Title: Geometric Machine Learning for cosmological galaxy models

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Collection/Series: Cosmology and Gravitation

Subject: Cosmology

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Abstract:

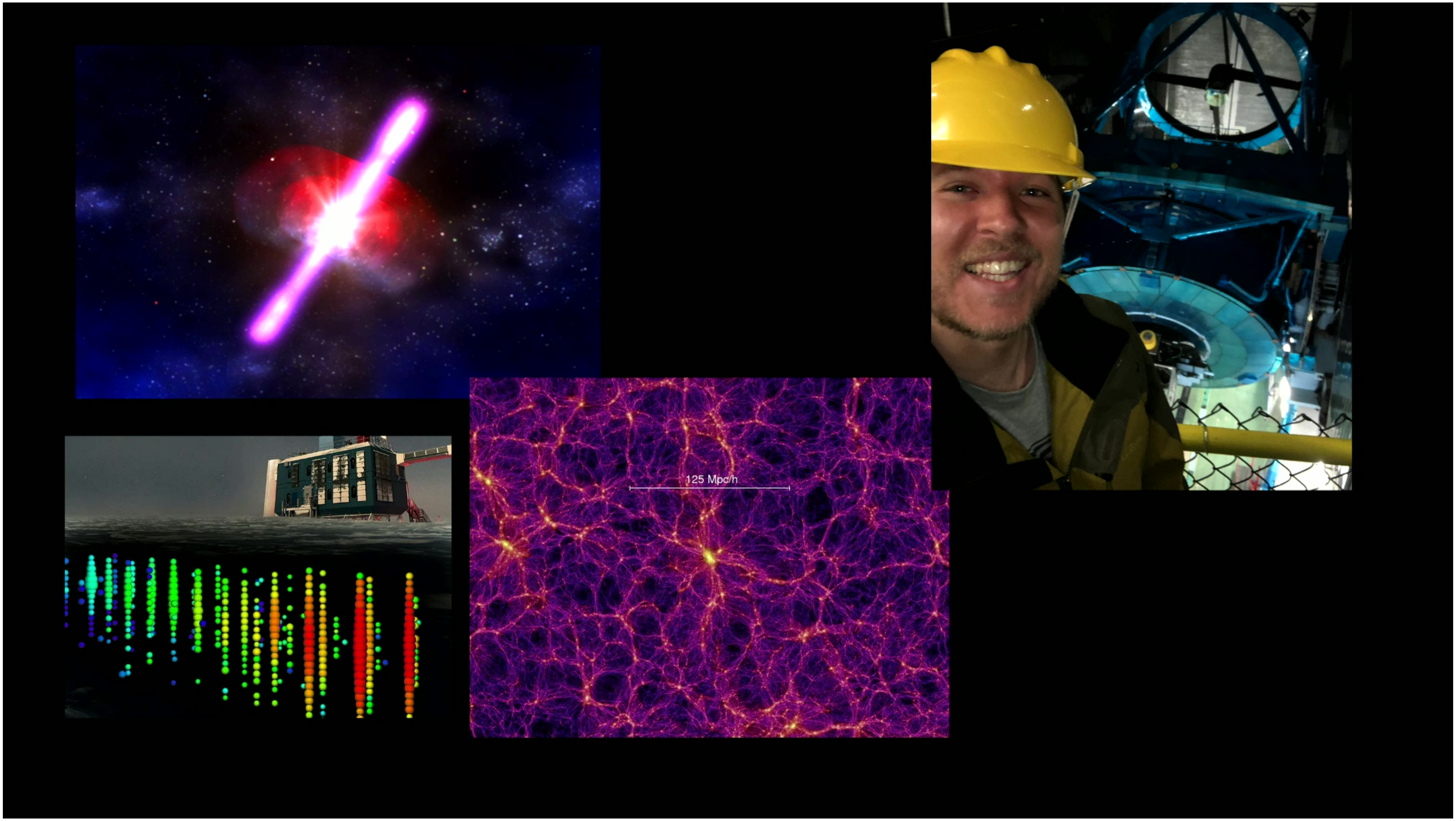
Galaxies are the medium through which we study the structure of the universe. However, widely applied statistical models of galaxies are generally over-simplified: even recently proposed models cannot capture the dependencies on environment or formation history. To solve this problem, I will introduce Graph Neural Networks (GNNs), a general and ideal tool for physical modelling. Geometrically constrained GNNs vastly improve our models, and allow us to ask detailed questions about the importance of formation history and environment for cosmological galaxy modeling. I will also prove a surprising equivalence between these two aspects of galaxy formation.

Geometric Machine Learning for cosmological galaxy models

Christian Kragh Jespersen

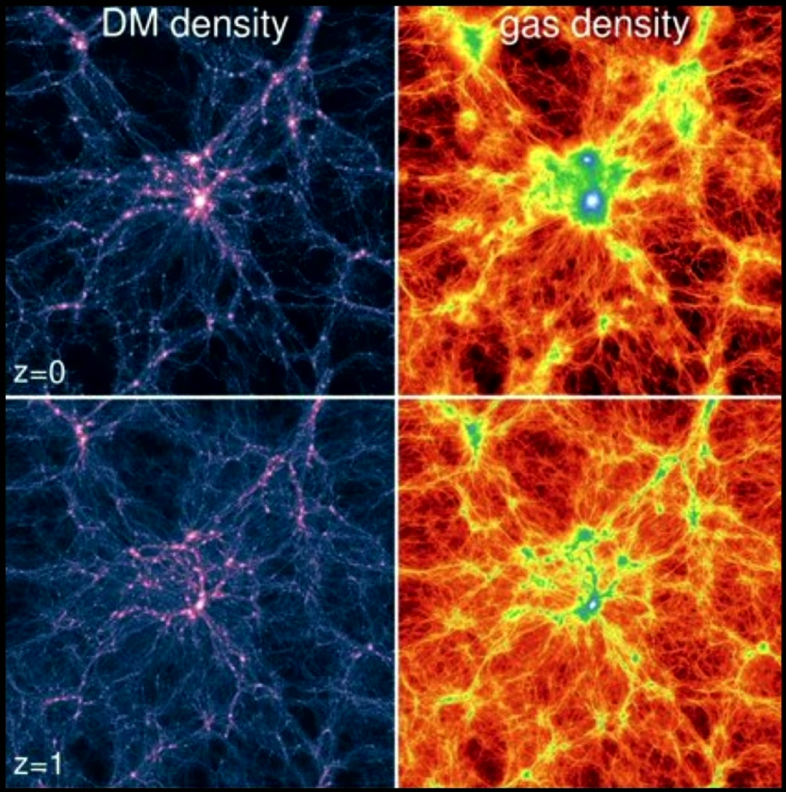
Perimeter Institute, 05/11/2024

with John F. Wu, Chen-Yu Chuang, **Peter Melchior, David N. Spergel,** Miles Cranmer, Shirley Ho, Rachel Somerville, Risa Wechsler, Shy Genel, and Yen-Ting Lin


125 Mpc/h




$$\text{Galaxy} = f(\boxed{\ldots})$$



$$\xi_{gg} \propto \xi_{mm}$$

Galaxy ~ f(Halo)

ML for galaxy-halo connection is common

MNRAS **000**, 000–000 (0000) Preprint 3 May 2018 Compiled using MNRAS LaTeX style file v3.0

Painting galaxies into dark matter halos using machine learning

MNRAS **000**, 1–18 (2015) Preprint 20 August 2018 Compiled using MNRAS LaTeX style file v3.0

Machine Learning and Cosmological Simulations I: Semi-Analytical Models

MNRAS **000**, 1–15 (2021) Preprint 19 January 2022 Compiled using MNRAS LaTeX style file v3.0

Mimicking the halo–galaxy connection using machine learning

MNRAS **000**, 1–16 (2021) Preprint 4 November 2021 Compiled using MNRAS LaTeX style file v3.0

A machine learning approach to mapping baryons onto dark matter haloes using the EAGLE and C-EAGLE simulations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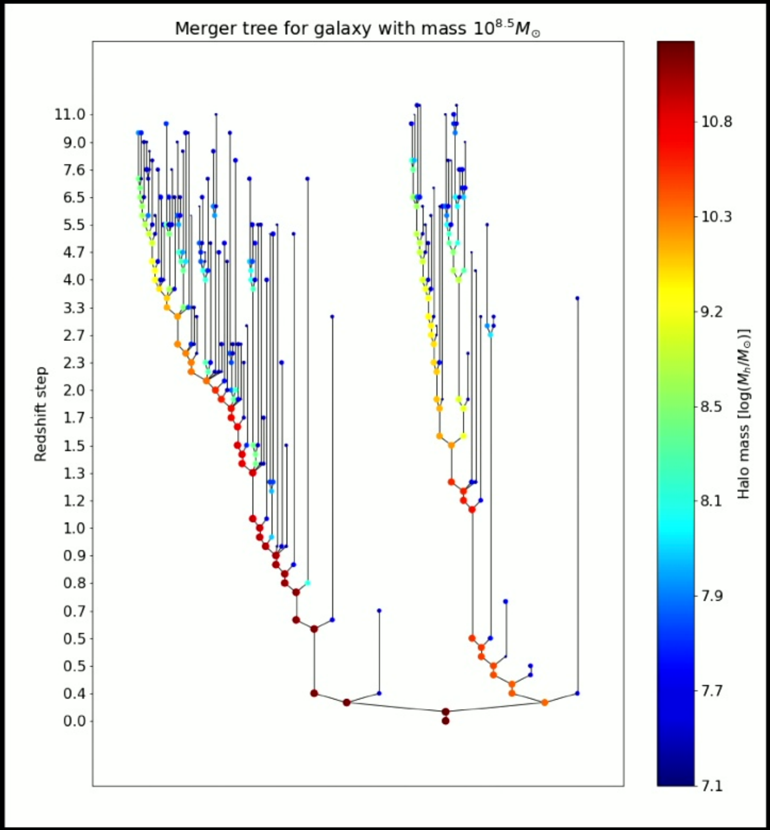
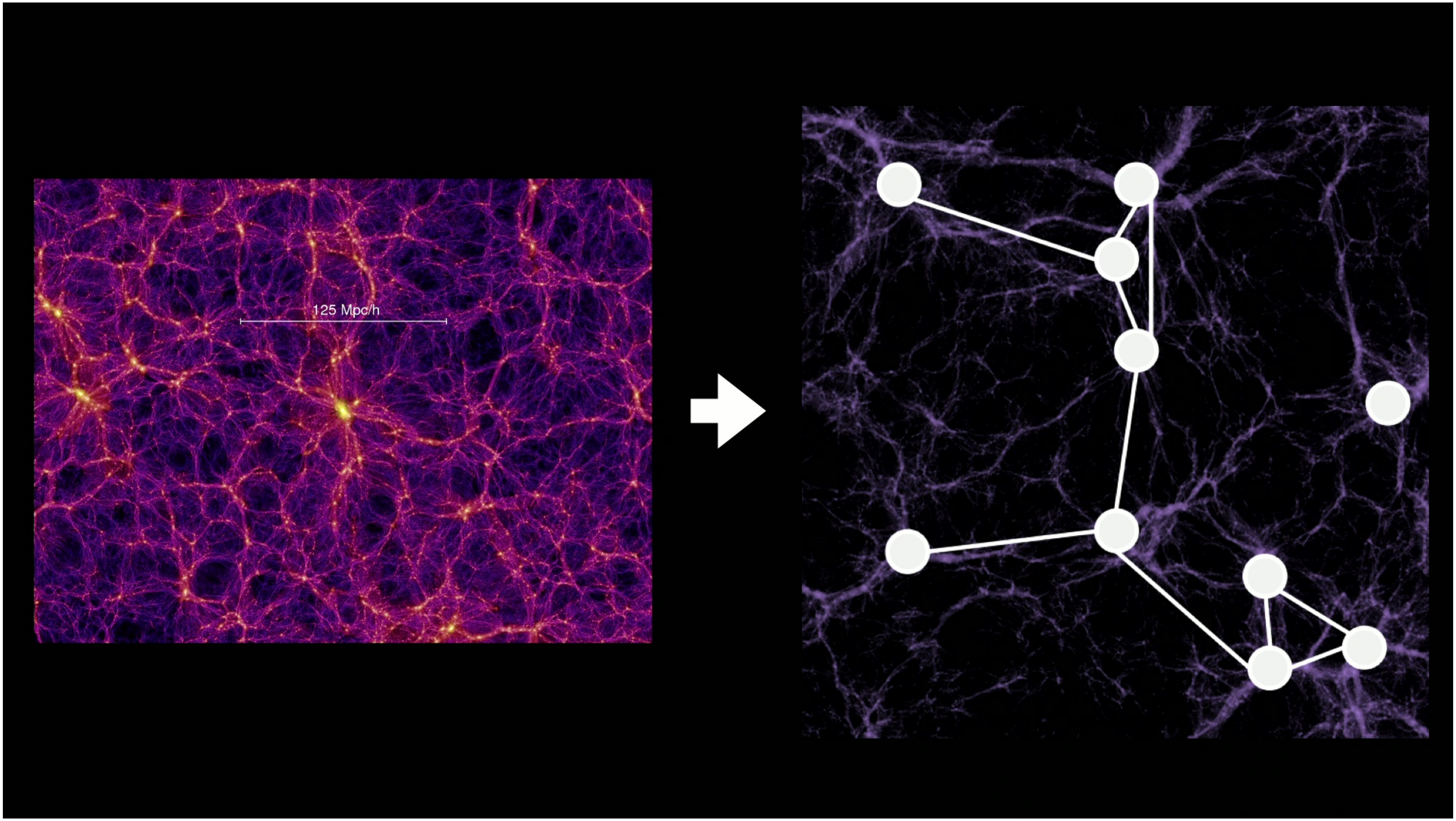
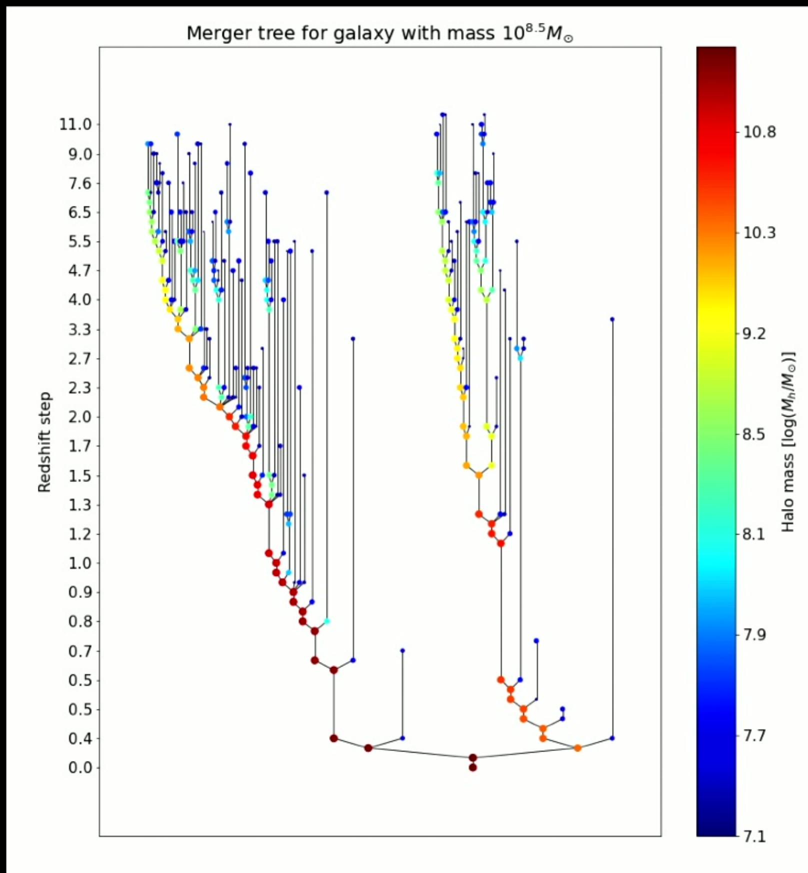

