

The AI Discovery Revolution in Astronomy

Cecilia Garraffo & the AstroAI team

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Bill Freeman

Melanie Weber

David Alvarez-Melis

Robin Walters

Katie Bouman





Fig: Ashley Miller



Fig: Ashley Villar

We will observe more data in one year than all our observations so far

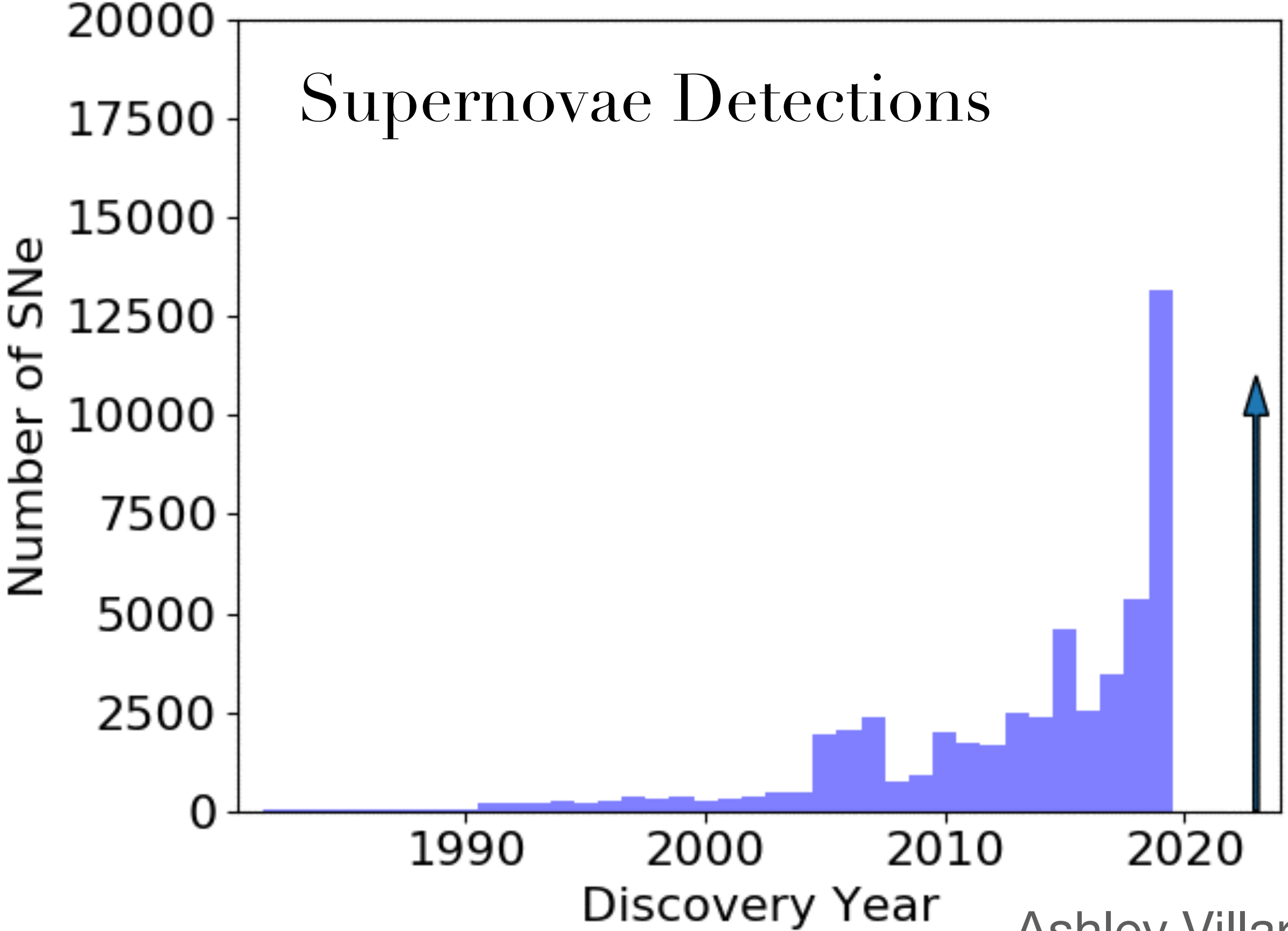
Vera Rubin Observatory

A night sky photograph showing the Milky Way galaxy in full view, stretching across the upper two-thirds of the frame. The galaxy's core is bright and yellowish, with various spiral arms and dark dust lanes. In the lower right foreground, the Vera Rubin Observatory building is visible, a large, multi-tiered structure with a white, angular facade. Some windows are illuminated from within, showing warm yellow and red light. The building is situated on a dark, rocky hillside. The sky is filled with numerous stars, and a faint horizon line is visible at the bottom left.

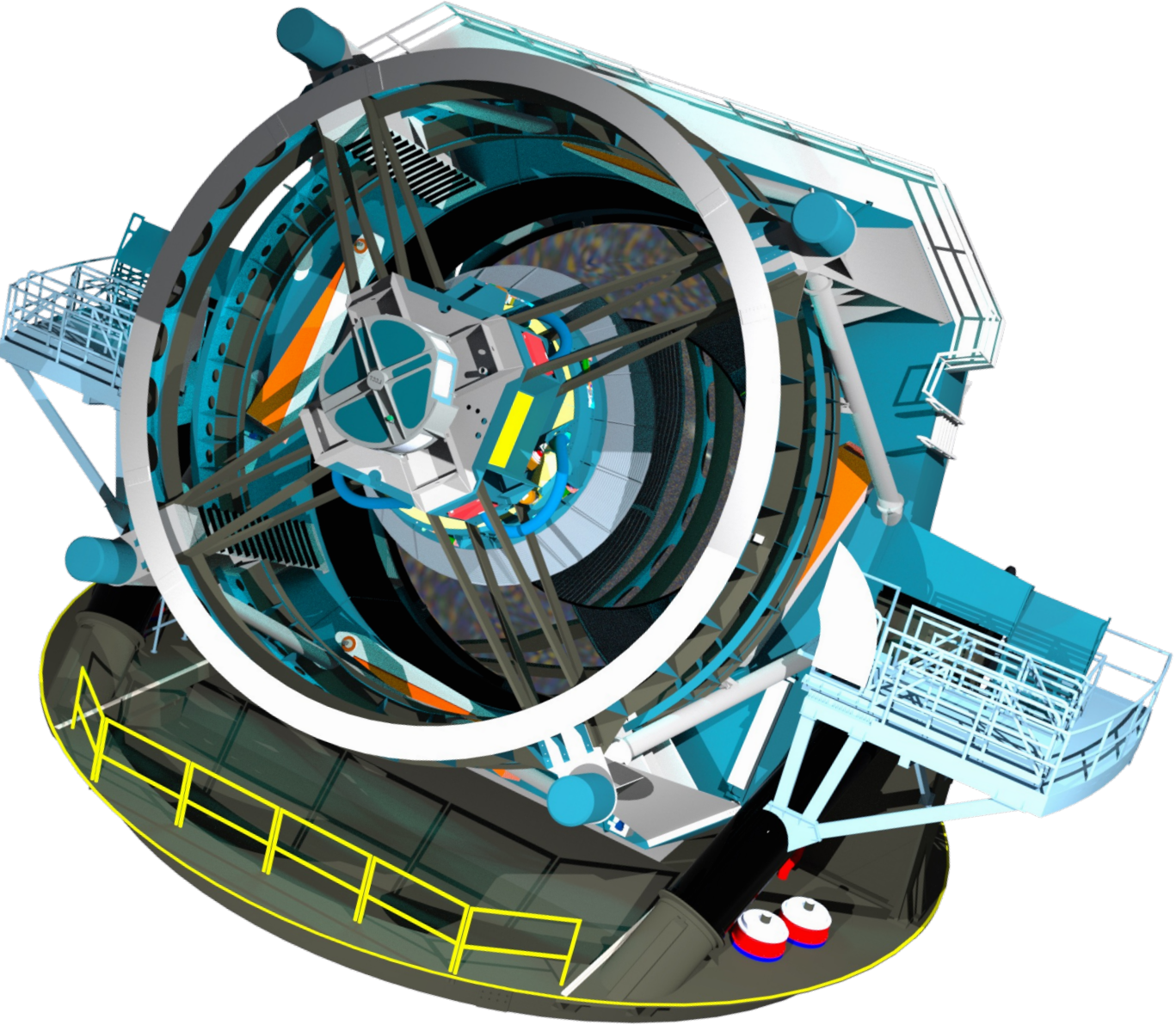
Fig: Ashley Villar

We will observe more data in one year than all our observations so far

Big Data Revolution in *Astrophysics*



Ashley Villar





Radio

Infrared

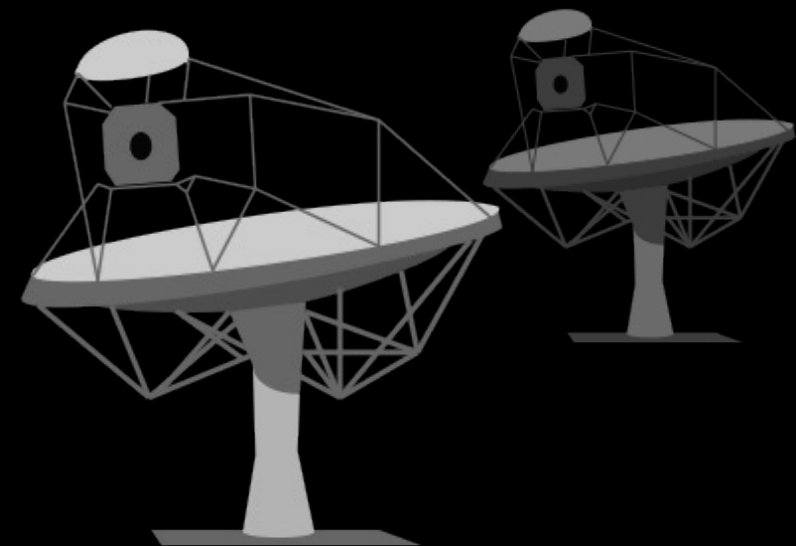
Visible

Ultra-violet

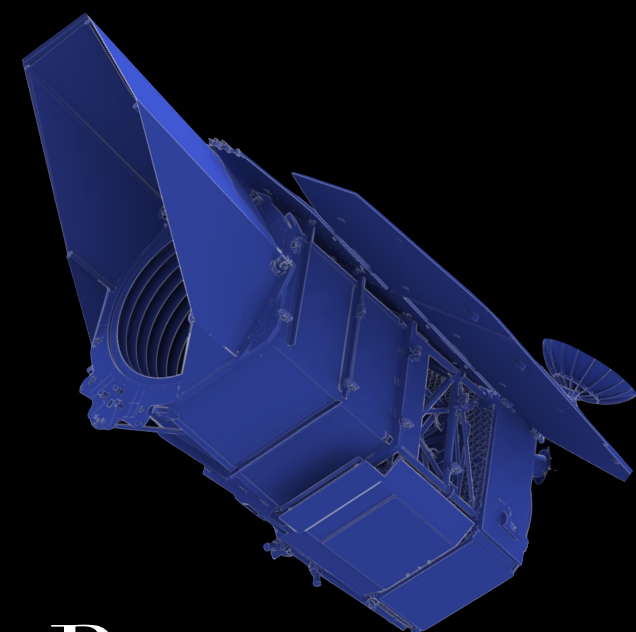
X-ray



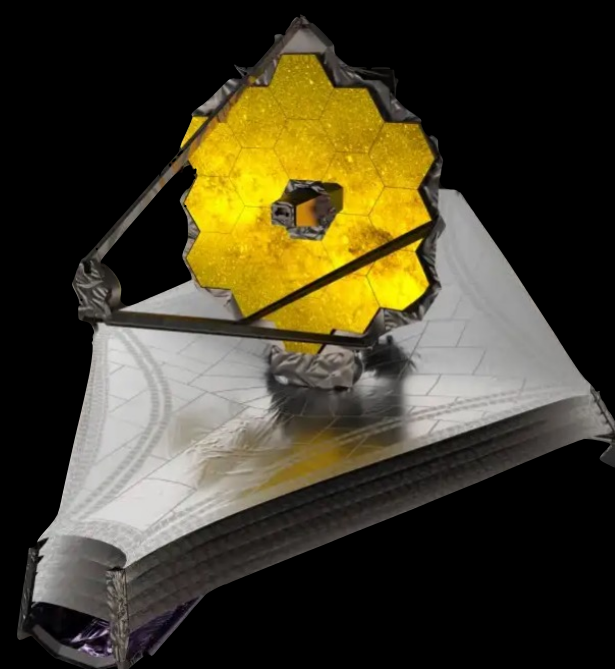
Spectrum



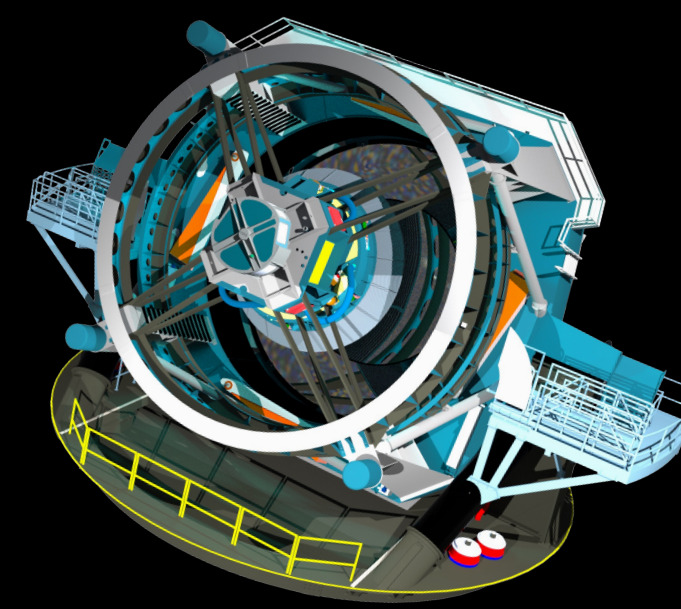
Ska



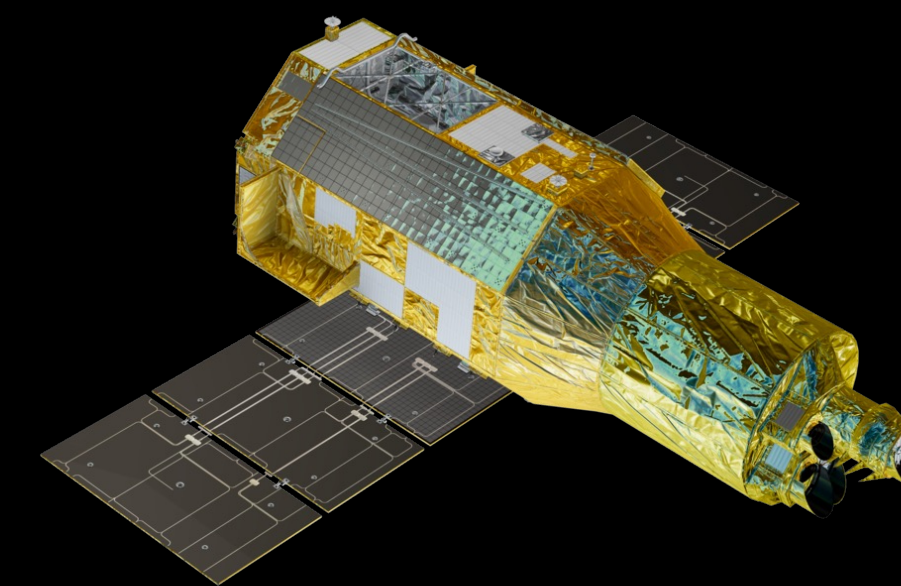
Roman



Webb



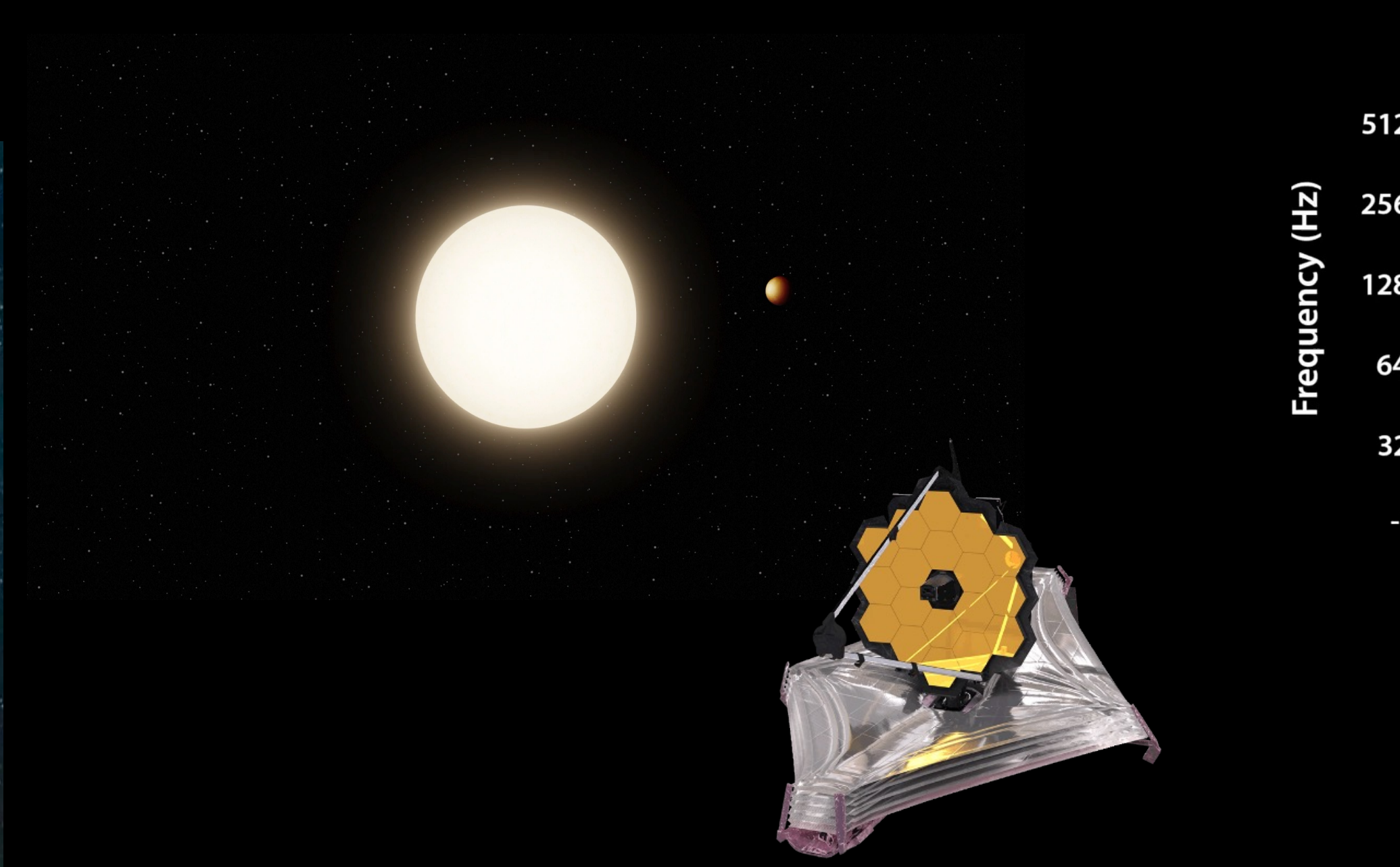
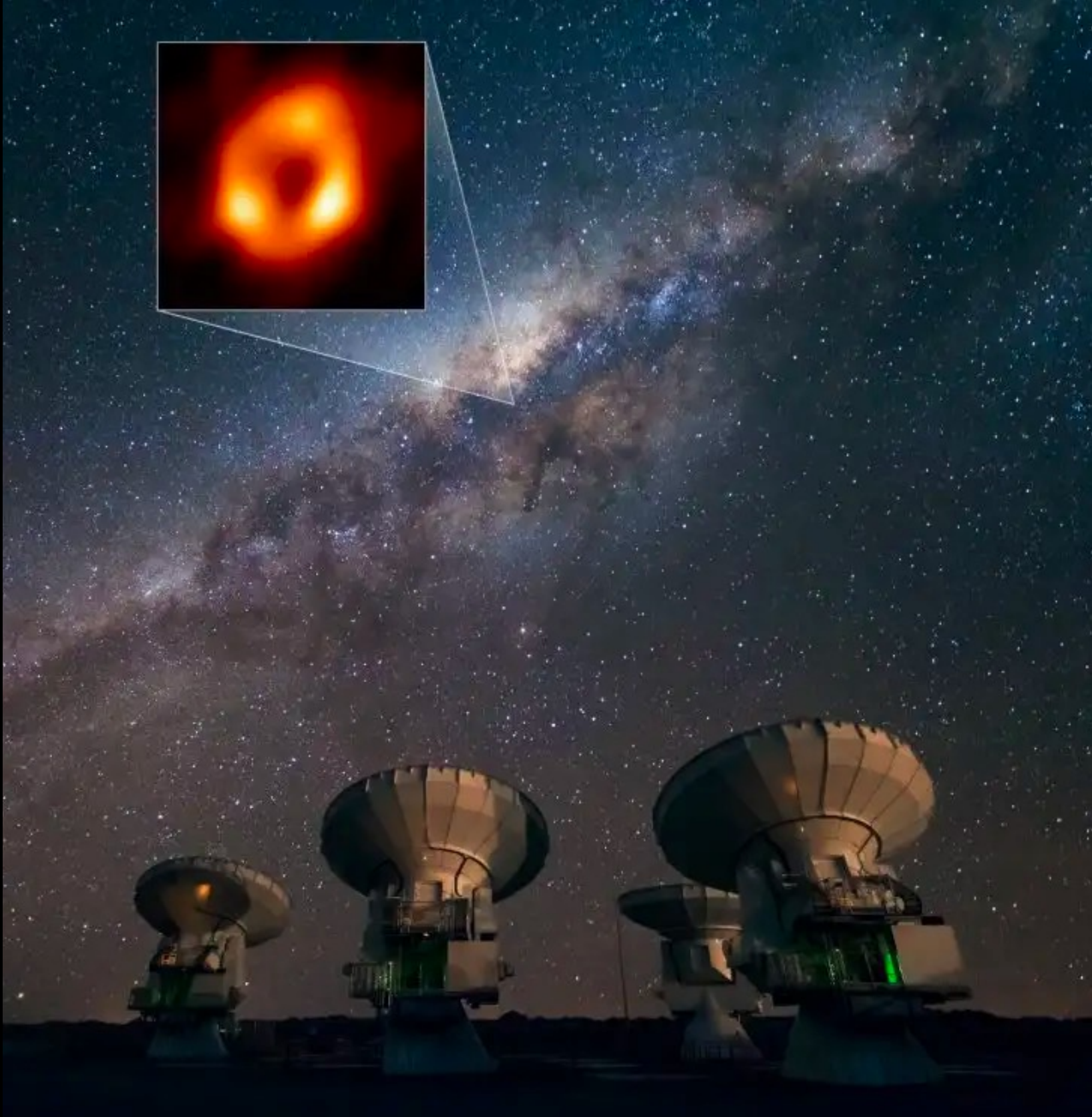
Rubin



