Simulations & AI for fundamental physics

Francisco Villaescusa-Navarro

SIMONS FOUNDATION — FLATIRON INSTITUTE — PRINCETON UNIVERSITY

Swiss SKA days 2024

Outline

- Motivation
- Numerical simulations
- The role of AI

Cosmology

Branch of Astrophysics that studies the Universe's:

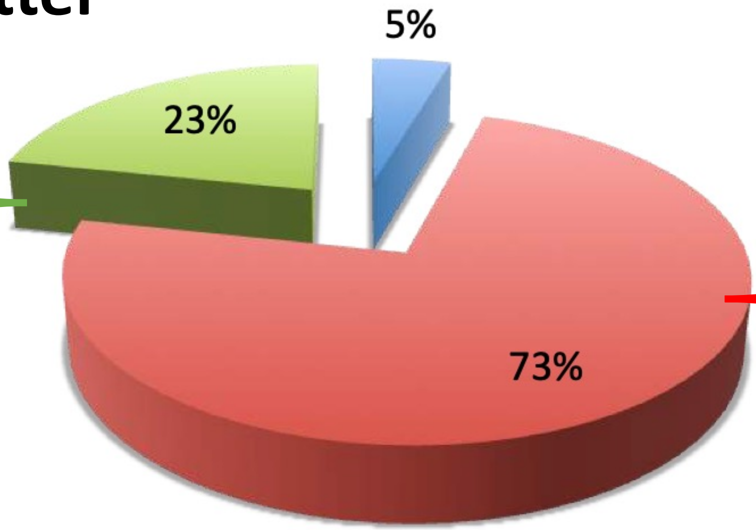
- Origin and fate
- Composition
- Laws
- Structure
- Dynamics

Our Universe

Dark Matter

- Cold dark matter
- Warm dark matter
- Atomic dark matter
- …

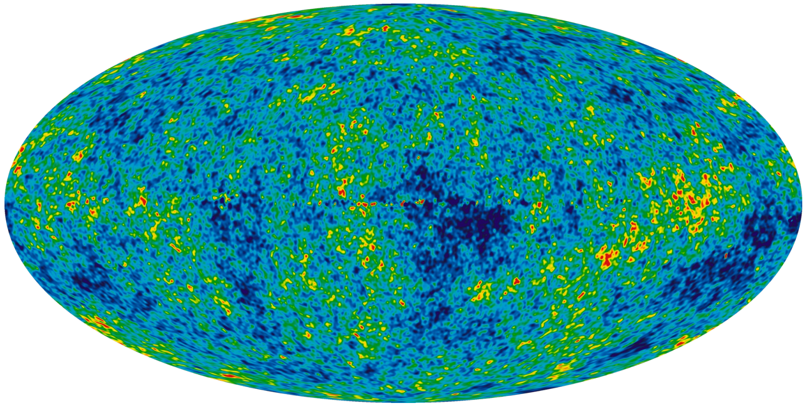
Baryons (Ordinary matter)

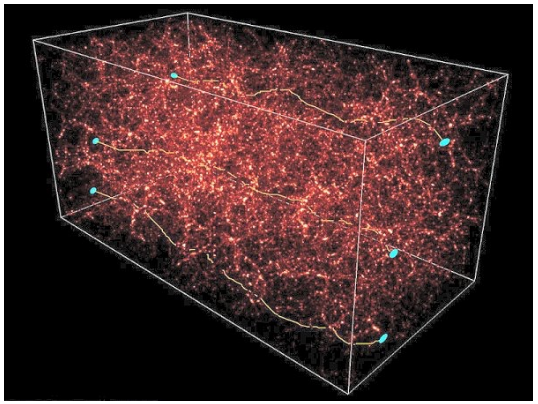


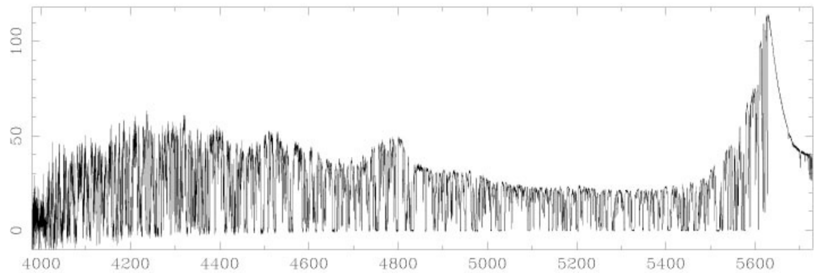
- General relativity (Λ)
- Modified gravity
- …

Dark Energy

The ΛCDM model







$$\Omega_b \pm \delta\Omega_b$$

$$\Omega_m \pm \delta\Omega_m$$

$$h \pm \delta h$$

$$w_0 \pm \delta w_0$$

$$w_a \pm \delta w_a$$

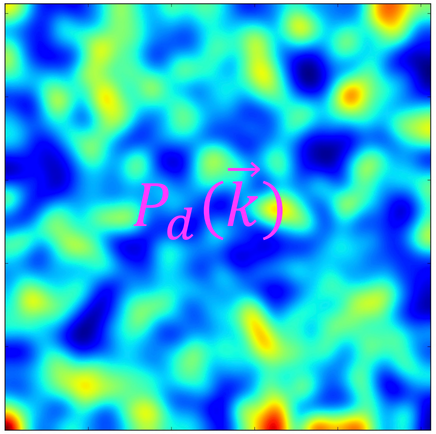
$$n_s \pm \delta n_s$$

$$\sigma_8 \pm \delta\sigma_8$$

$$M_\nu \pm \delta M_\nu$$

$$N_{\rm eff} \pm \delta N_{\rm eff}$$

Parameter inference

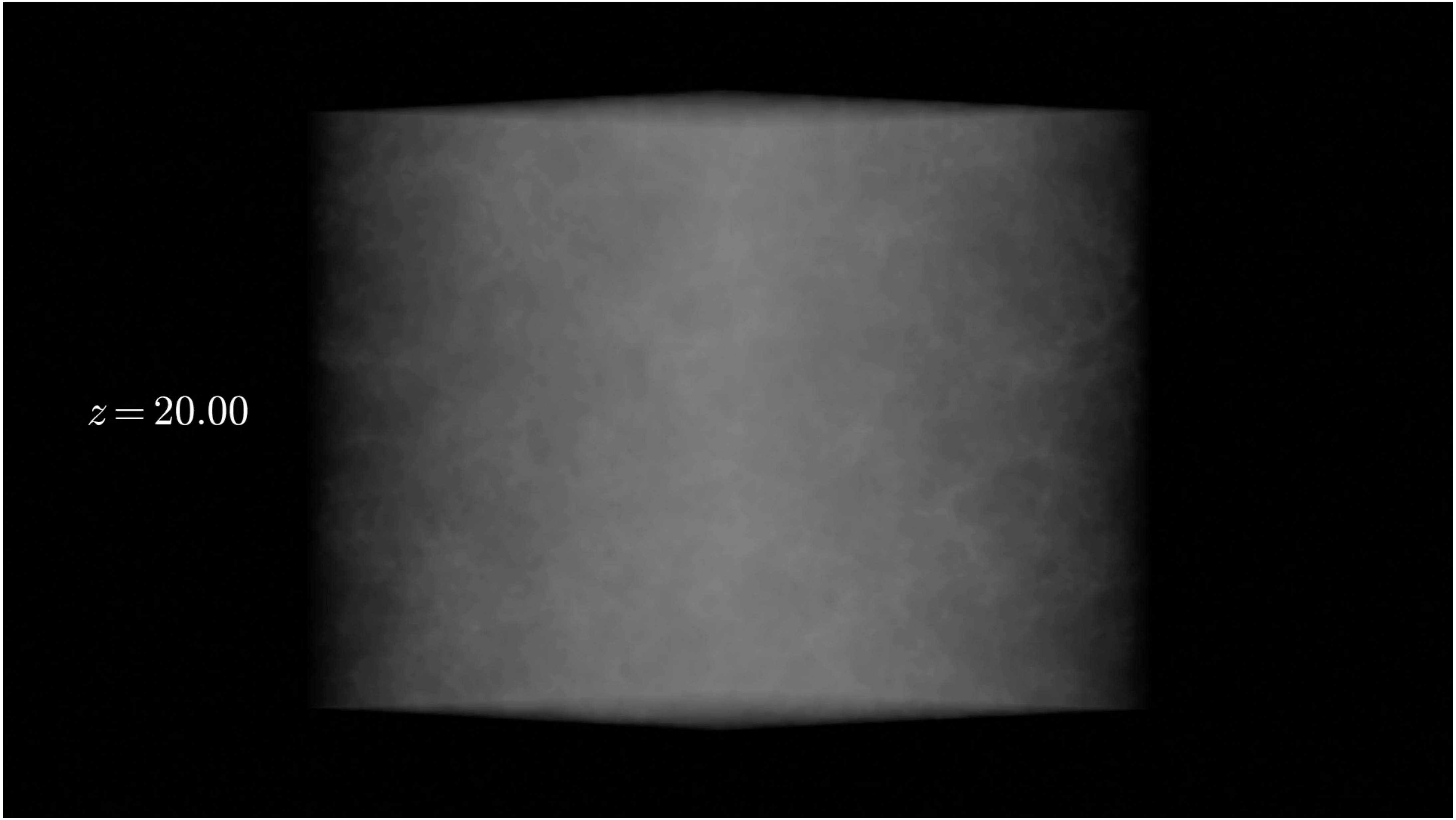
Observations	Theory
	$P_t(\vec{k}\vert\vec{\theta})$