Merger tree for galaxy with mass $10^{8.5} M_\odot$
Redshift step
11.0
9.0
7.6
6.5
5.5
4.7
4.0
3.3
2.7
2.3
2.0
1.7
1.5
1.3
1.2
1.0
0.9
0.8
0.7
0.5
0.5
0.4
0.0
Halo mass [$\log(M_h/M_\odot)$]
10.8
10.3
9.2
8.5
8.1
7.9
7.7
7.1



125 Mpc/h


Merger tree for galaxy with mass $10^{8.5} M_\odot$
Redshift step
11.0
9.0
7.6
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4.7
4.0
3.3
2.7
2.3
2.0
1.7
1.5
1.3
1.2
1.0
0.9
0.8
0.7
0.5
0.5
0.4
0.0
Halo mass [$\log(M_h/M_\odot)$]
10.8
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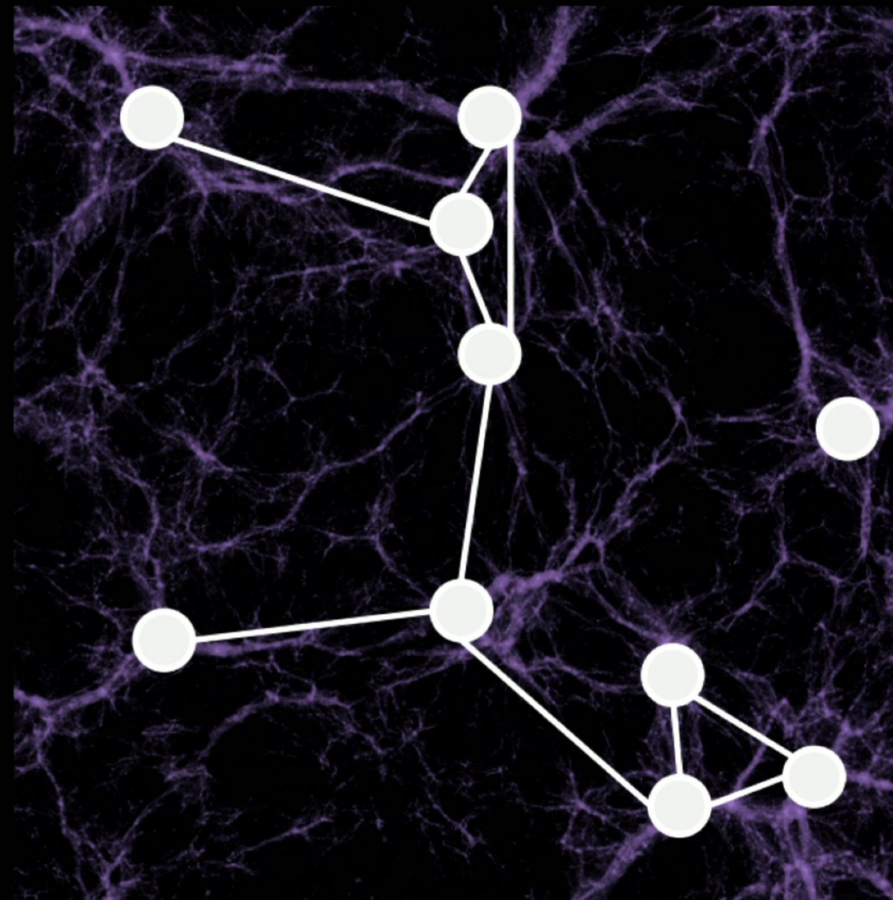
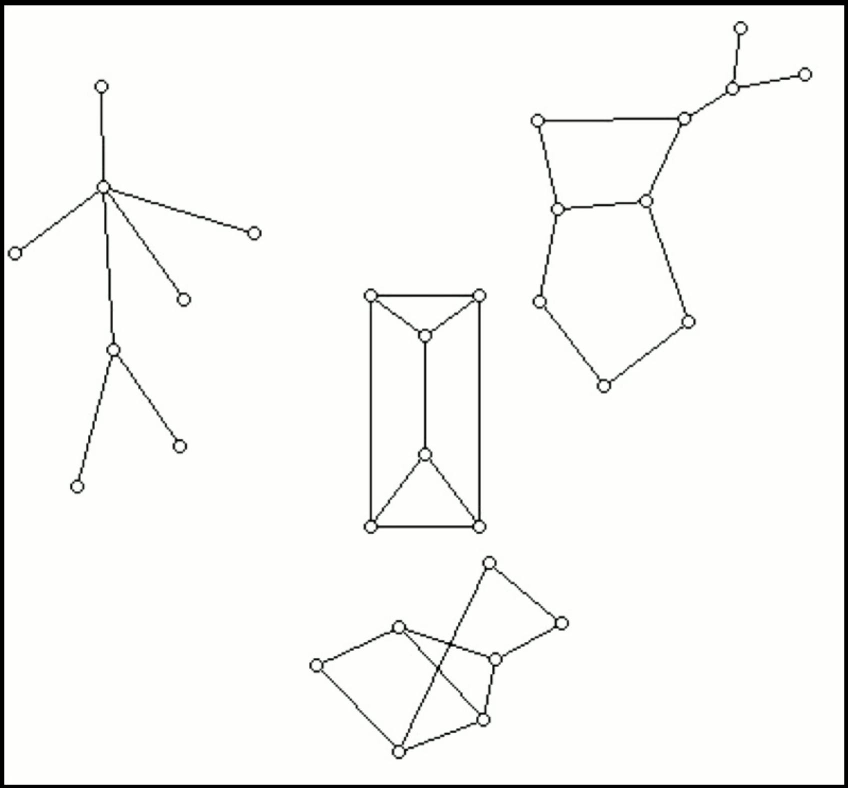
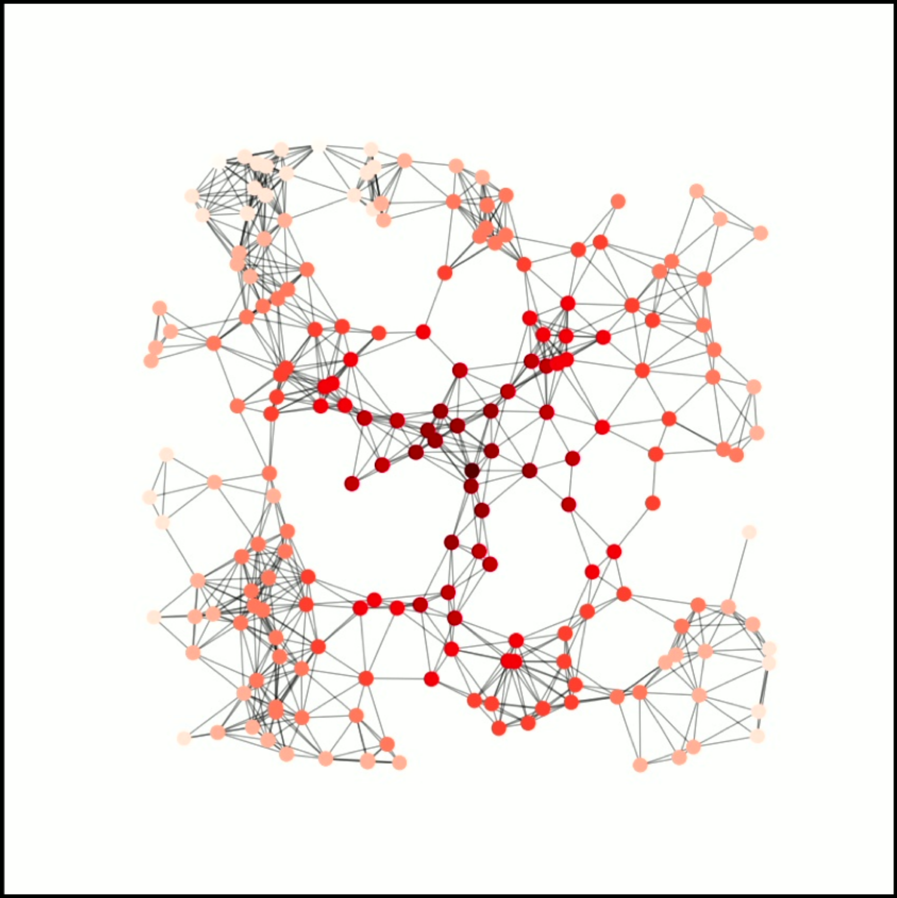
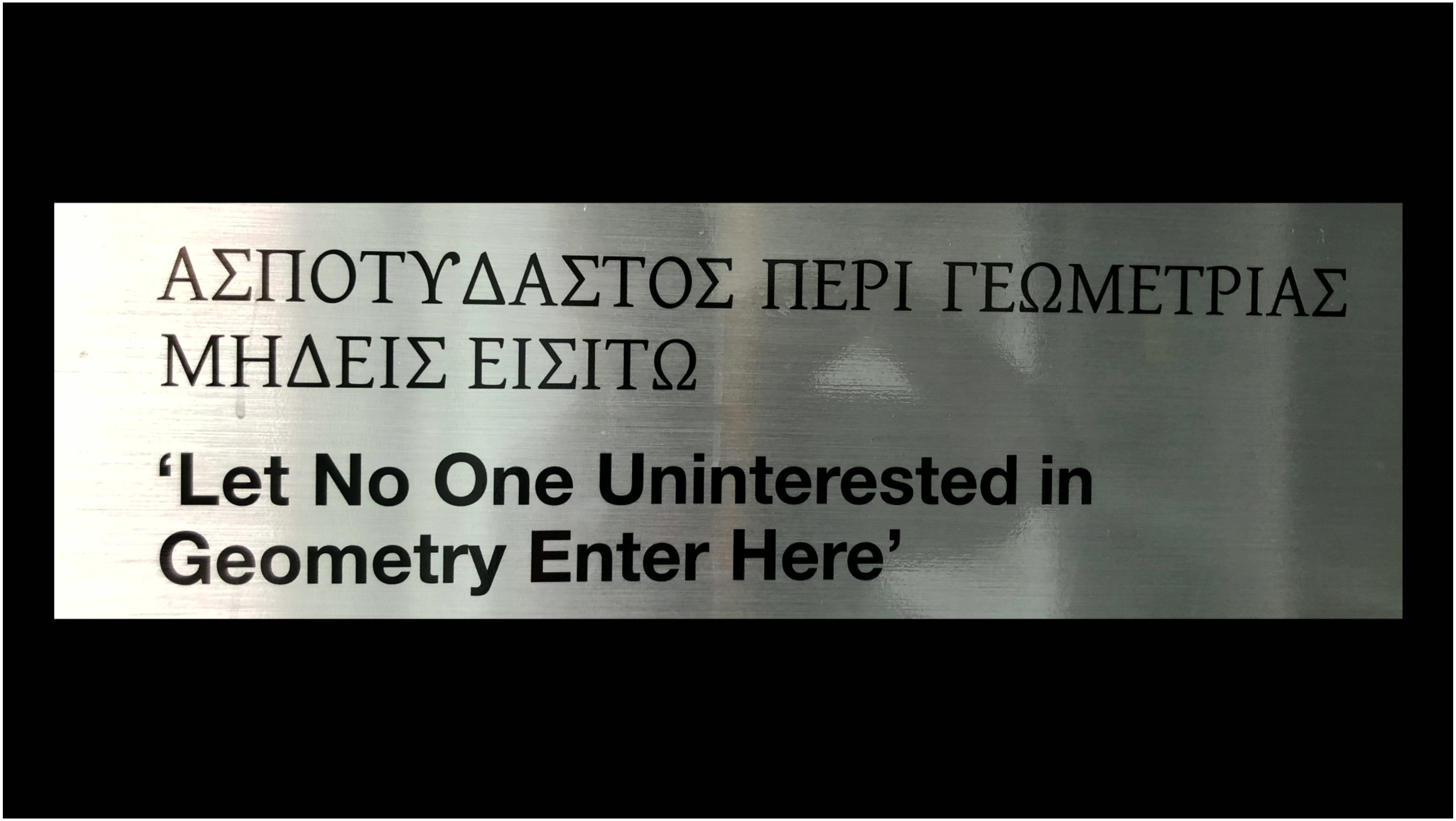
8.1
7.9
7.7
7.1



