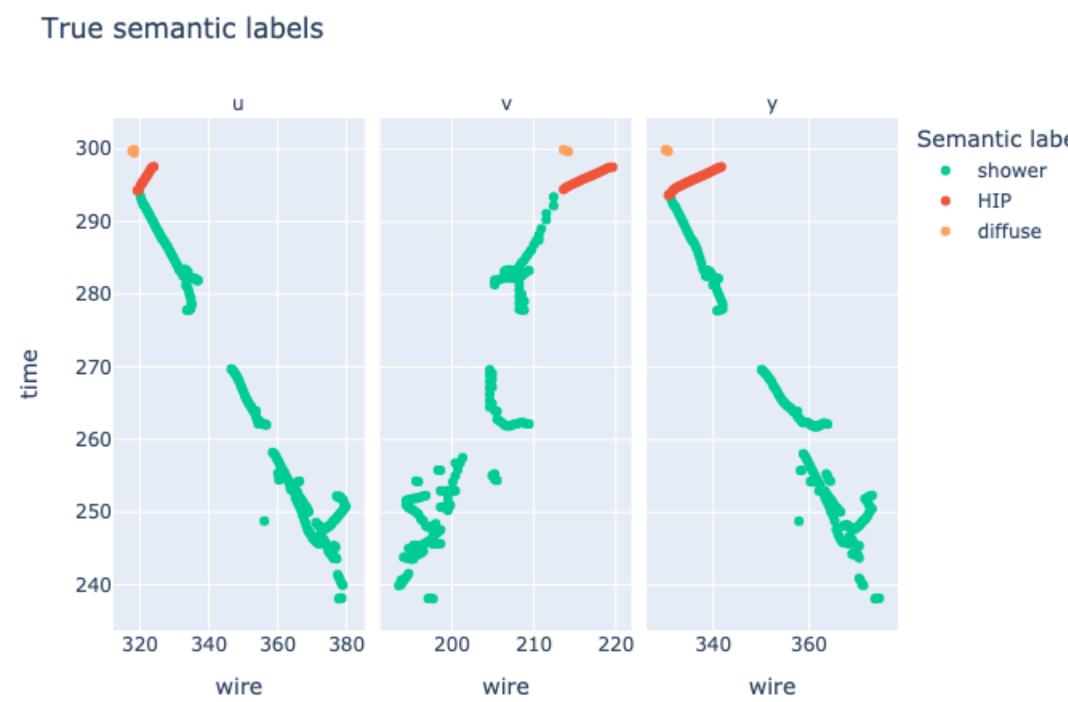

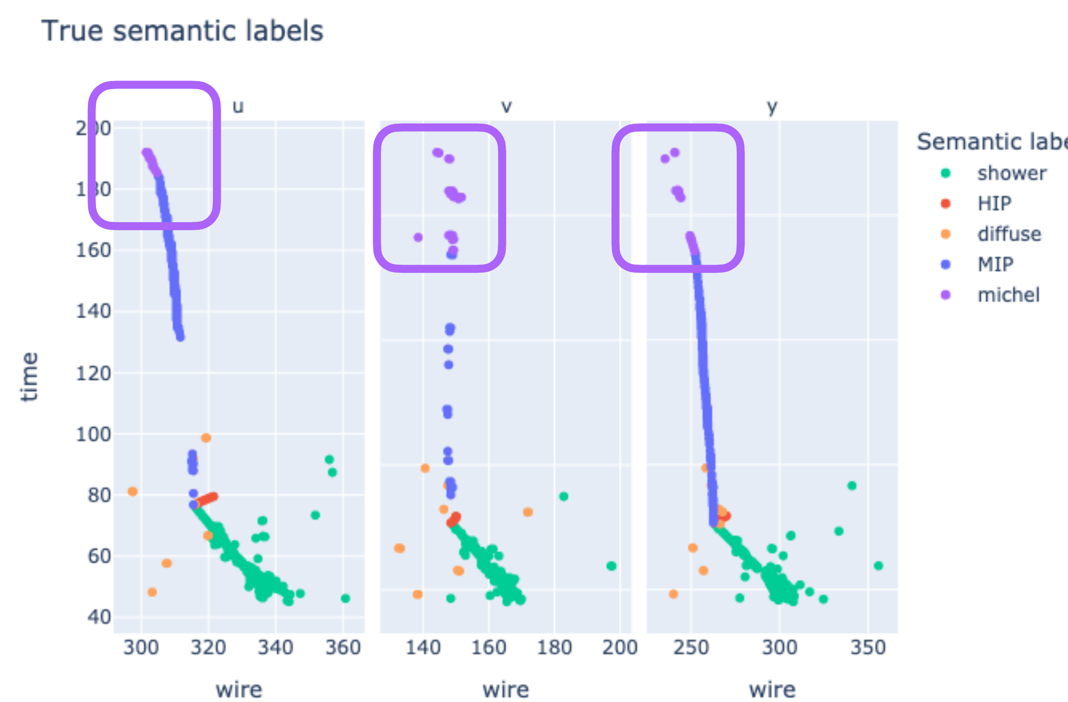

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