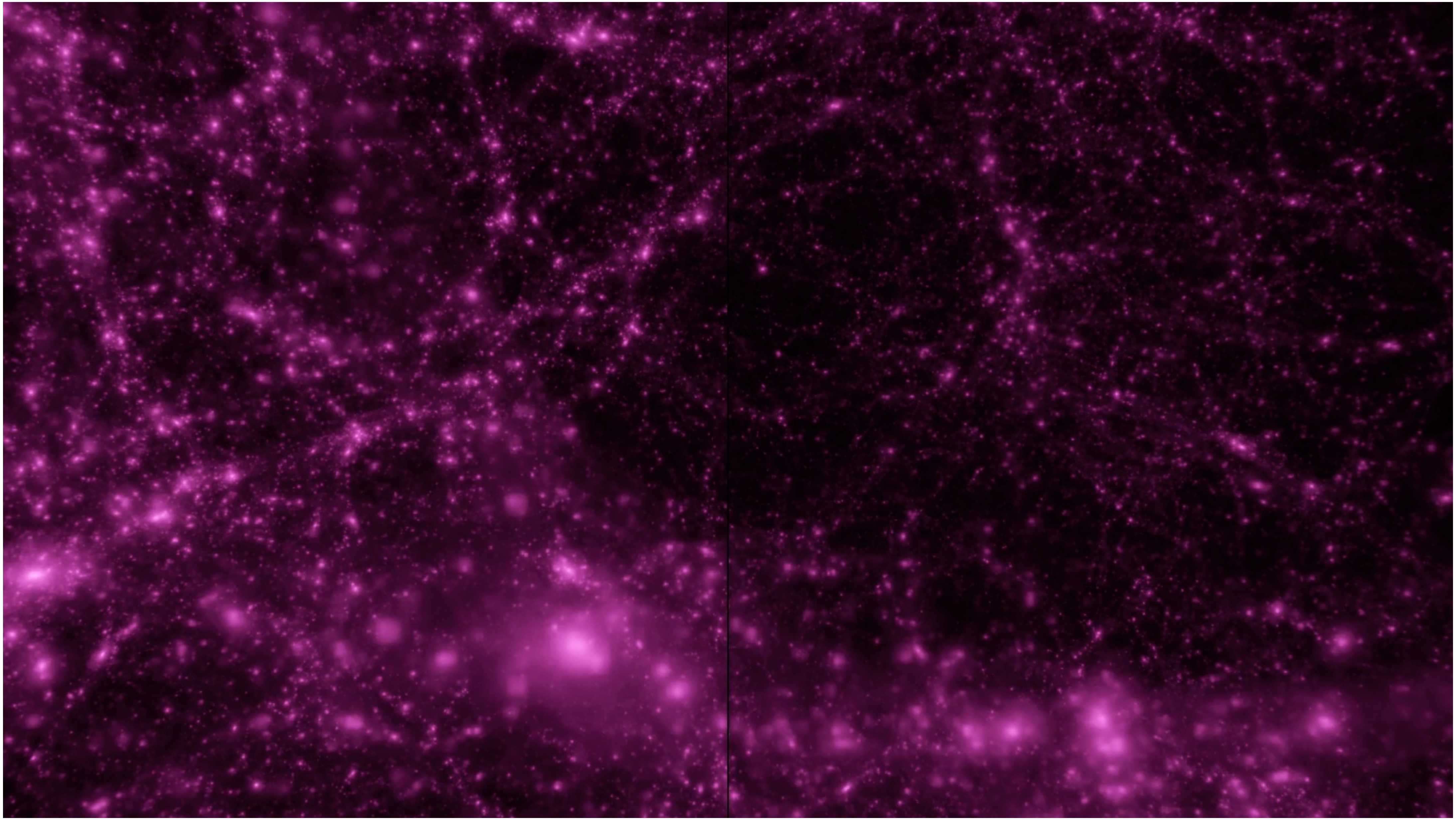
Summary

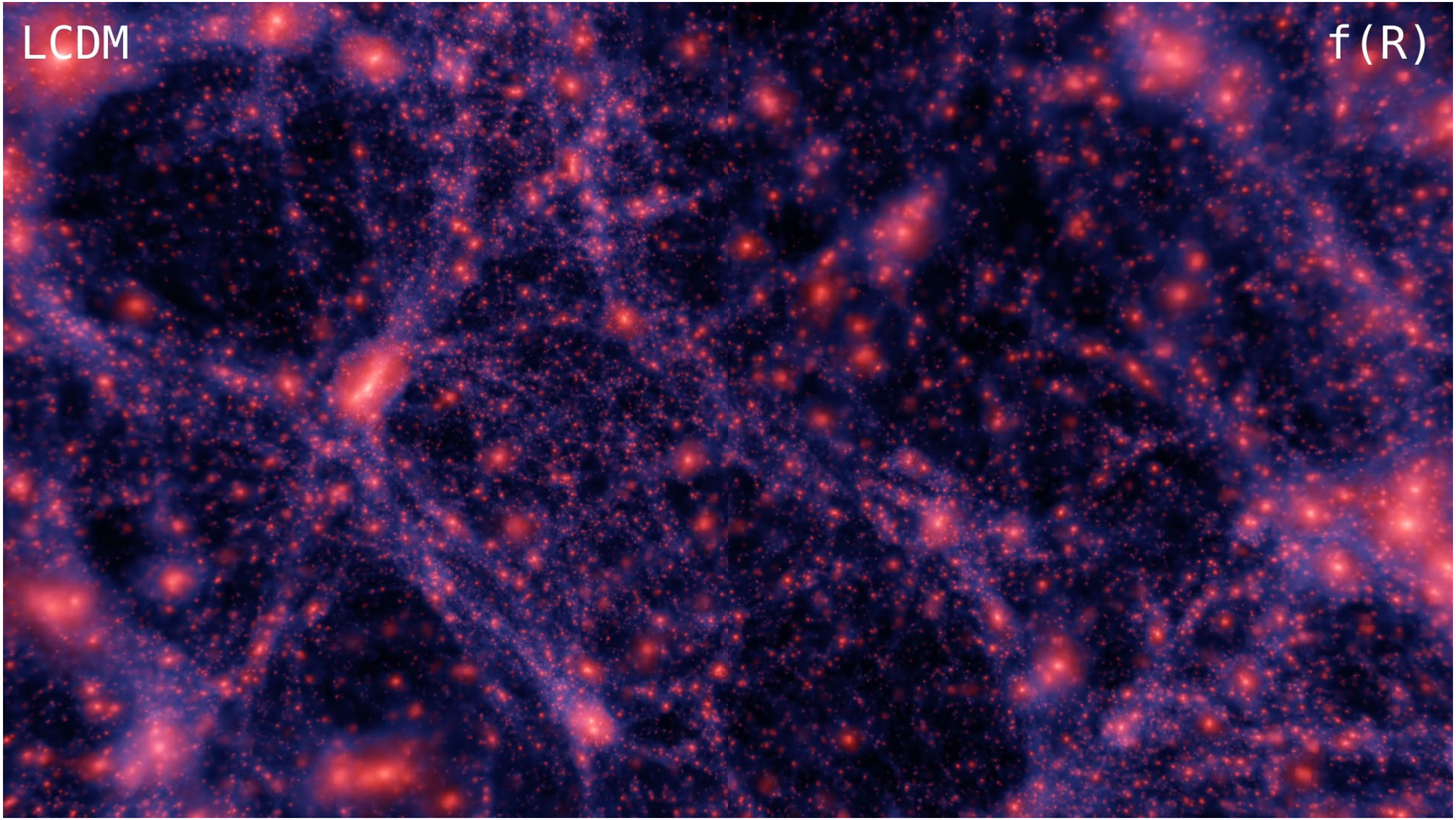
- <u>Motivation</u>

- Numerical simulations

- The role of AI


$z = 20.00$





LCDM
f(R)

The Quijote Simulations

(https://quijote-simulations.readthedocs.io)

- A set of 87,000 full N-body simulations
- More than 40,000 cosmologies in $\{\Omega_m, \Omega_b, h, n_s, \sigma_8, M_\nu, w_0, \delta_b, f_{NL}, g_{NL}, f(R)\}$
- 12+ trillion particles over a volume larger than entire observable Universe
- Catalogs with billions of halos, voids (Gigantes), and galaxies (Molino). WL maps (Ulagam)
- 50 Million CPU hours; 1+ Petabyte of data
- 180+ papers written using this data
- All data publicly available (binder & globus)

Generic conclusion:
Lots of information on small scales beyond P(k)