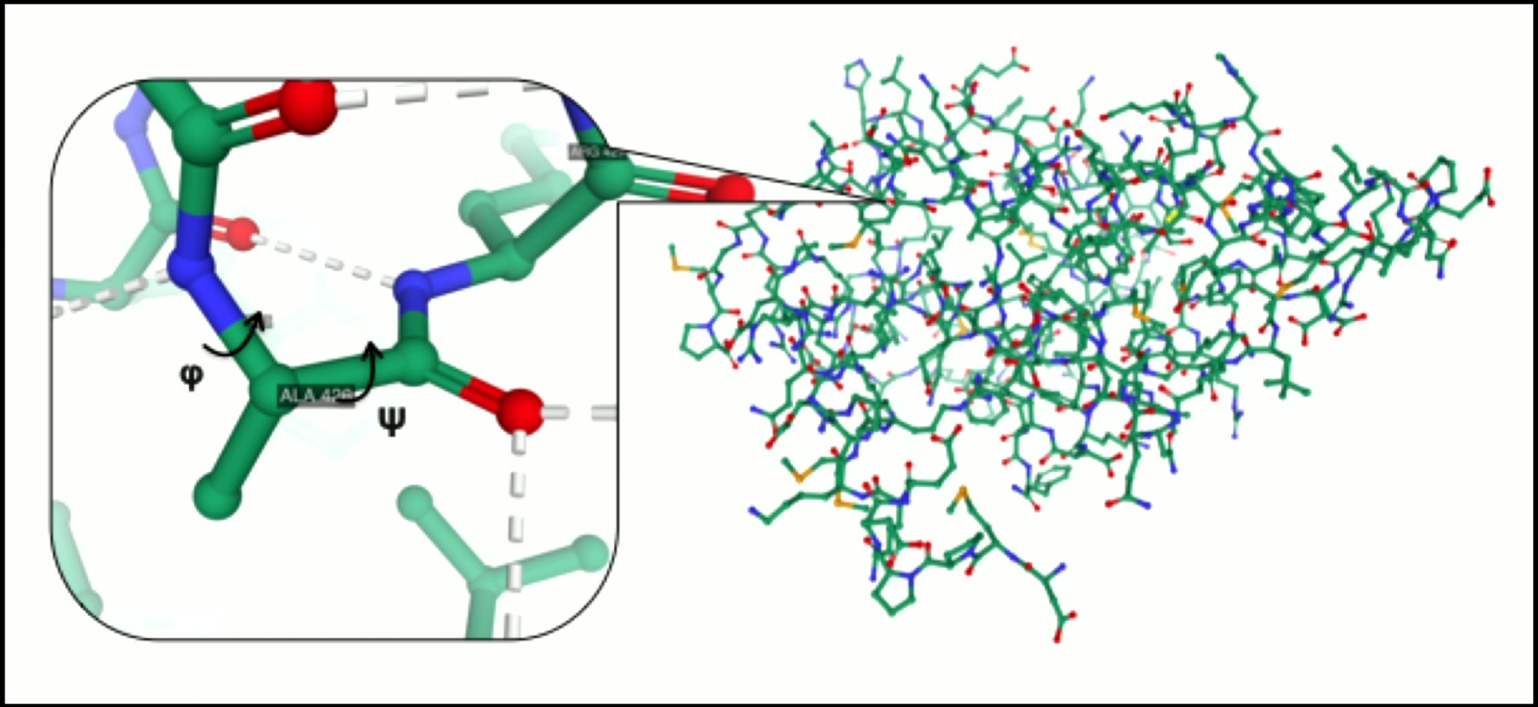




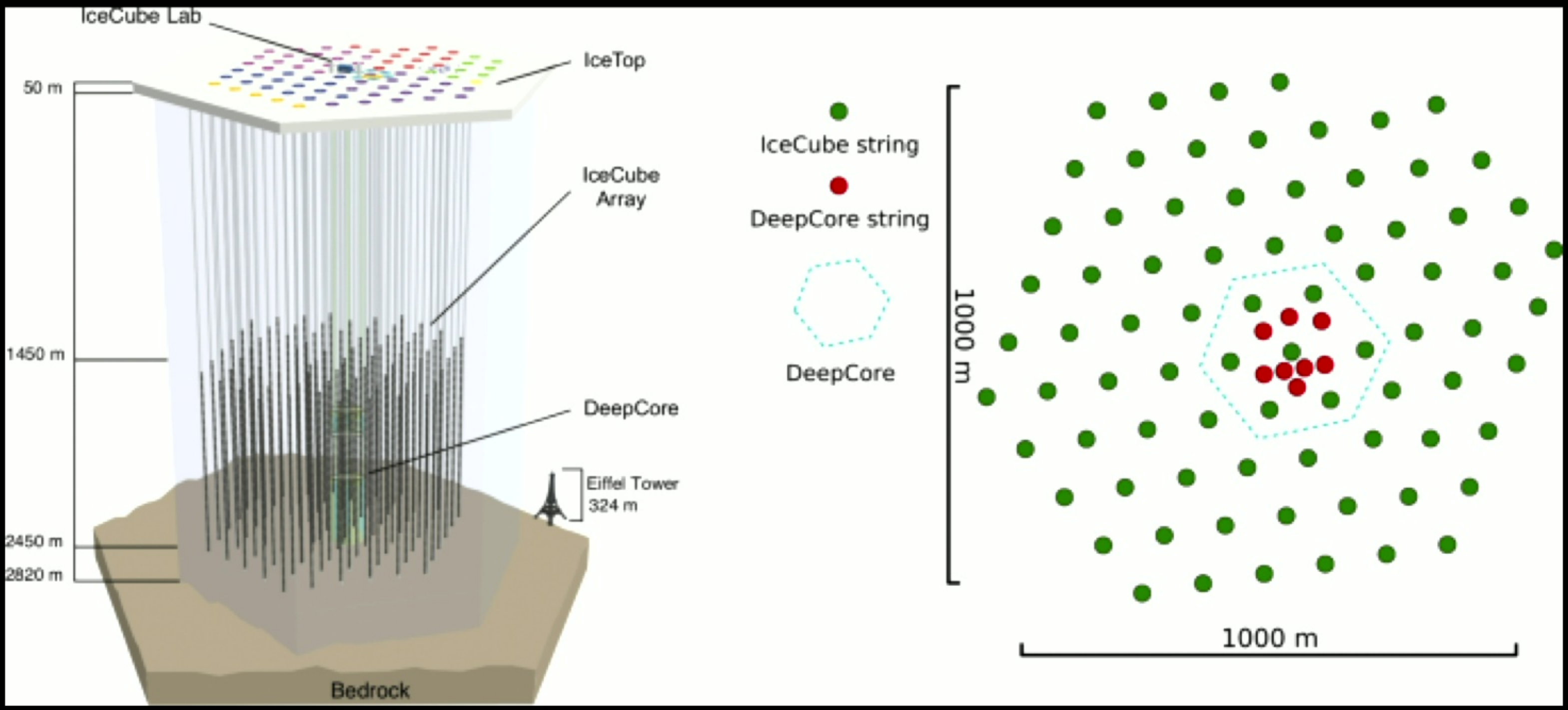
In modern physics … a central theme will be a Geometric Principle: The laws of physics must all be expressible as geometric (coordinate-independent and referenceframe-independent) relationships between geometric objects (scalars, vectors, tensors, ...) that represent physical entities.