Rayos X

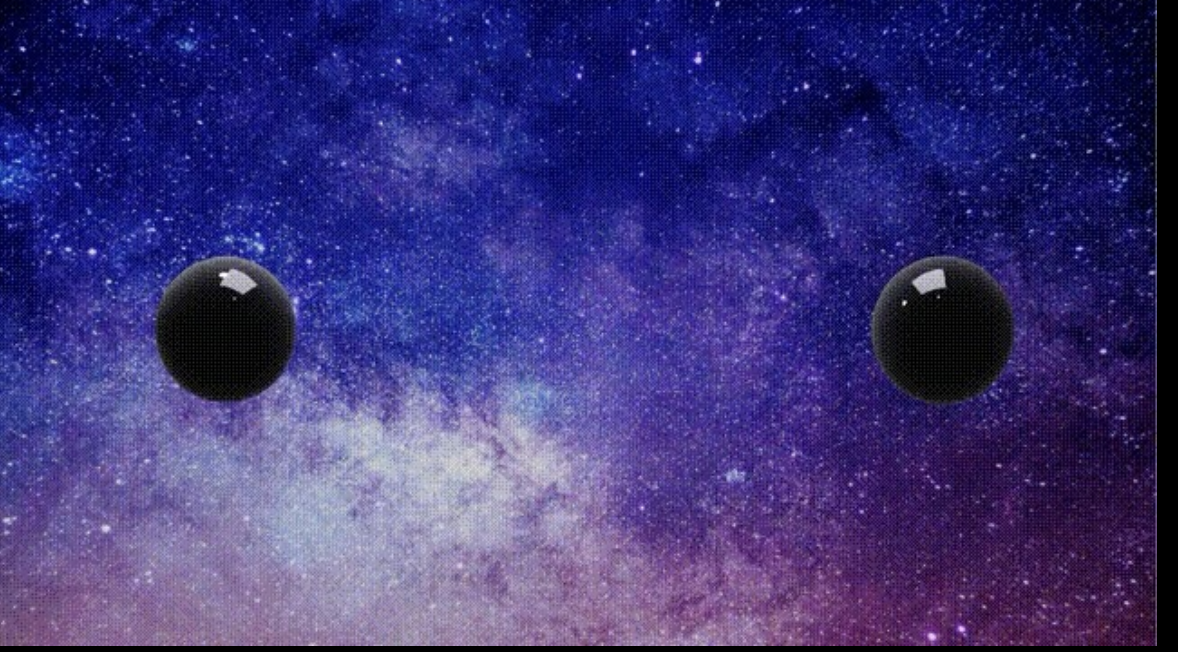
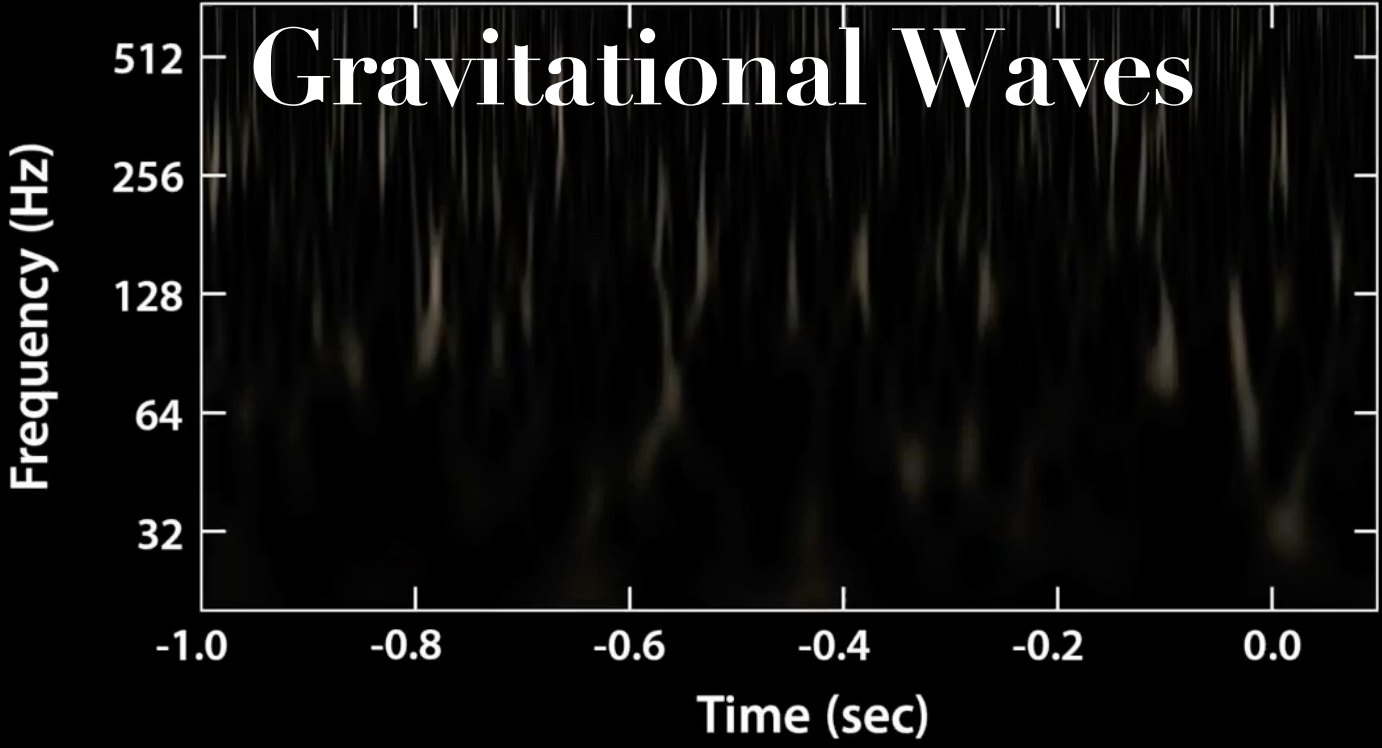
New Windows into the Universe

Event Horizon Telescope



James Webb Space Telescope

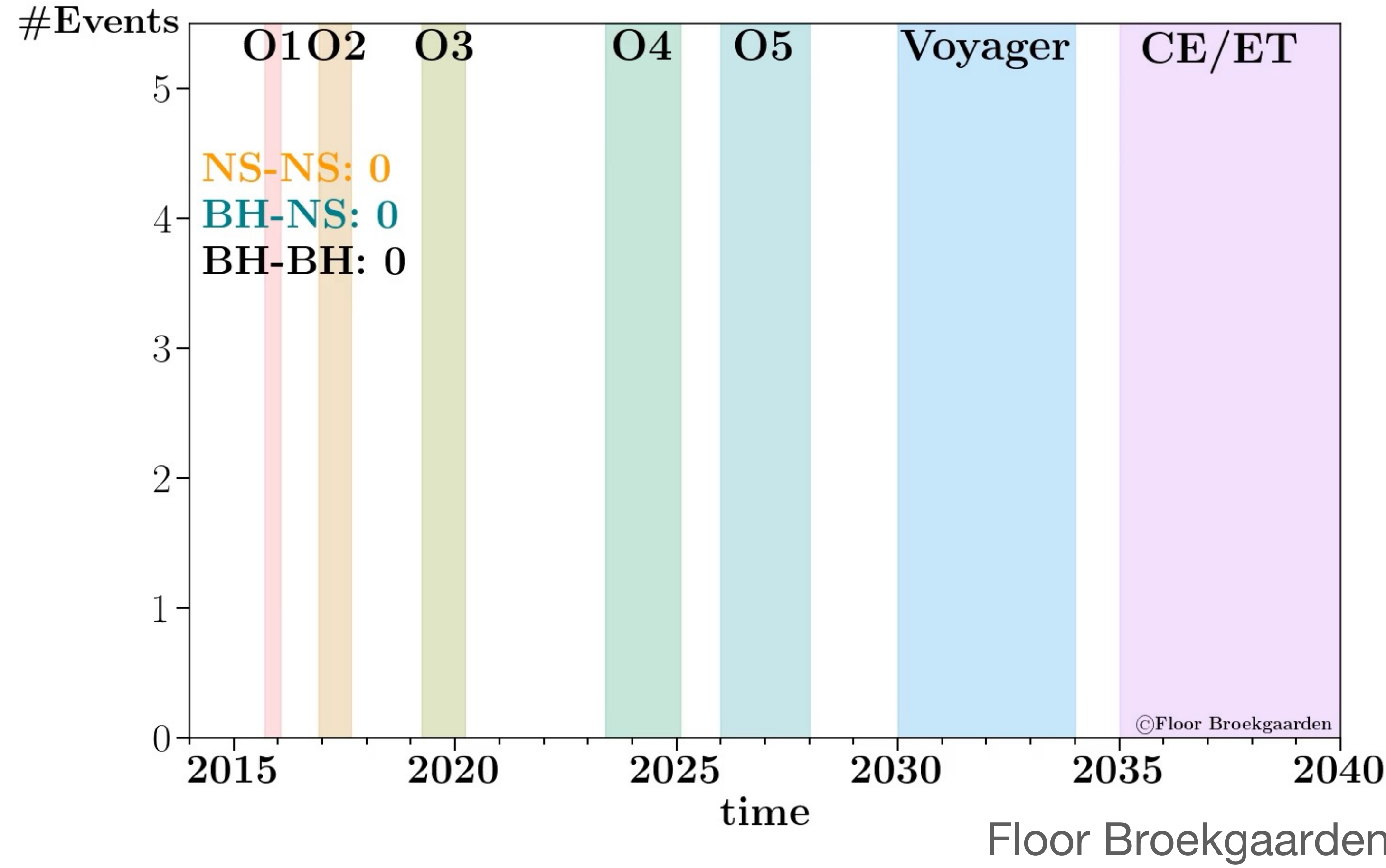
September 14, 2015 Hanford Observatory
Natural Pitch

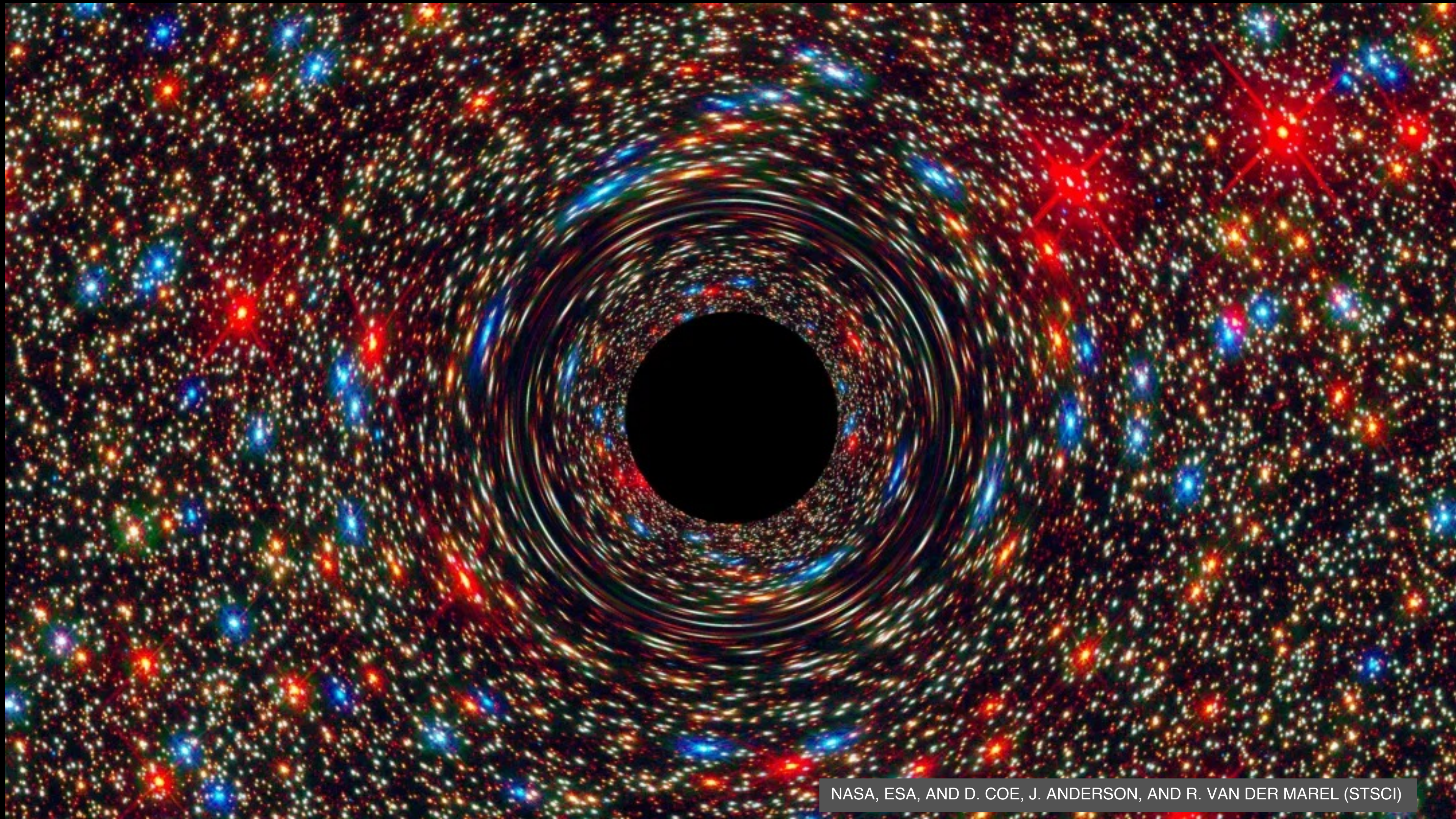


NEUTRINOS Ice Cube

New Windows into the Universe

Gravitational Wave Detections





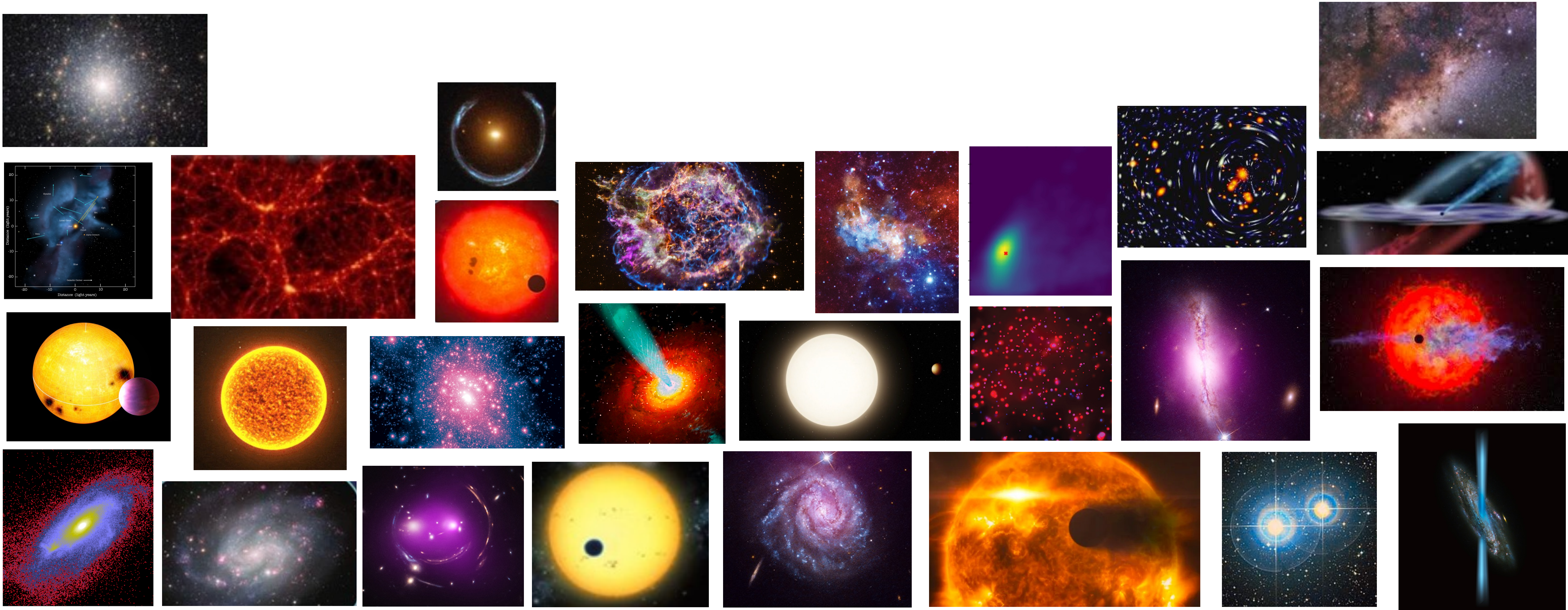
NASA, ESA, AND D. COE, J. ANDERSON, AND R. VAN DER MAREL (STSCI)

Search for the unexpected

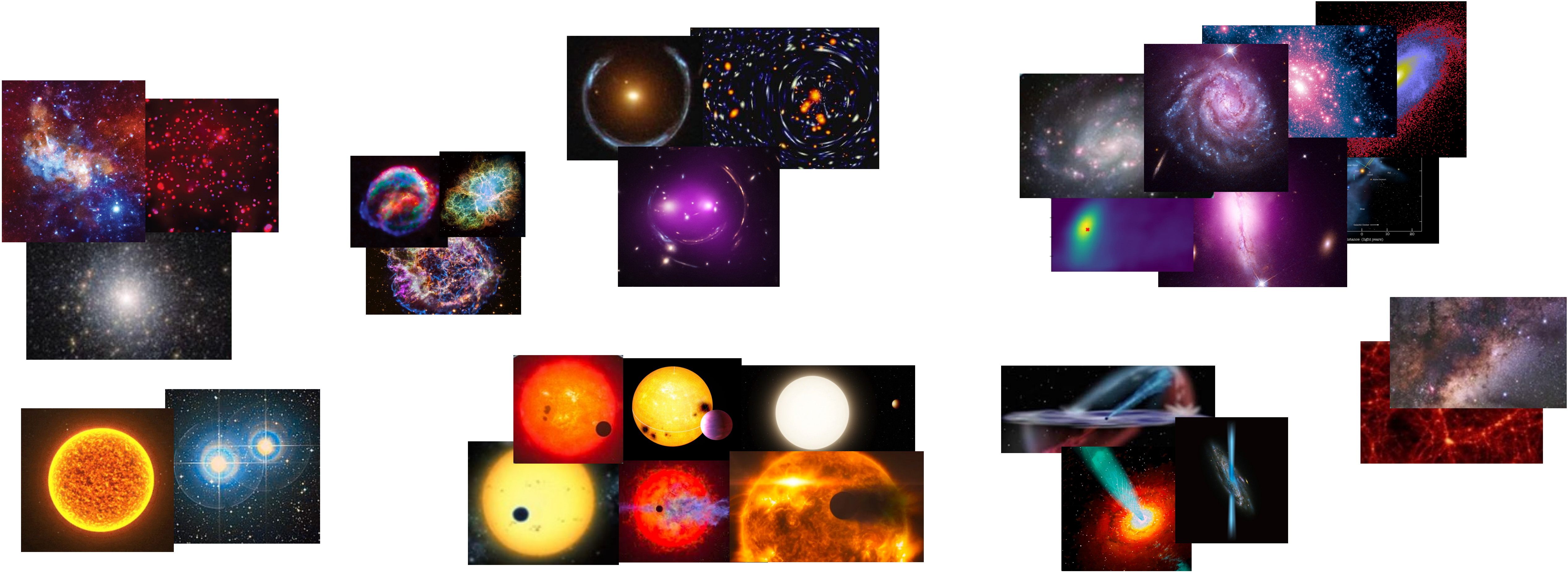


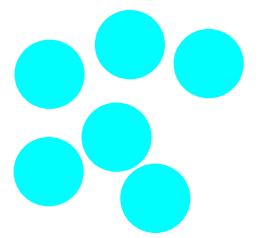
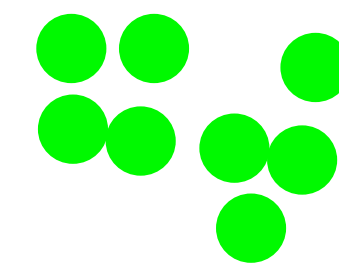
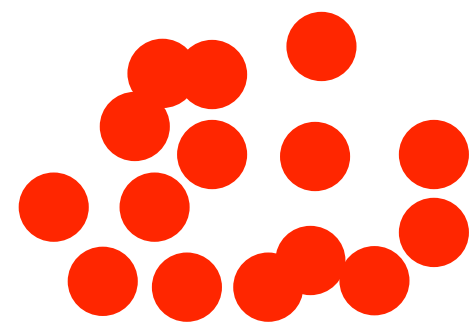
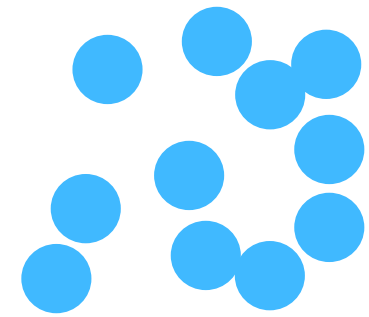
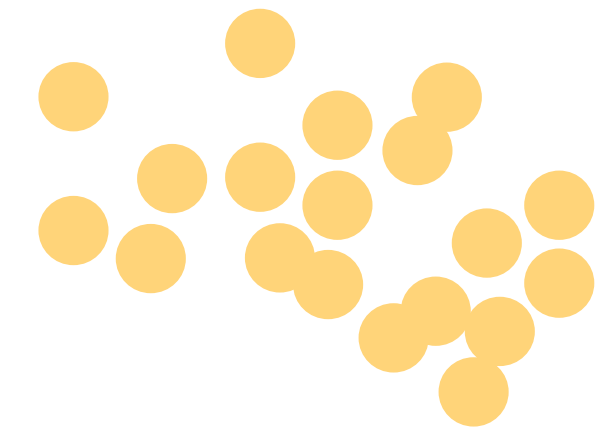
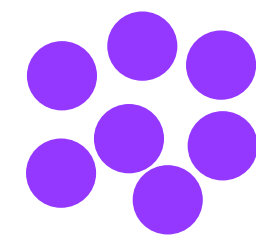
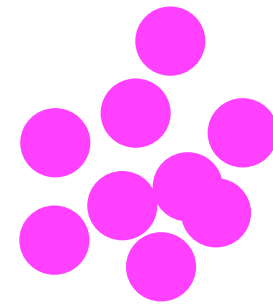
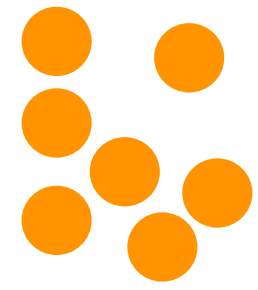
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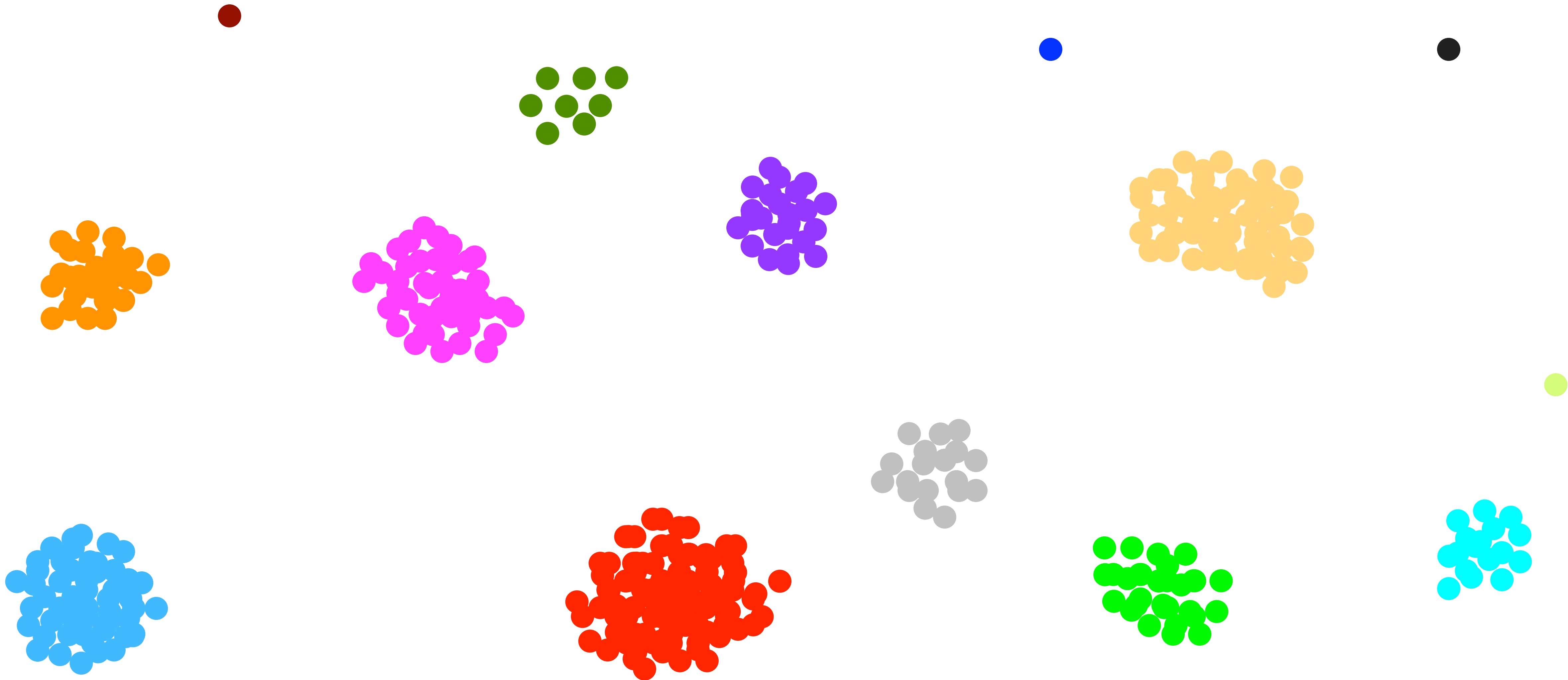
Search for the unexpected