Benefits: Lots of information

Problems: Non-linearities & baryonic effects

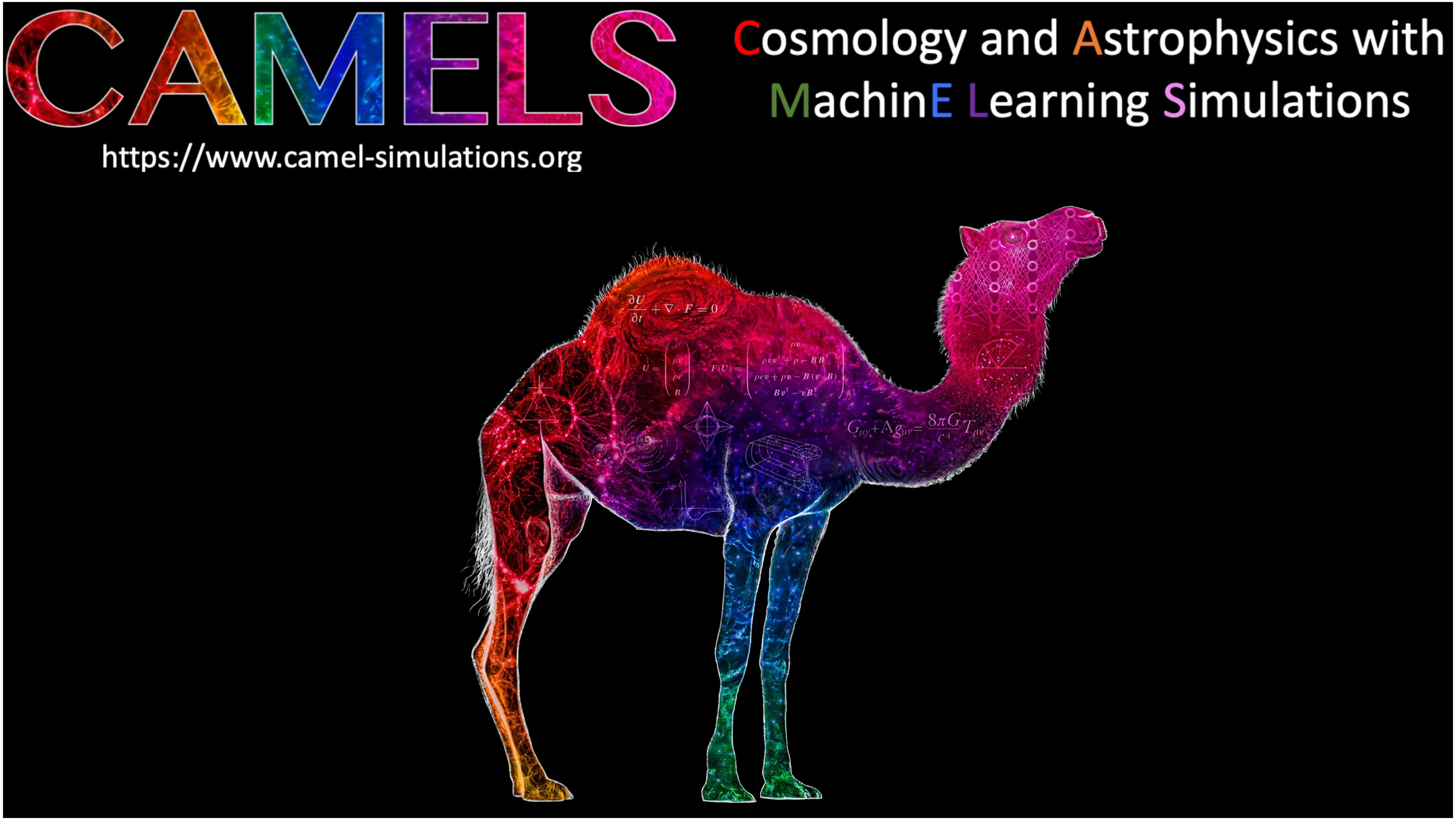
$z = 9.94$

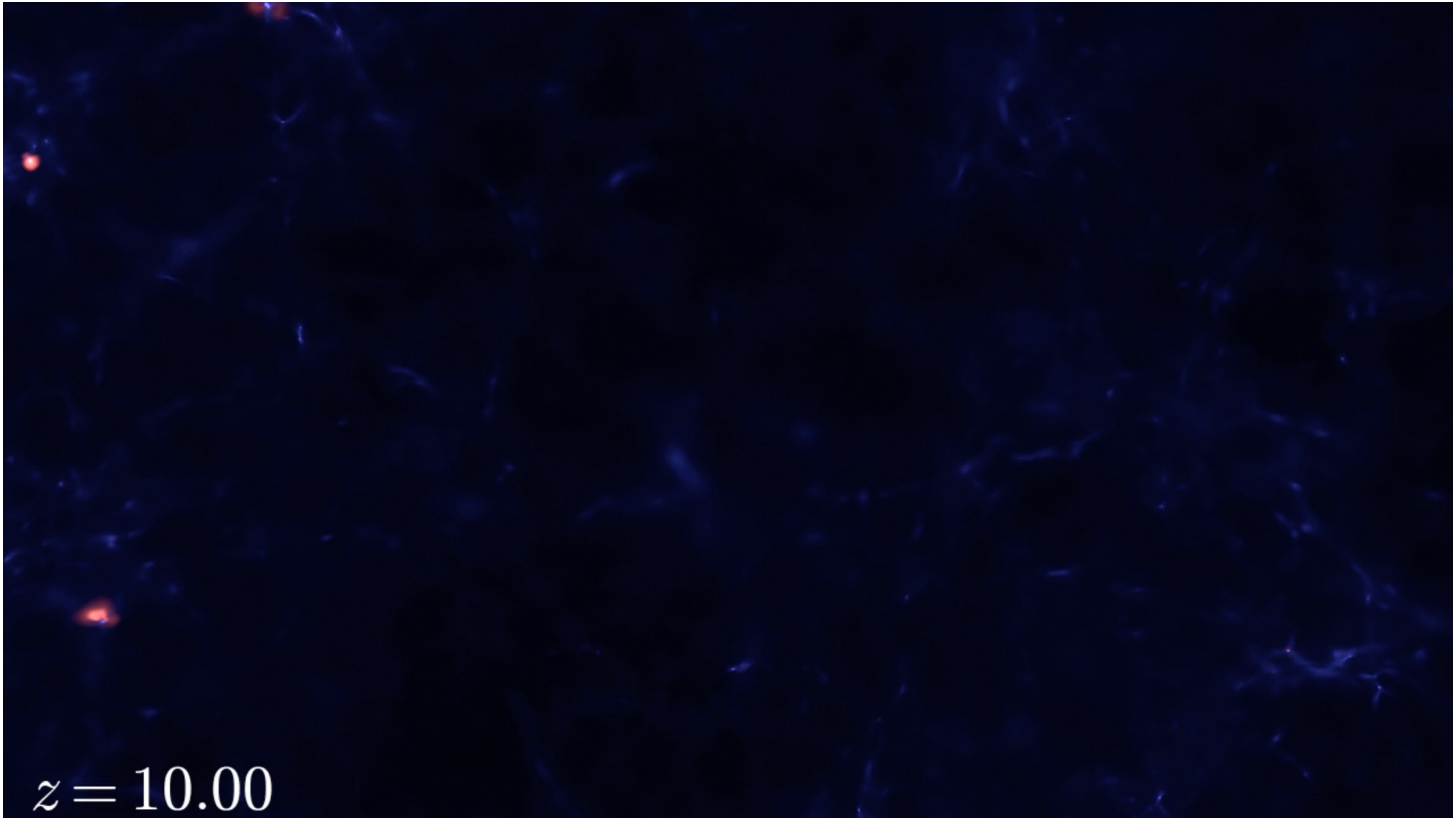
Summary

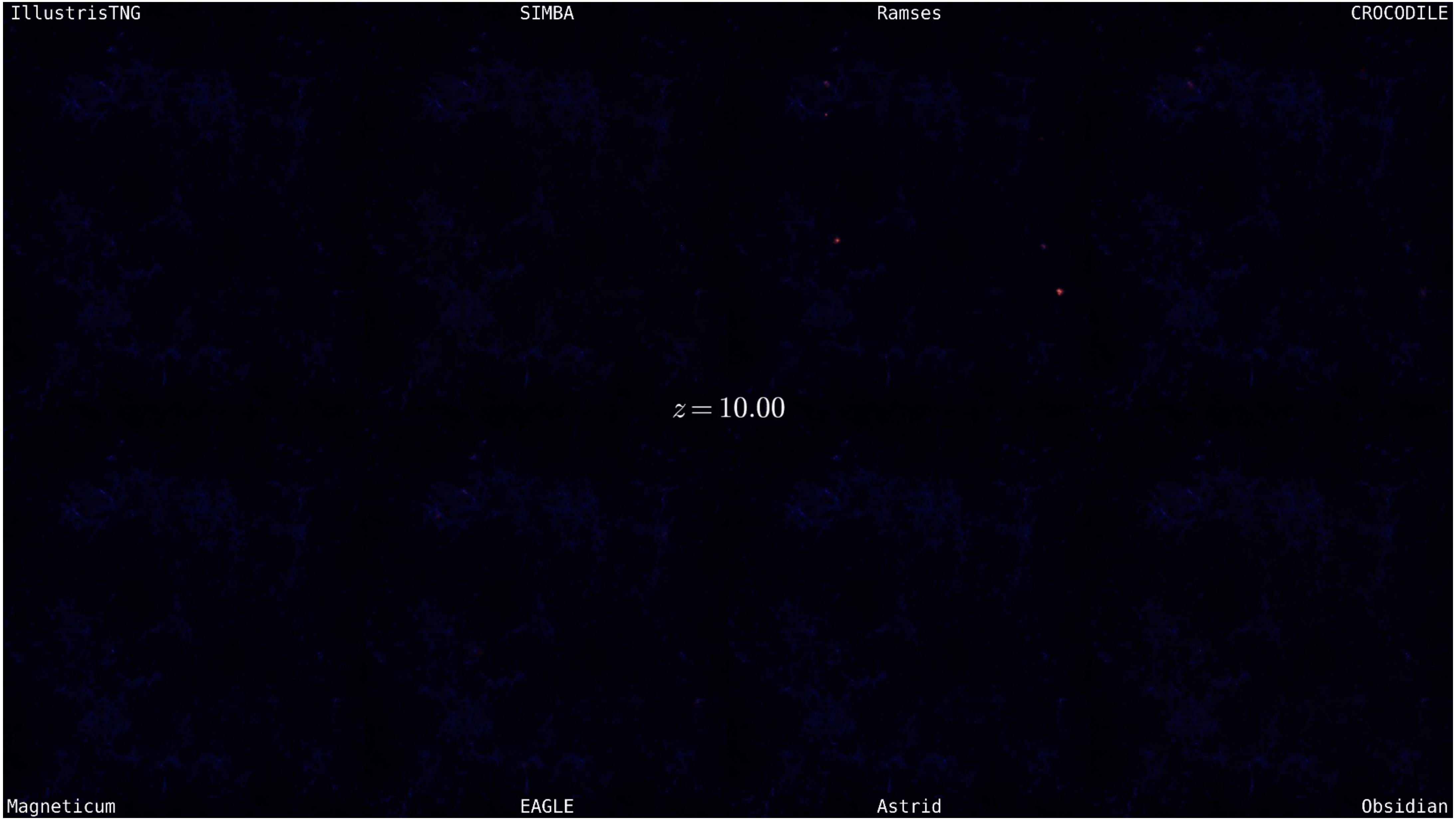
- <u>Motivation</u>

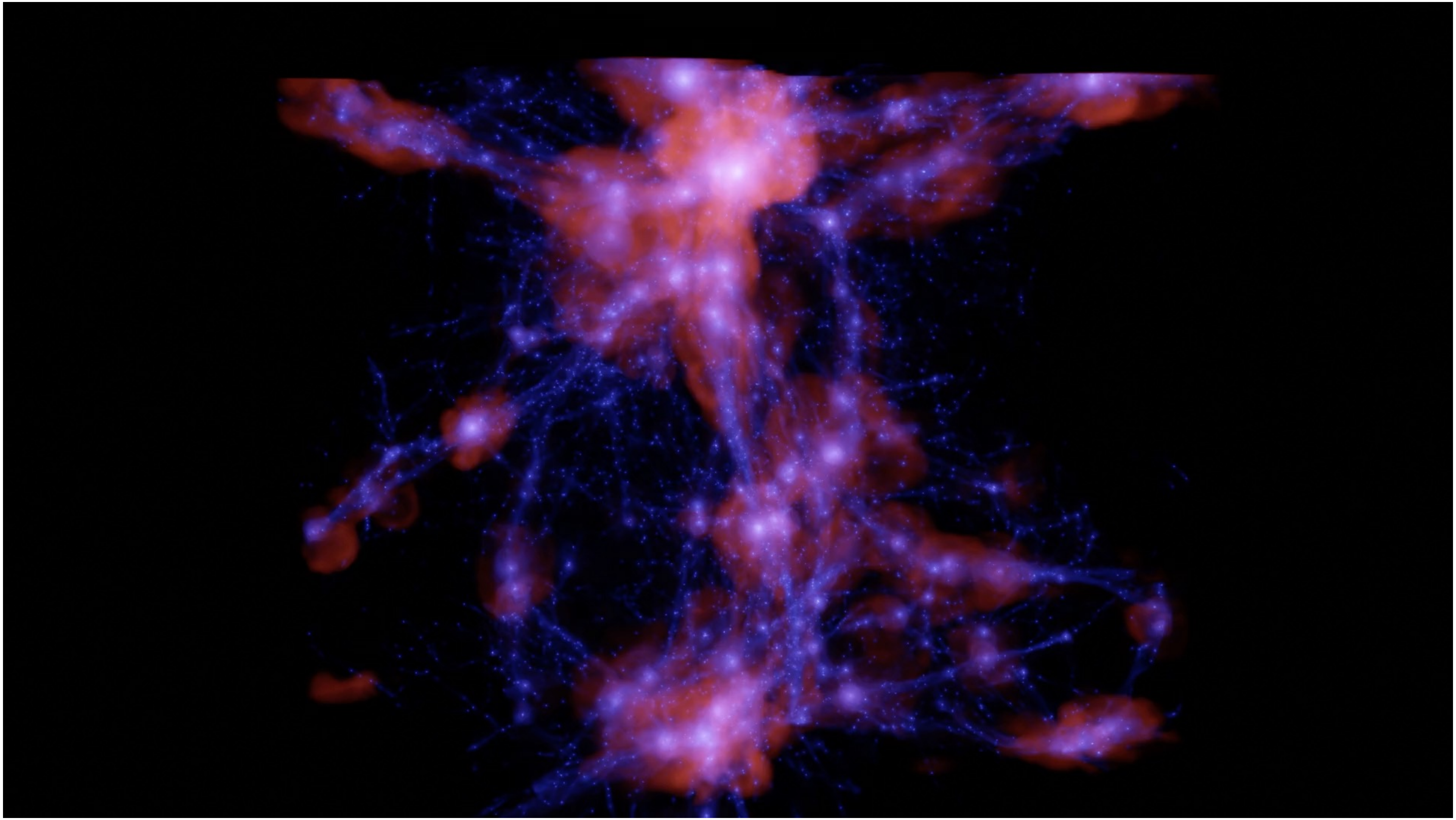
- <u>Numerical simulations</u>

- The role of AI

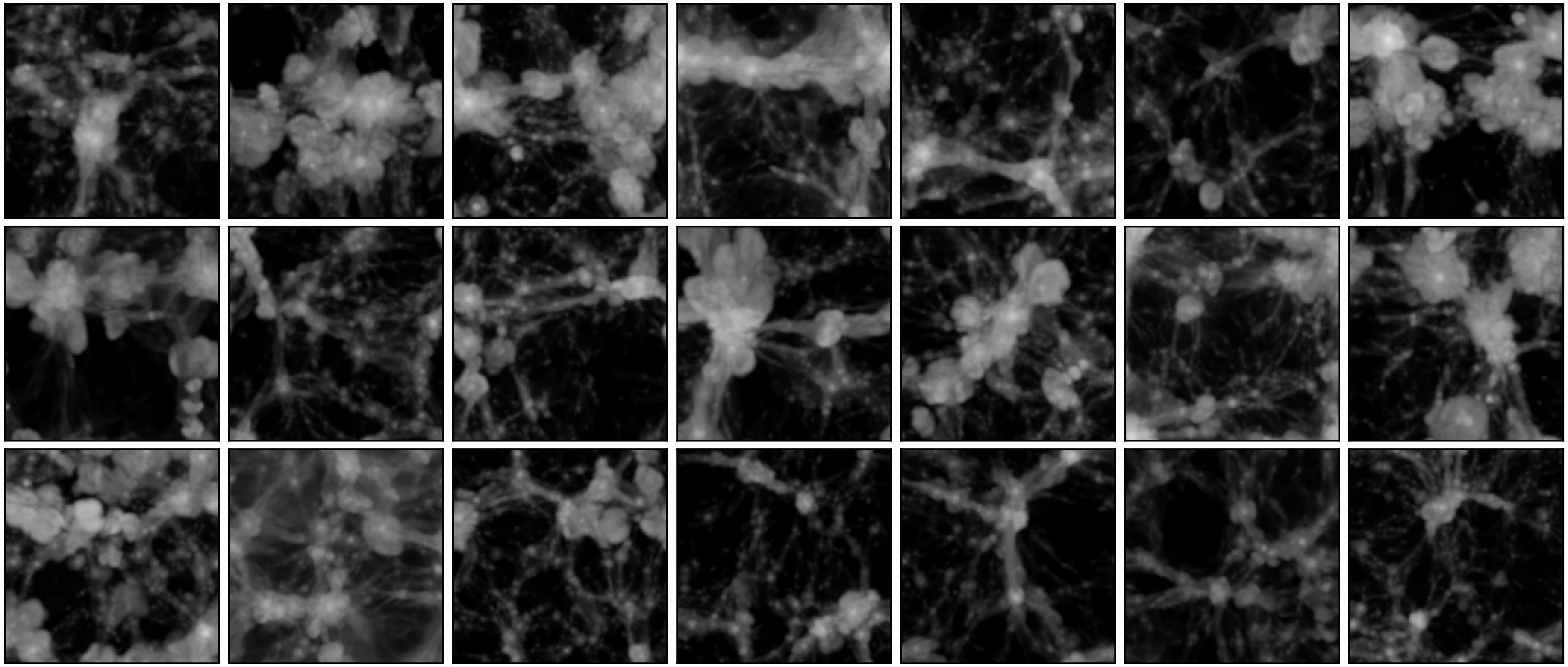

CAMELS
https://www.camel-simulations.org
Cosmology and Astrophysics with