ΑΣΠΟΤΥΔΑΣΤΟΣ ΠΕΡΙ ΓΕΩΜΕΤΡΙΑΣ
ΜΗΔΕΙΣ ΕΙΣΙΤΩ
‘Let No One Uninterested in
Geometry Enter Here’

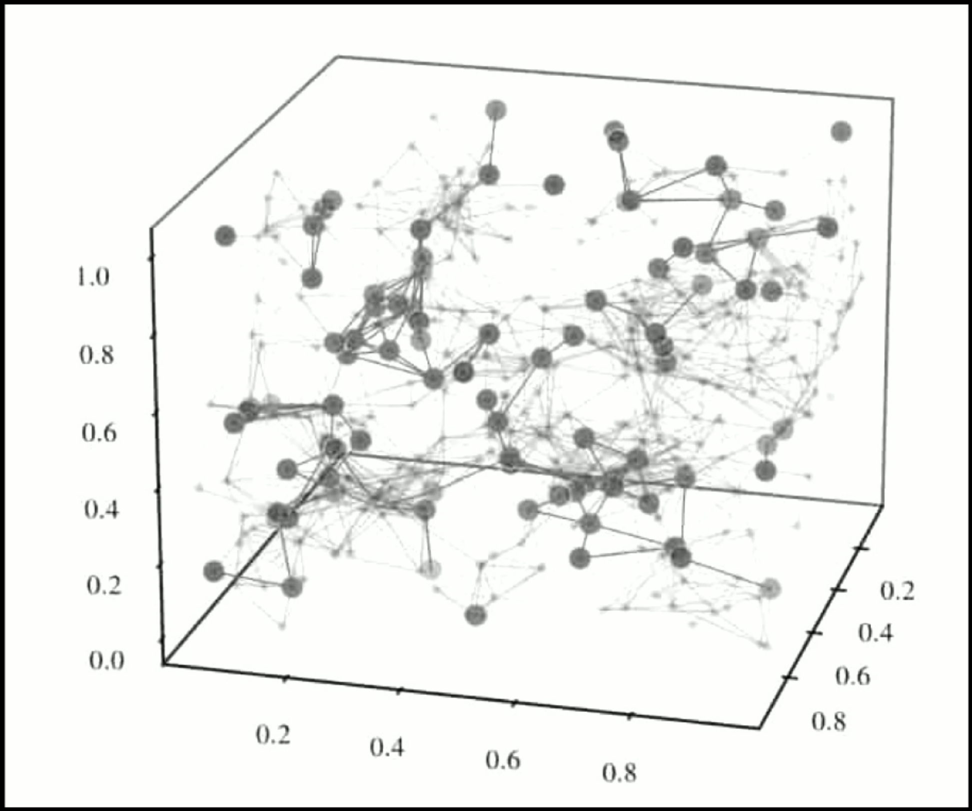
Molecules are Graphs



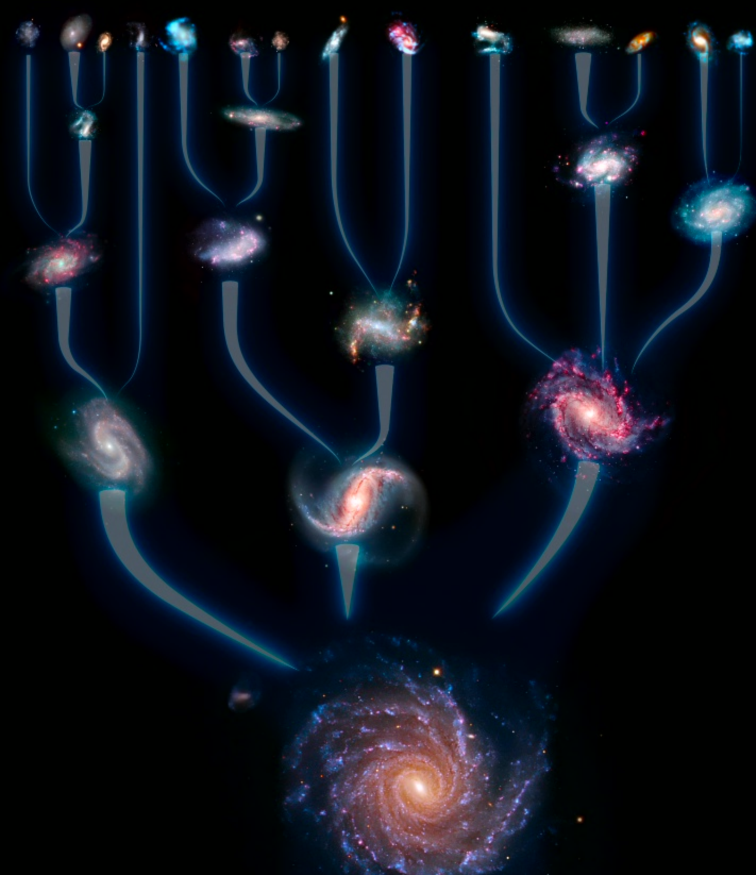
Neutrino Observatories are Graphs

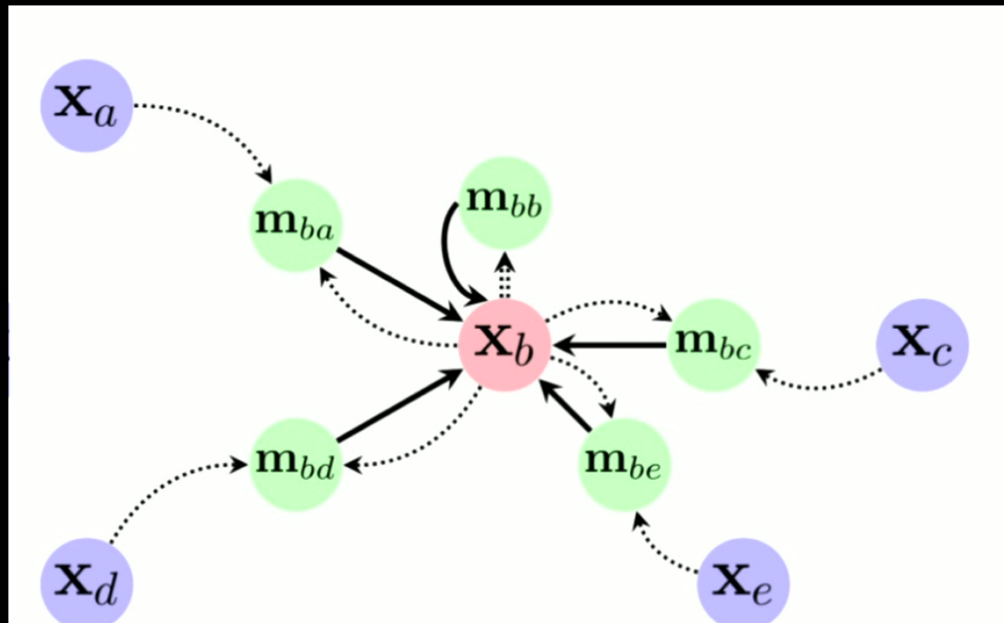


Large Scale Structure is a Graph



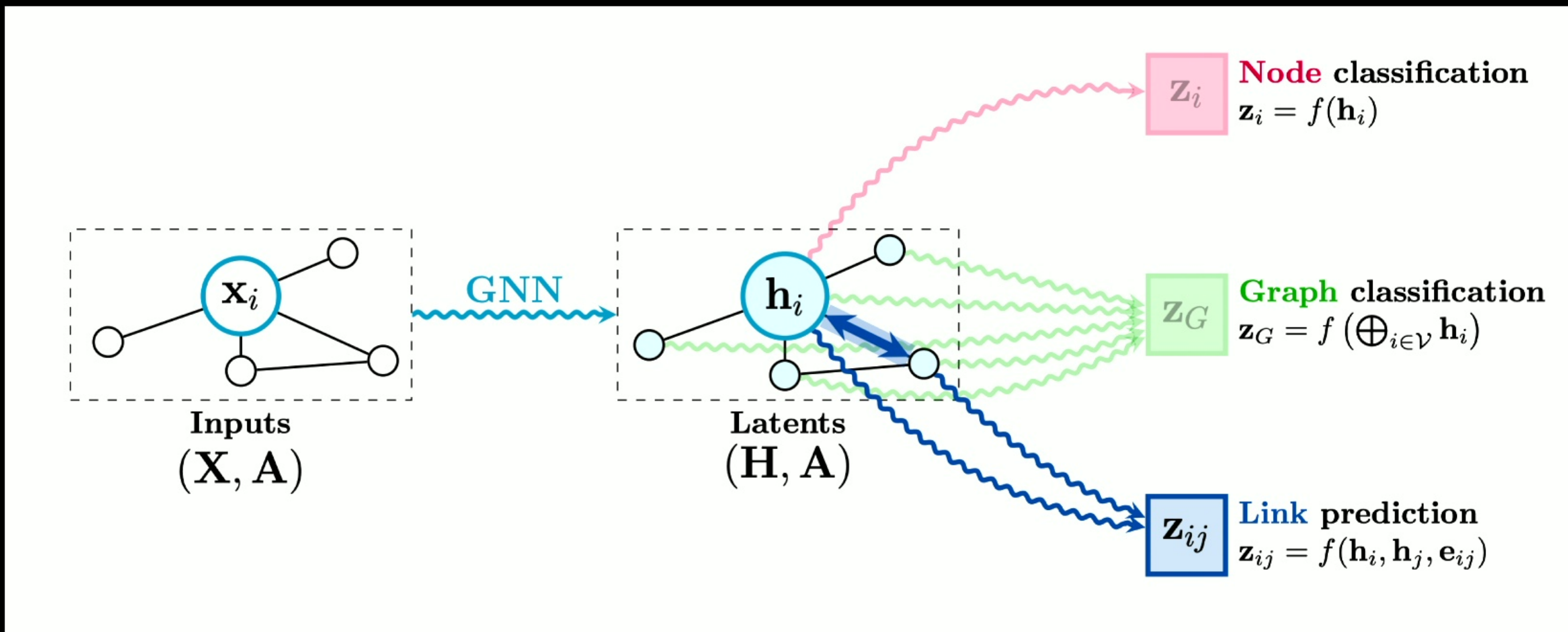
Galaxy Evolution is a Graph





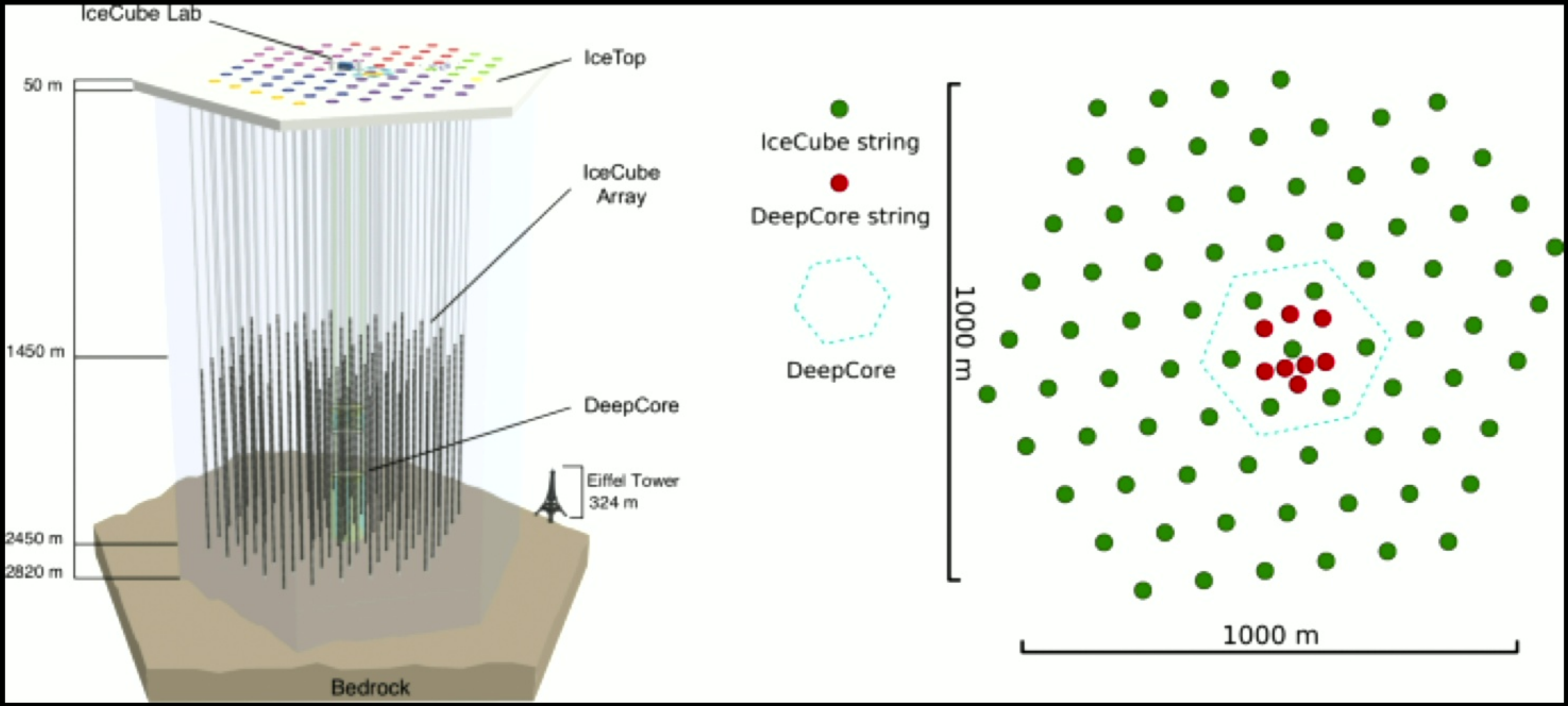
Message-passing

$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi\left(\mathbf{x}_u, \mathbf{x}_v, \mathbf{e}_{uv}\right)\right)$$



Node classification
$\mathbf{z}_i = f(\mathbf{h}_i)$
Graph classification
$\mathbf{z}_G = f\left(\bigoplus_{i\in\mathcal{V}} \mathbf{h}_i\right)$
Link prediction
$\mathbf{z}_{ij} = f(\mathbf{h}_i, \mathbf{h}_j, \mathbf{e}_{ij})$
GNN
Inputs
$(\mathbf{X}, \mathbf{A})$
Latents
$(\mathbf{H}, \mathbf{A})$

How would you fit this on a grid?