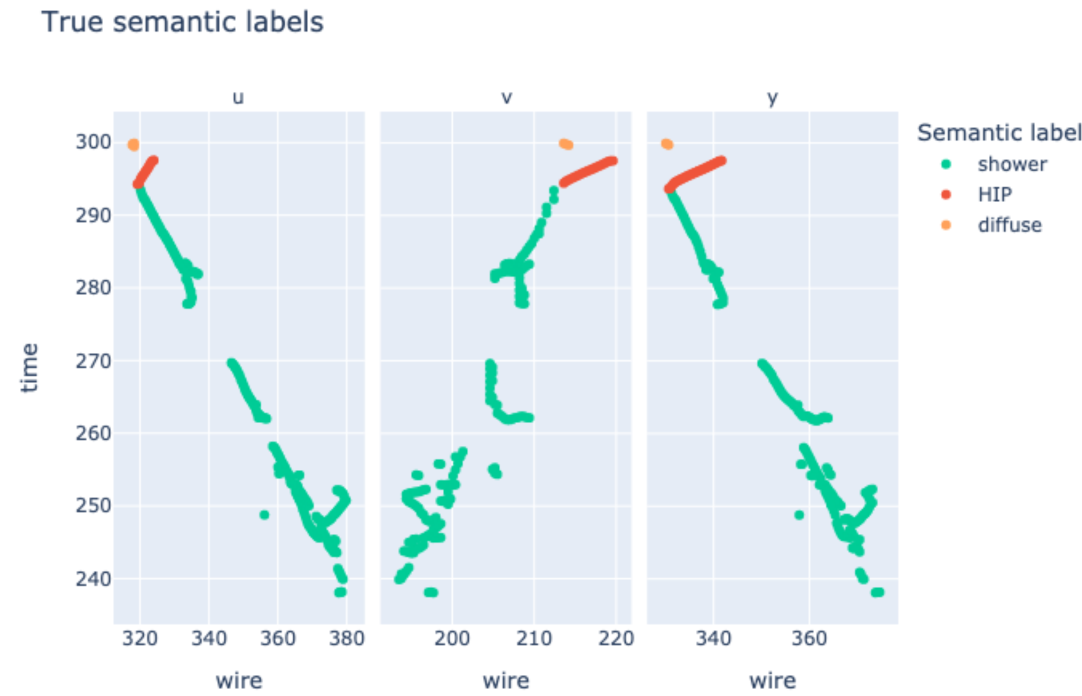
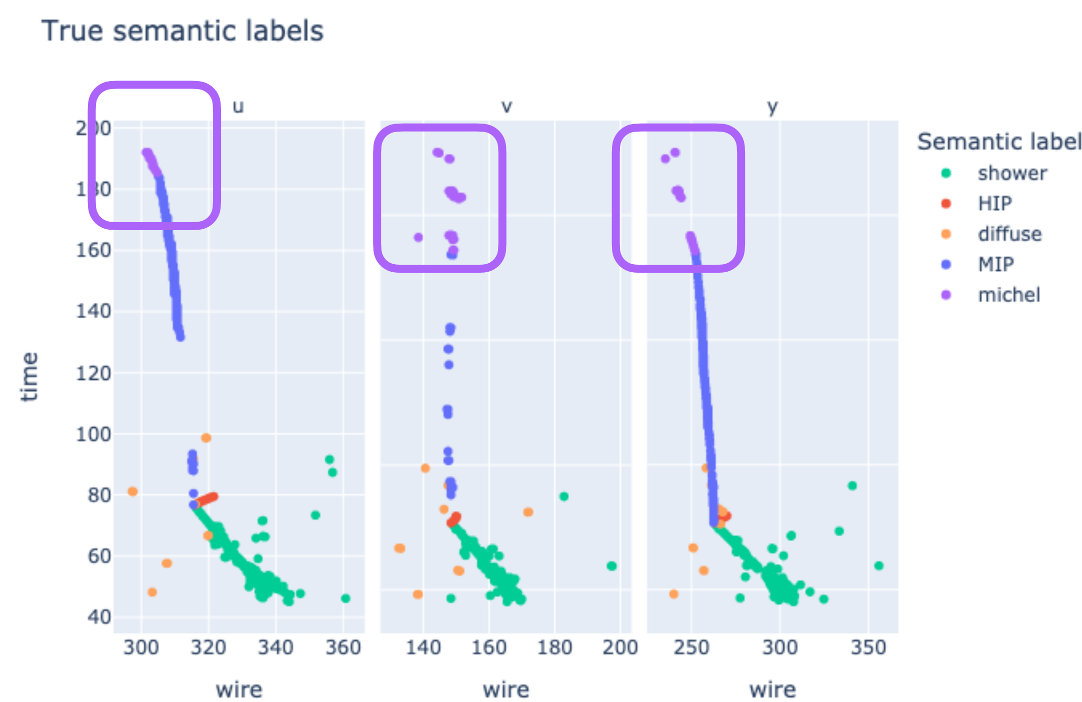