Search for the unexpected



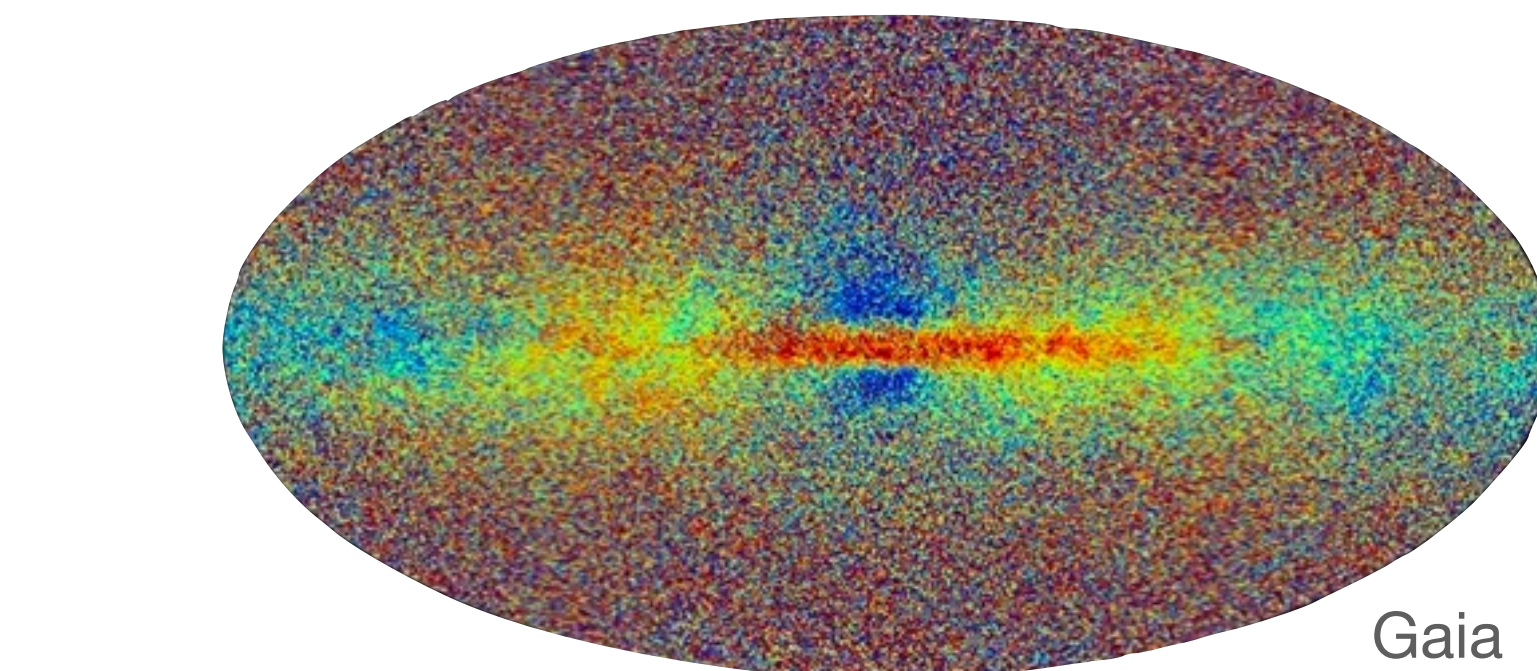




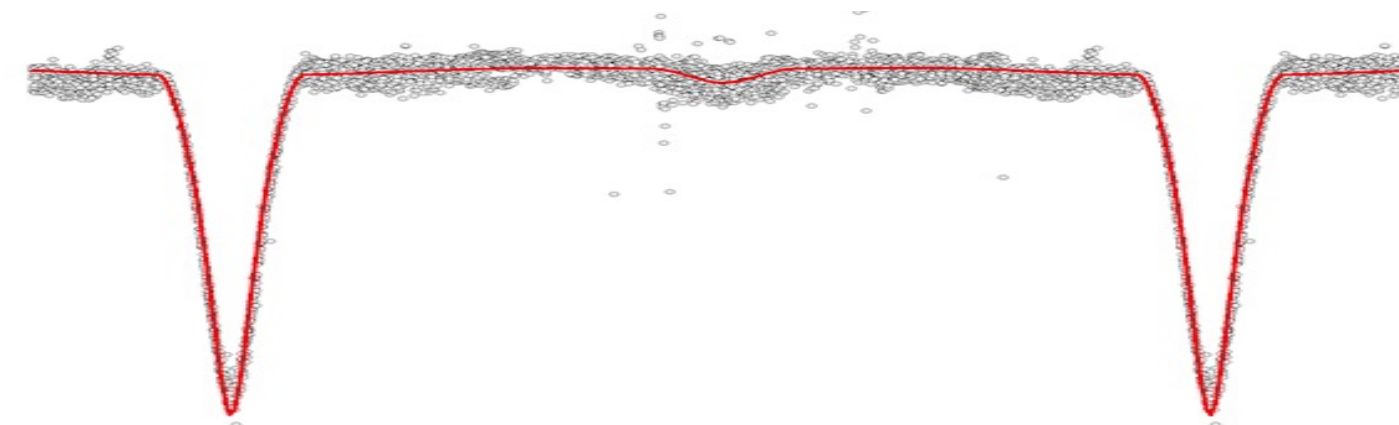
The need for new AI for Astronomy

1. The Complex Nature of Astronomical Data

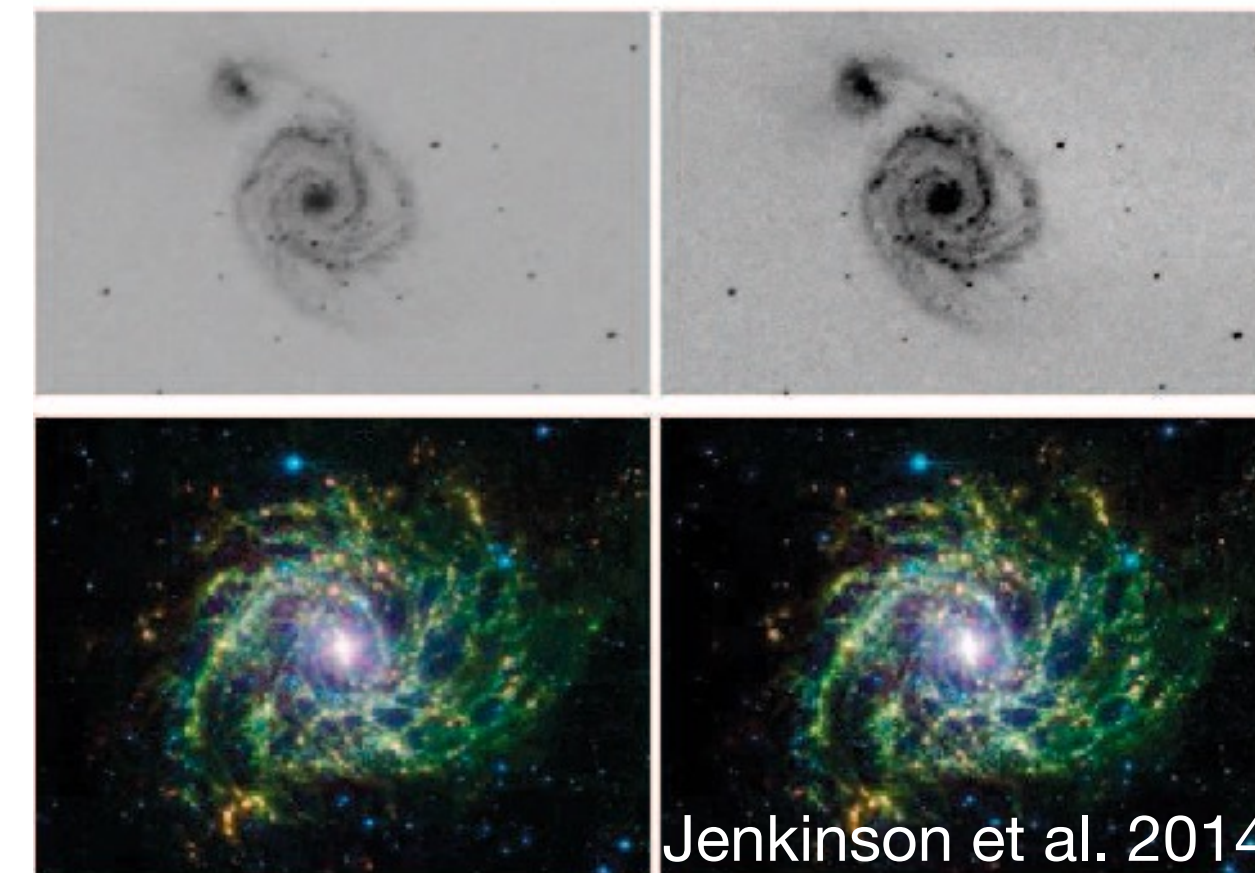
The Complex Nature of Astronomical Data



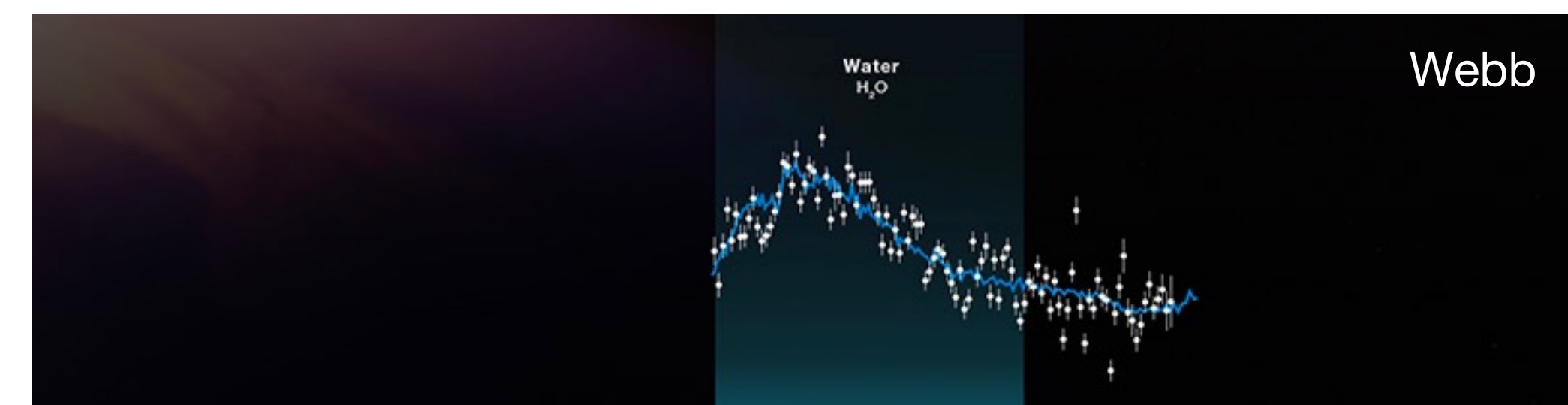
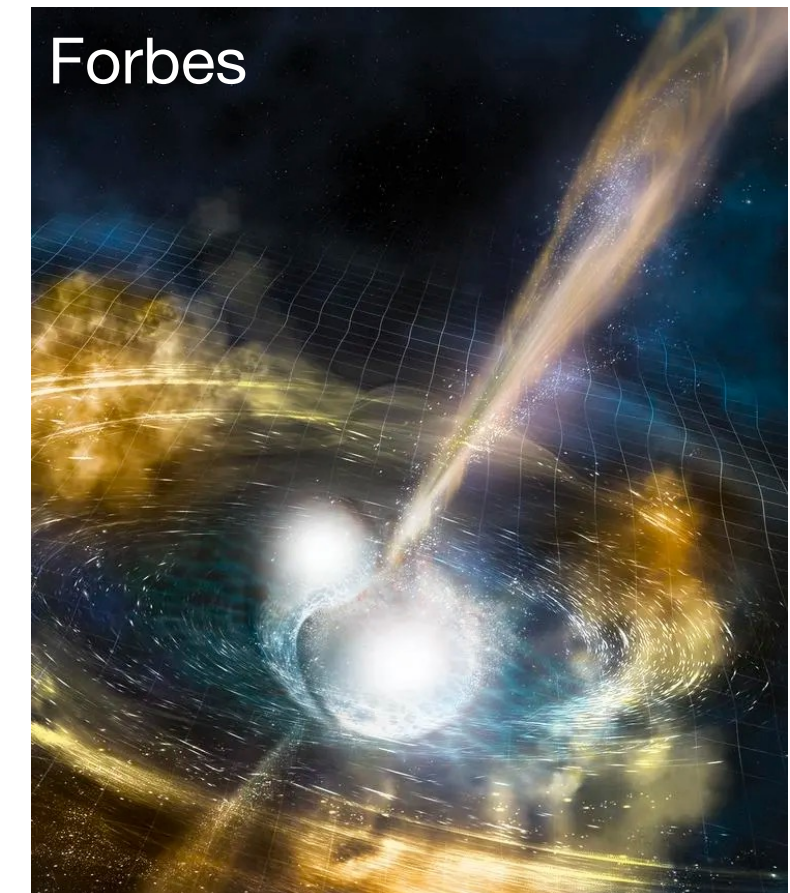
Gaia



Manzoori et al. 2017

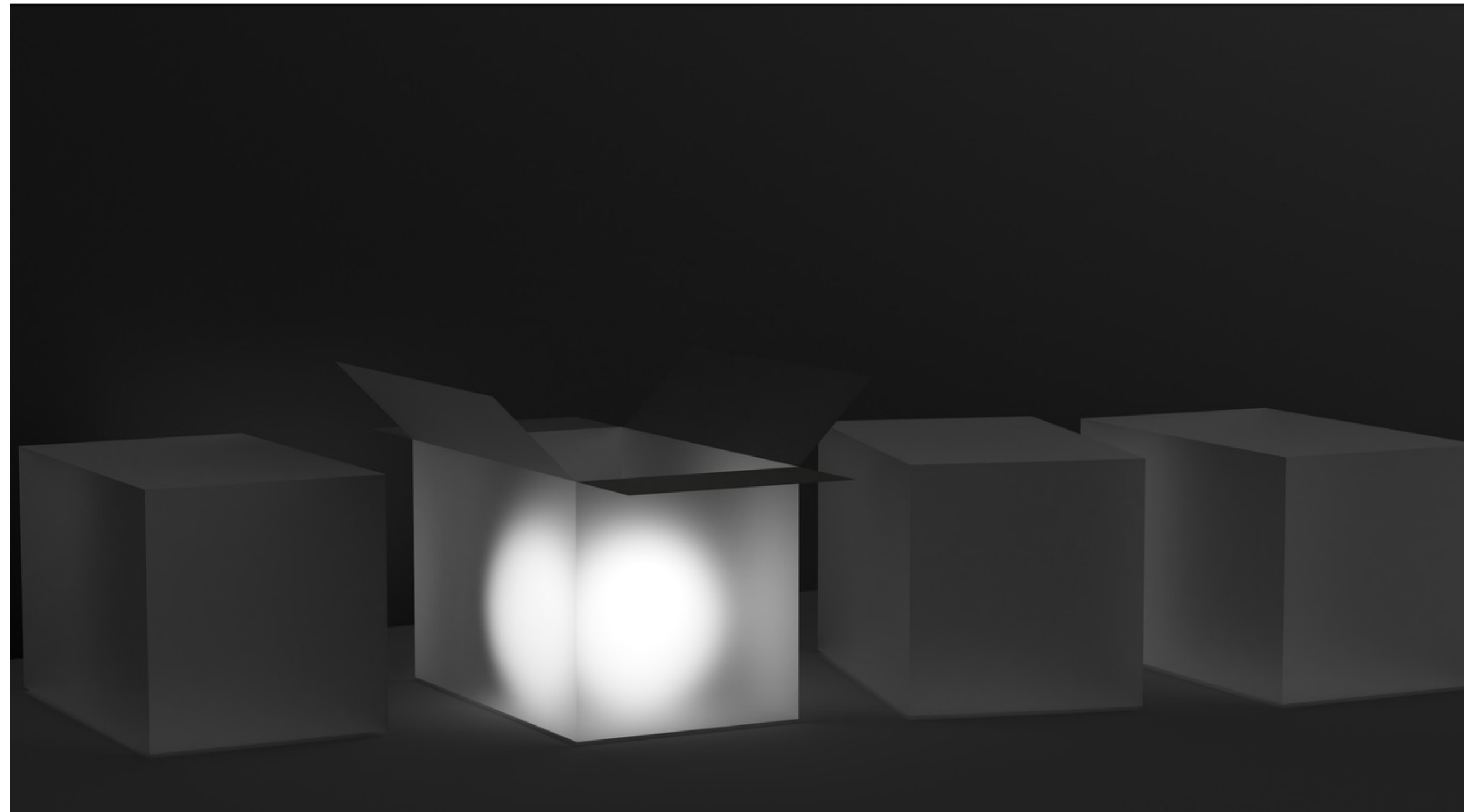


Jenkinson et al. 2014



Webb

2. The Complex Nature of the Task

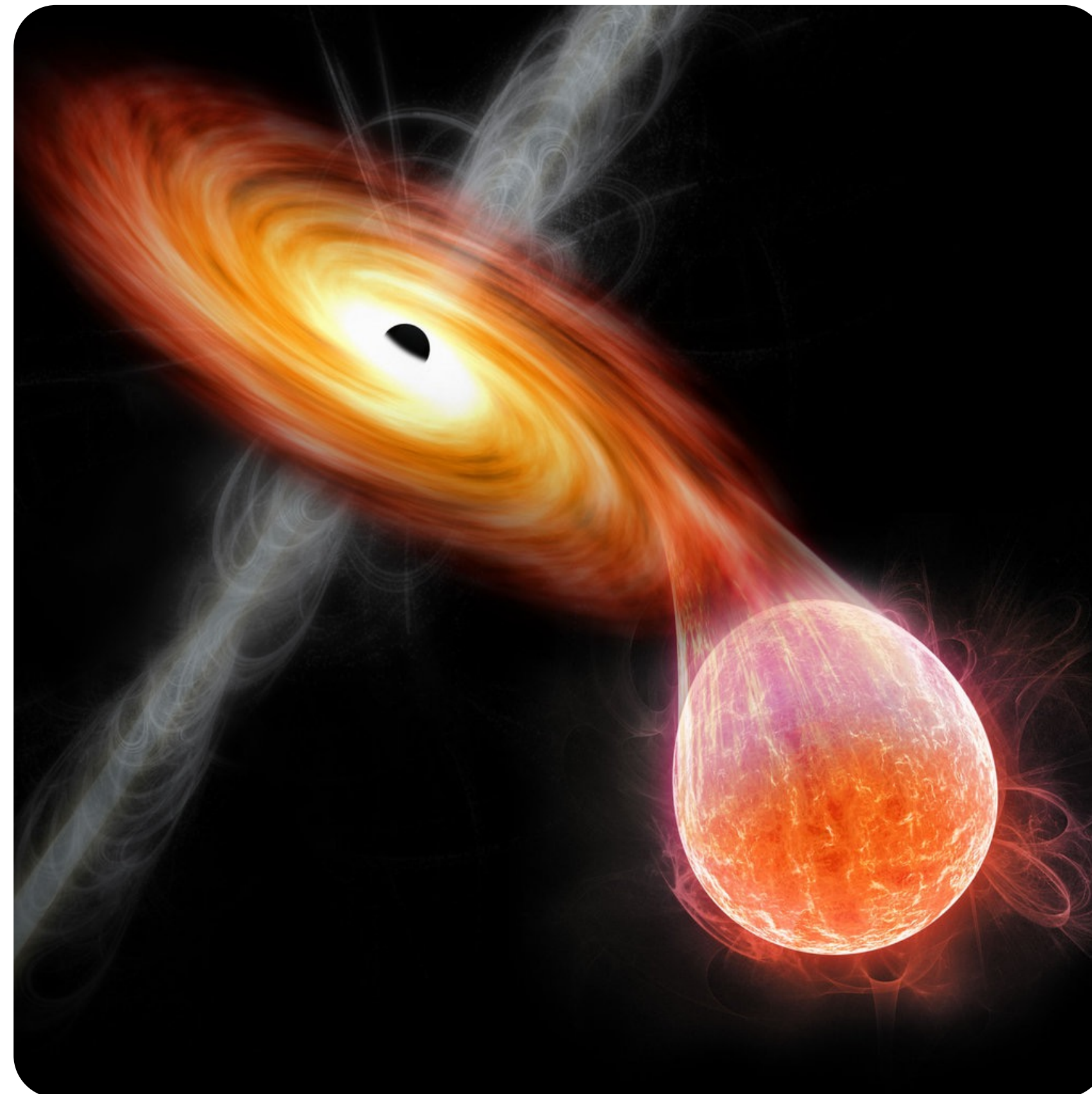


Physical AI Models

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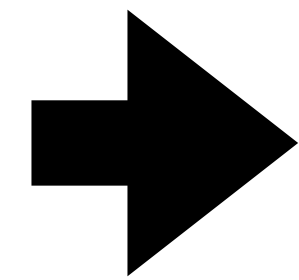
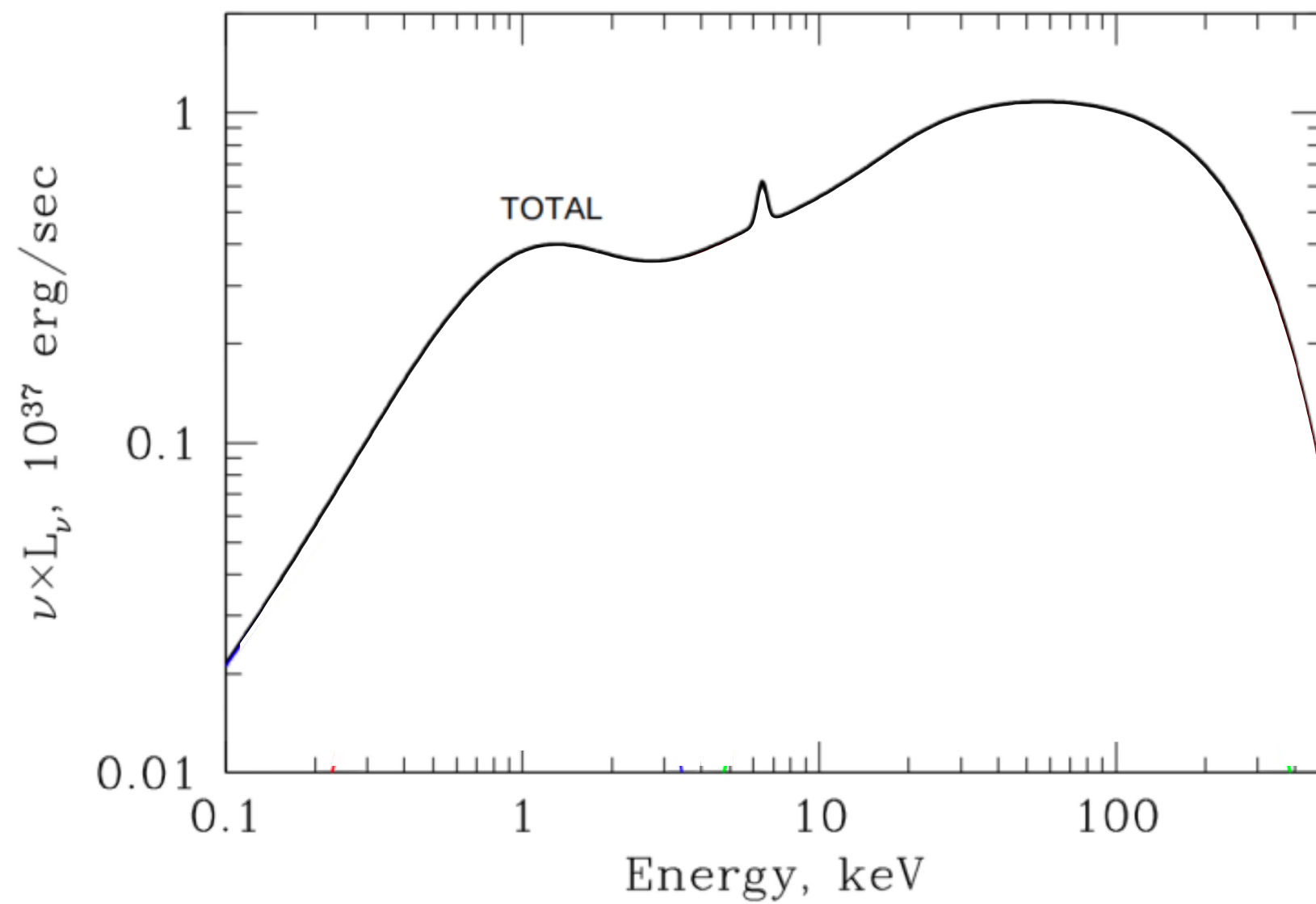
Enabling Next Generation Astrophysics