MachinE Learning Simulations


$z = 10.00$


IllustrisTNG
SIMBA
Ramses
CROCODILE
$z = 10.00$
Magneticum
EAGLE
Astrid
Obsidian



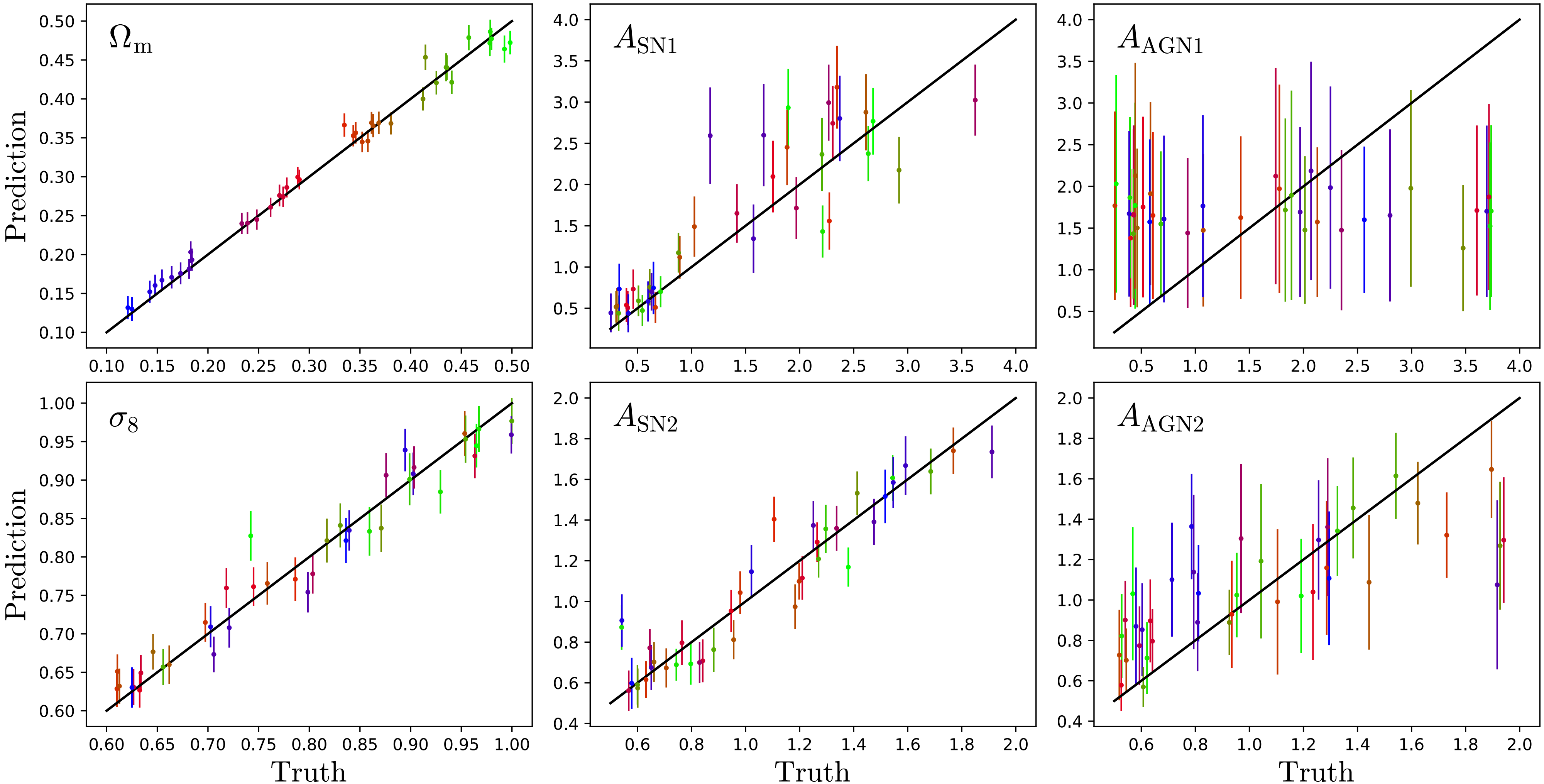
Example I: Gas temperature



Every map has $256{\times}256$ pixels, covers an area of $25{\times}25$ $(h^{-1}\mathrm{Mpc})^2$, and has a different cosmology & astrophysics. 15,000 images in total.

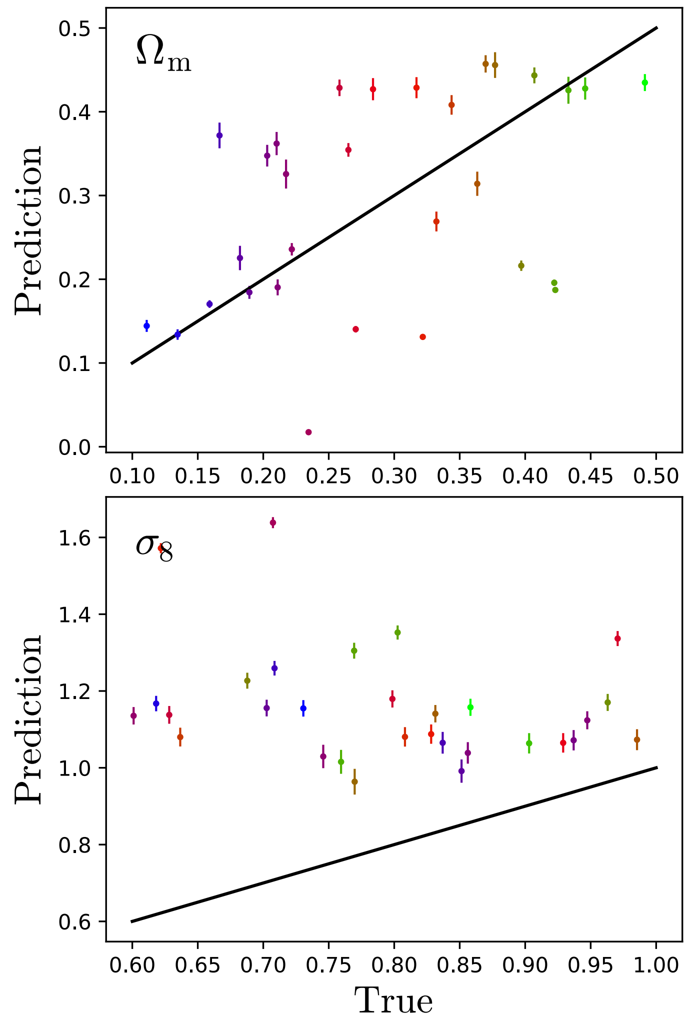
Likelihood-free inference: gas temperature