Must-have symmetries

Given some permutation matrix **P**, we want some properties:

For scalar output functions, **invariance** when acting with **P**

$$f\left(\mathbf{PX}, \mathbf{PAP}^\top\right) = f(\mathbf{X}, \mathbf{A}) \text{ (Invariance)}$$

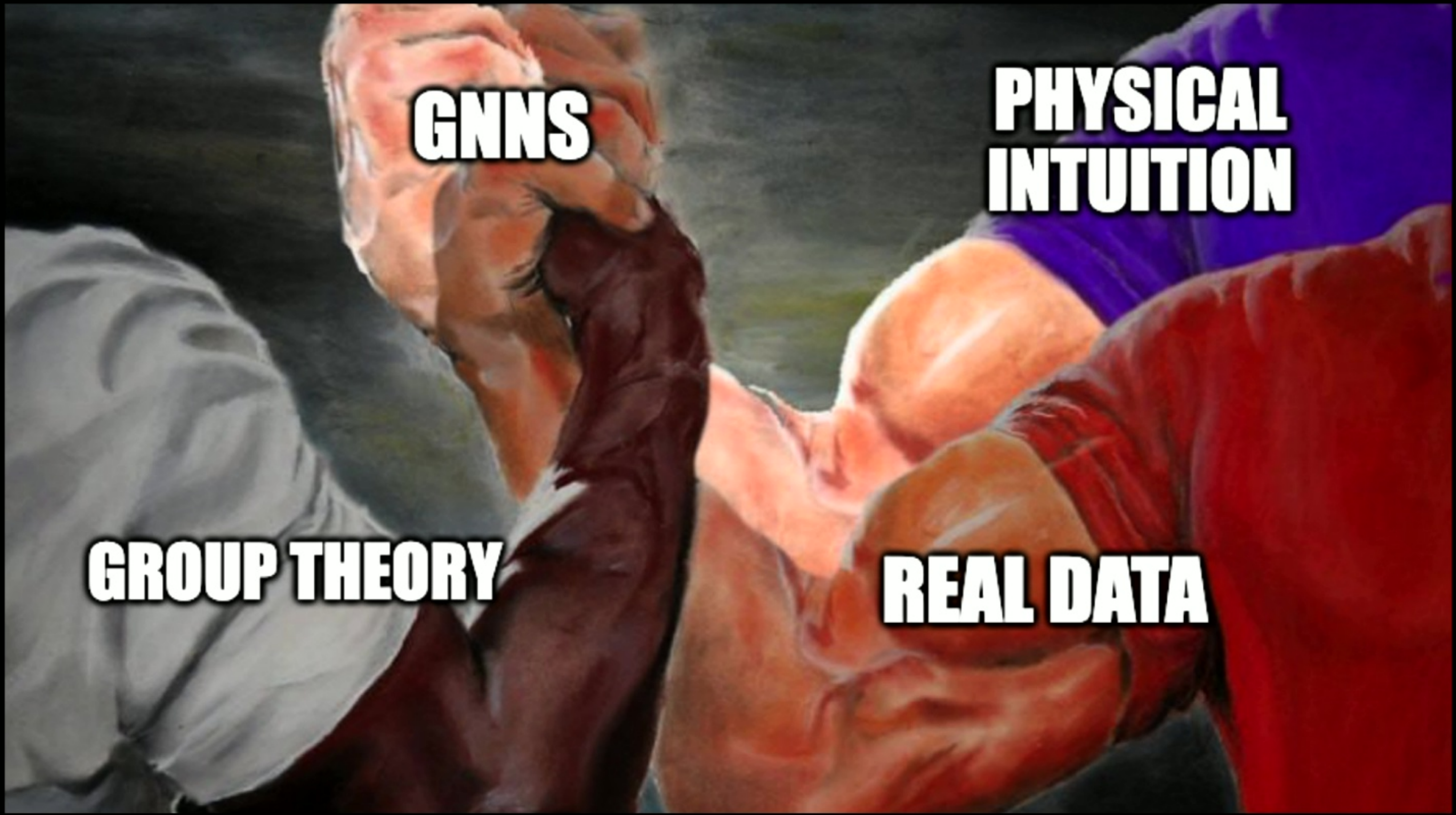
For vector output functions, **equivariance** when acting with **P**

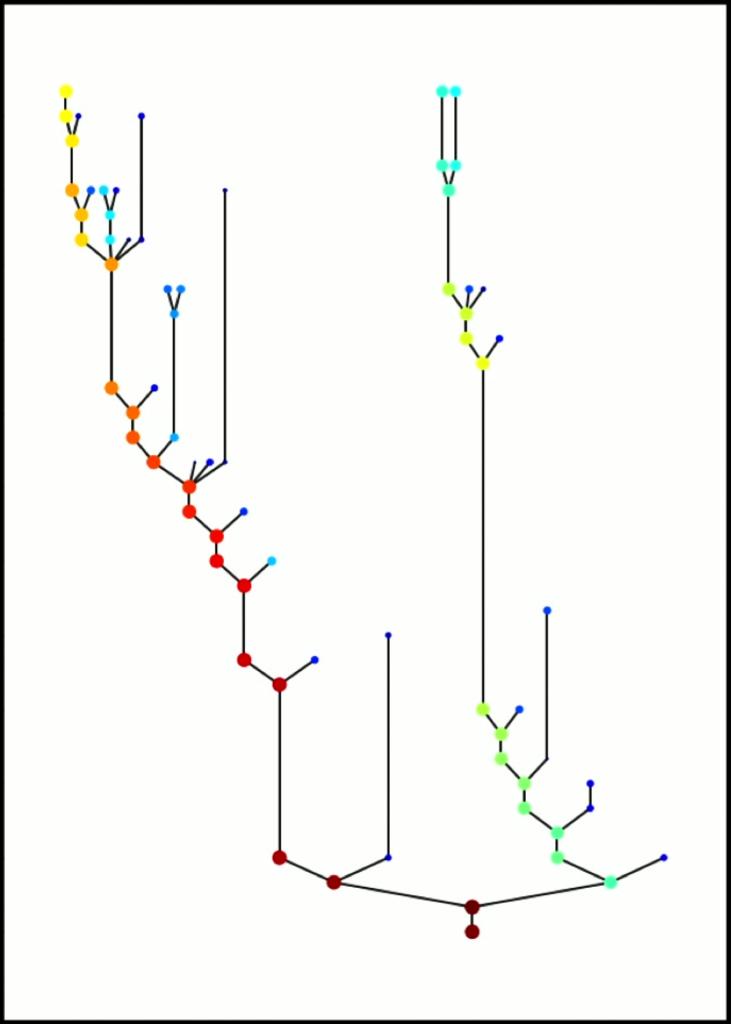
$$\mathbf{F}\left(\mathbf{PX}, \mathbf{PAP}^\top\right) = \mathbf{PF}(\mathbf{X}, \mathbf{A}) \text{ (Equivariance)}$$

Physics with GNNs

- A natural abstraction of physical systems and inherently local -> easier physical interpretations + separability
- Can embed almost arbitrary symmetries
- Embeds inductive biases easily by restructuring the graph -> more efficient learning and no need to learn things we already know