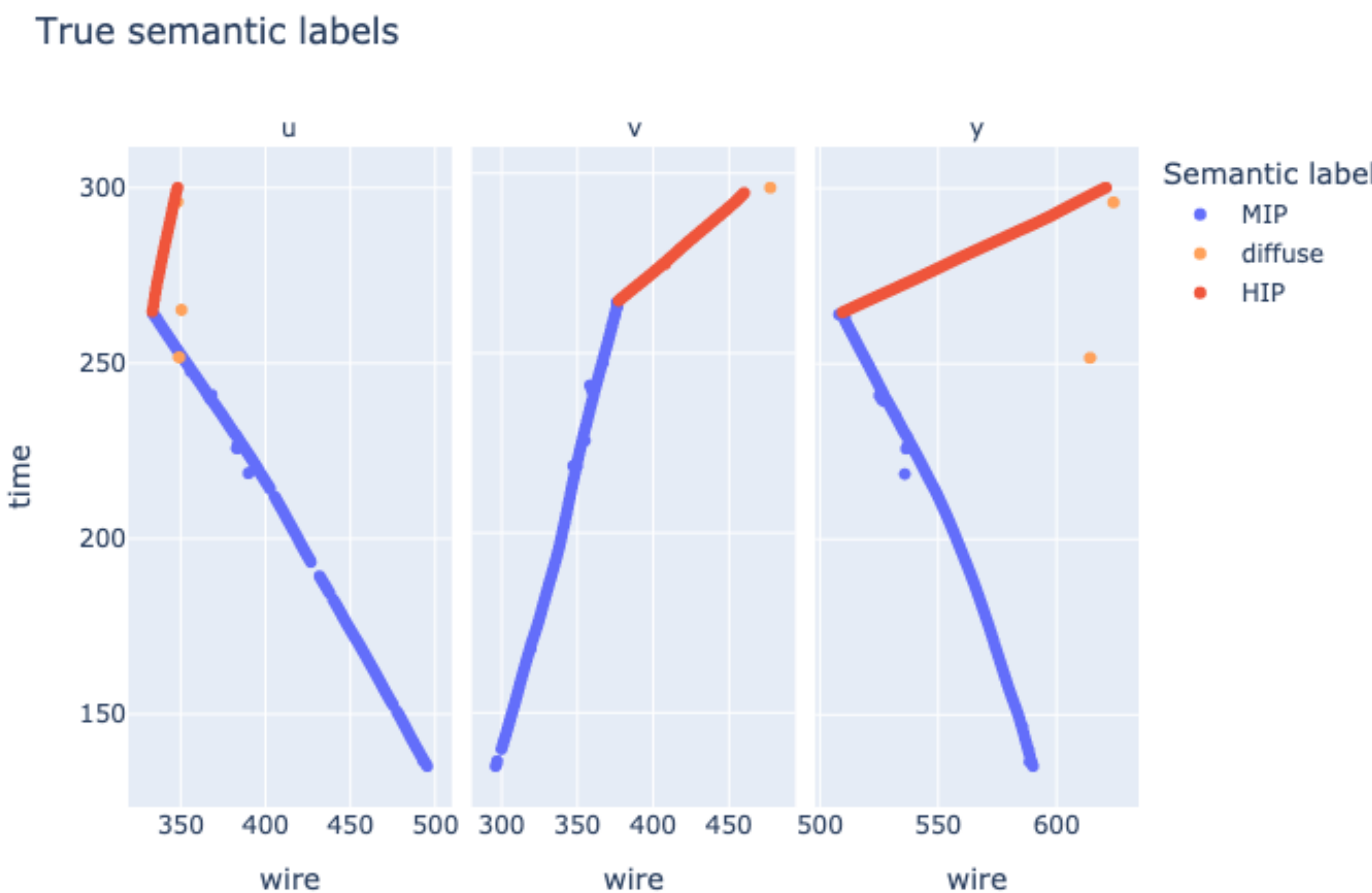
  - Combine instance and semantic segmentation for **full particle reconstruction**.