FVN et al. 2021a



Robustness: gas temperature

FVN et al. 2021a

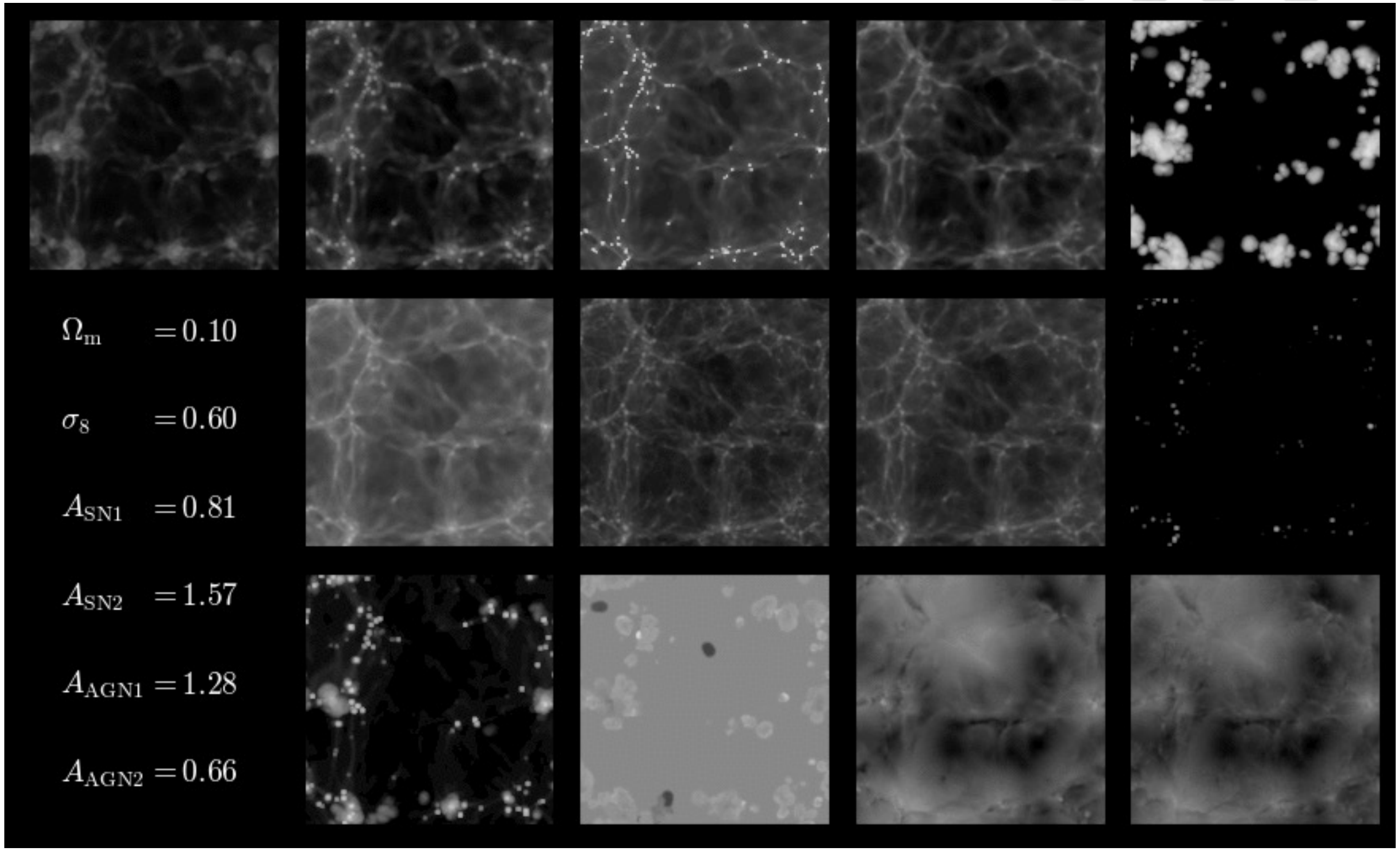


CAMELS Multifield Dataset

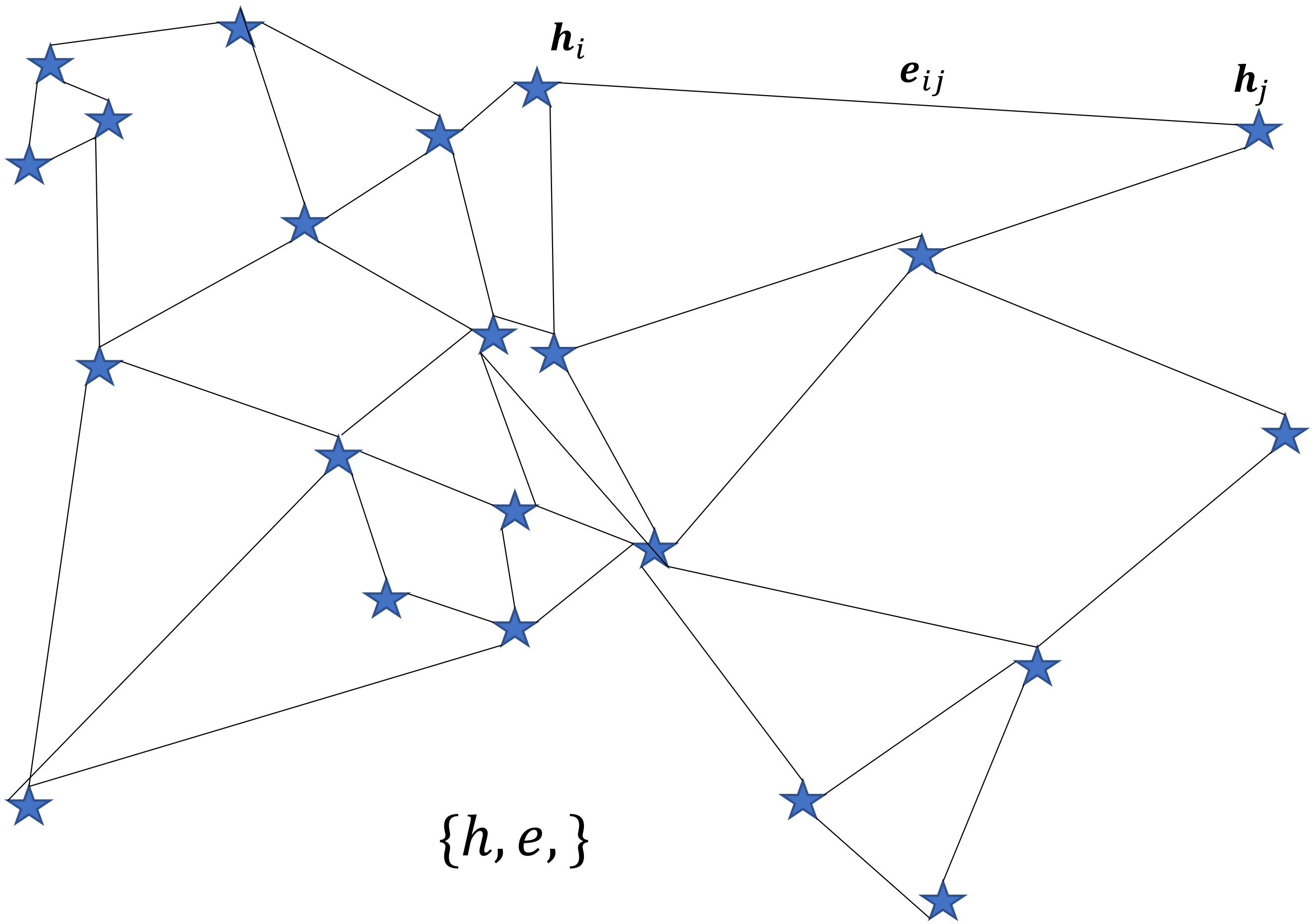
FVN et al. 2021c

https://camels-multifield-dataset.readthedocs.io

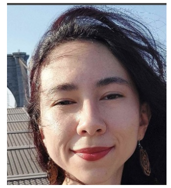
- Hundreds of thousands of labeled 2D maps and 3D grids
- Several redshifts: 0, 0.5, 1, 1.5, 2
- Three different resolutions
- 13 different fields:
    1. Gas density
    2. Gas temperature
    3. Gas metallicity
    4. Gas pressure
    5. Neutral hydrogen density
    6. Electron number density
    7. Dark matter density
    8. Total matter density
    9. Stellar mass density
    10. Gas velocity
    11. Dark matter velocity
    12. Magnetic fields
    13. Mg/Fe
- 70 Tb of data; Publicly available
- The MNIST of cosmology



Graphs and Graph neural networks




Pablo Villanueva-Domingo
(Barcelona)


Natali de Santi
(Flatiron/Sao Paolo)


Helen Shao
(Princeton)

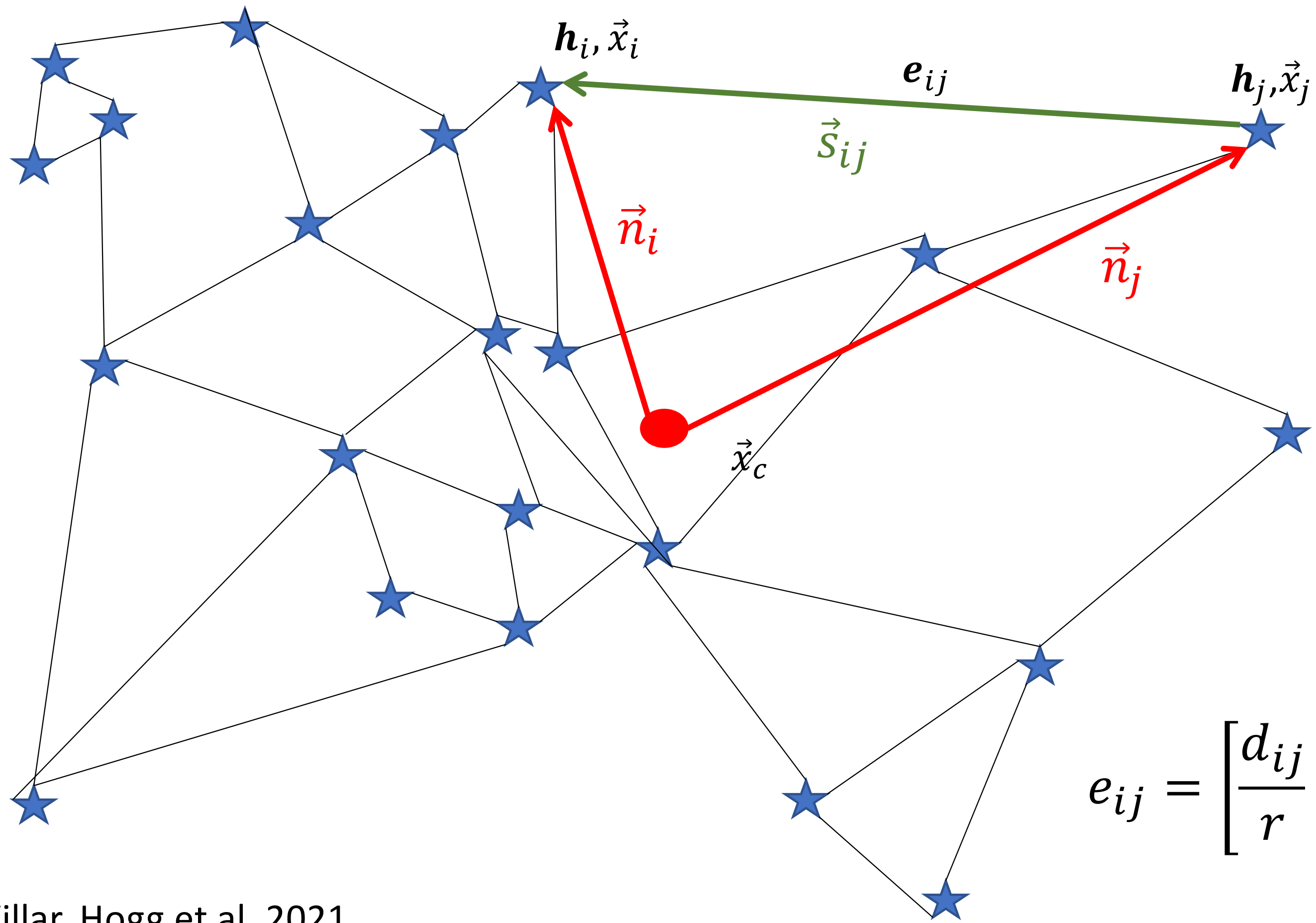
$$\mathbf{e}_{ij}^{(l+1)} = \phi_{l+1}([\mathbf{h}_i^{(l)}, \mathbf{h}_j^{(l)}, \mathbf{e}_{ij}^{(l)}])$$

$$\mathbf{h}_i^{(l+1)} = \psi_{l+1}([\mathbf{h}_i^{(l)}, \bigoplus_{j \in \mathcal{N}_i} \mathbf{e}_{ij}^{(l+1)}, \mathbf{u}])$$

$$\mathbf{y} = \xi([\bigoplus_{i \in \mathcal{G}} \mathbf{h}_i^{(L)}, \mathbf{u}])$$