X-ray binary



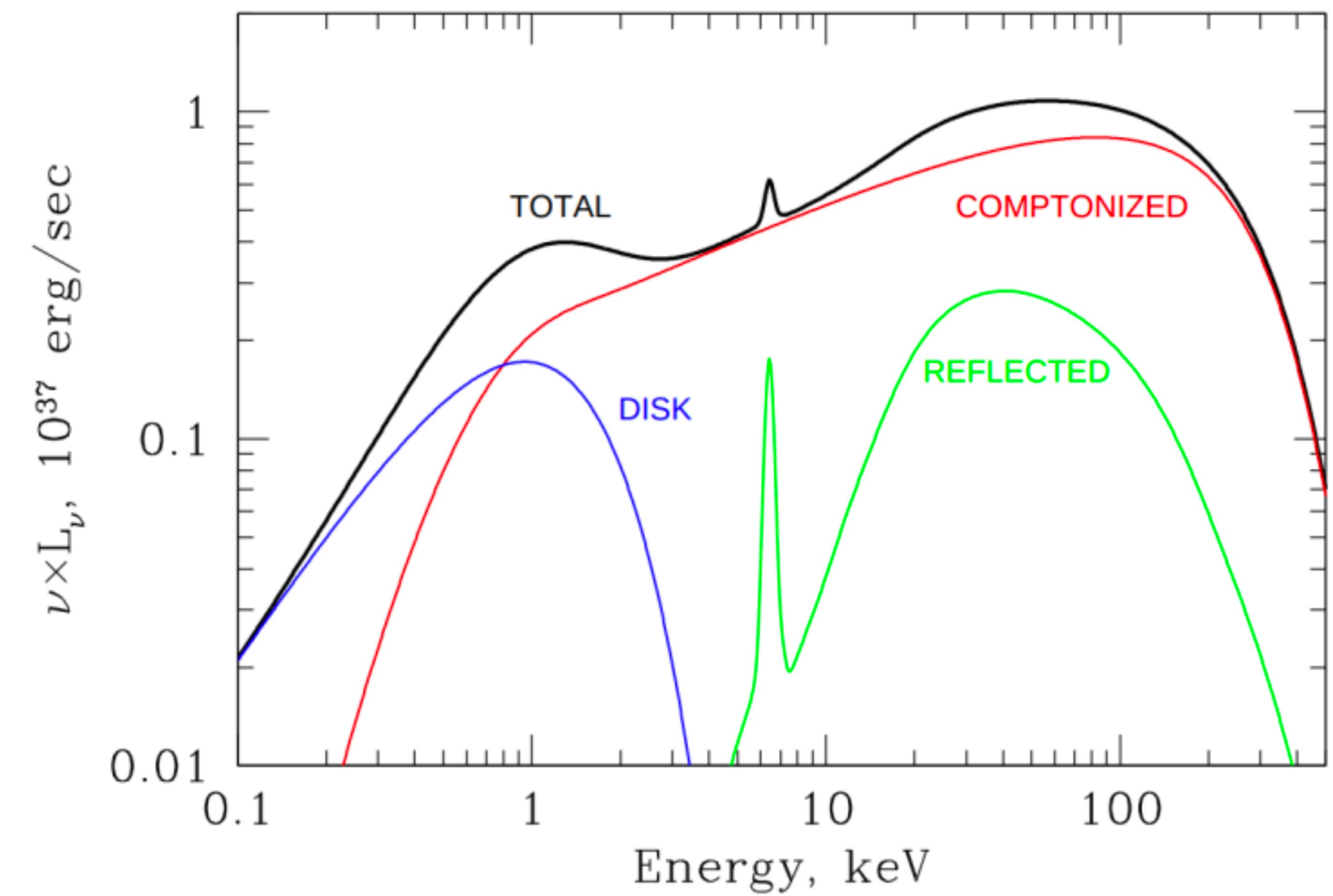
ASTROAI

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Expert

**10,000 spectra
24 hours of work**



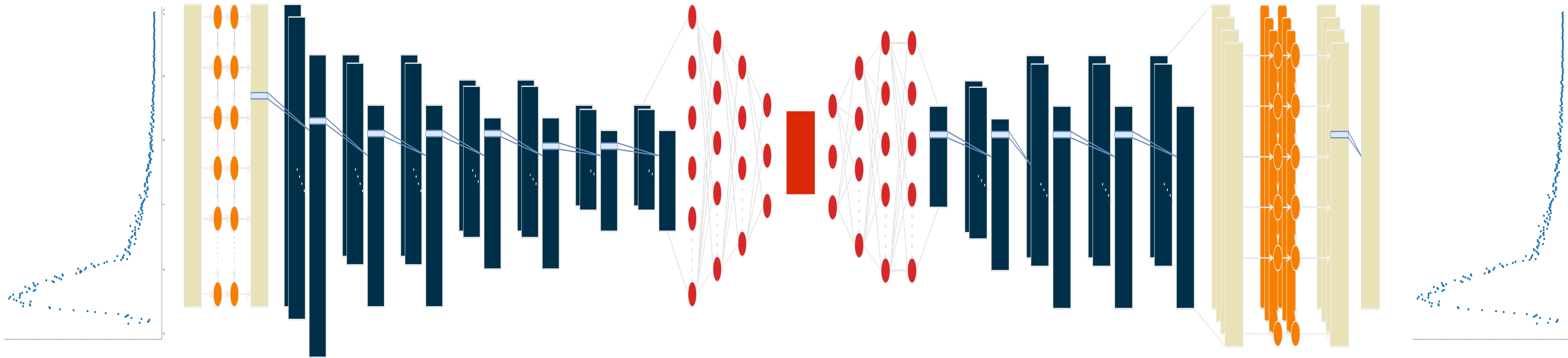
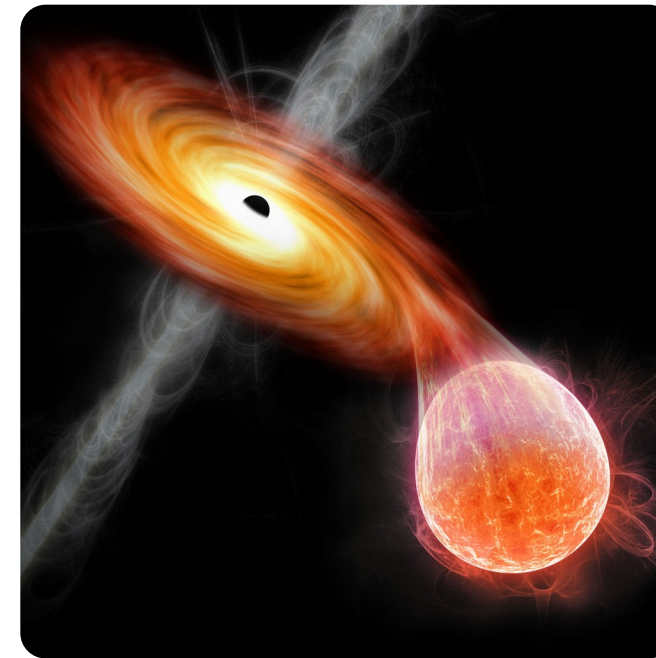
**Physical Parameters:
T, M, Spin**

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Ethan
Tregigda

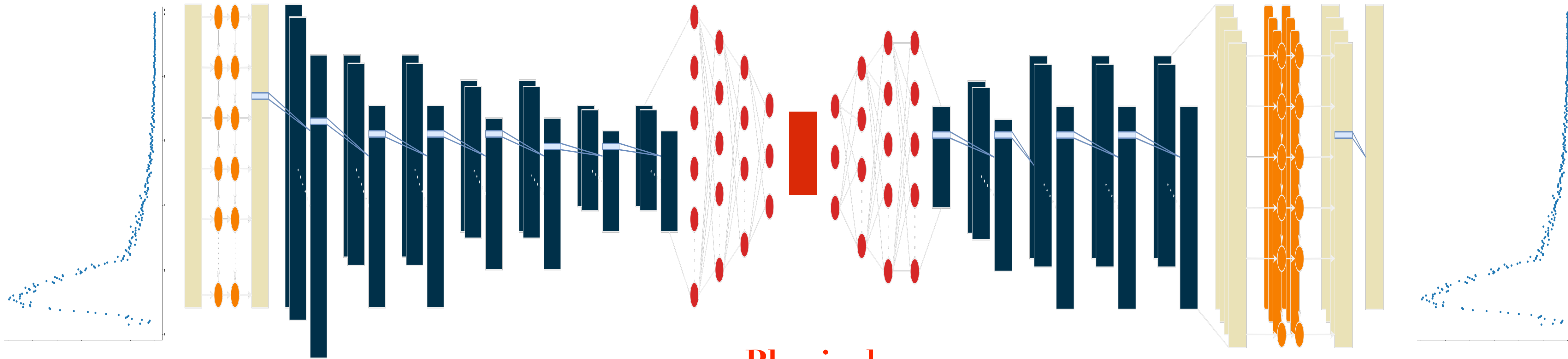
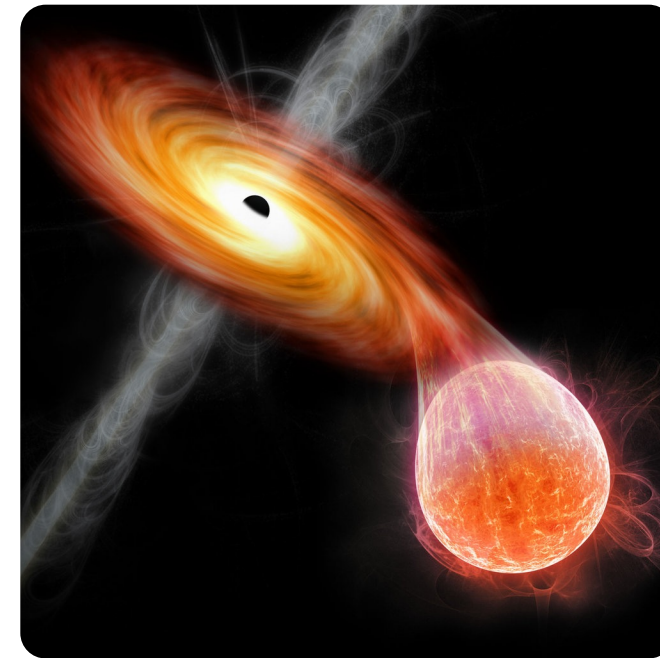


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Ethan
Tregigda

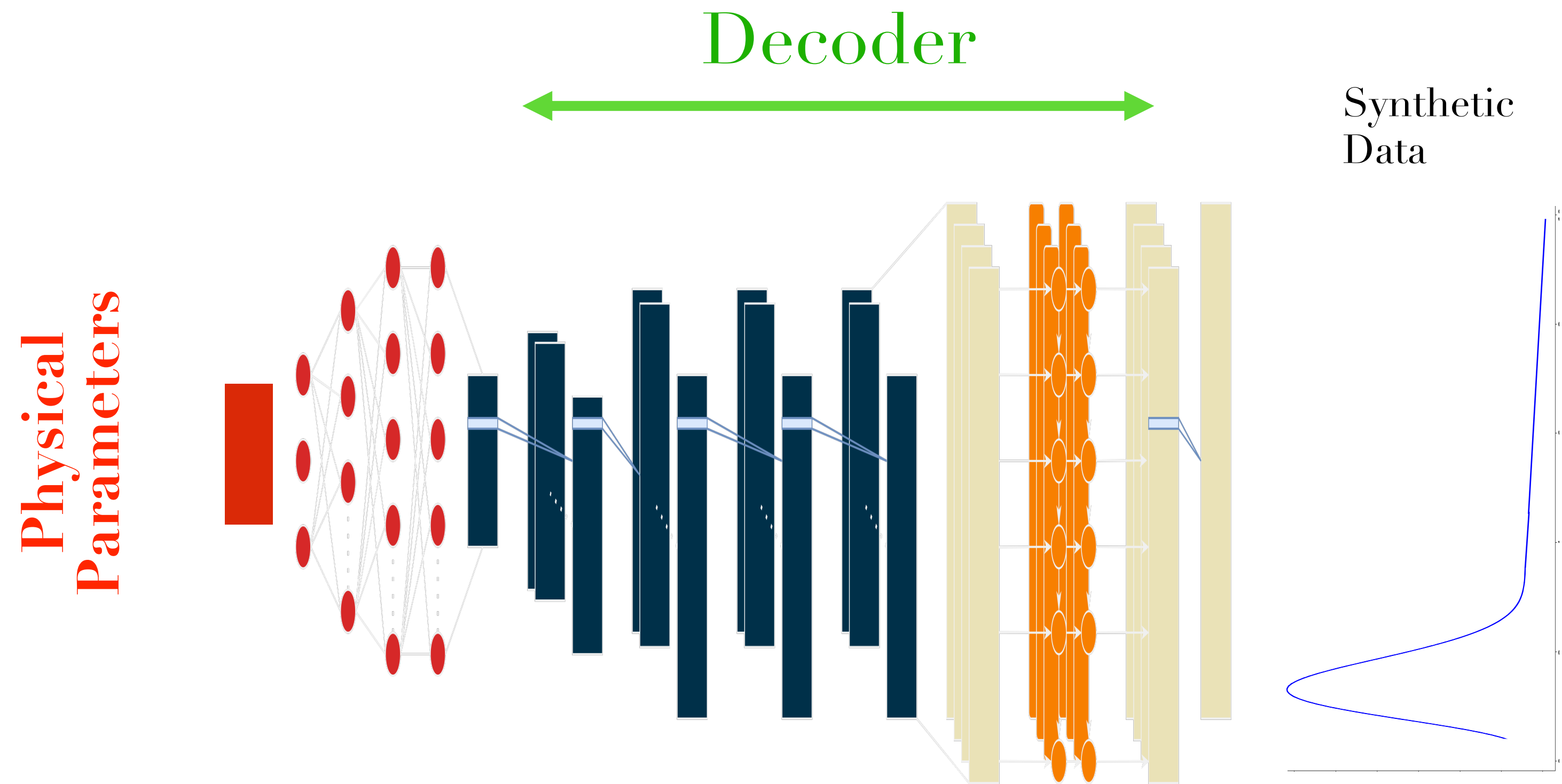


**Physical
Parameters**

Tregidga et al. 2023

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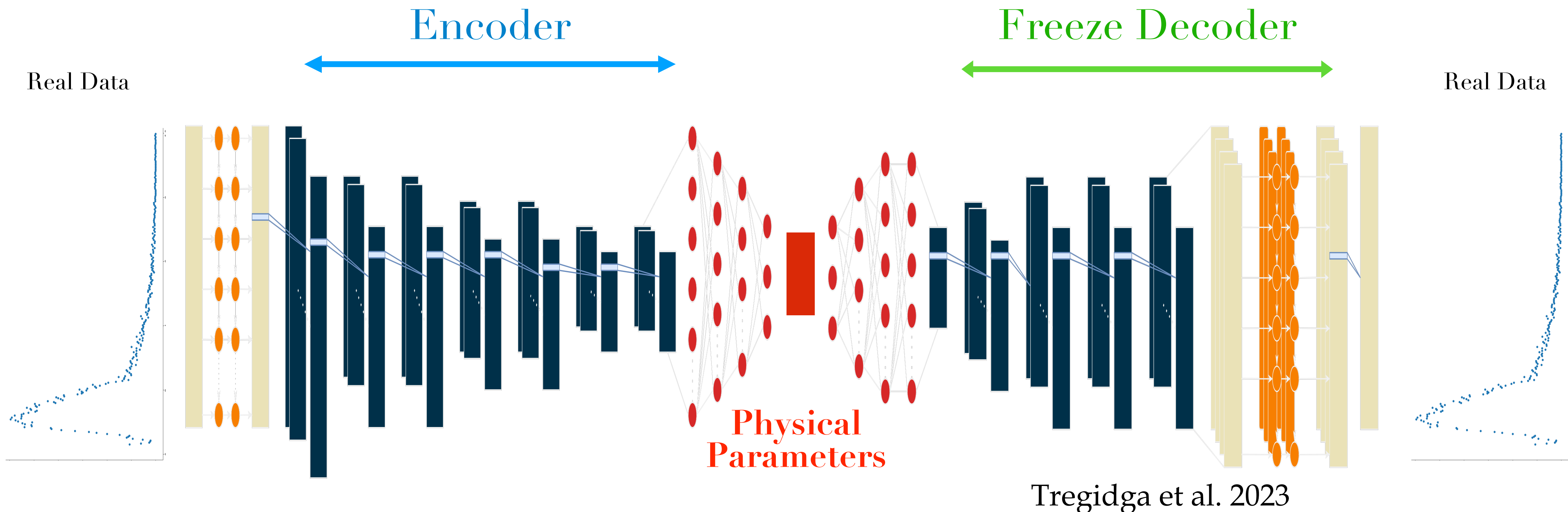
Enabling Next Generation Astrophysics



Tregidga et al. 2023

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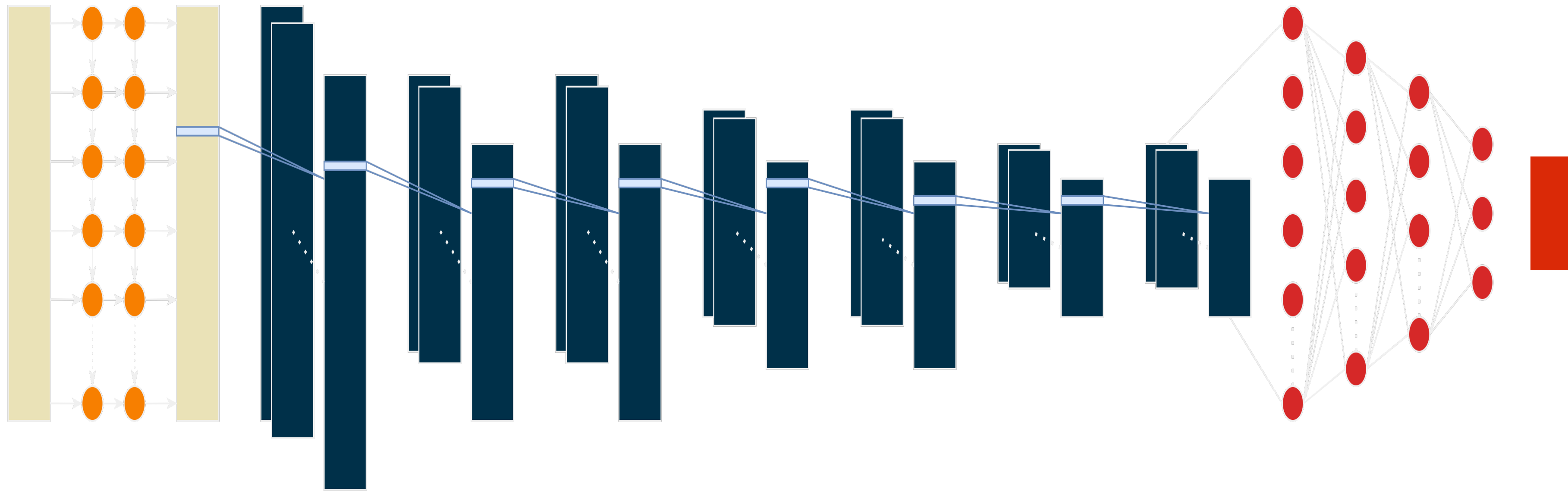
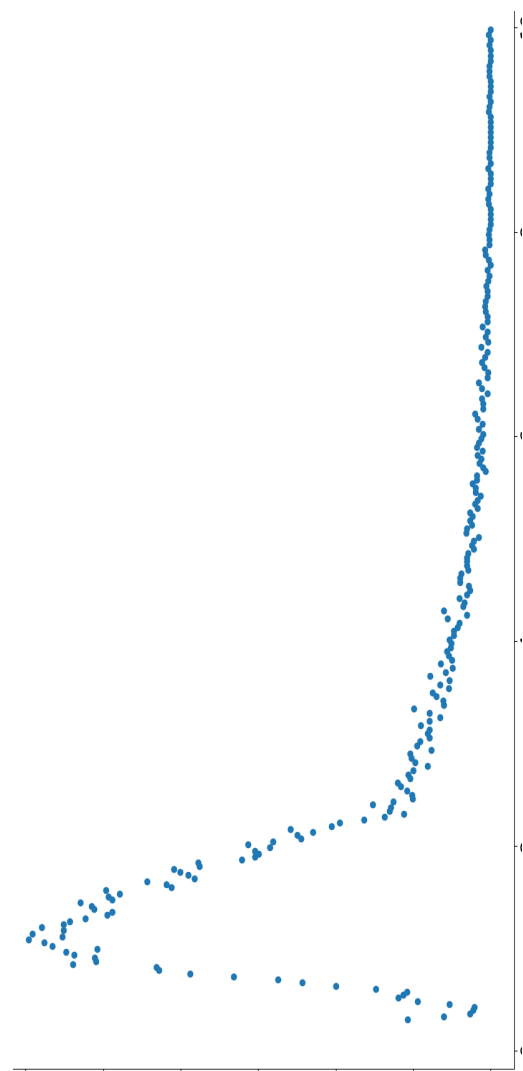
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Encoder