The Unreasonable Efficiency of GNNs for Physics





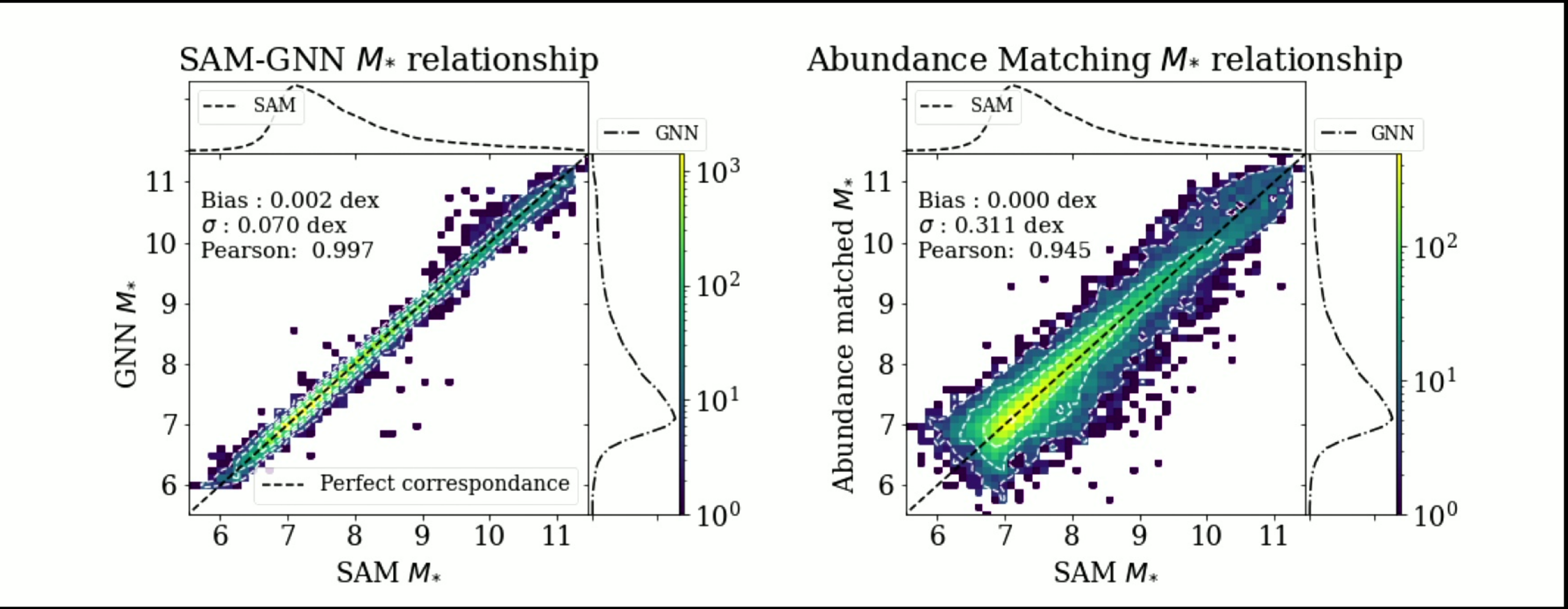
= Graph -> Graph Neural Network

Jespersen+ 22

arxiv.org/abs/2210.13473

MANGROVE

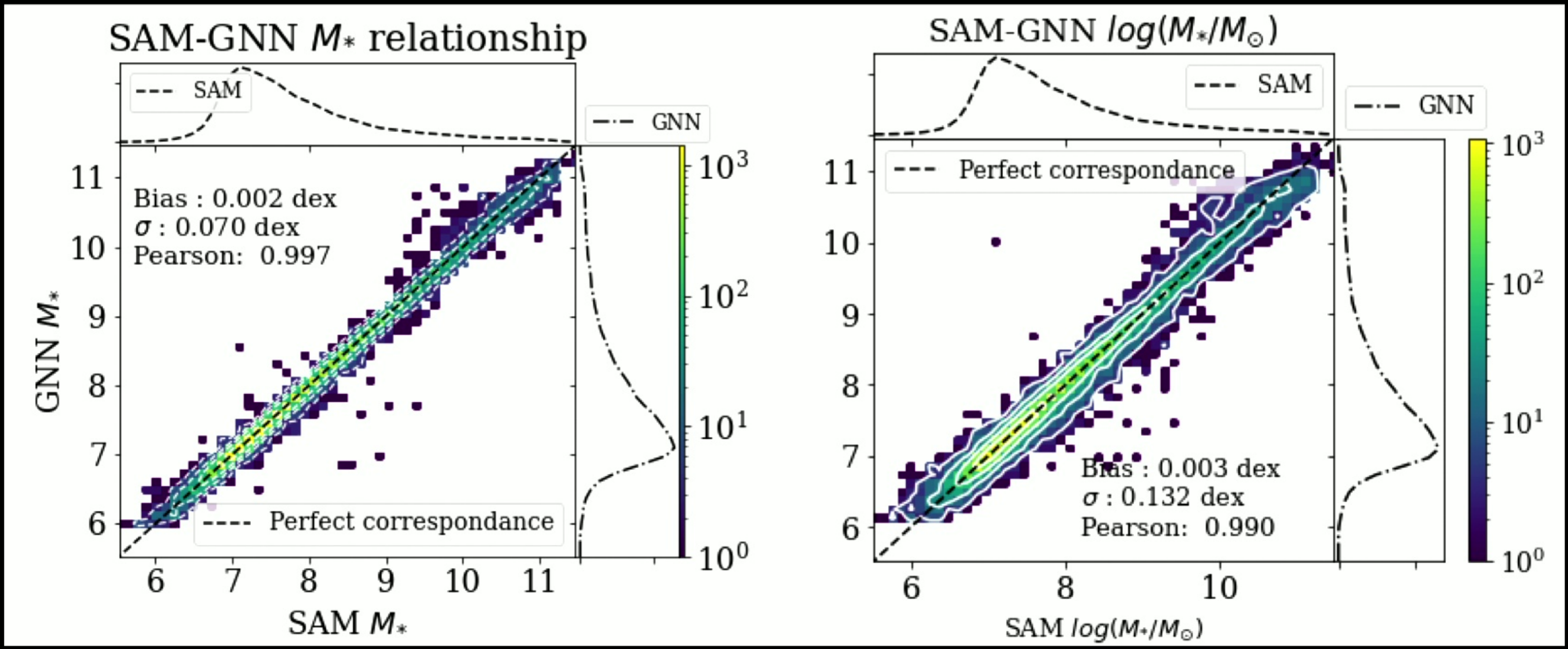
Jespersen+ 22



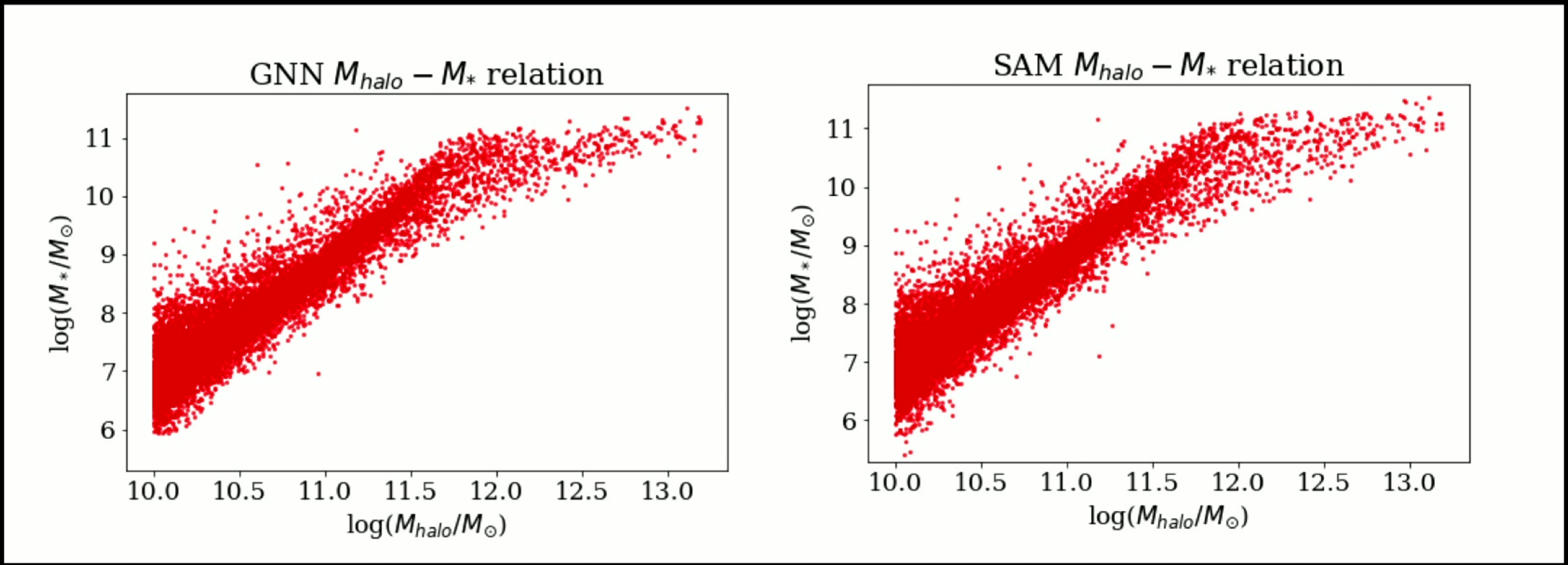
What about only all the final features?

Equivalent to the approach used in litterature

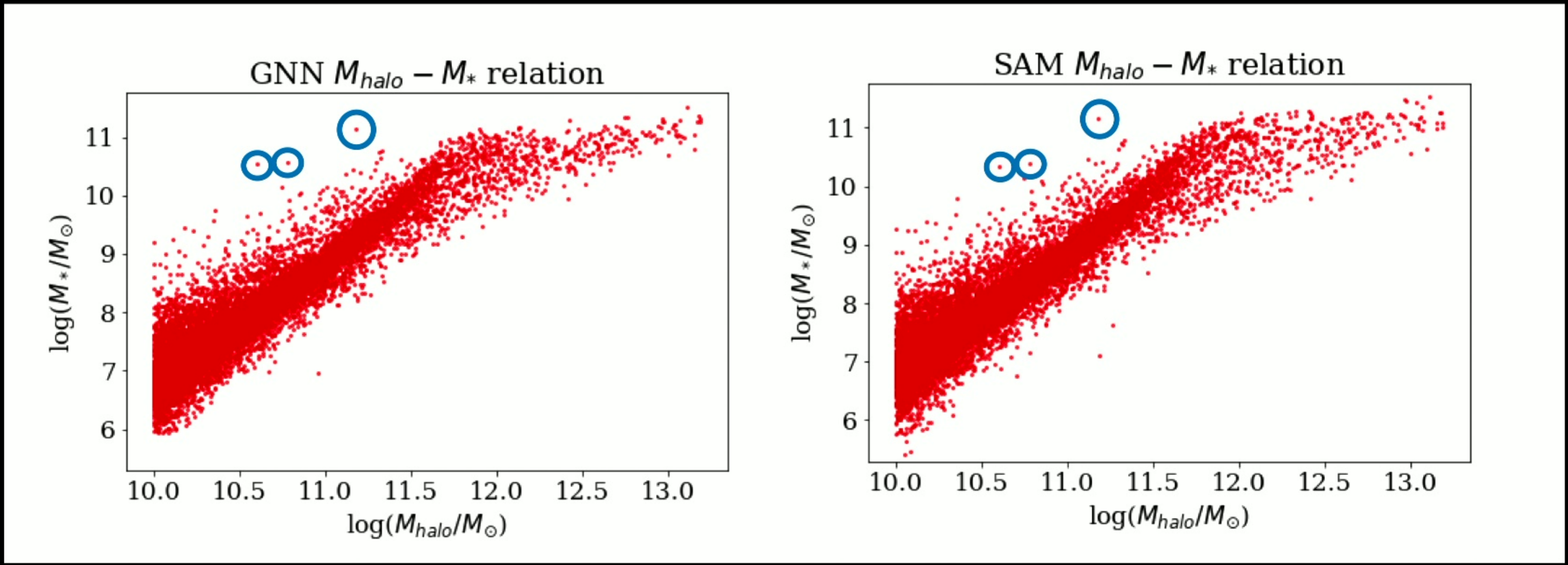
Jespersen+ 22



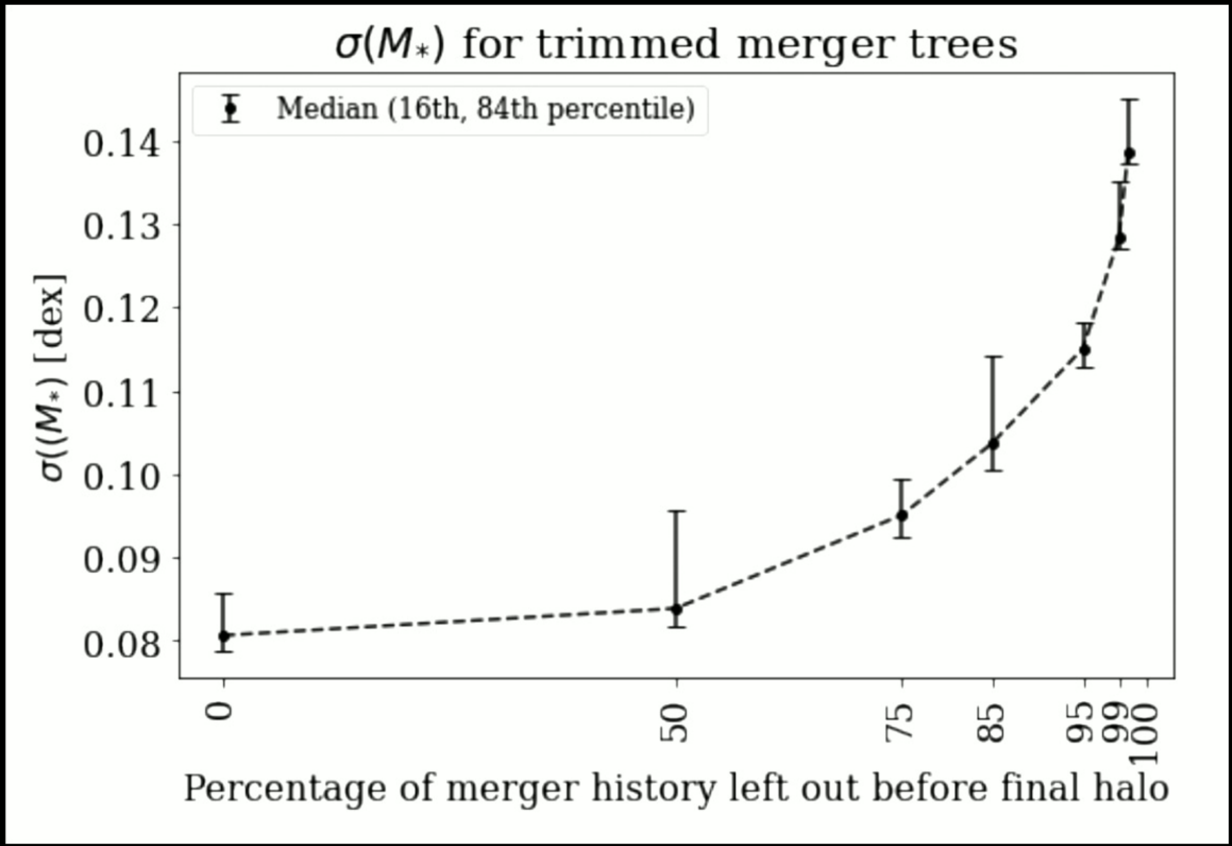
Eye test


GNN $M_{halo} - M_*$ relation
SAM $M_{halo} - M_*$ relation
$\log(M_*/M_\odot)$
$\log(M_{halo}/M_\odot)$
6
7
8
9
10
11
10.0
10.5
11.0
11.5
12.0
12.5
13.0

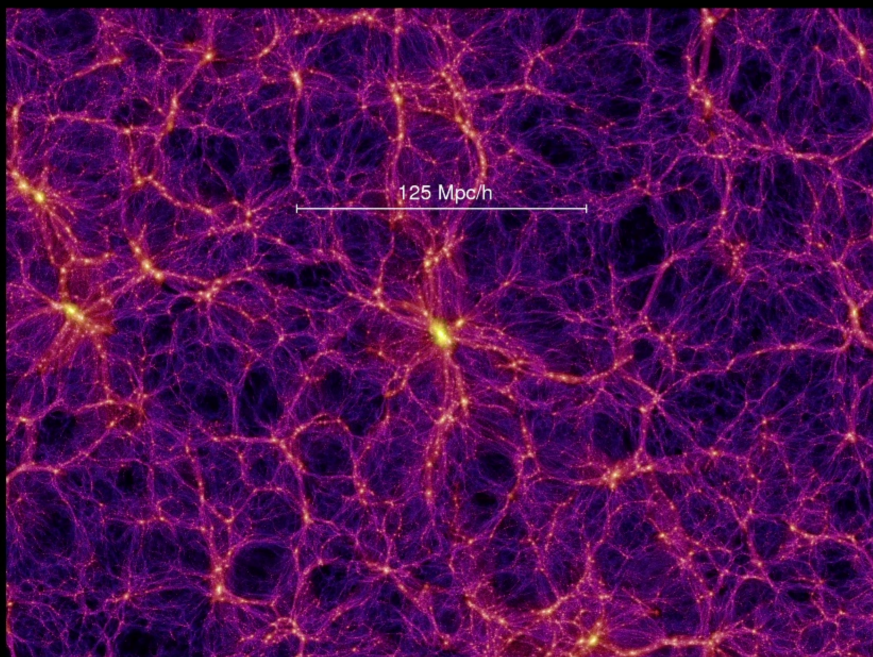
Outliers are dead on!