Example ν_μ interaction



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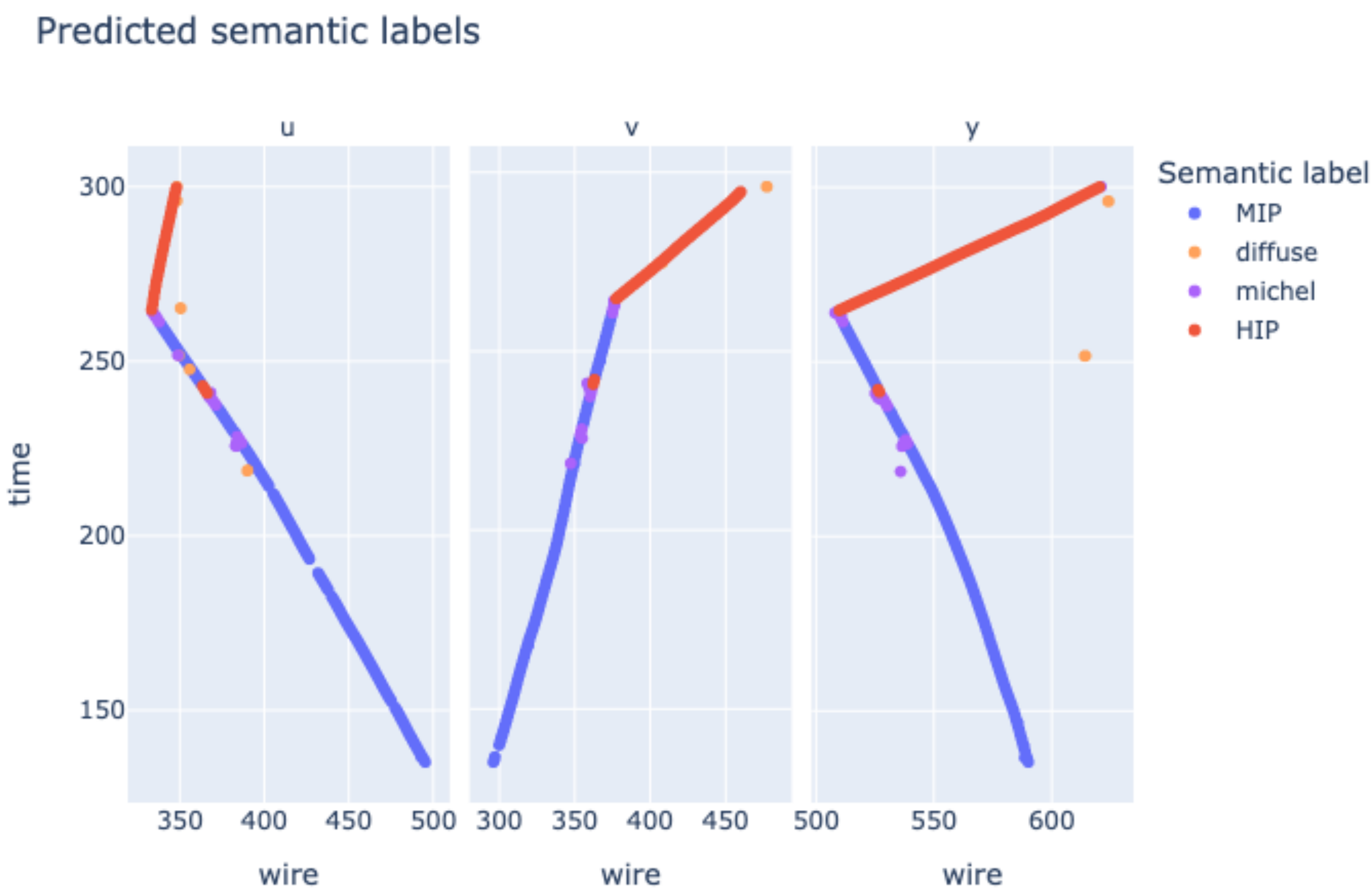