Real Data



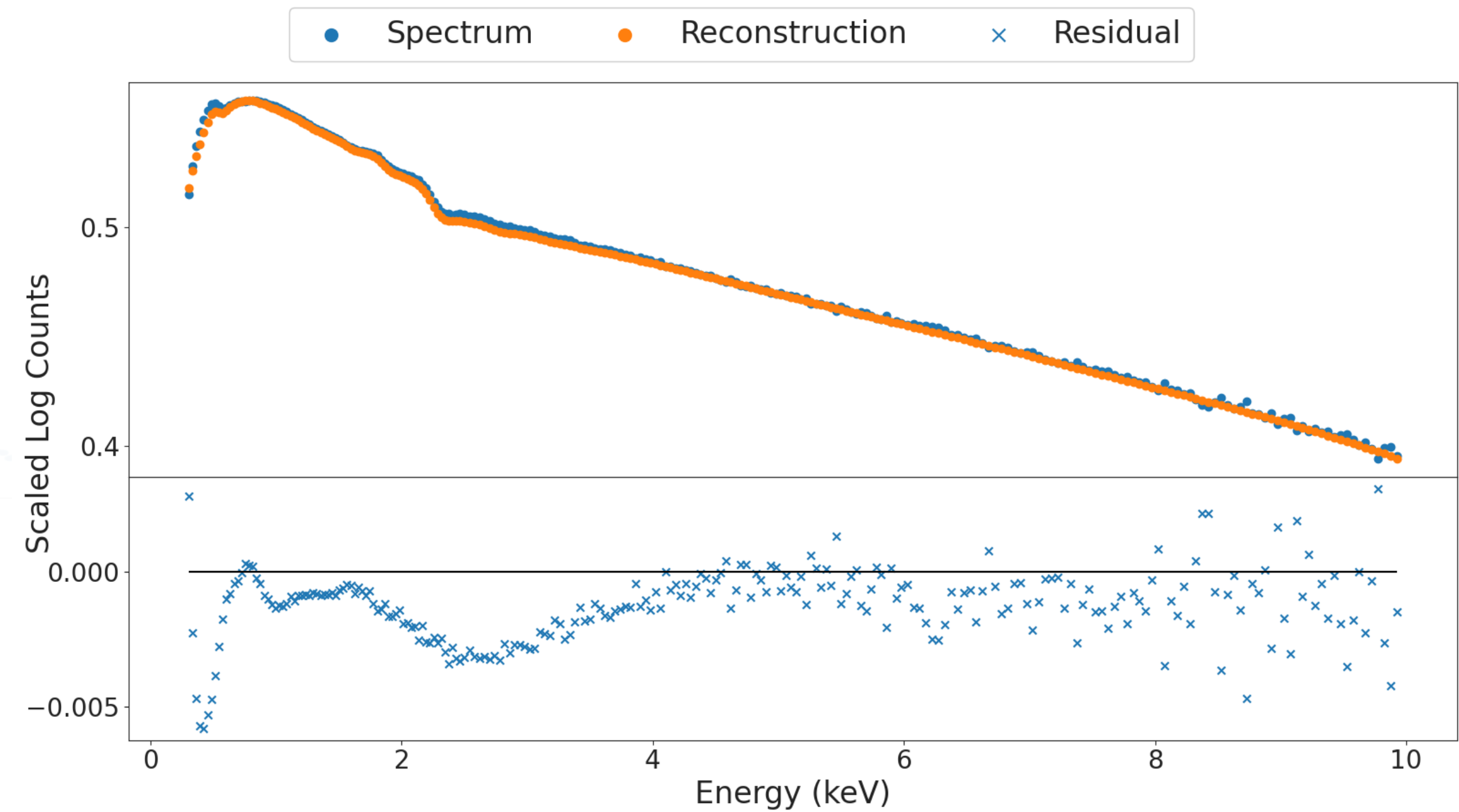
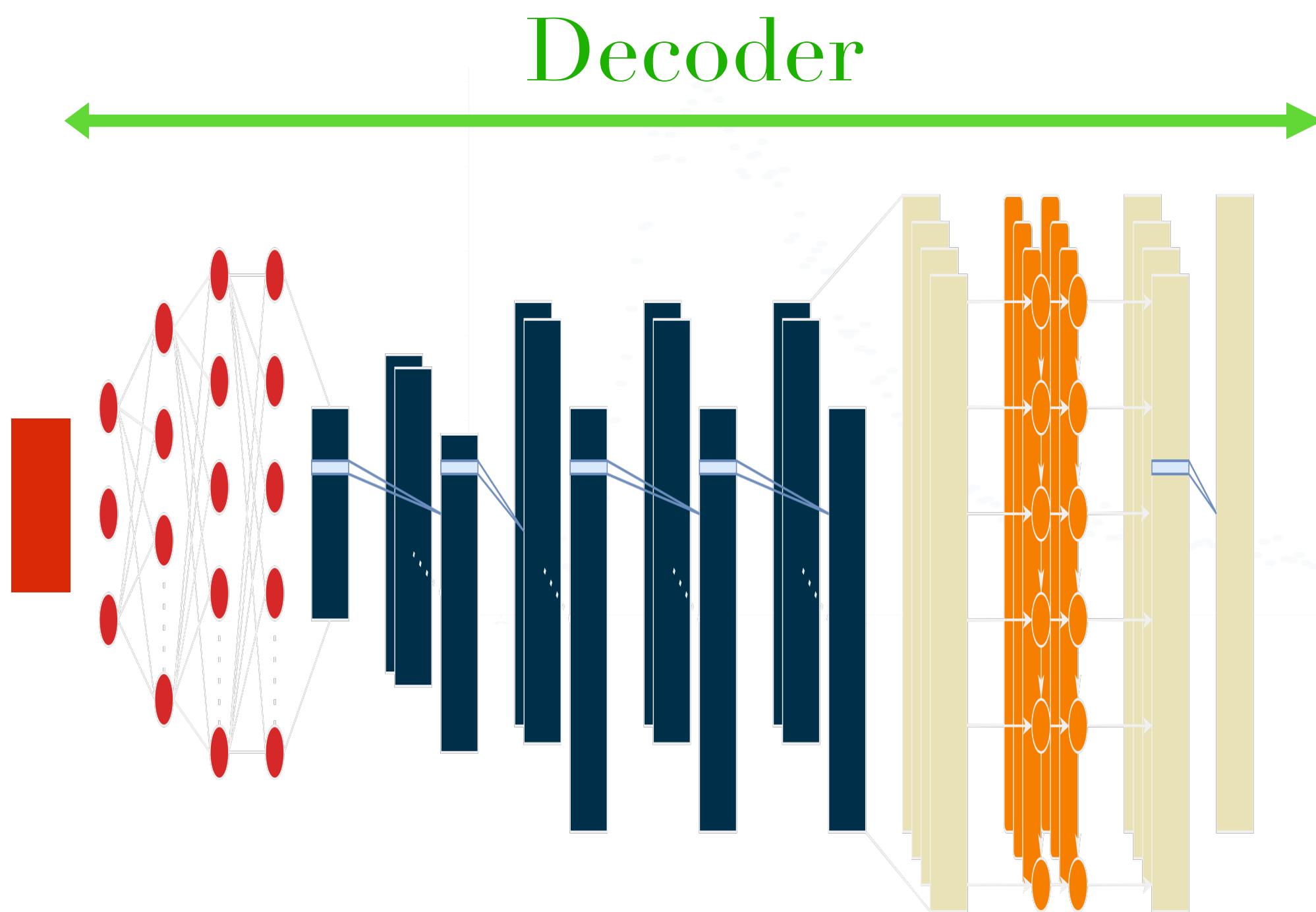
Physical Parameters

Tregidga et al. 2023

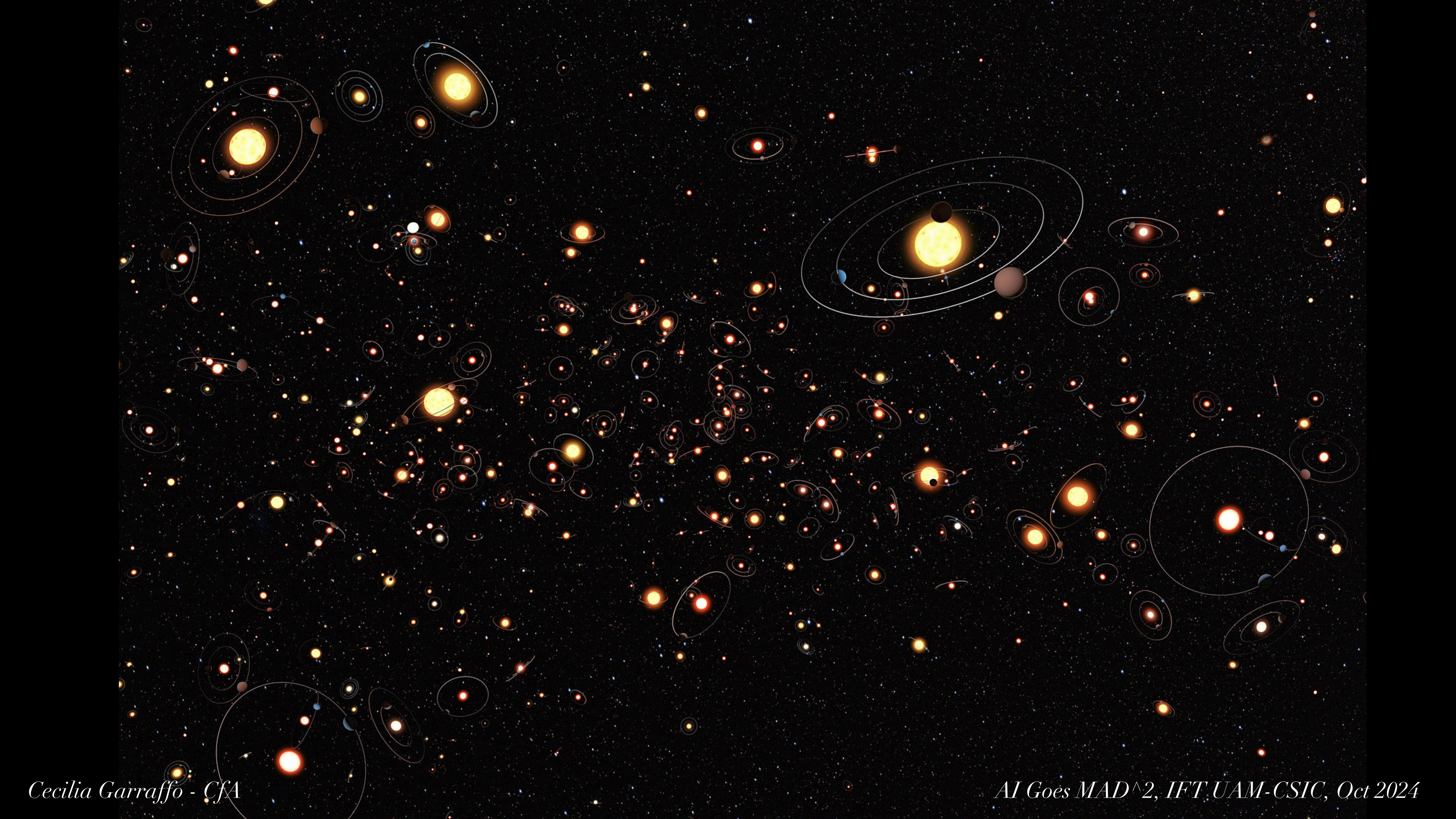
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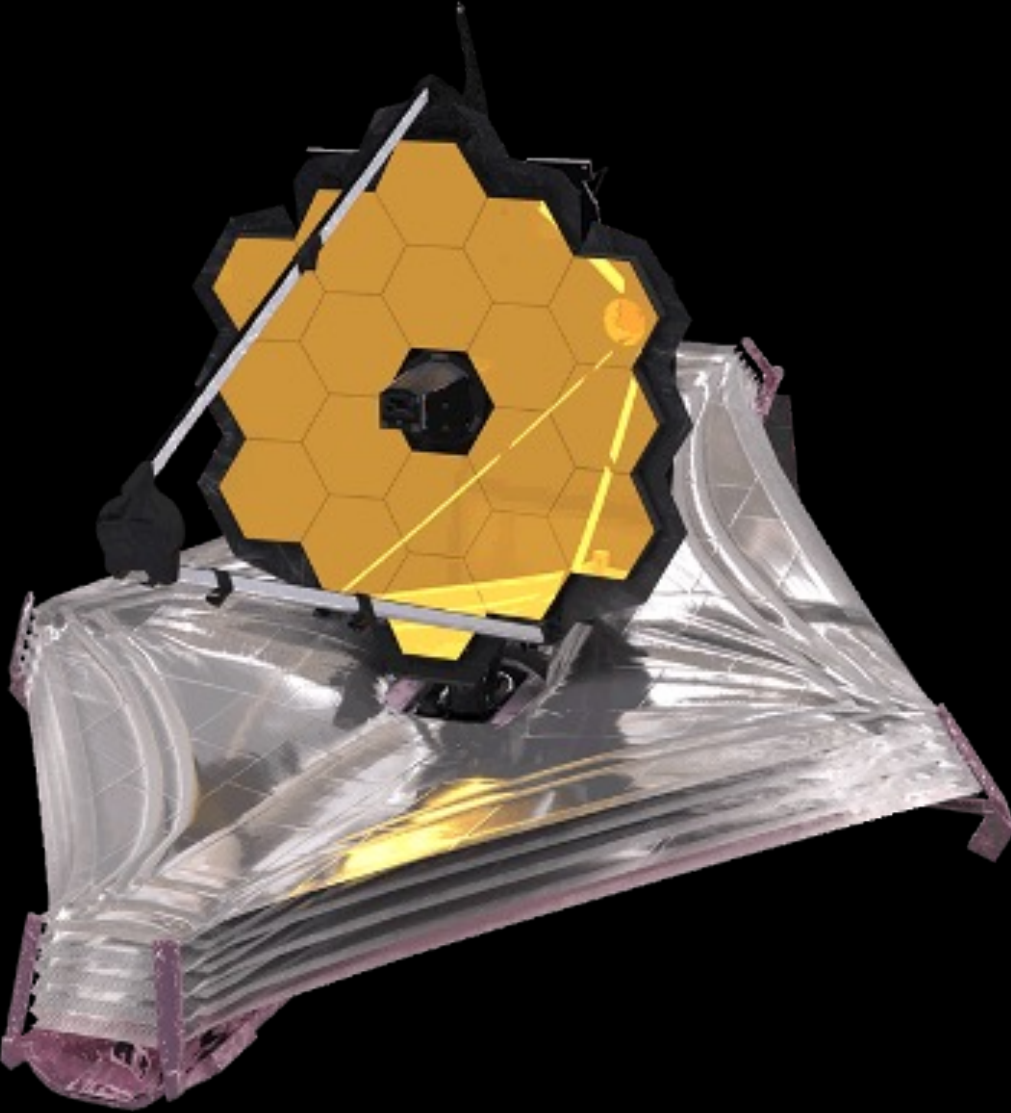
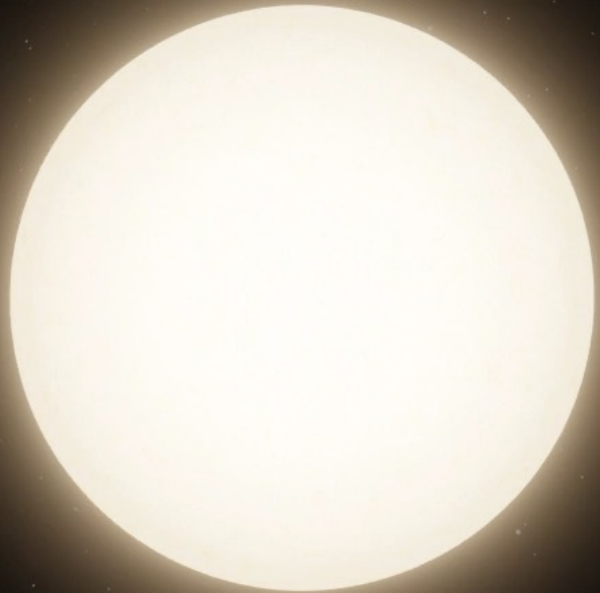
Physical Parameters

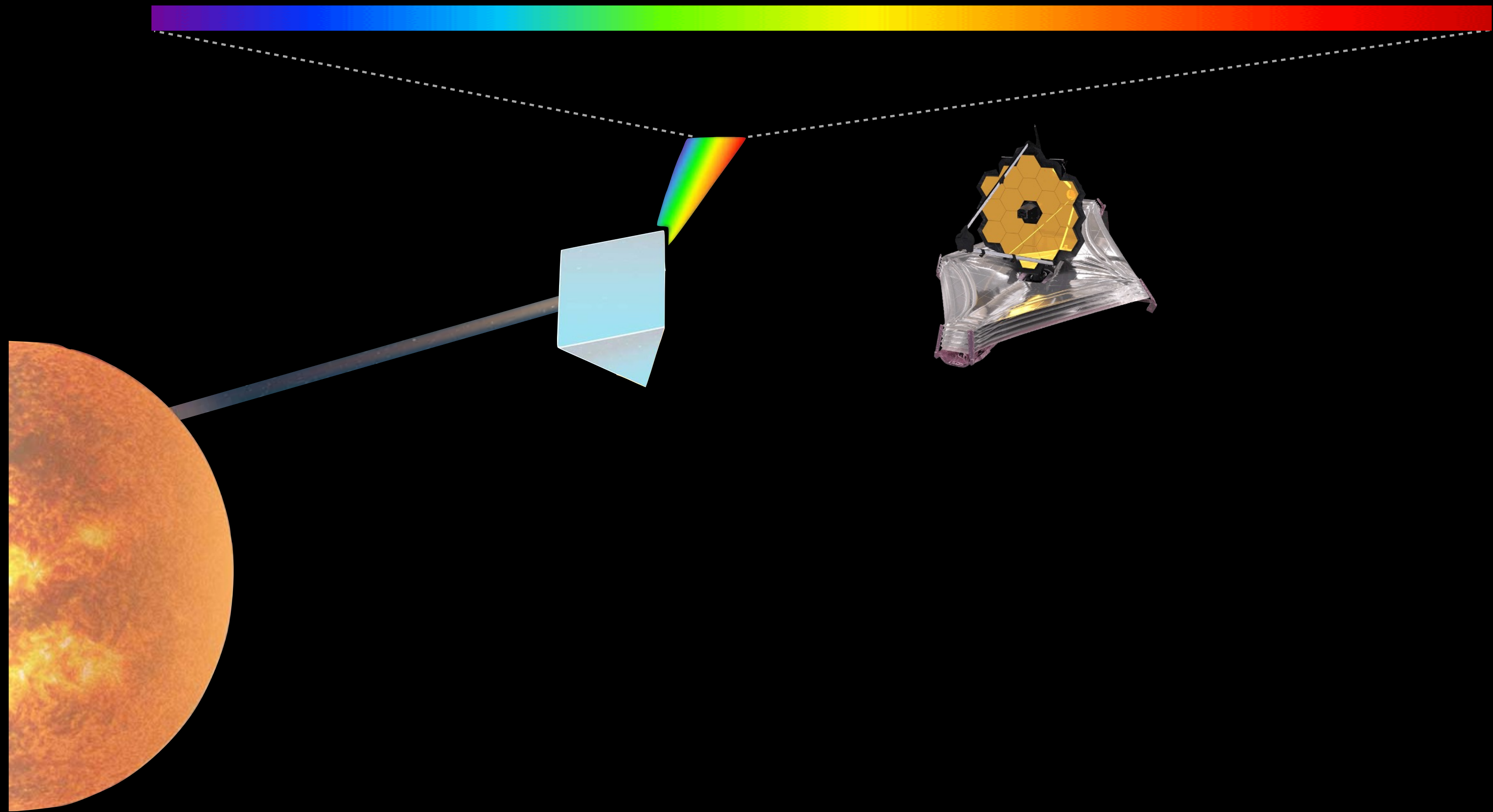


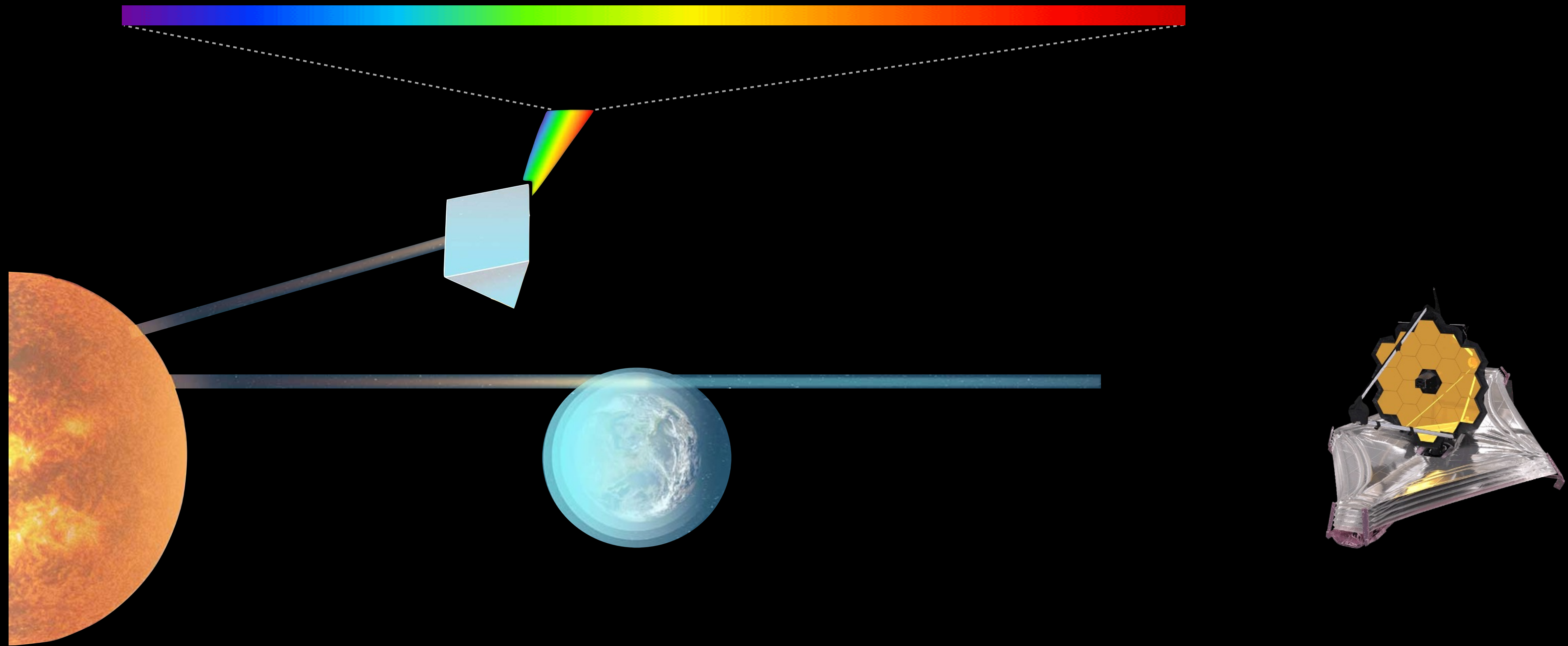
Tregidga et al. 2023

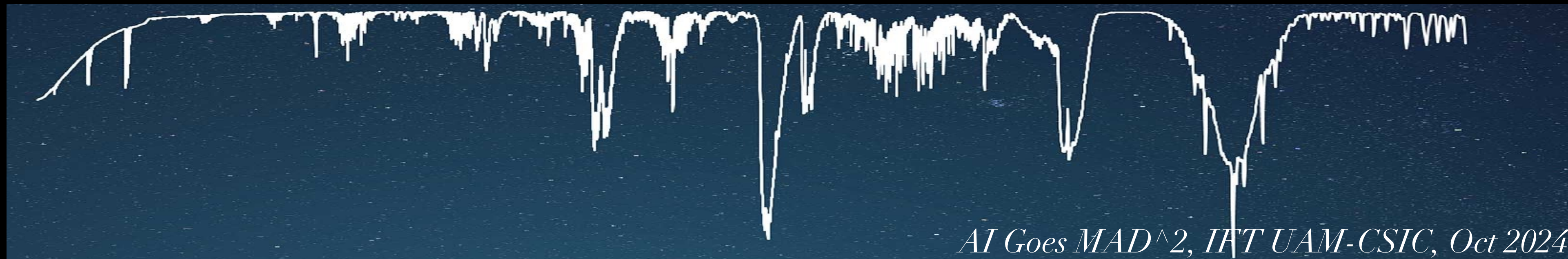
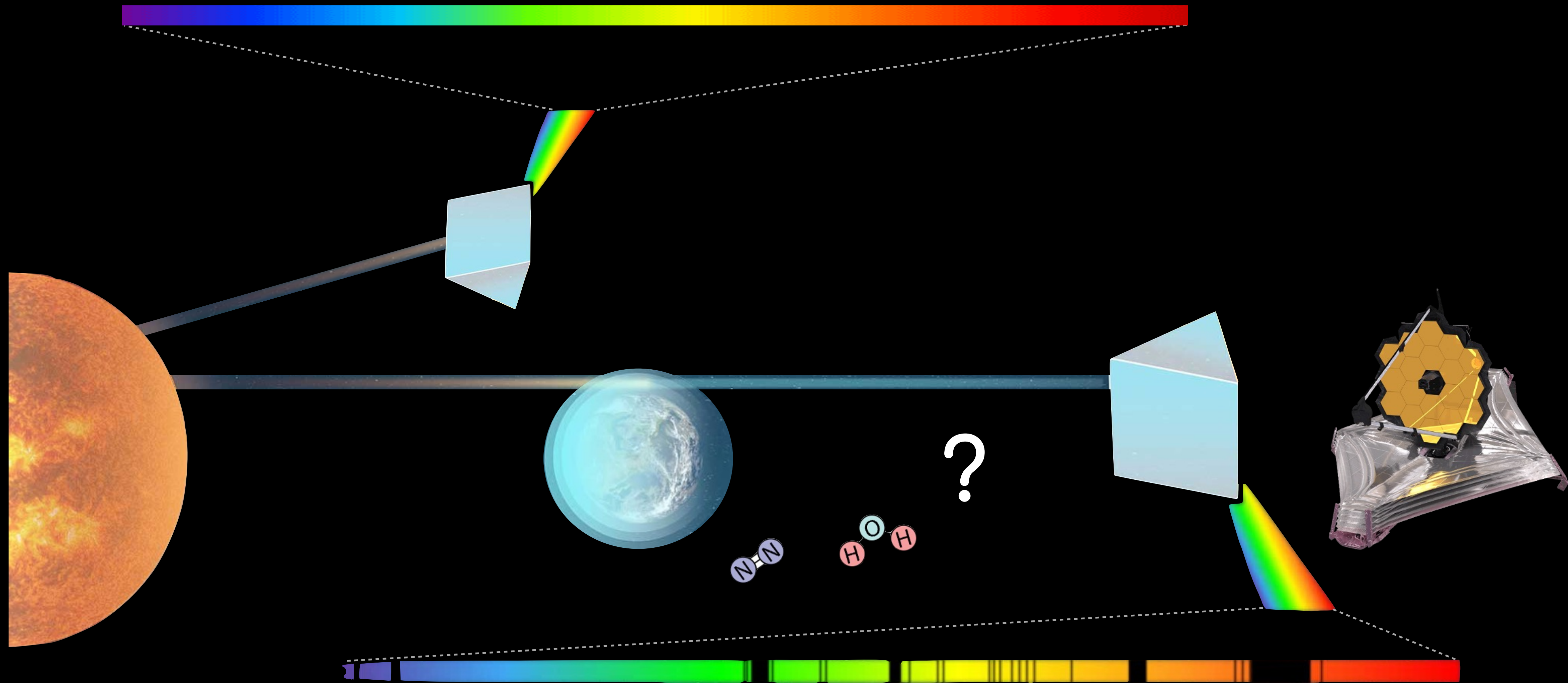