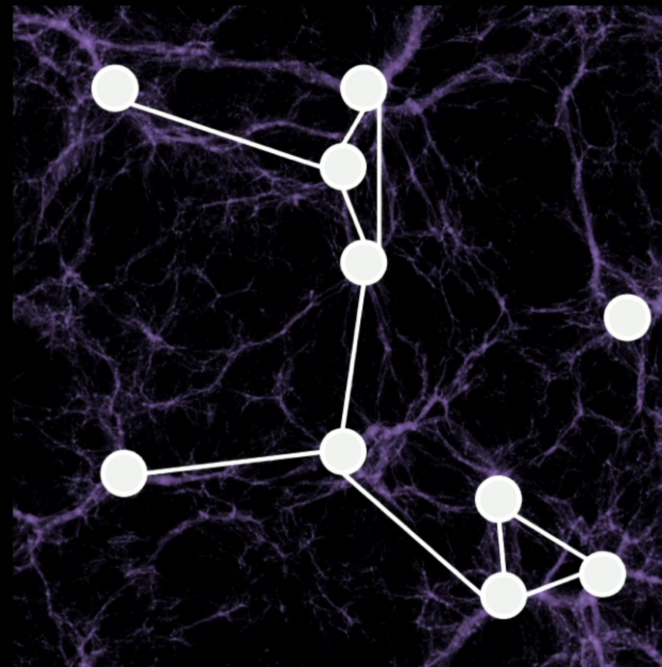


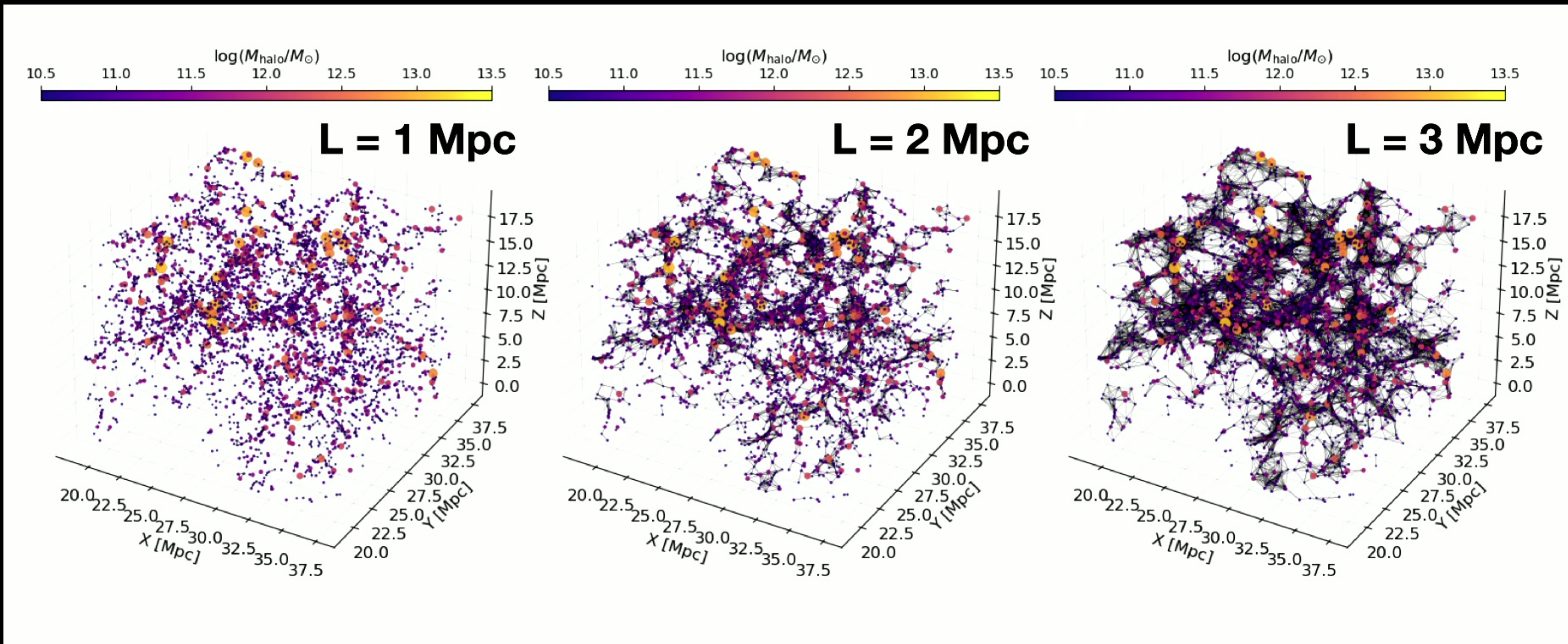
What part of the merger history is most important?

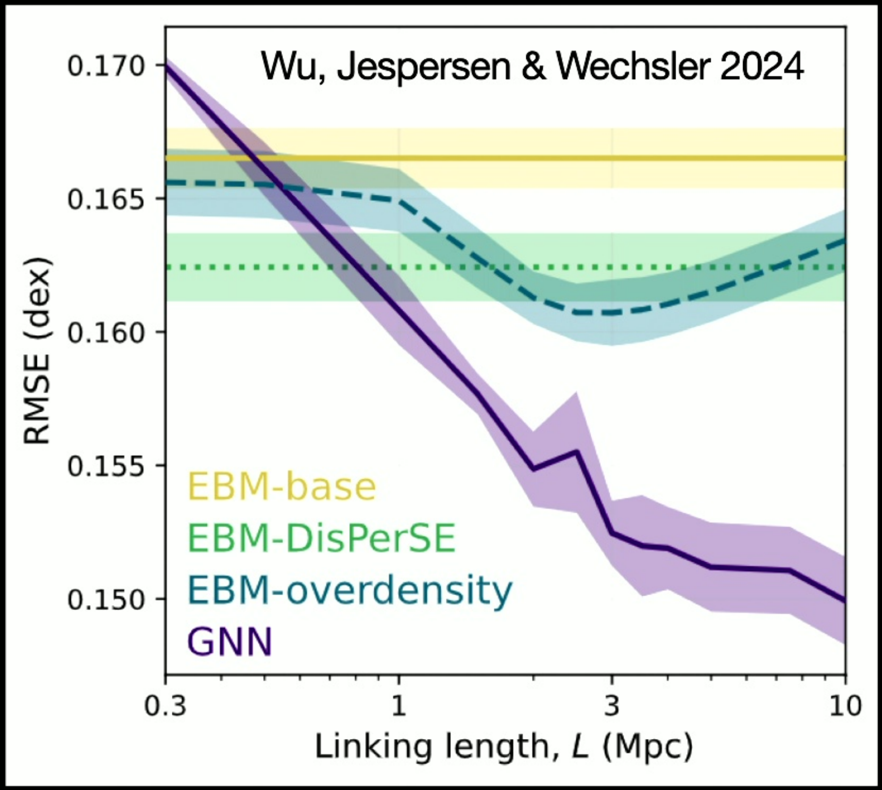


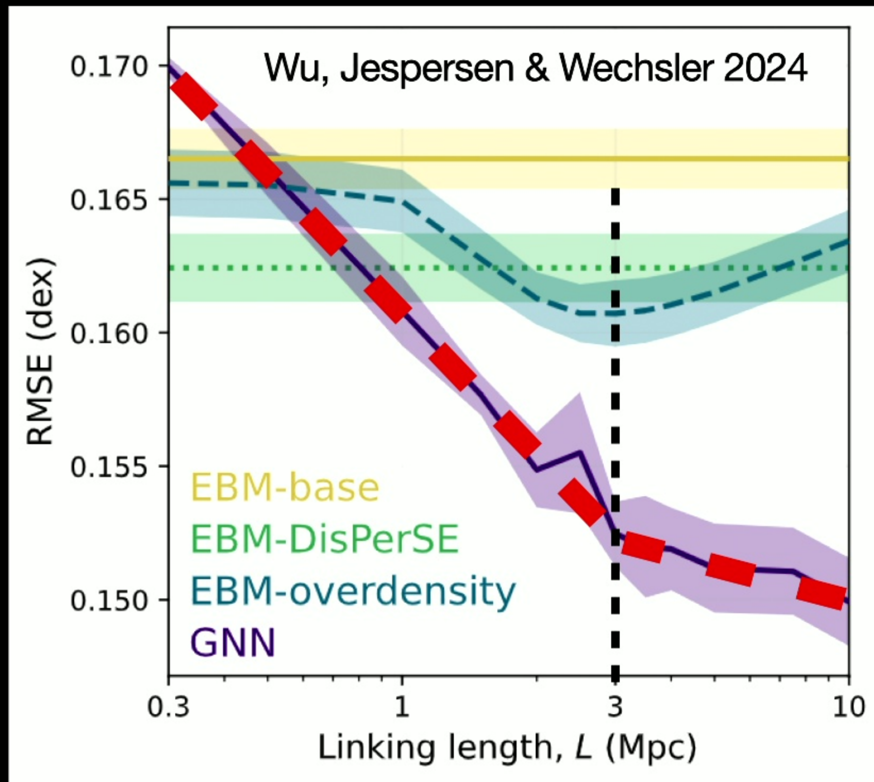
$$\text{Galaxy} \sim f(\text{Halo}, \text{History})$$