E(3)-invariant GNN

2204.13713



$$\vec{n}_i = \frac{\vec{x}_i - \vec{x}_c}{|\vec{x}_i - \vec{x}_c|} \qquad \vec{s}_{ij} = \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|}$$

$$\alpha_{ij} = \vec{s}_{ij} \cdot \vec{s}_{ij}$$

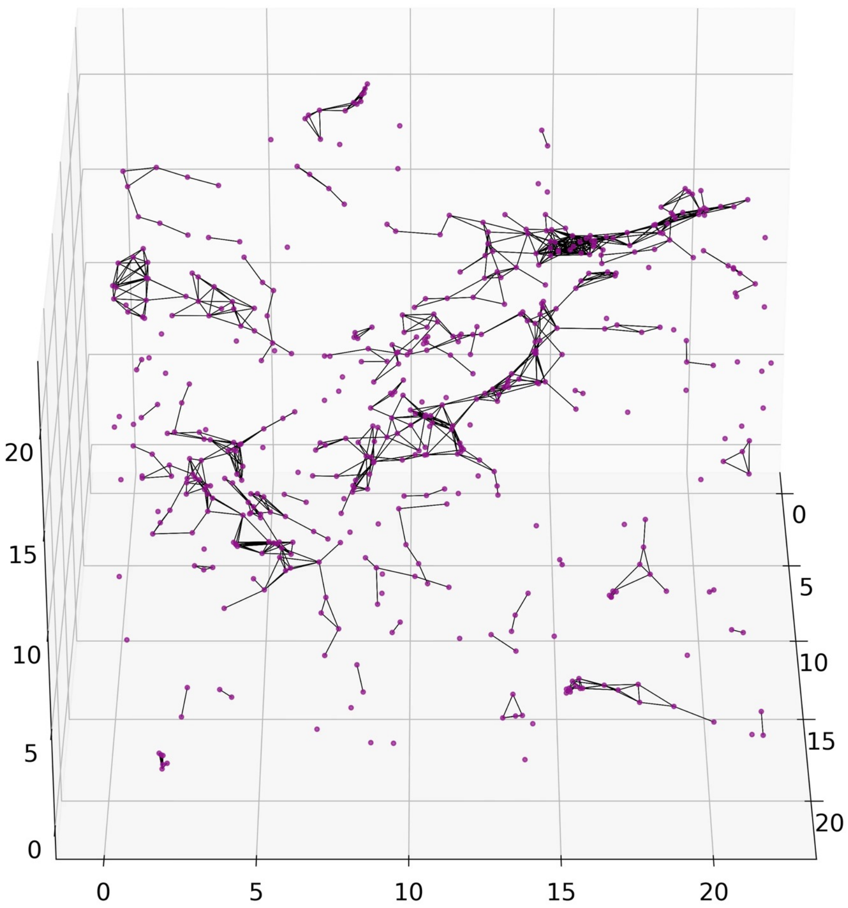
$$e_{ij} = \left[\frac{d_{ij}}{r}, \alpha_{ij}, \beta_{ij}\right] \in \mathbb{R}^3 \qquad \alpha_{ij} = \vec{n}_i \cdot \vec{n}_j$$

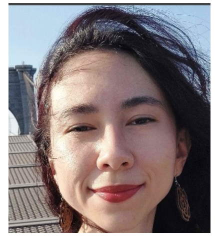
$$\beta_{ij} = \vec{n}_i \cdot \vec{s}_{ij}$$

Villar, Hogg et al. 2021
Scalars are universal

Galaxy catalogs as cosmic graphs

2302.14101

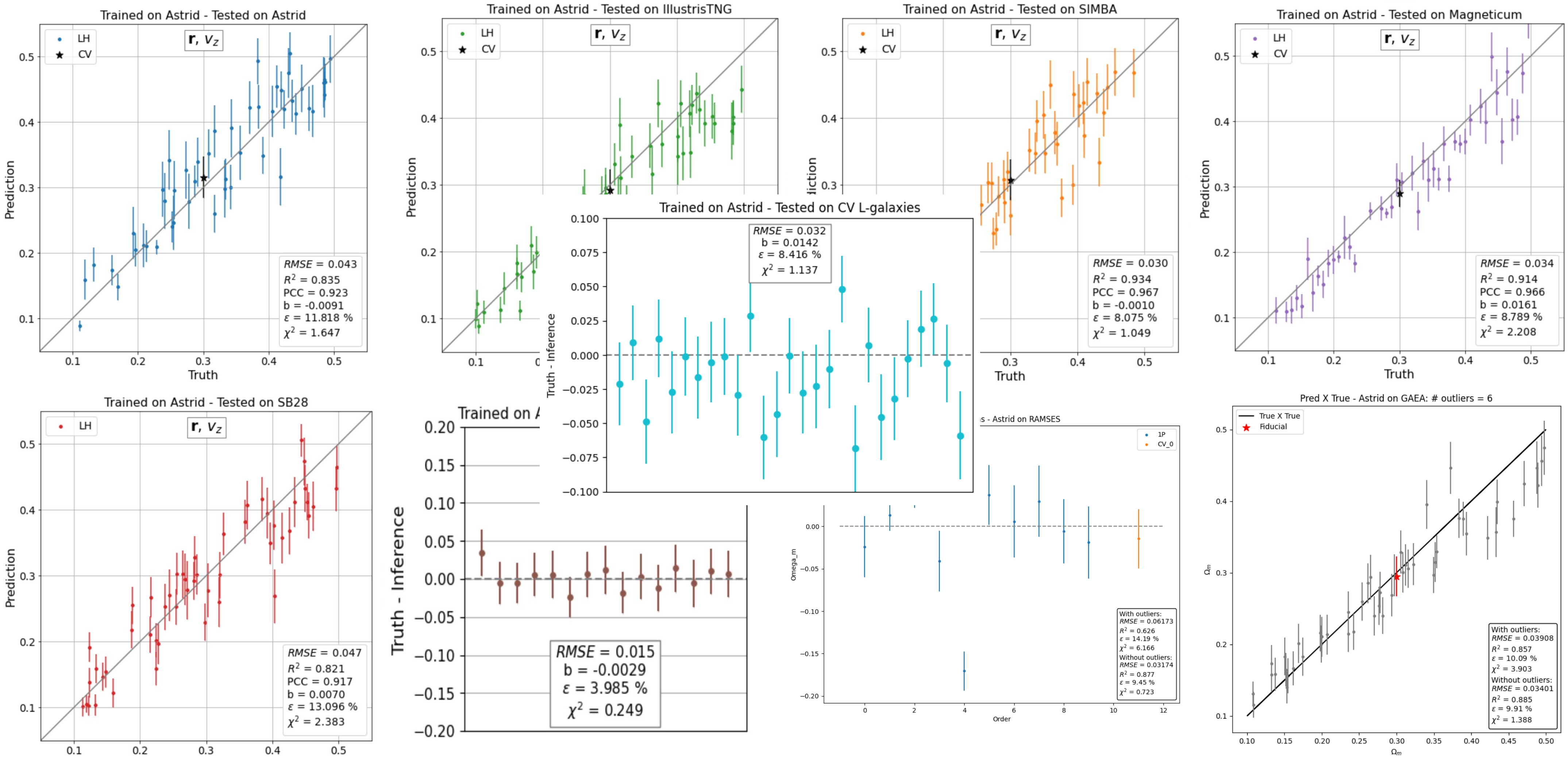




Natali de Santi
(Flatiron/Sao Paolo)

- 2 galaxies are linked if their distance is smaller than r_{link}
- Field-level and no cut on scale: $k_{\max}{\sim}100\ \mathrm{h/Mpc}$
- <u>By construction, rotational and translational invariant</u>

Robust field-level inference with GNNs



Robust field-level inference with GNNs: Interpretability

Helen Shao
(Princeton)

$$\mathbf{e}_{ij}^{(l+1)} = \phi_{l+1}([\mathbf{h}_i^{(l)}, \mathbf{h}_j^{(l)}, \mathbf{e}_{ij}^{(l)}])$$

$$\mathbf{h}_i^{(l+1)} = \psi_{l+1}([\mathbf{h}_i^{(l)}, \bigoplus_{j \in \mathcal{N}_i} \mathbf{e}_{ij}^{(l+1)}, \mathbf{u}])$$

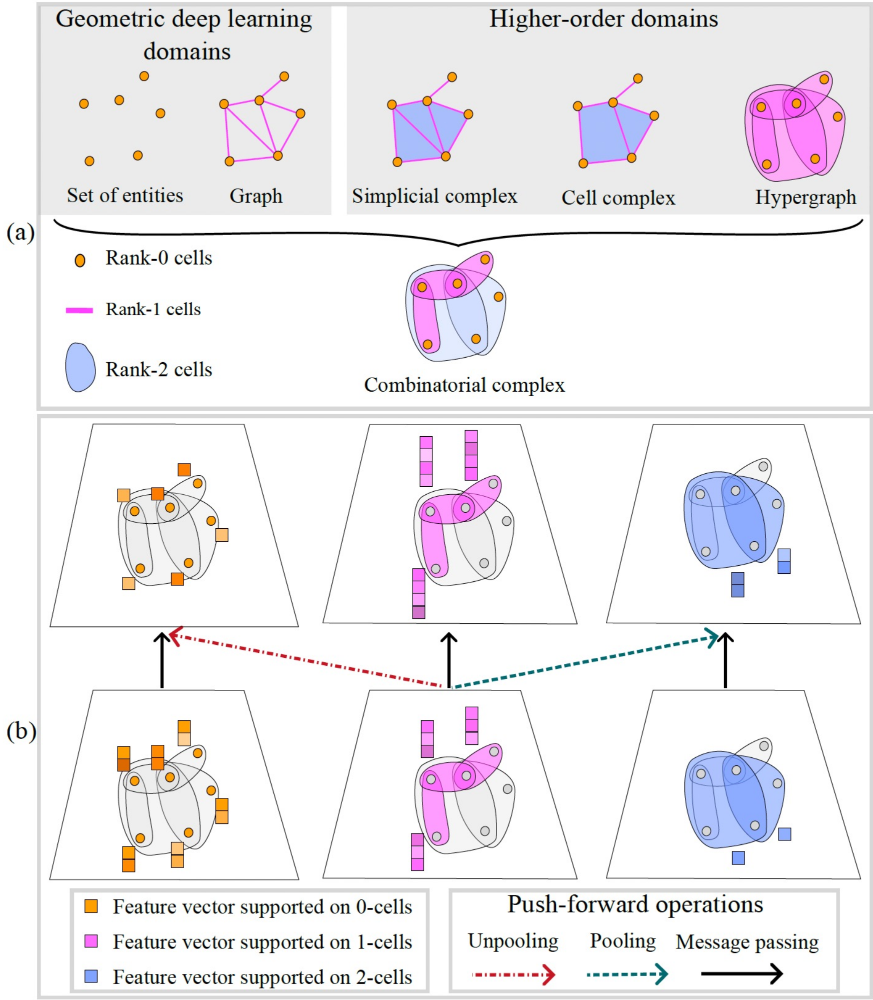
$$\mathbf{y} = \xi([\bigoplus_{i \in \mathcal{G}} \mathbf{h}_i^{(L)}, \mathbf{u}])$$

GNN Component	Formula
Edge Model: $e_1^{(1)}$	$1.32\lvert v_i - v_j + 0.21\rvert + 0.12(v_i - v_j) - 0.12(\gamma_{ij} + \beta_{ij} - 1.73)$
Edge Model: $e_2^{(1)}$	$\lvert 1.62(v_i - v_j) + 0.45\rvert + 1.98(v_i - v_j) + 0.55$
Node Model: $v_1^{(1)}$	$1.21^{v_i}(0.77^{3.29\sum_{j\in\mathcal{N}_j} e_1^{(1)} + \sum_{j\in\mathcal{N}_j} e_2^{(1)}}) + 0.12$
Node Model: $v_1^{(1)} + v_2^{(1)}$	$0.78 - \sqrt{\log(0.16^{\sum_{j\in\mathcal{N}_j} e_2 + \sum_{j\in\mathcal{N}_j} e_1 - 0.41 v_i - 1.05}) + 1.45}$
Final MLP: μ_{Ω_m}	$4 \times 10^{-4} \cdot (-5.5\sum_{i\in\mathcal{G}} v_2^{(1)} + 2.21\sum_{i\in\mathcal{G}} v_1^{(1)} + \lvert 0.96\sum_{i\in\mathcal{G}} v_2^{(1)} + 0.82\sum_{i\in\mathcal{G}} v_1^{(1)}\rvert) - 0.103$