James Webb Space Telescope





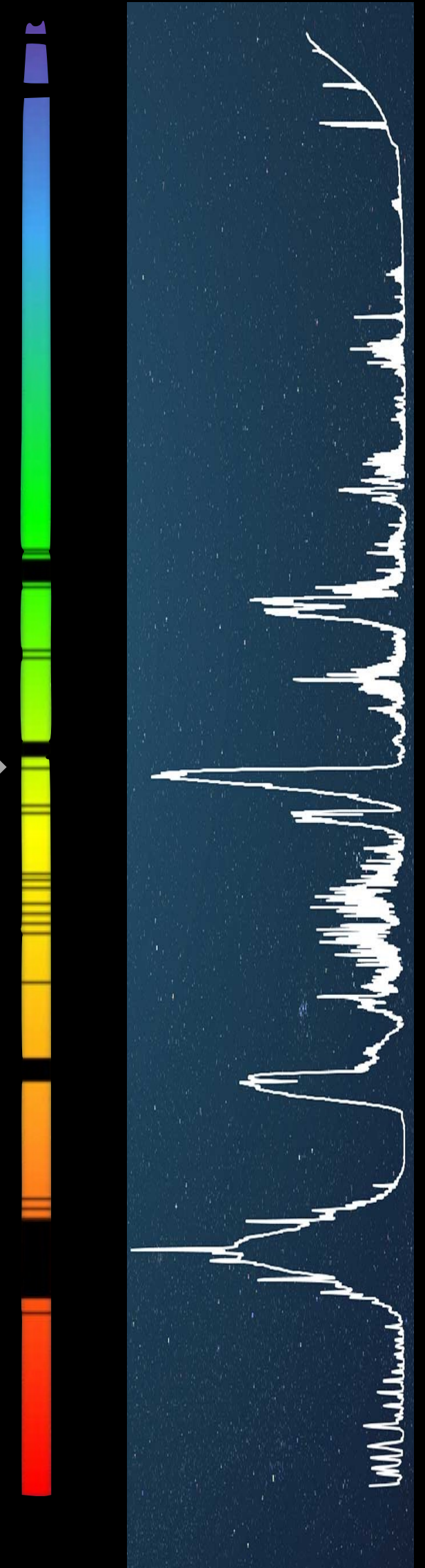
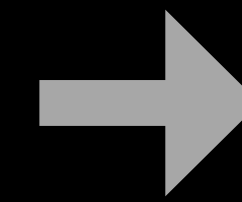
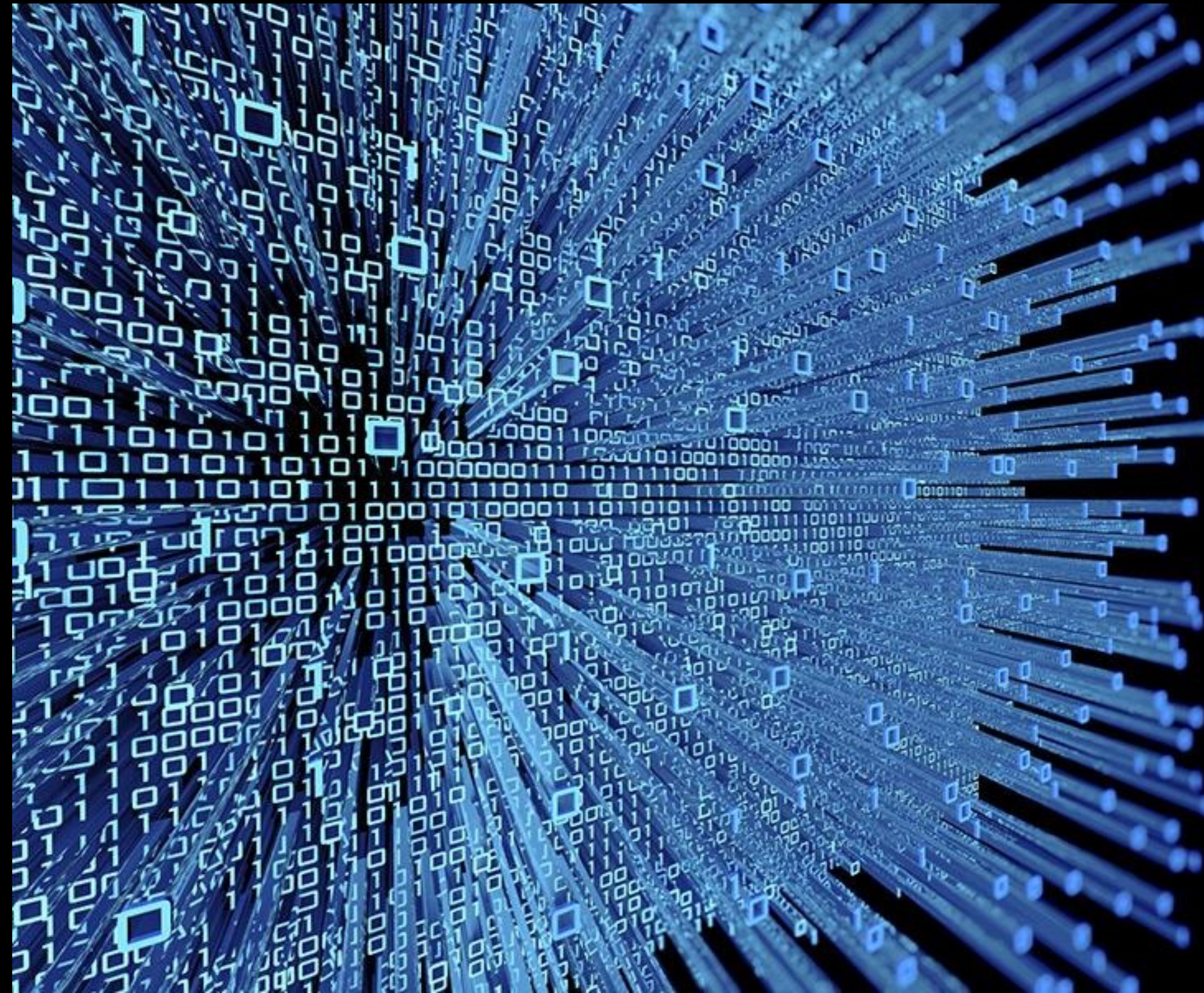
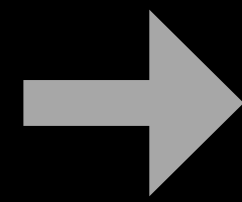
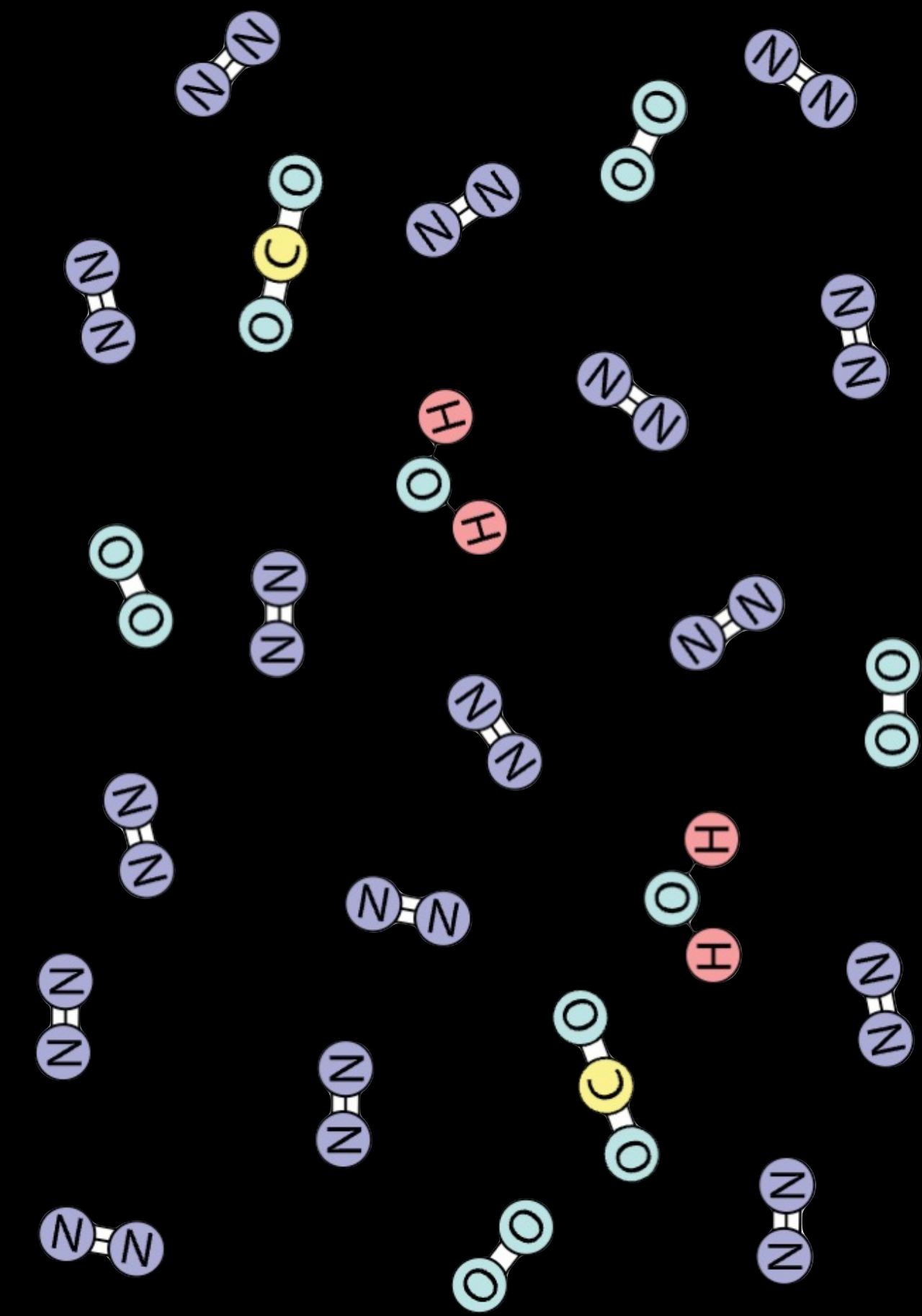




Chemical Composition

Simulation

Spectrum

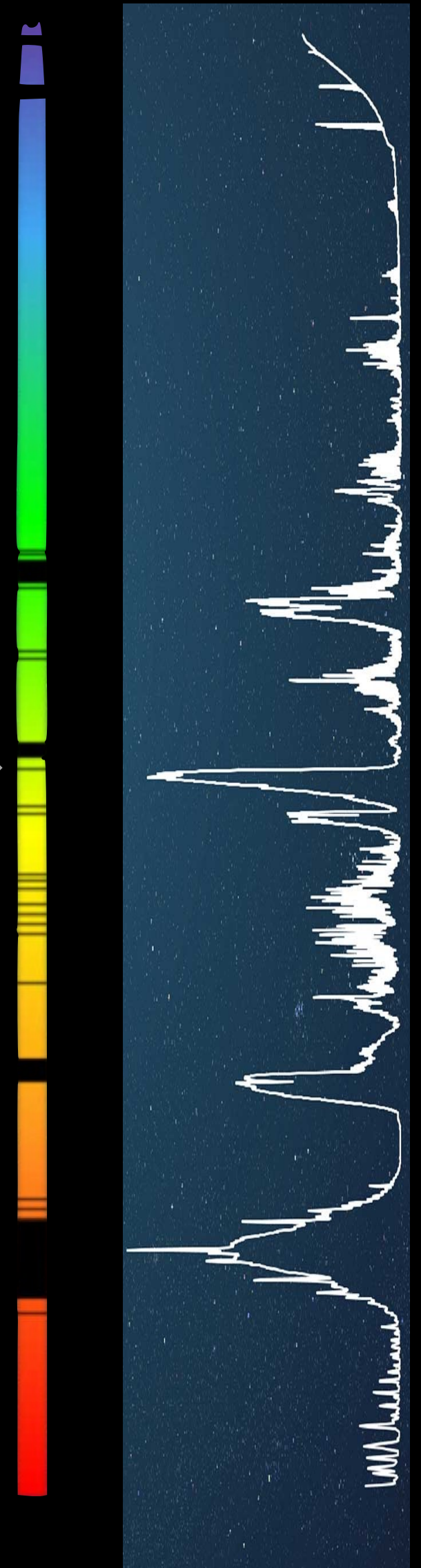
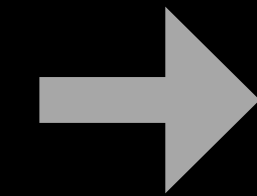
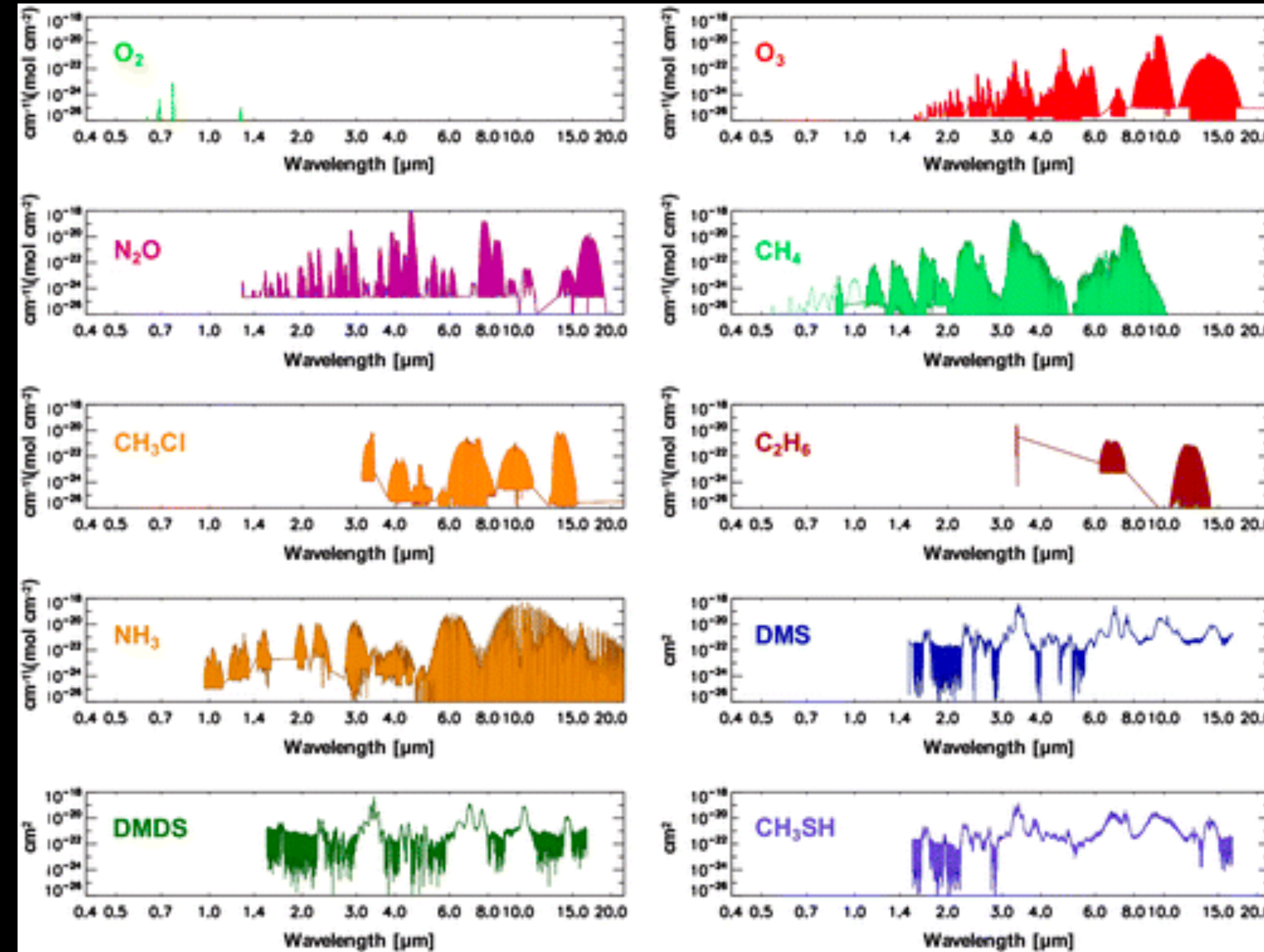
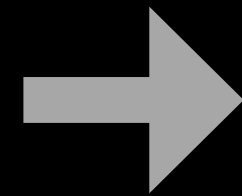
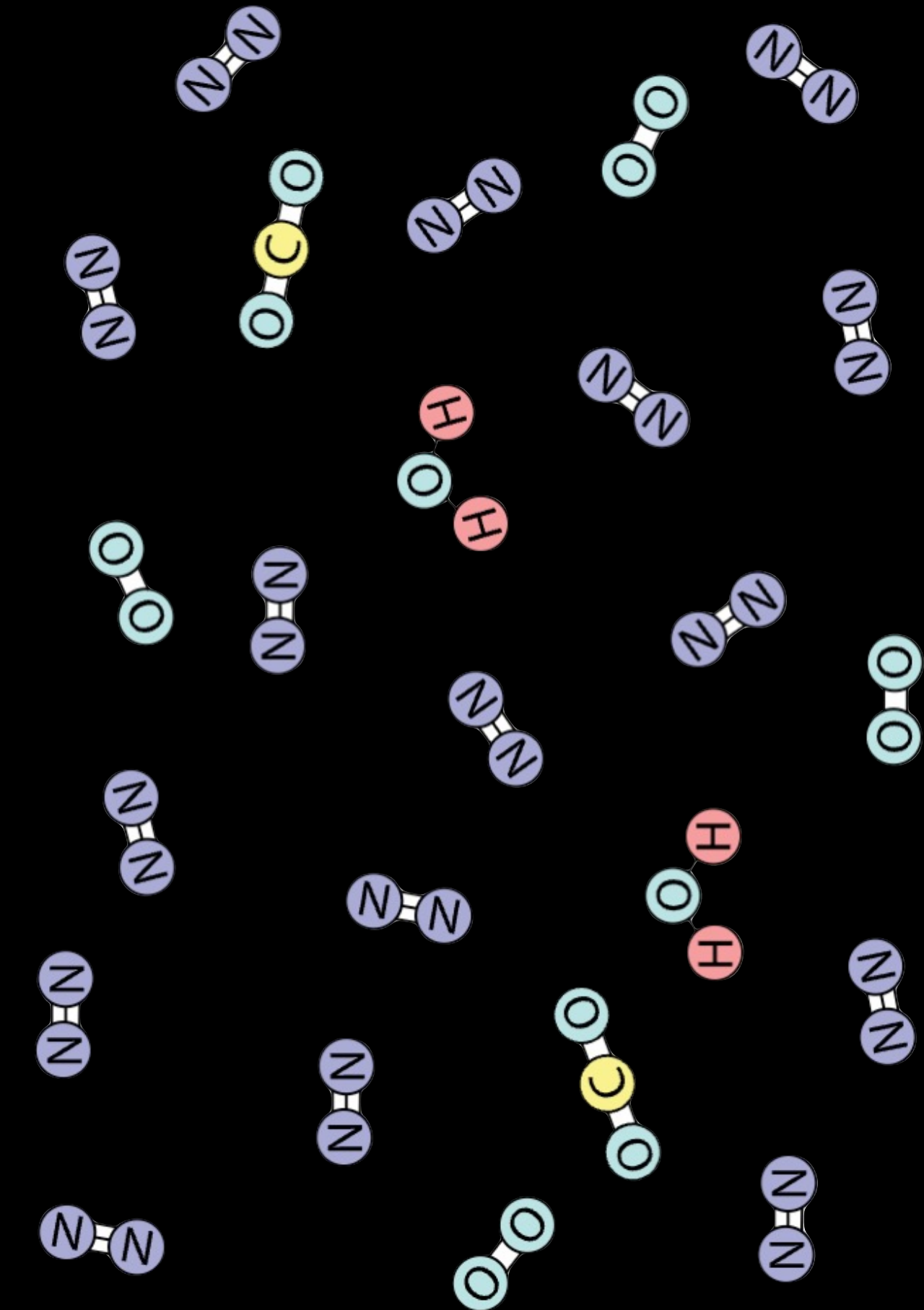