125 Mpc/h

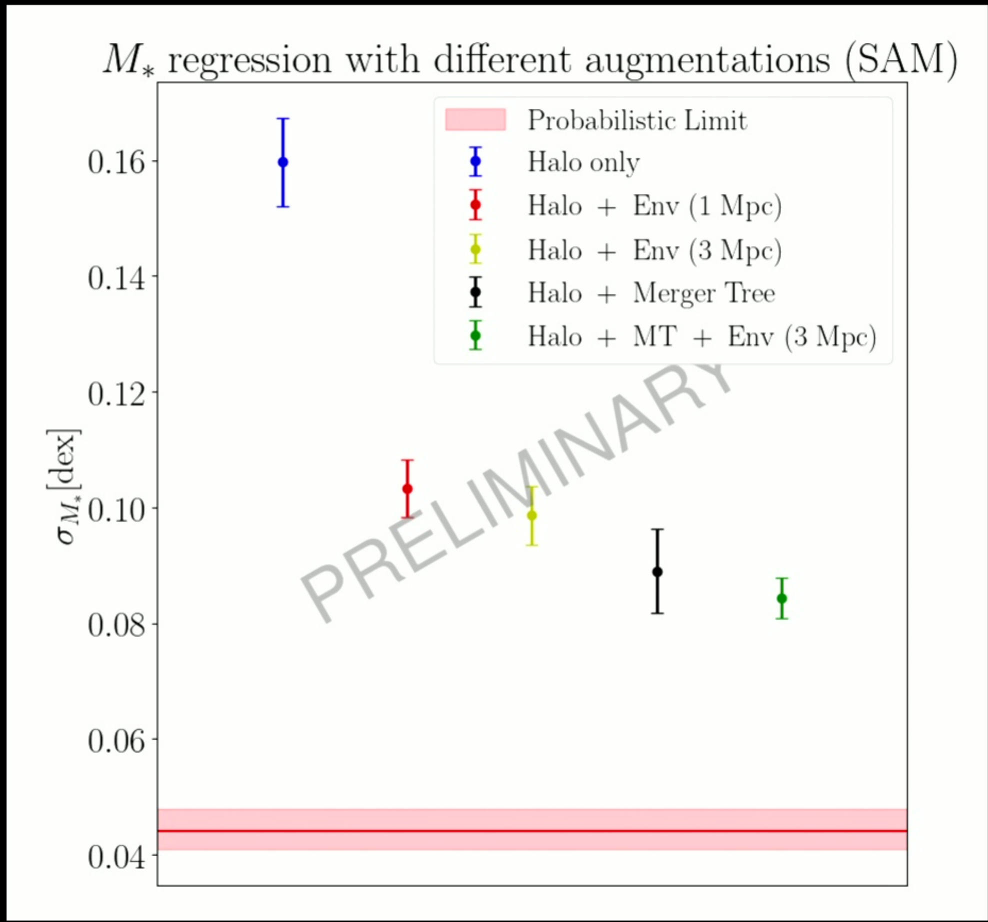



log($M_{\rm halo}/M_\odot$)
10.5 11.0 11.5 12.0 12.5 13.0 13.5
L = 1 Mpc
L = 2 Mpc
L = 3 Mpc
X [Mpc]
Y [Mpc]
Z [Mpc]
20.0 22.5 25.0 27.5 30.0 32.5 35.0 37.5
0.0 2.5 5.0 7.5 10.0 12.5 15.0 17.5


Wu, Jespersen & Wechsler 2024
0.170
0.165
0.160
0.155
0.150
RMSE (dex)
EBM-base
EBM-DisPerSE
EBM-overdensity
GNN
0.3
1
3
10
Linking length, L (Mpc)

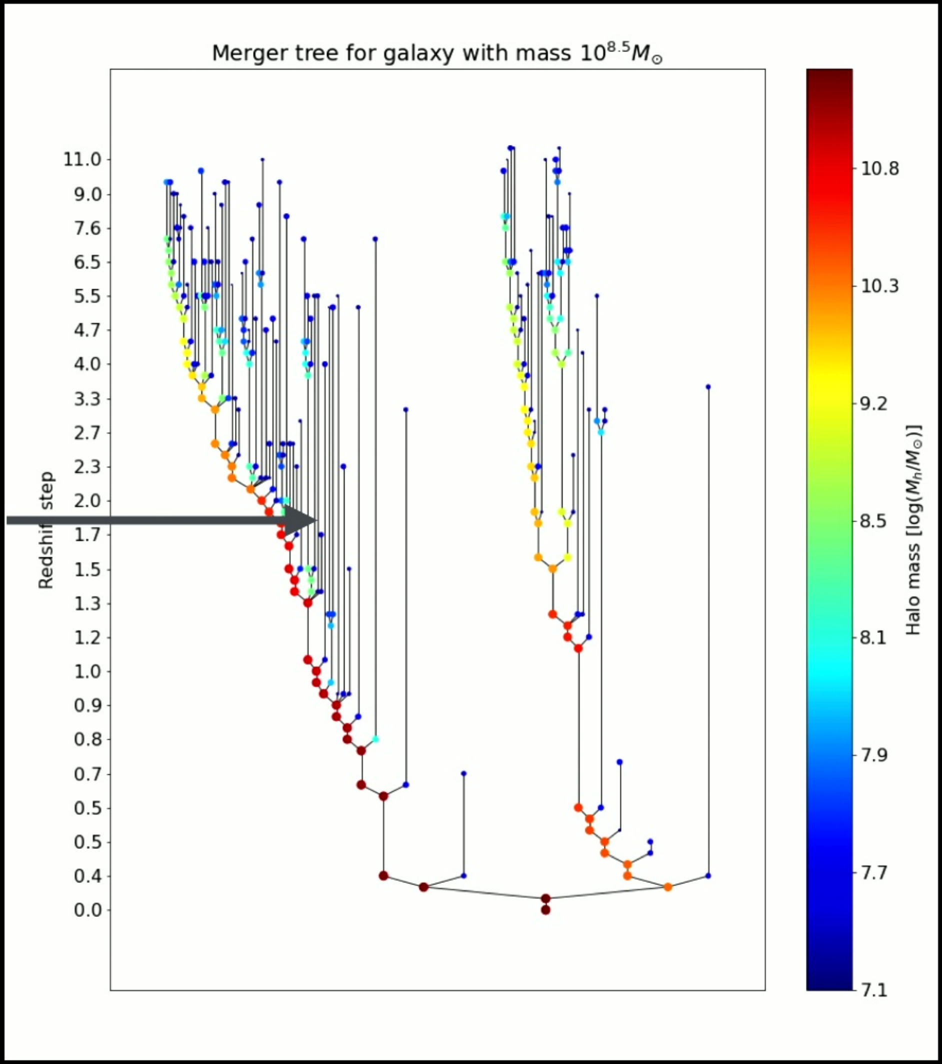

Wu, Jespersen & Wechsler 2024
0.170
0.165
0.160
0.155
0.150
RMSE (dex)
EBM-base
EBM-DisPerSE
EBM-overdensity
GNN
0.3
1
3
10
Linking length, L (Mpc)

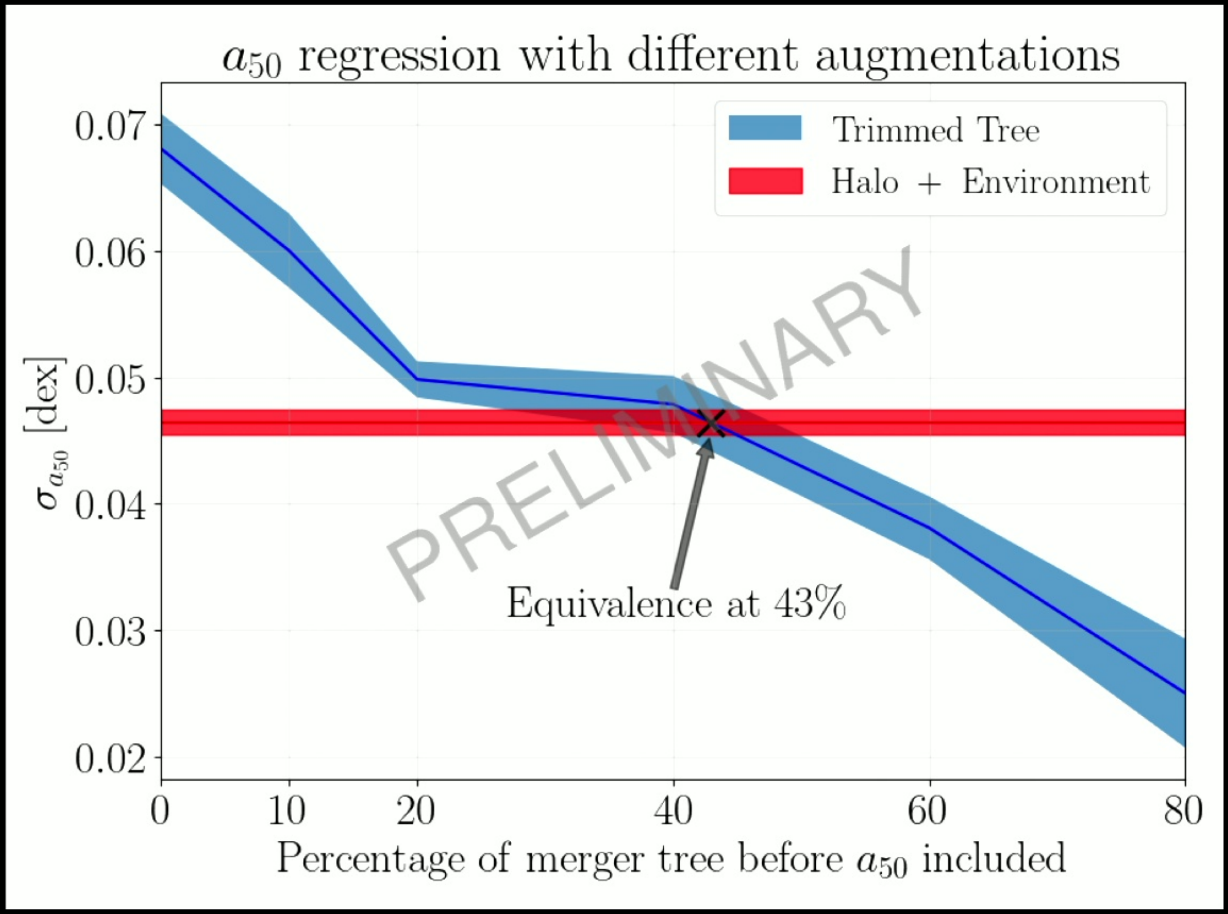
$$\text{Galaxy} \sim f(\text{Halo}, \text{History}, \text{Environment})$$



M_* regression with different augmentations (SAM)
σ_{M_*}[dex]
0.16
0.14
0.12
0.10
0.08
0.06
0.04
Probabilistic Limit
Halo only
Halo + Env (1 Mpc)
Halo + Env (3 Mpc)
Halo + Merger Tree
Halo + MT + Env (3 Mpc)
PRELIMINARY

50% of mass accumulated

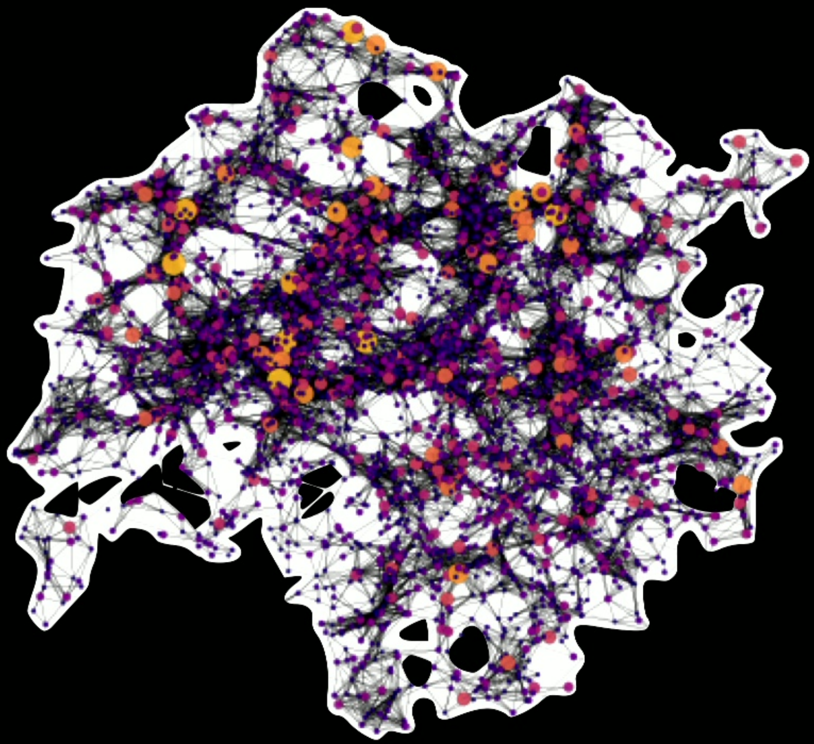




a_{50} regression with different augmentations
Trimmed Tree
Halo + Environment
$\sigma_{a_{50}}$ [dex]
0.07
0.06
0.05
0.04
0.03
0.02
0
10
20
40
60
80
Percentage of merger tree before a_{50} included
Equivalence at 43%
PRELIMINARY

So what did we learn?

- GNNs are a natural fit for physics
- Applying GNNs, we find that:
  - History is important for galaxies
  - Environment is important for galaxies
- These are important in the **same way**



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