https://arxiv.org/abs/2302.14591

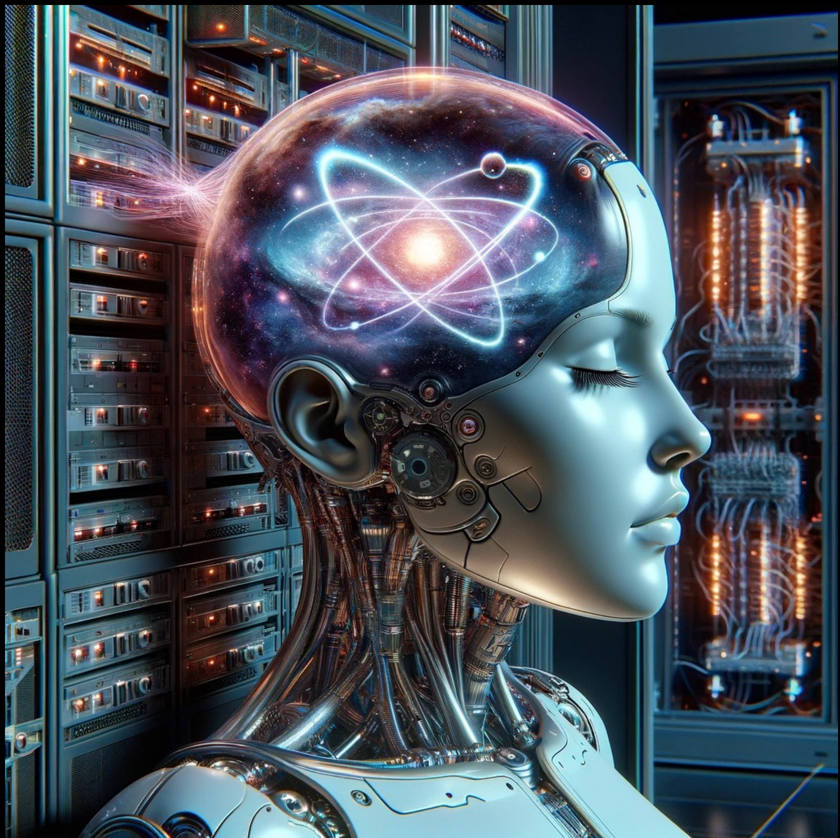
Beyond graphs: Topological deep learning

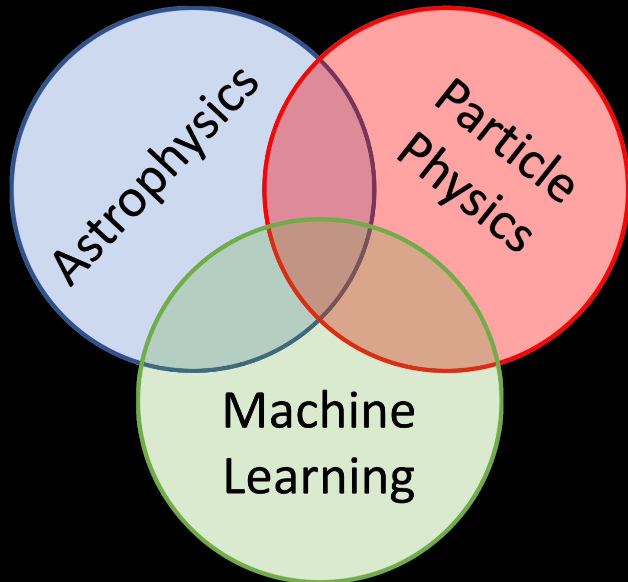
Hajij et al. 2022

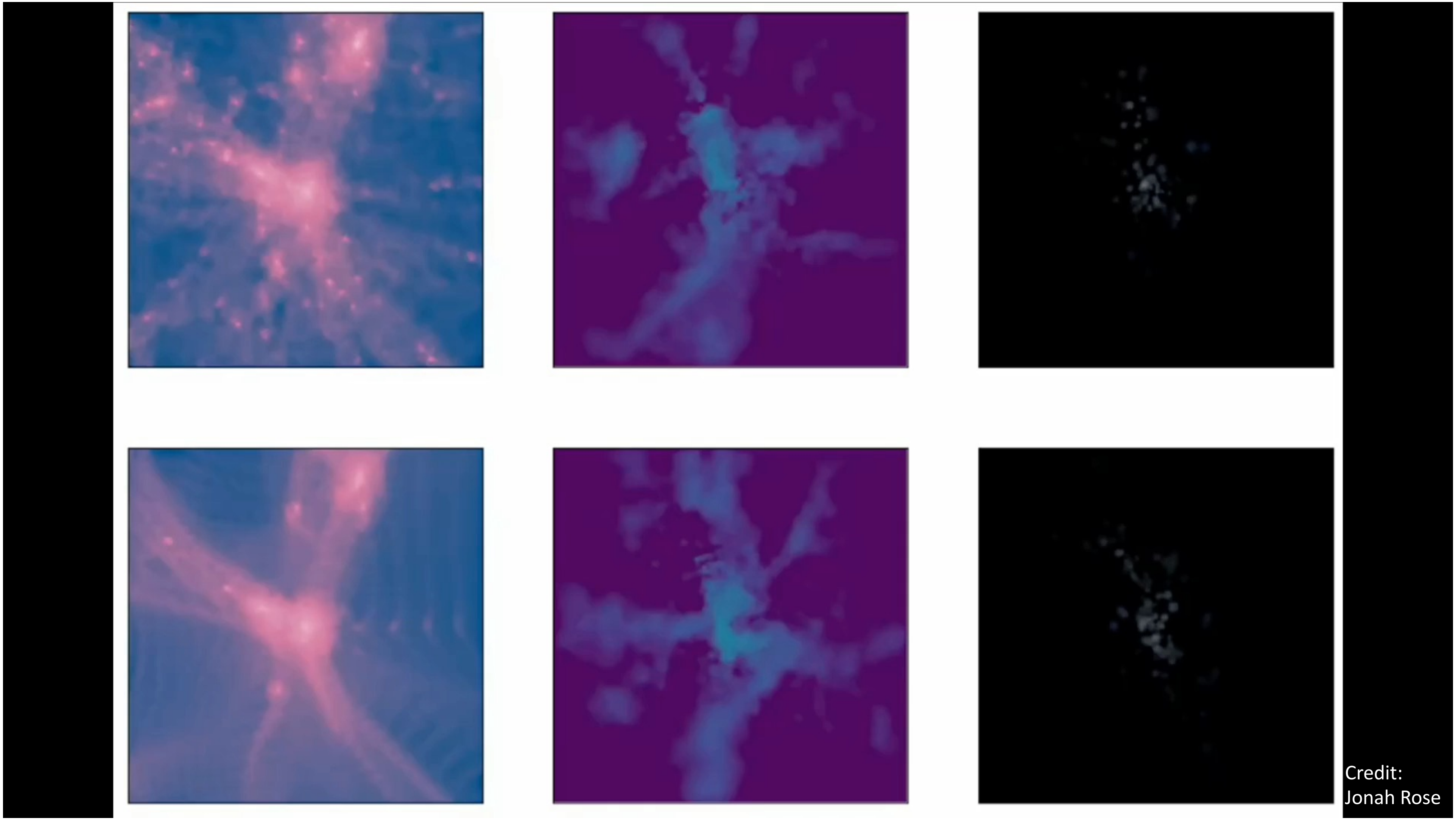


The DREAMS project

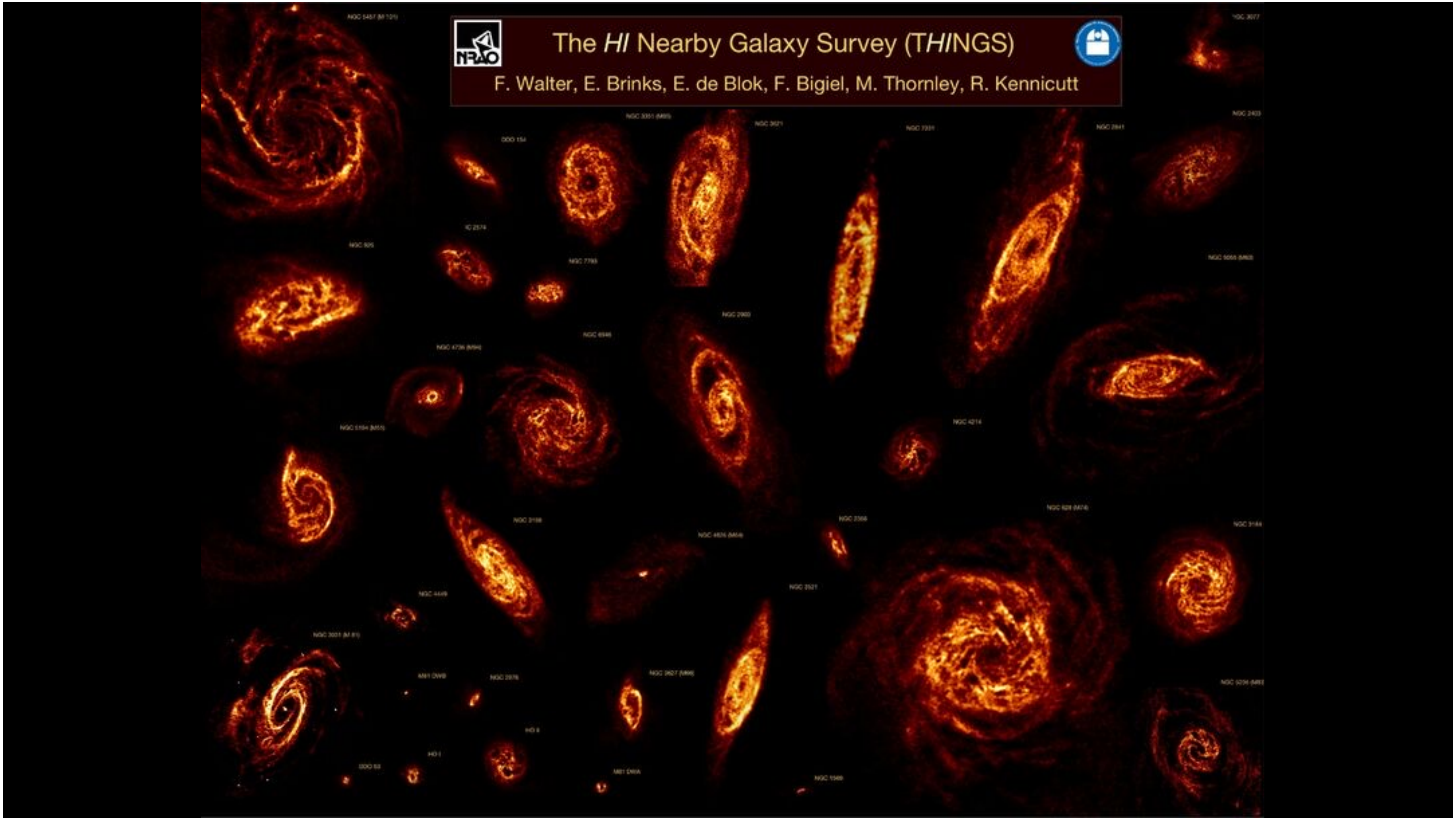
DaRk mattEr with AI and siMulationS





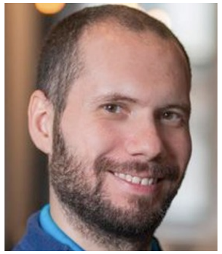

Credit:
Jonah Rose

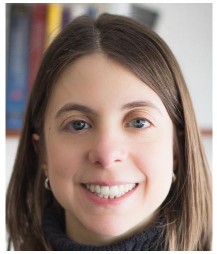

Credit:
Jonah Rose


The *HI* Nearby Galaxy Survey (TH*I*NGS)
F. Walter, E. Brinks, E. de Blok, F. Bigiel, M. Thornley, R. Kennicutt
NRAO


Jonah Rose
(Florida)


Paul Torrey
(Virginia)


Francisco Villaescusa-Navarro
(CCA/Princeton)


Mariangela Lisanti
(Princeton/CCA)


Sandip Roy
(Princeton)