Chemical Composition



Spectrum

Simulation

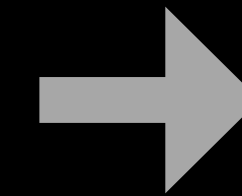
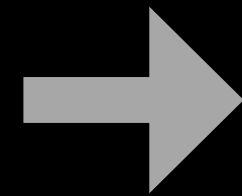
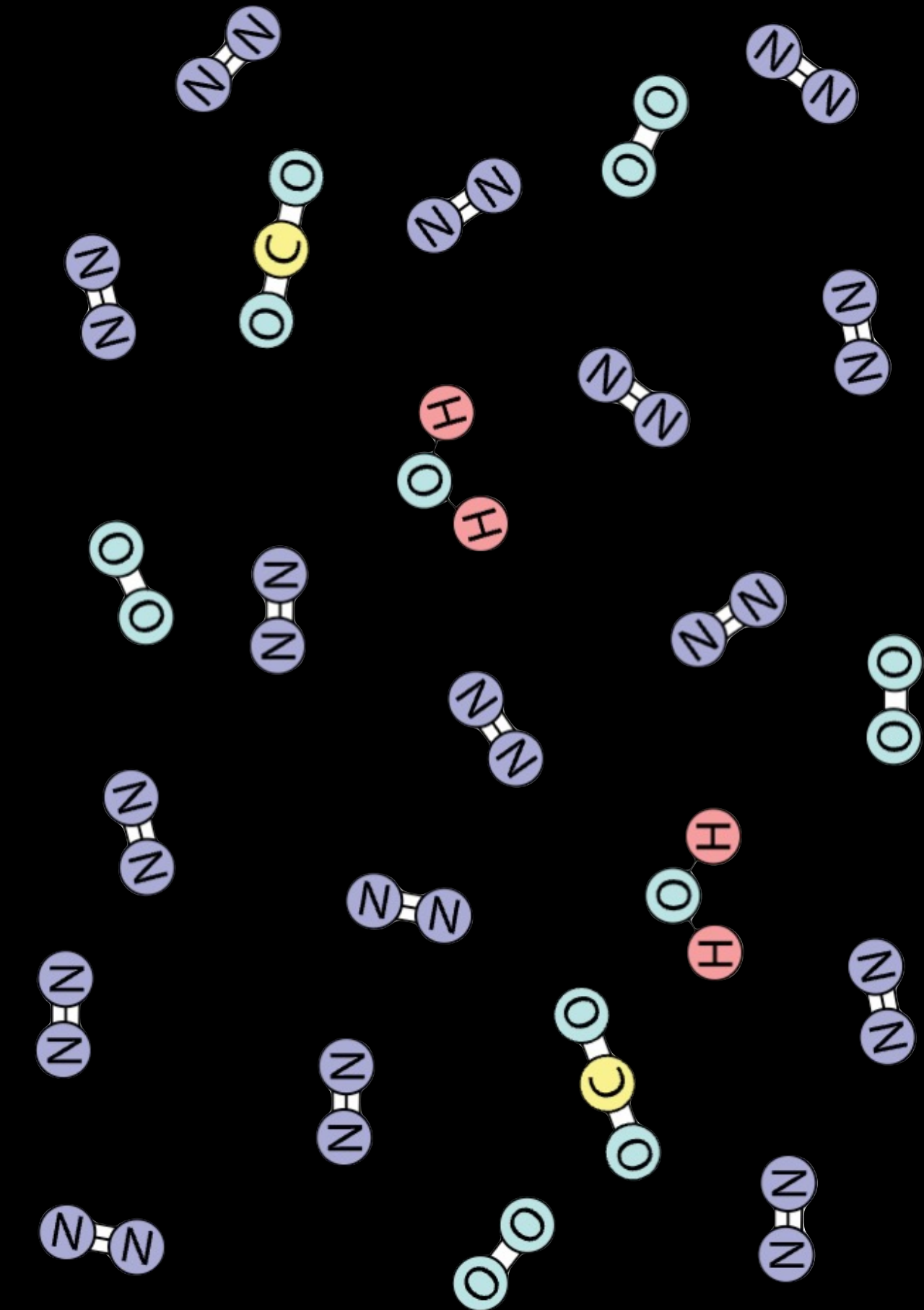


Chemical Composition



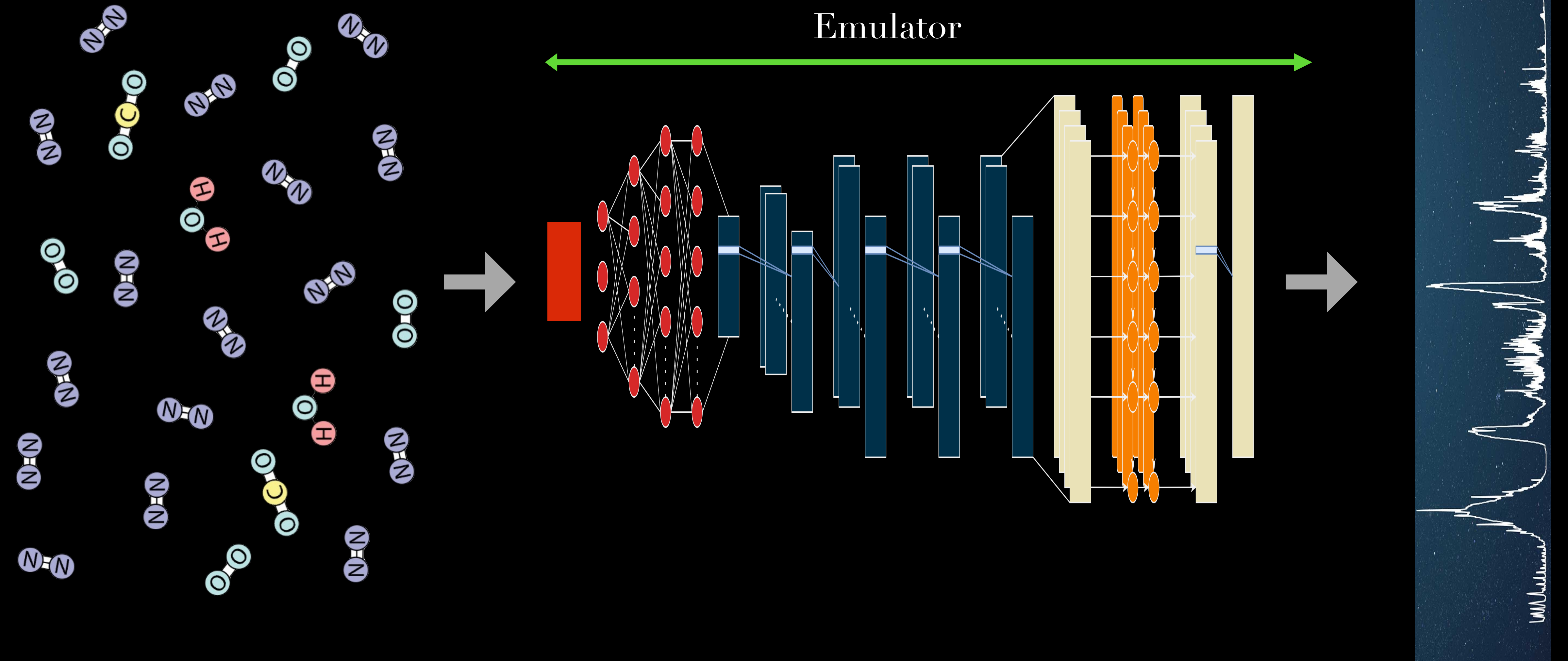
Spectrum

Simulation



Chemical Composition

Spectrum

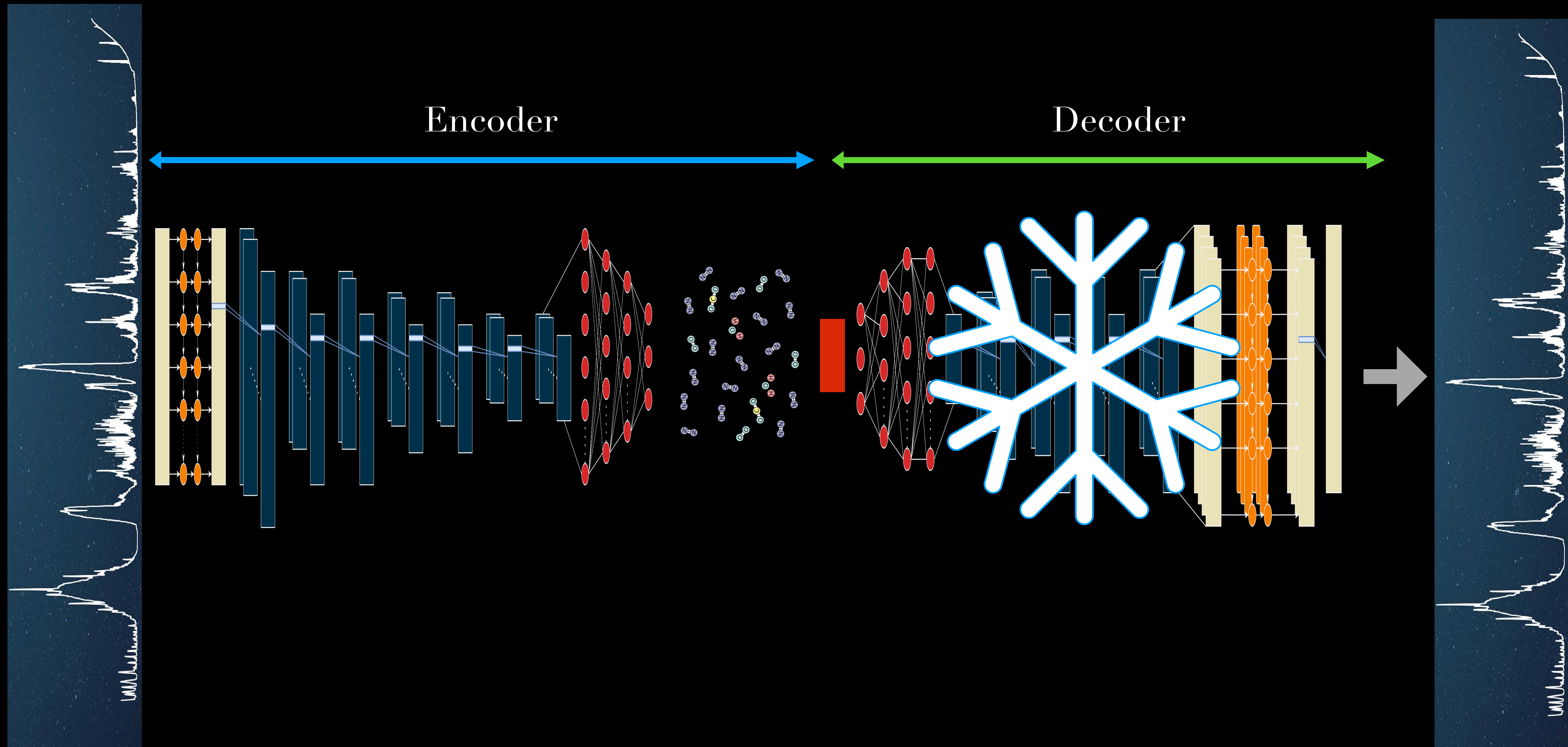


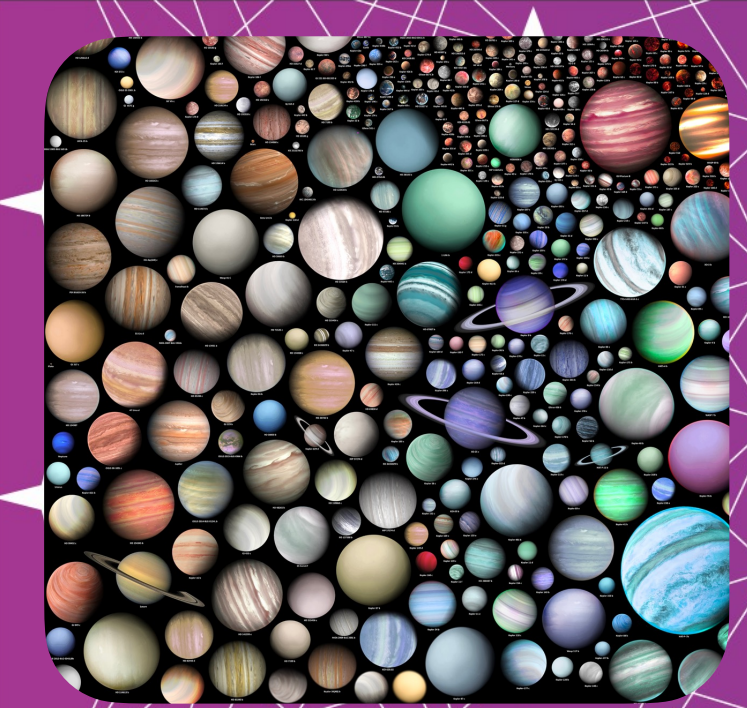
Chemical Composition

Spectrum

Encoder

Decoder



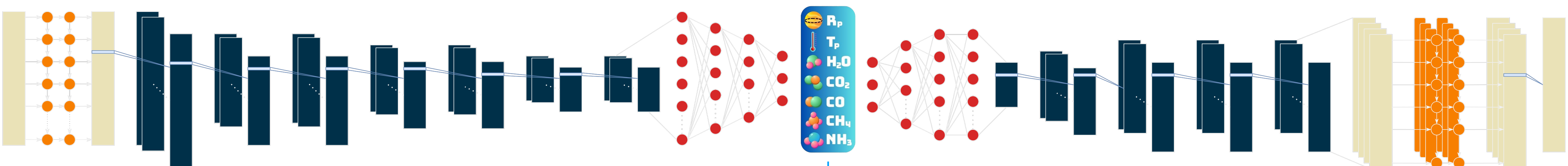


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Mayeul Aubin



● Spectrum

● Reconstruction

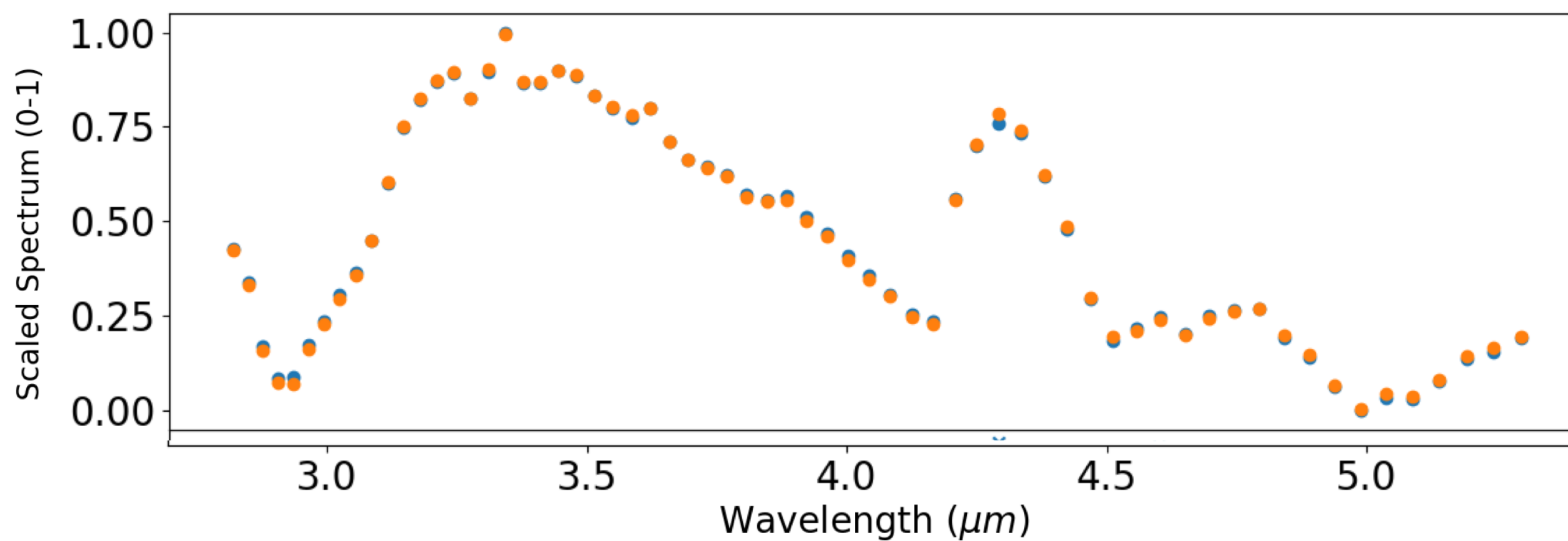
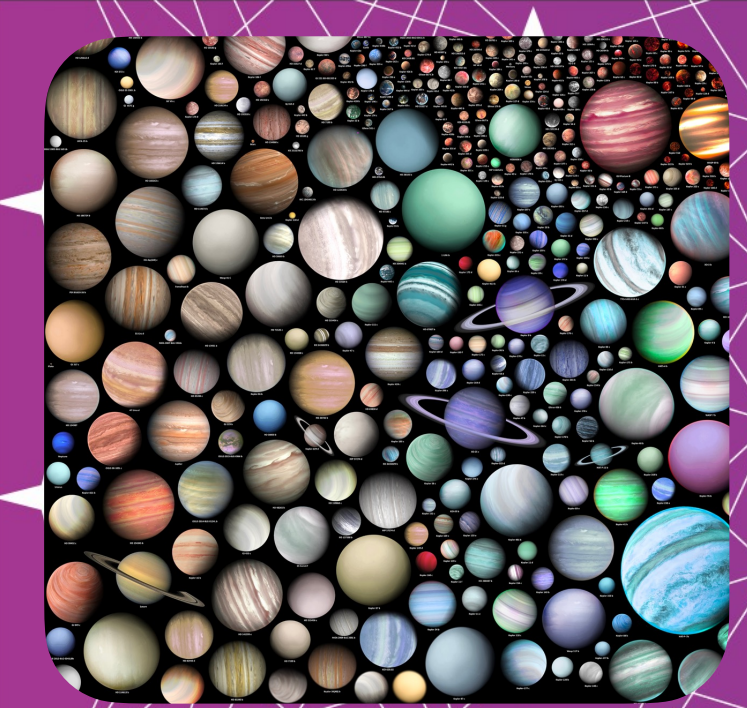


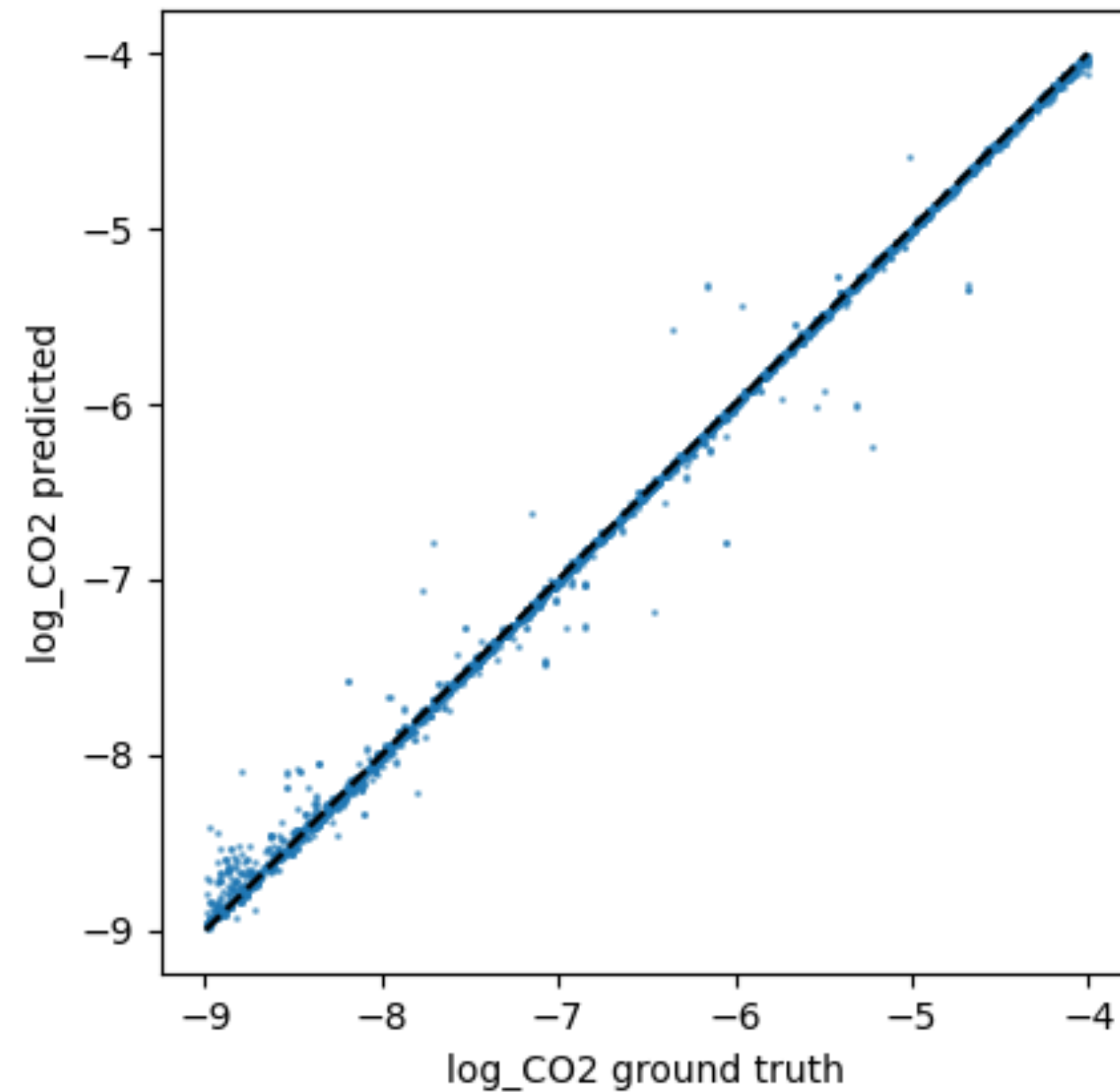
Figure 2: Reconstruction of a spectrum by the decoder



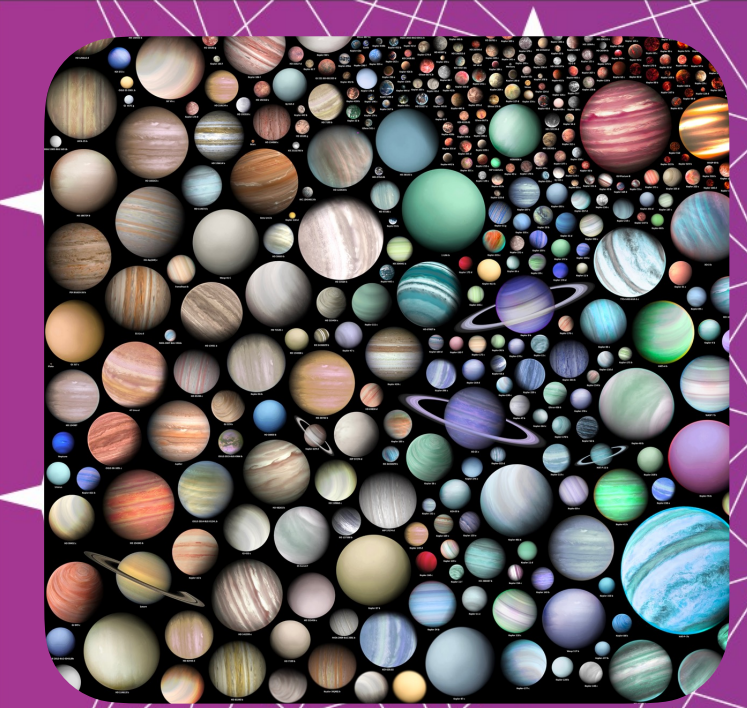
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The encoder can reliably predict the target parameters