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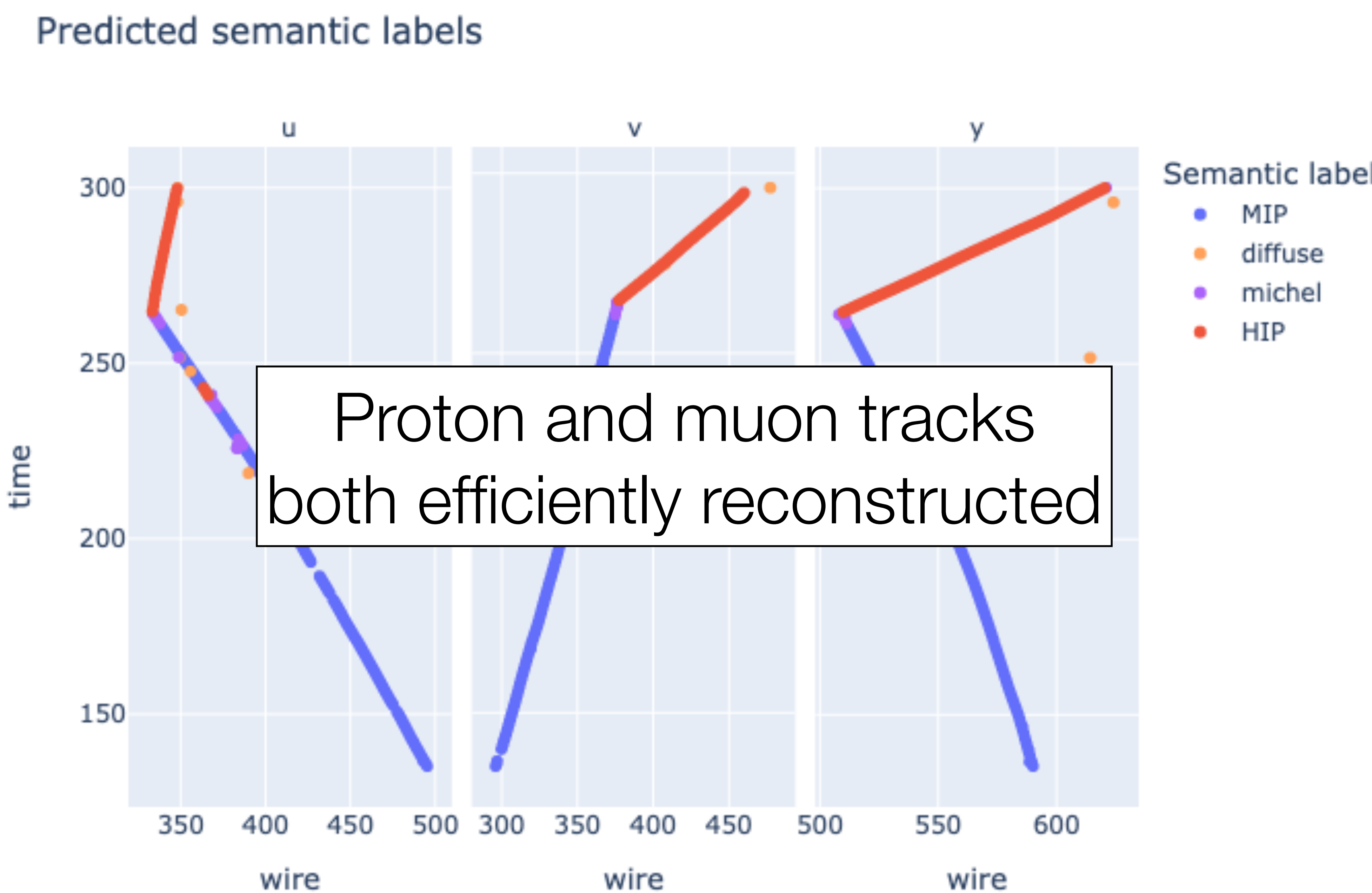
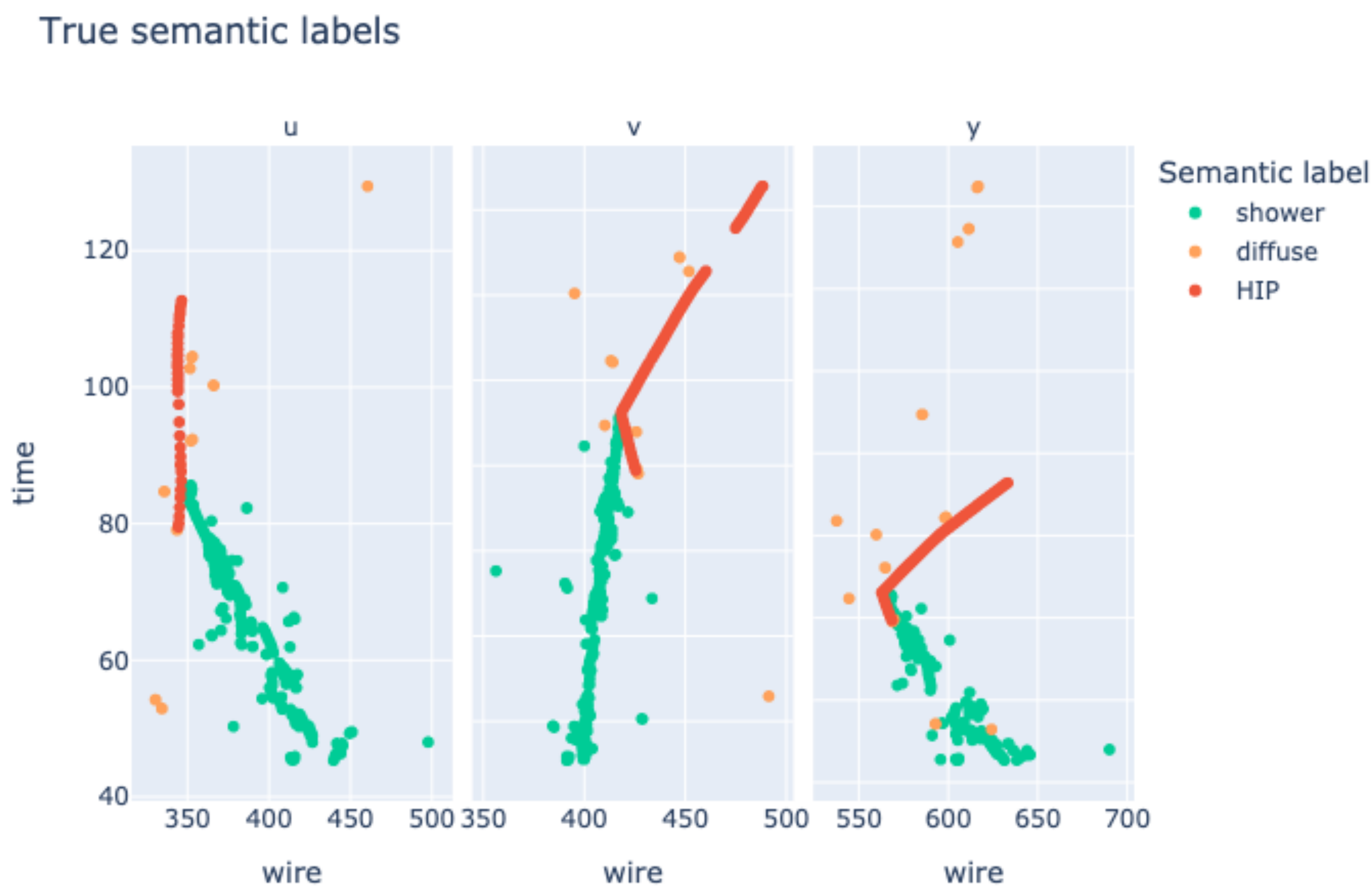