Tri Nguyen
(MIT)


Kassidy Kollmann
(Princeton)

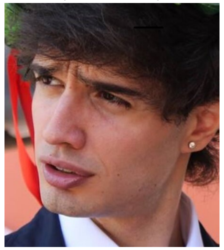

Alex Garcia
(Virginia)


Bonny Wang
(Carnegie Mellon)


Belen Costanza
(La plata)


Akaxia Cruz
(CCA)


Nitya Kallivayalil
(Virginia)


Andrea Caputo
(CERN)


Mikhail Medvedev
(Kansas/IAS/ITC)


Mark Vogelsberger
(MIT)


Arya Farahi
(UT Austin)


Soumyodita Karmakar
(New Mexico)


Francis-Yan Cyr-Racine
(New Mexico)


Cian Roche
(MIT)


Stephanie O'Neil
(MIT)


Shy Genel
(CCA/Columbia)


Lina Necib
(MIT)


Daniel Angles-Alcazar
(UConn)

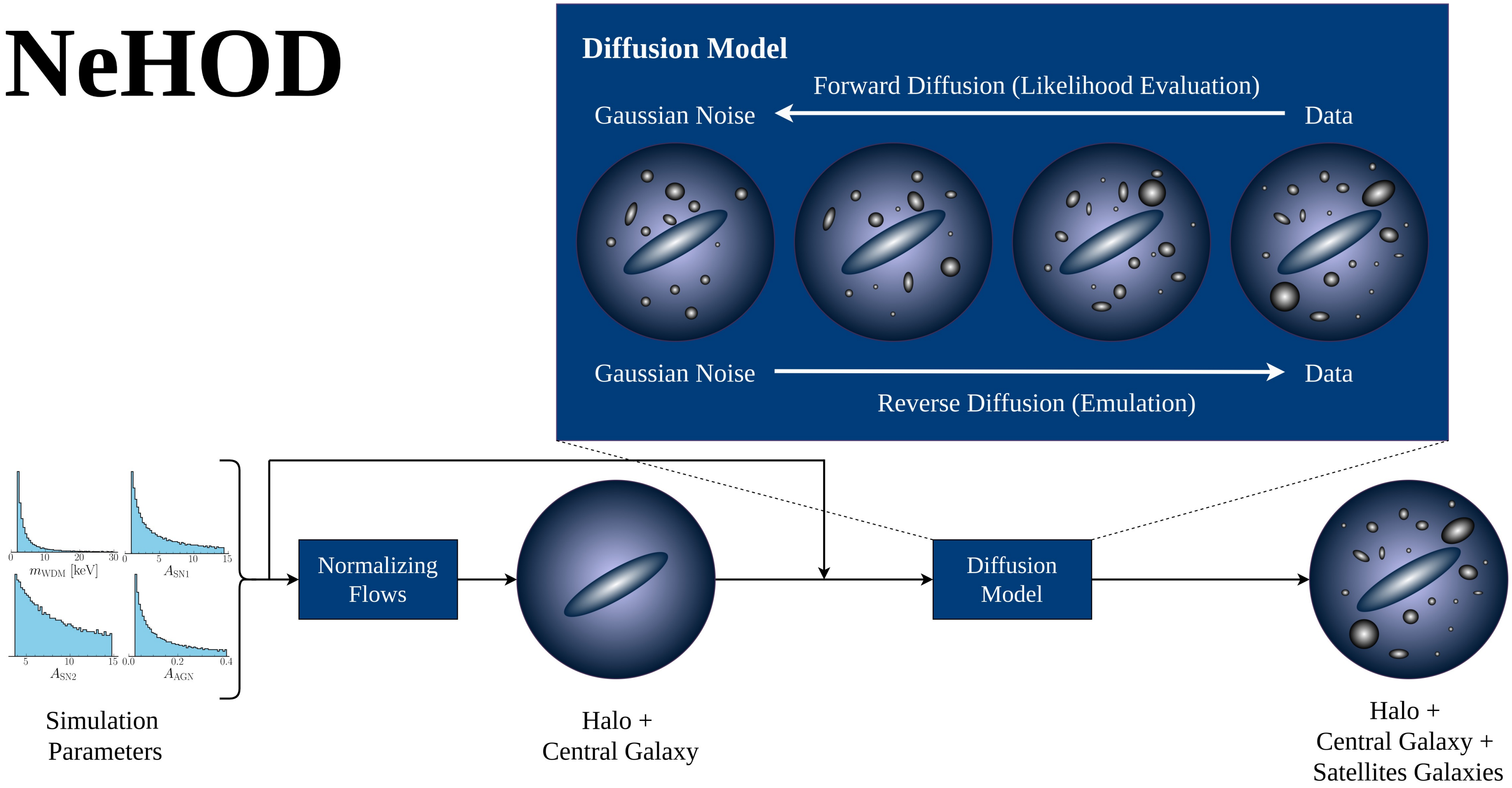

Julian Muñoz
(UT Austin)

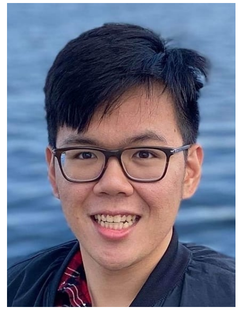

Romain Teyssier
(Princeton)


David Spergel
(Simons Foundation)


Julianne Dalcanton
(CCA)

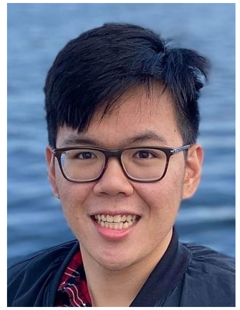
NeHOD



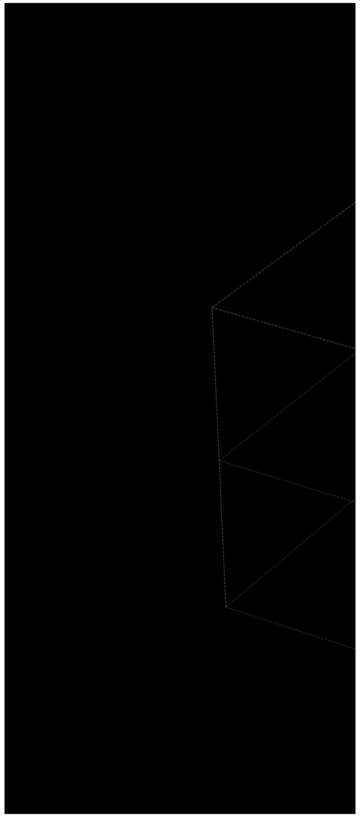


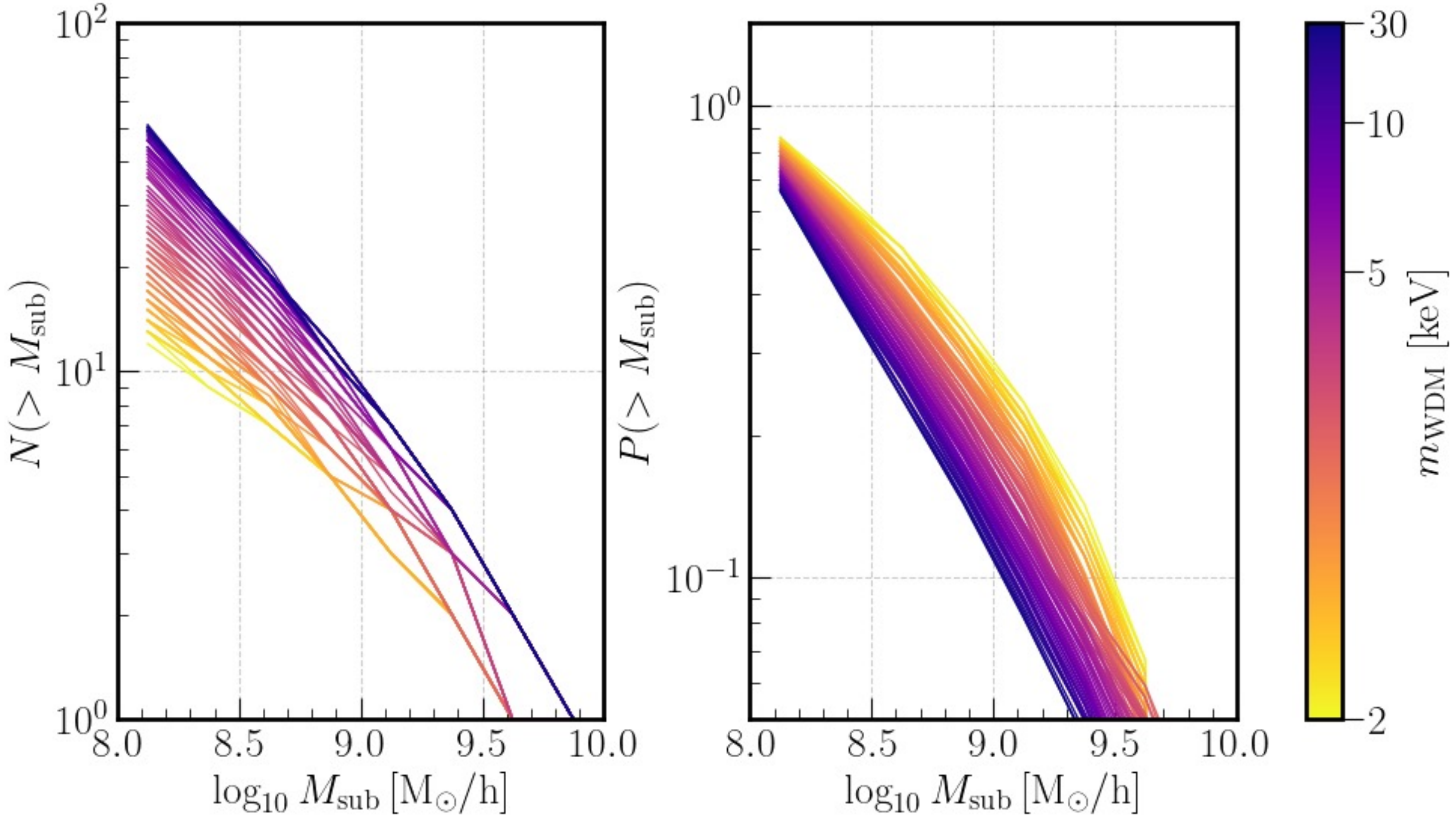
Tri Nguyen
(MIT)

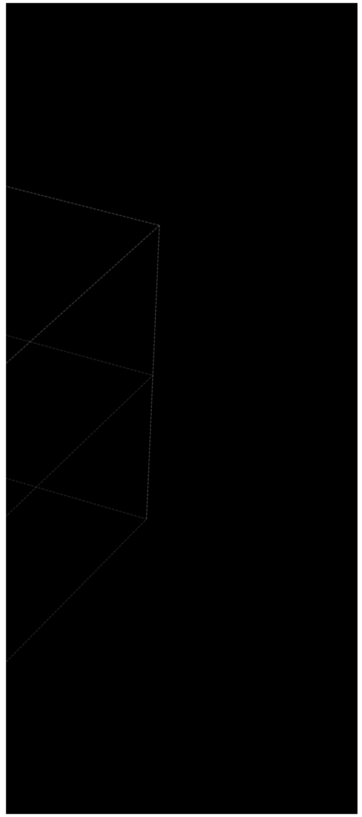
Neuro HOD



Tri Nguyen
(MIT)







Conclusions

- We want to know what are the laws and constituents of the Universe
- Traditionally, we have used analytic techniques for this
- Simulations allow us to make predictions over broader aspects
- Deep learning is a powerful tool to explore massive amounts of data