Example ν_e interaction



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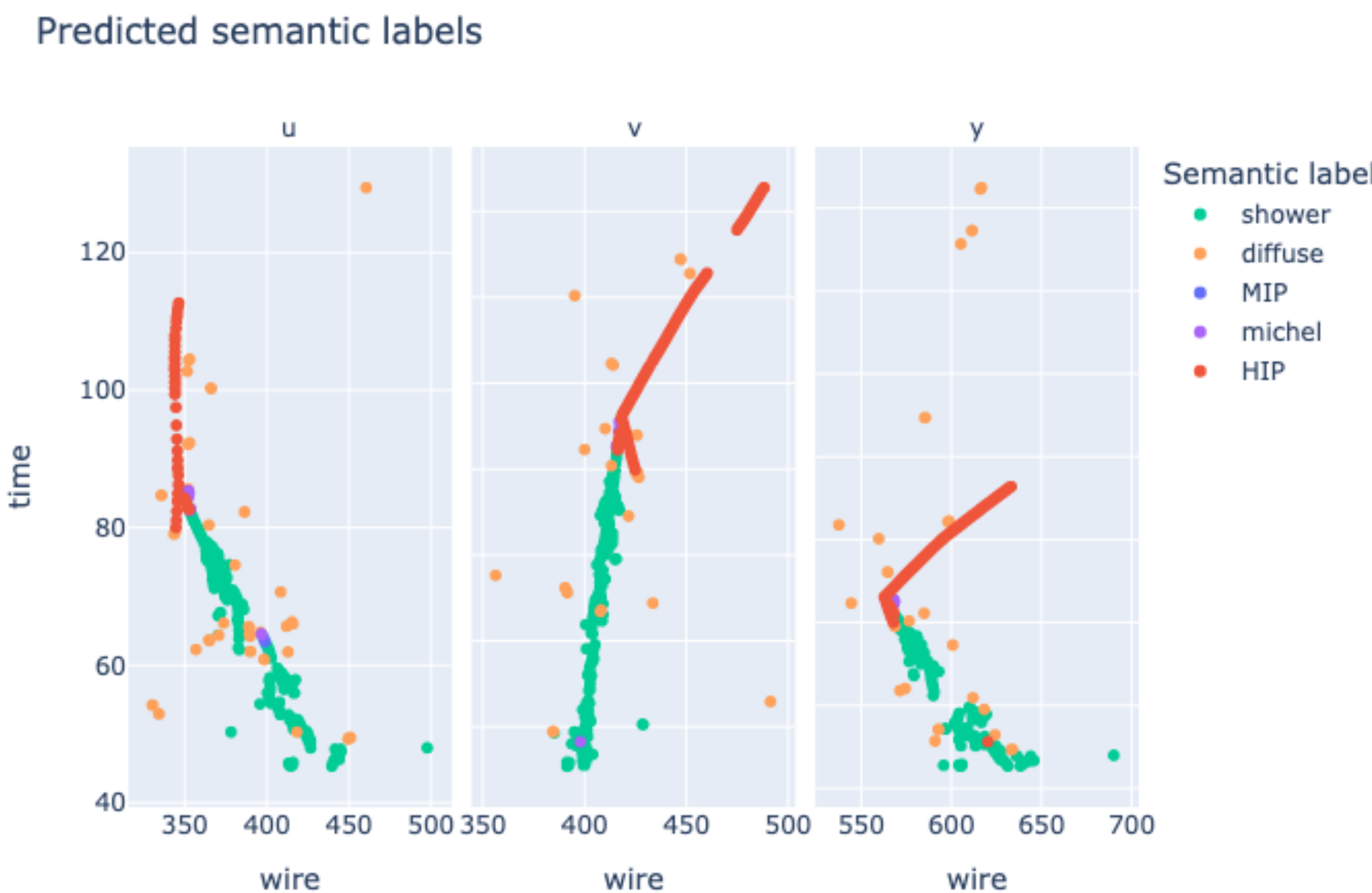

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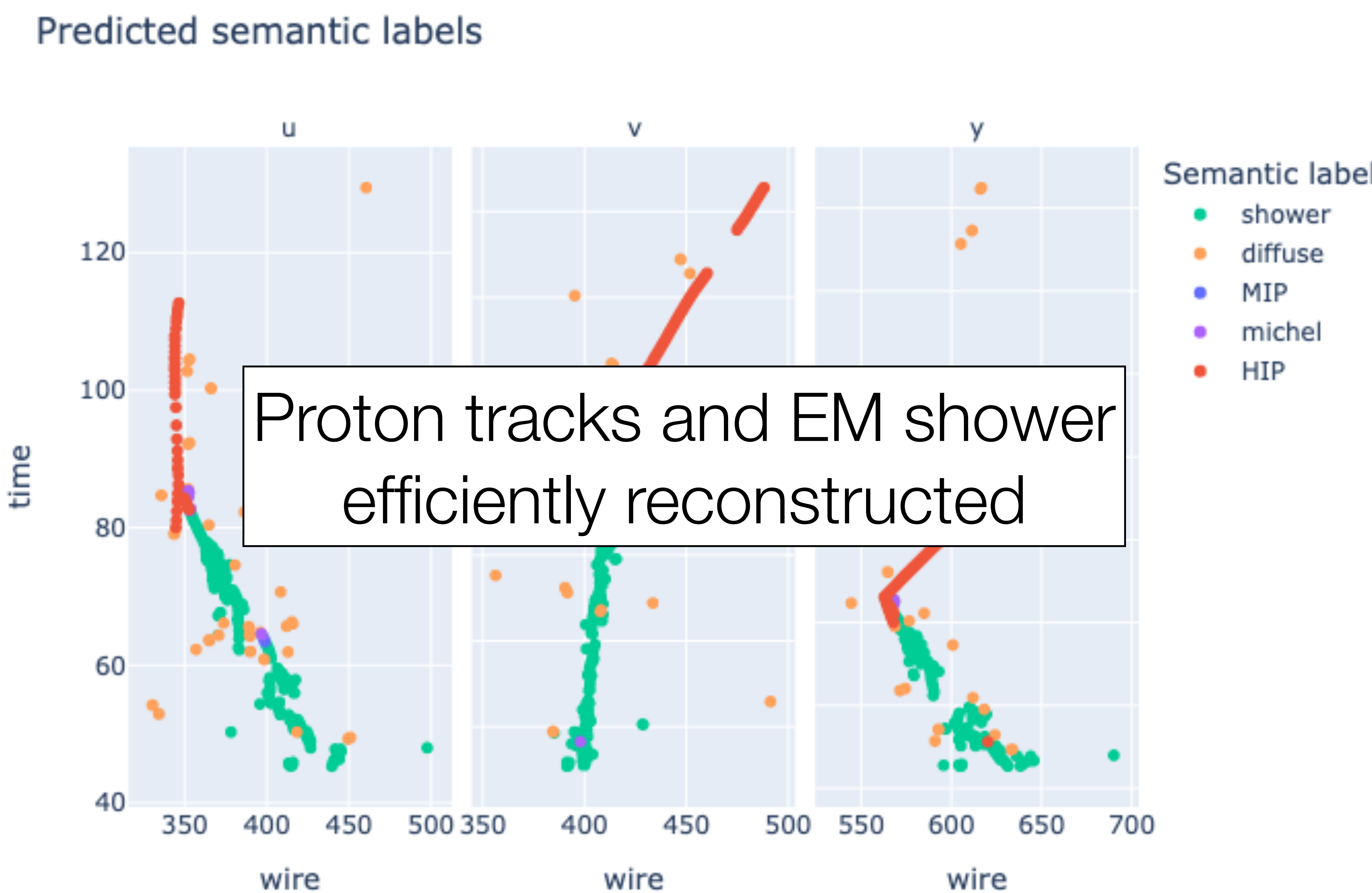
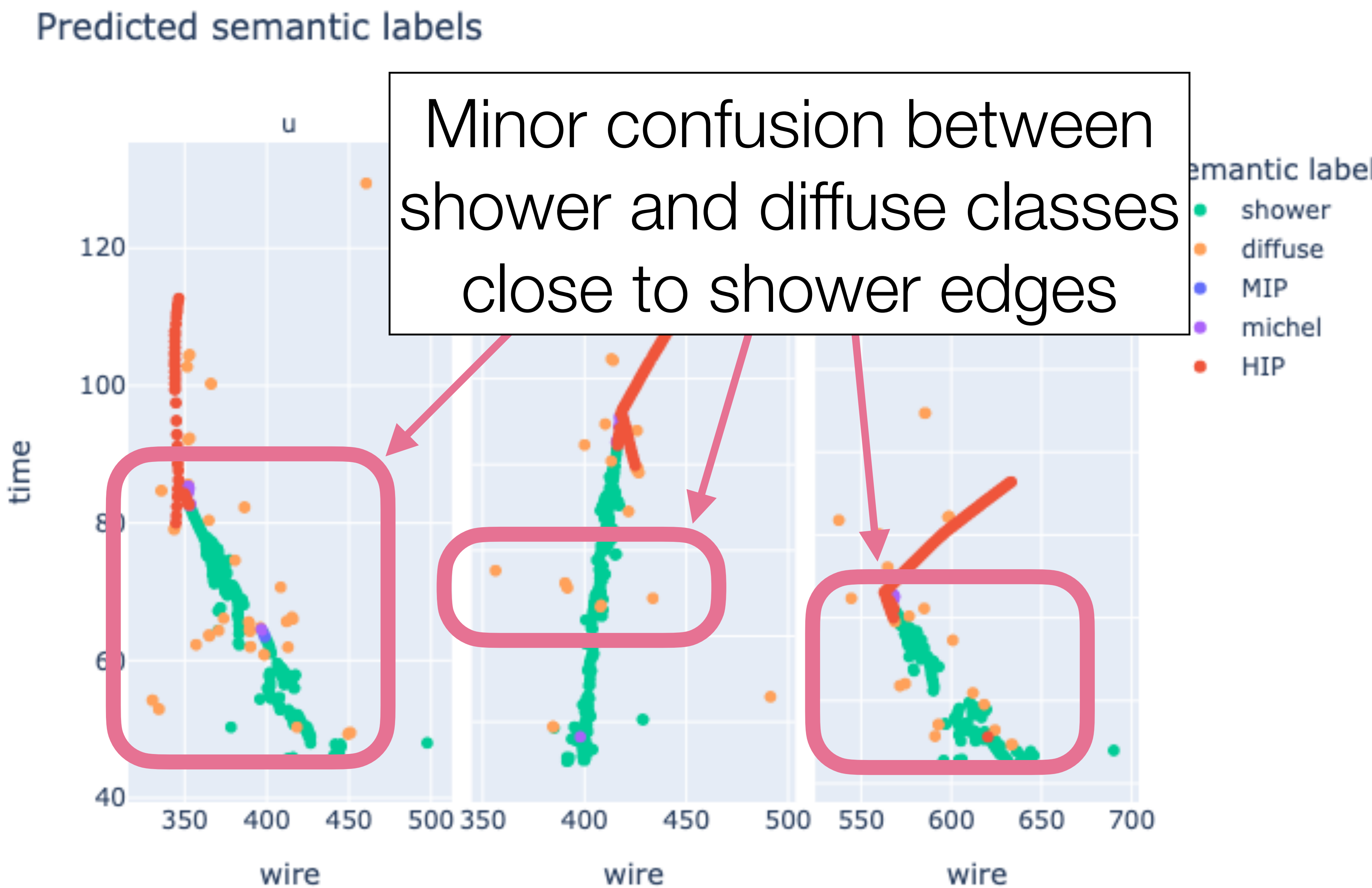


Proton tracks and EM shower efficiently reconstructed

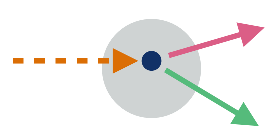
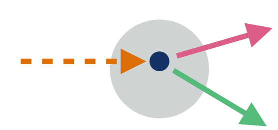
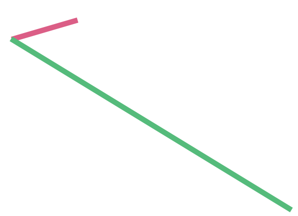
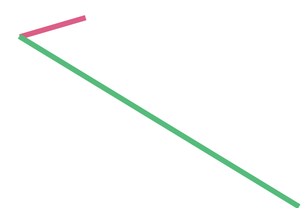
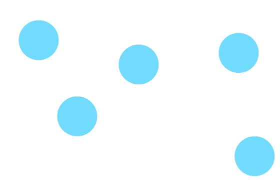
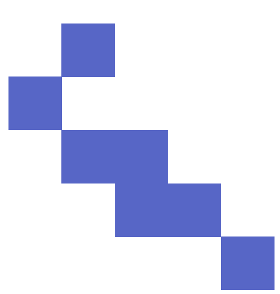
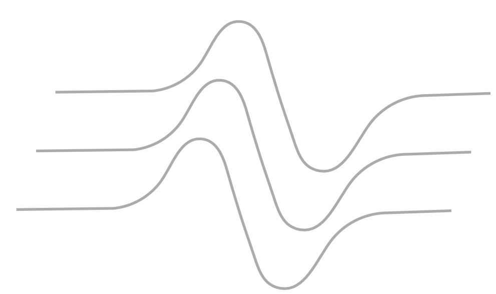
Example ν_e interaction



Minor confusion between shower and diffuse classes close to shower edges

Common abstraction for neutrino experiments

- Although the details of many neutrino physics experiments vary, the majority of them share a common paradigm at a high level.

NOvA		MicroBooNE		Shared structure
	Neutrino generator (GENIE)		Neutrino generator (GENIE)	**Event information**
	Particle simulation (Geant4)		Particle simulation (Geant4)	**True particles**
	True light depositions		True ionization electrons	**True energy deposits**
	Photoelectrons on APDs		Pulses on TPC wires	**Detector hits**

NuML & PyNuML

- The **NuML** package is a toolkit for writing **physics event records** to an **HDF5 file format**.
  - Hold low-level information such as **simulated particles**, **hits**, **true energy depositions** etc.
  - Generic data structure can be **shared across experiments**.
  - Common interface with **PandAna** analysis toolkit (see CHEP 2021 talk).
  - Available as LArSoft package on GitHub.

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- The **PyNuML** package is designed to provide a **generic**, **accessible**, **efficient** and **flexible** solution for many of the necessary tasks in leveraging ML for particle physics.
  - Define **particle ground truth labels** for Geant4-simulated particles.
  - **Arrange detector hits into ML objects**, ie. graphs, CNN pixel maps, etc.
  - Efficiently **preprocess ML inputs in parallel in HPC environments** using MPI.
  - Available as Python package on GitHub, or install with `pip install pynuml`!

Summary

- **NuGraph2** is a state-of-the-art graph neural network for semantically labelling detector hits in neutrino physics experiments.
  - Model developed and tested in MicroBooNE and DUNE, and designed to be utilised across many neutrino physics detectors.
  - Targeting full particle reconstruction for next generation architecture.

- Standardised process of producing ML inputs from HEP data for general use with **NeutrinoML** toolkit.
  - Toolkit utilised for MicroBooNE's public data release.
  - Open-source, easy-to-install code packages.