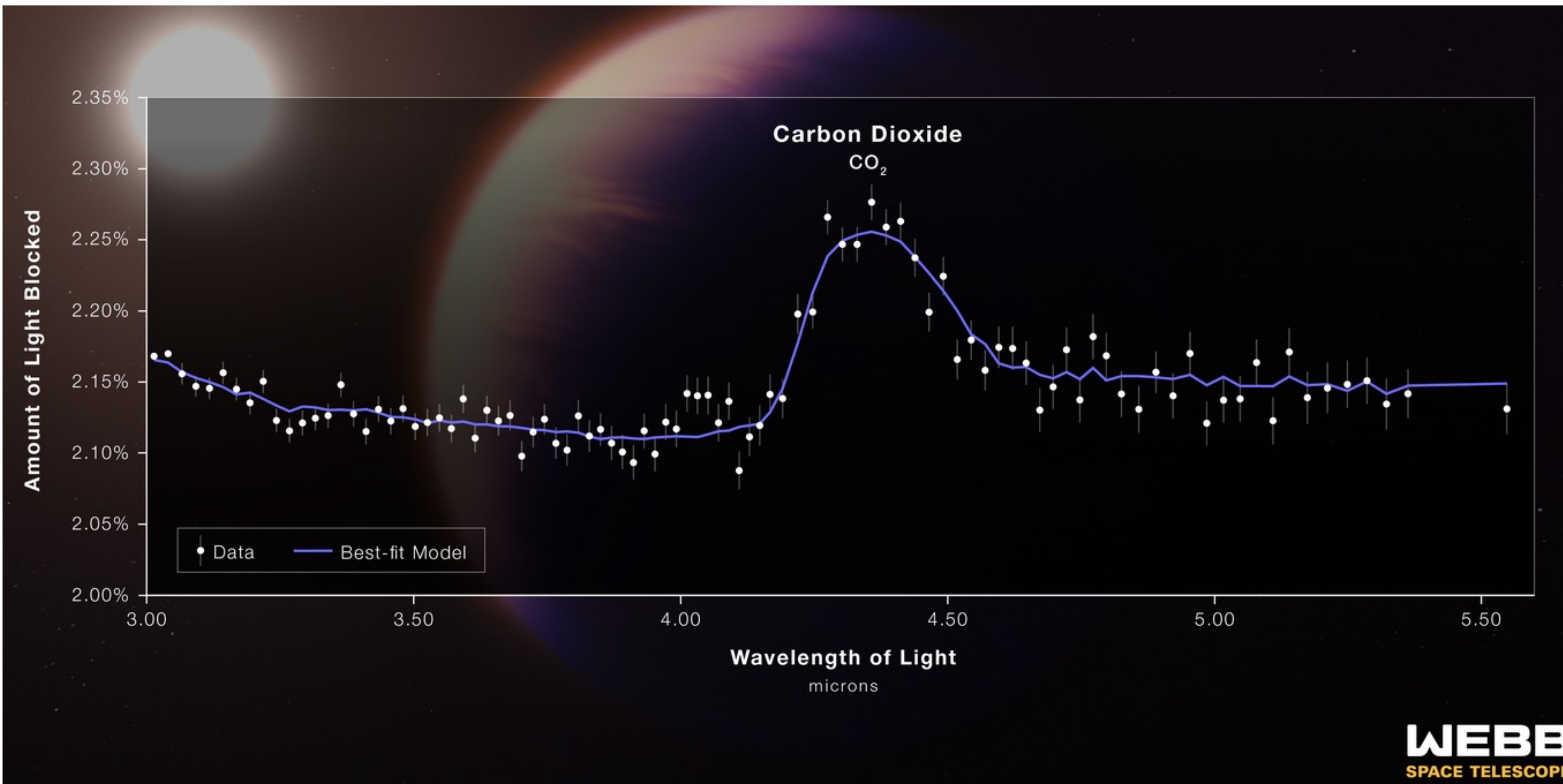


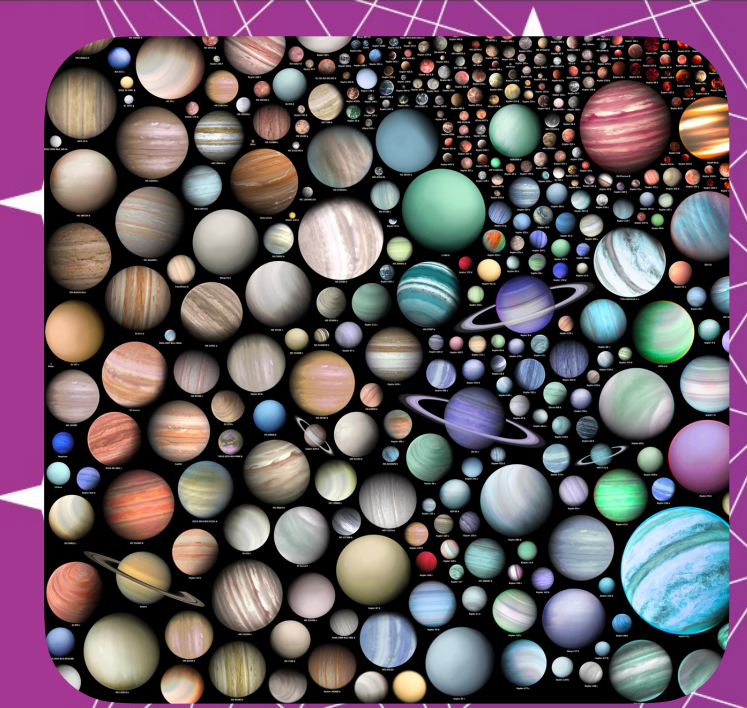
Prediction of the mass fraction of CO₂ in the atmosphere by the encoder



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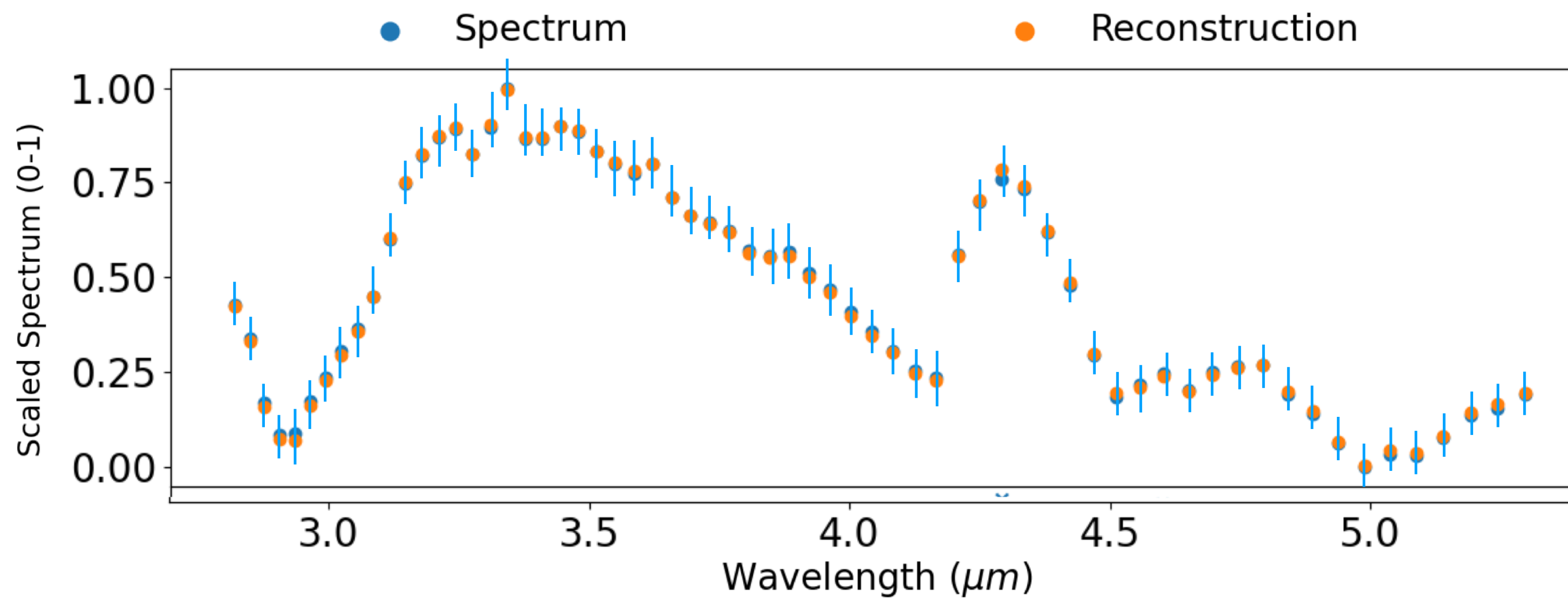
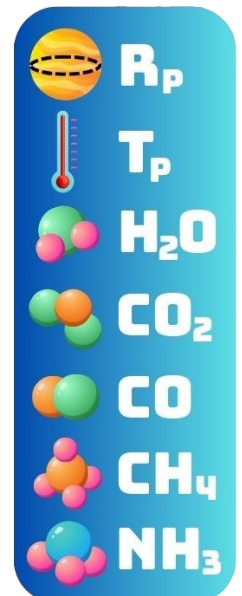
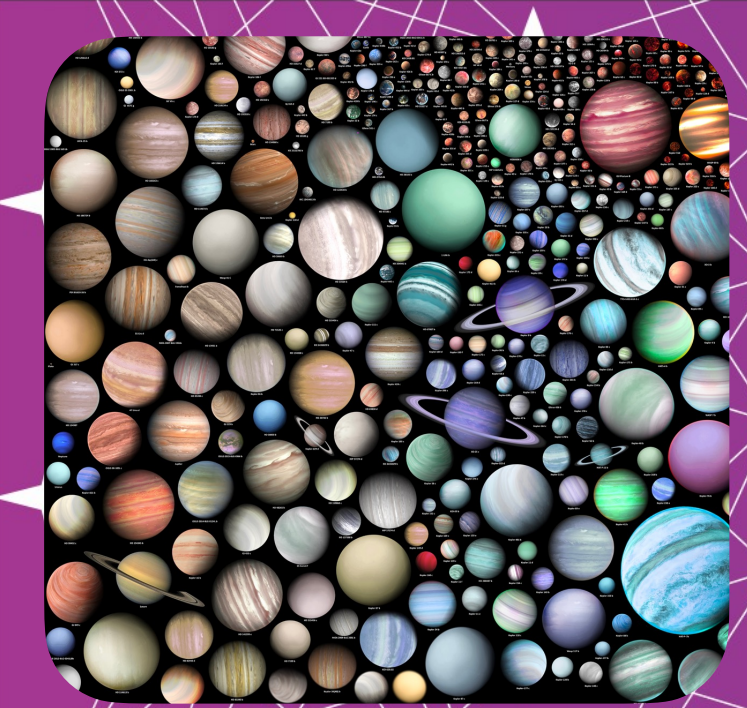


Figure 2: Reconstruction of a spectrum by the decoder



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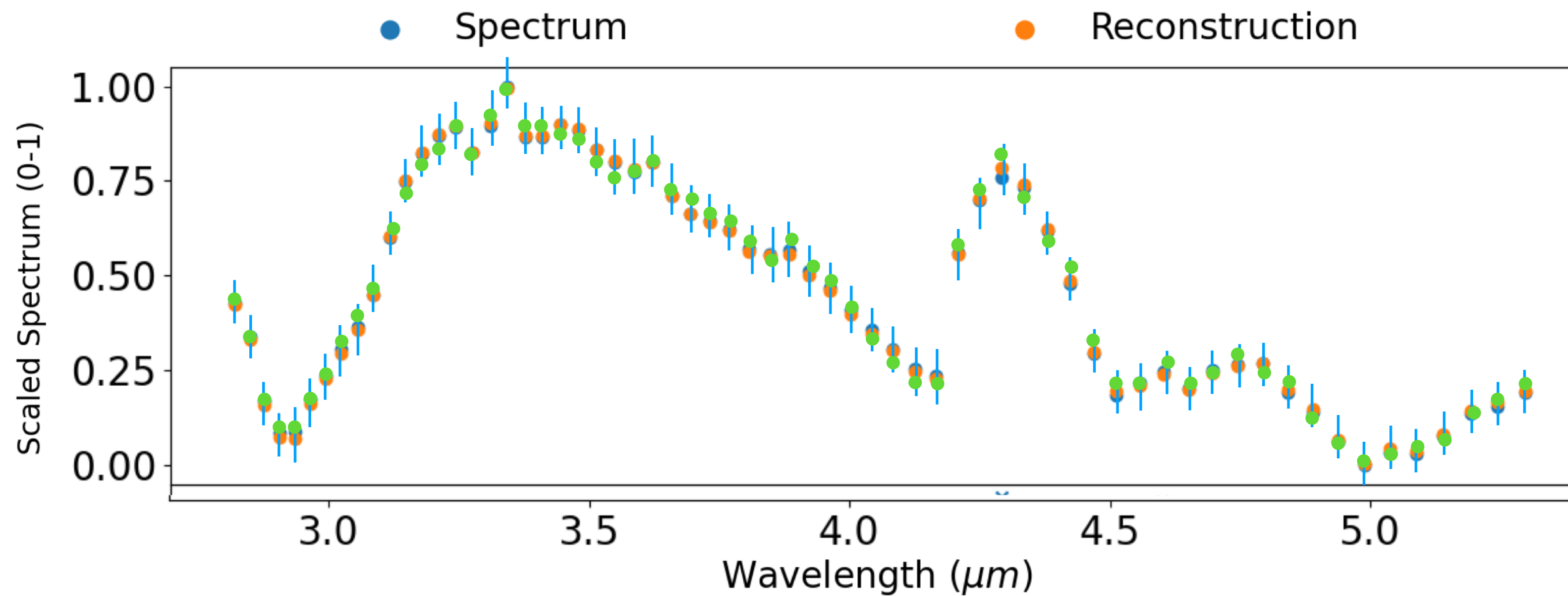
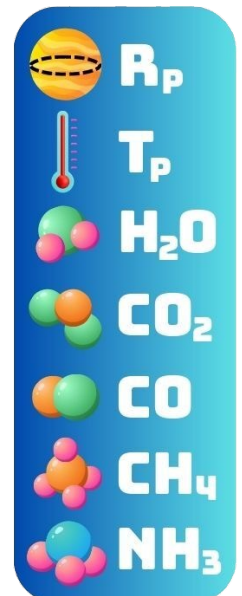
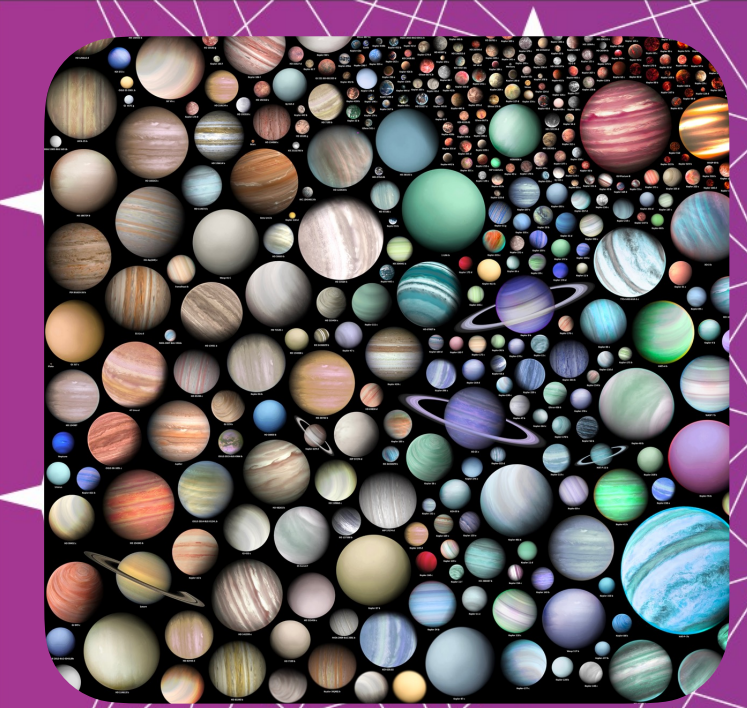
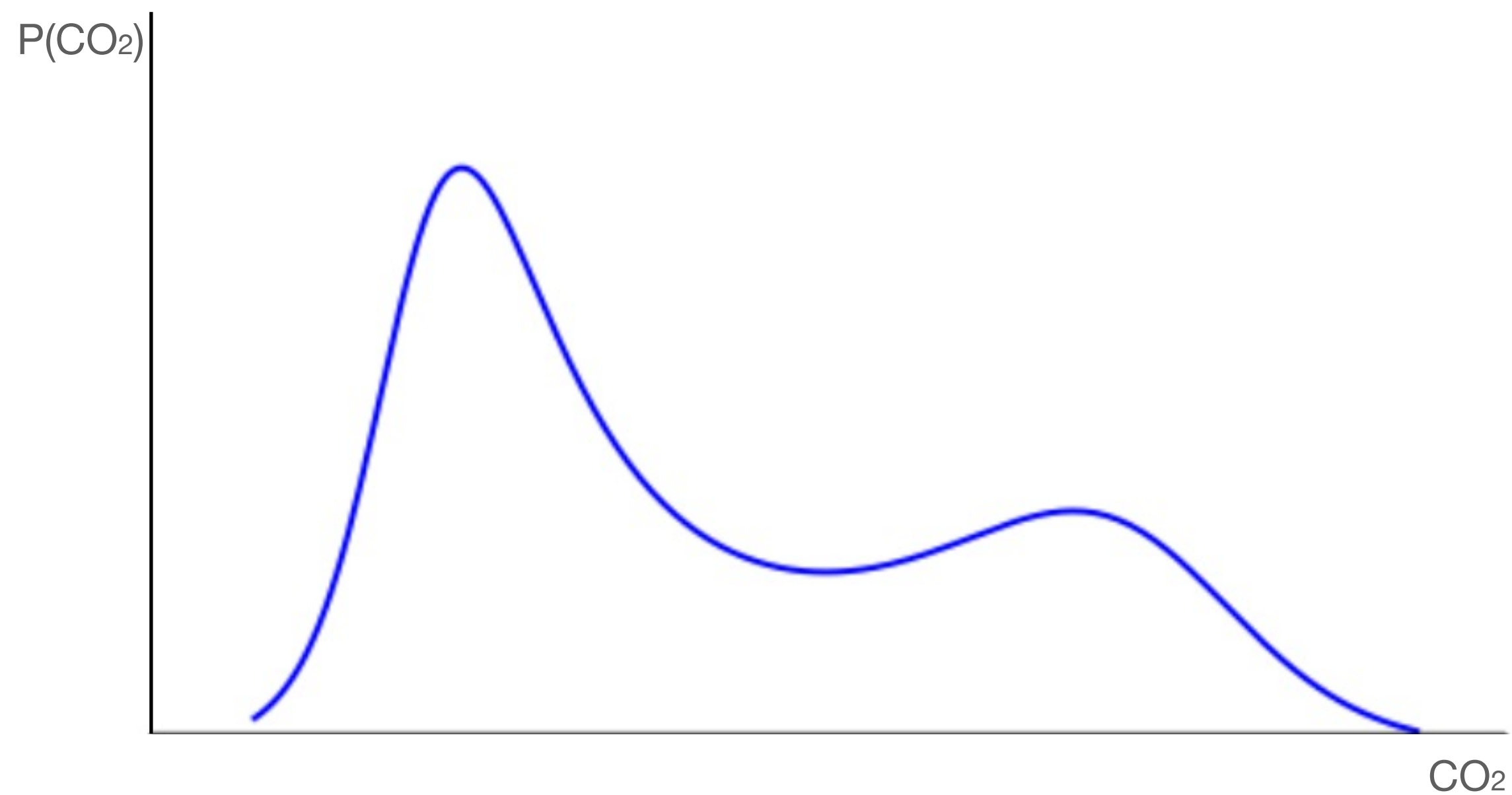


Figure 2: Reconstruction of a spectrum by the decoder

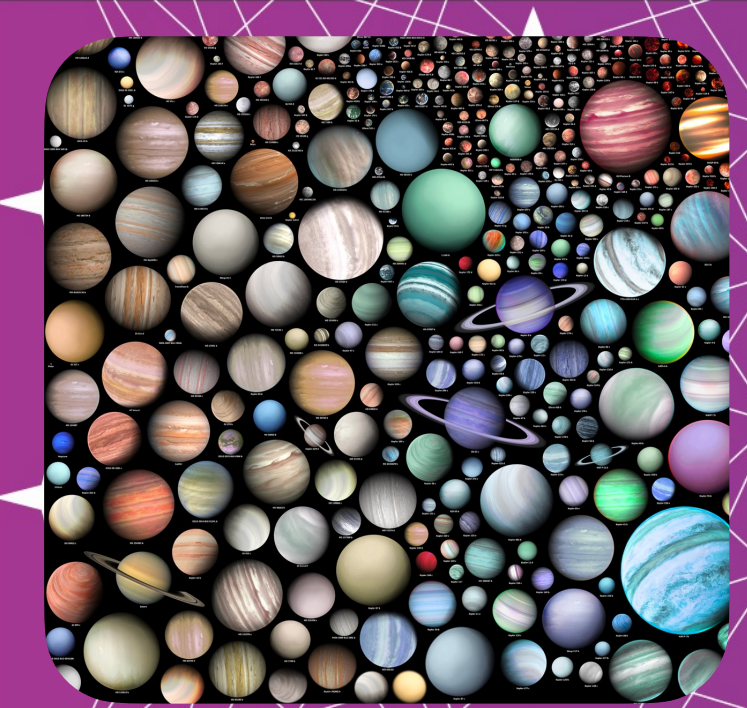


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Physical Probabilistic AI Models



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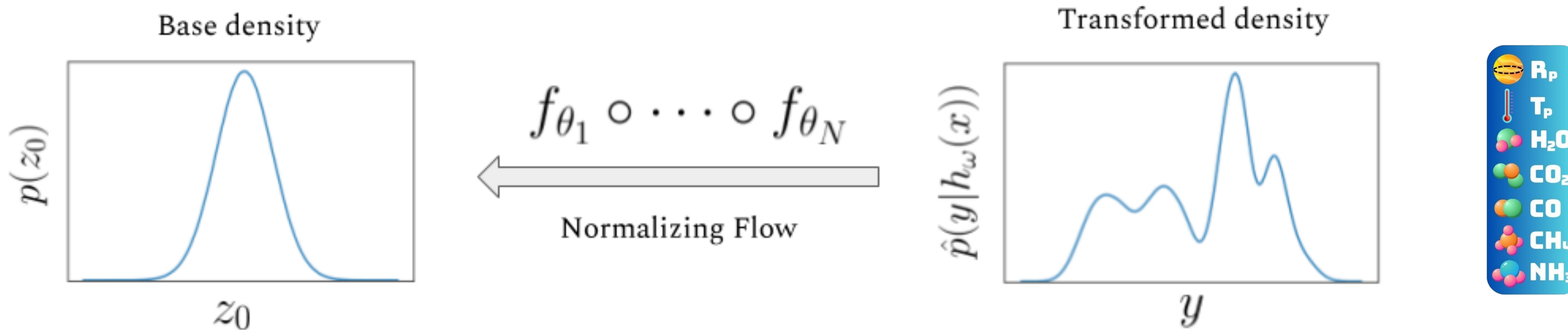
Enabling Next Generation Astrophysics

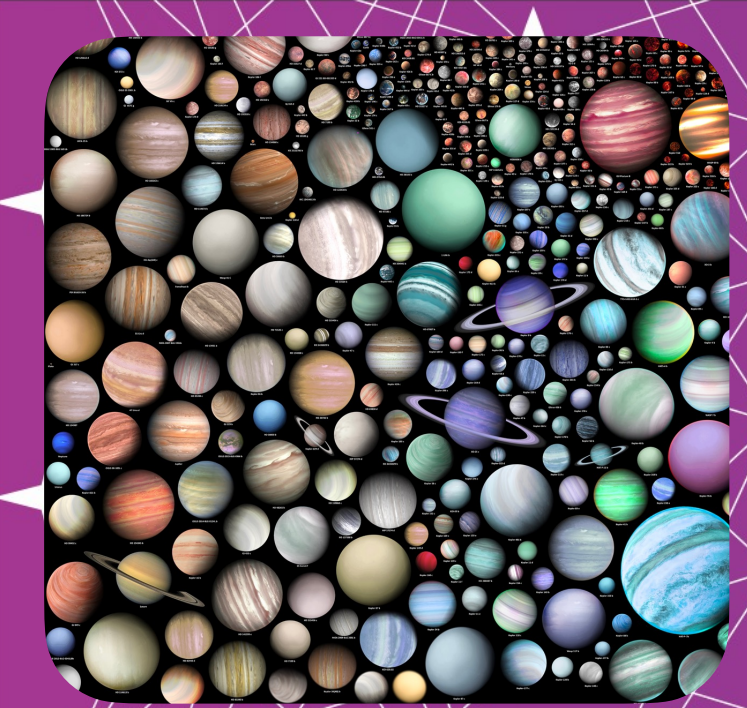


Mayeul Aubin

Carol Cuesta-Lázaro

Normalising Flows





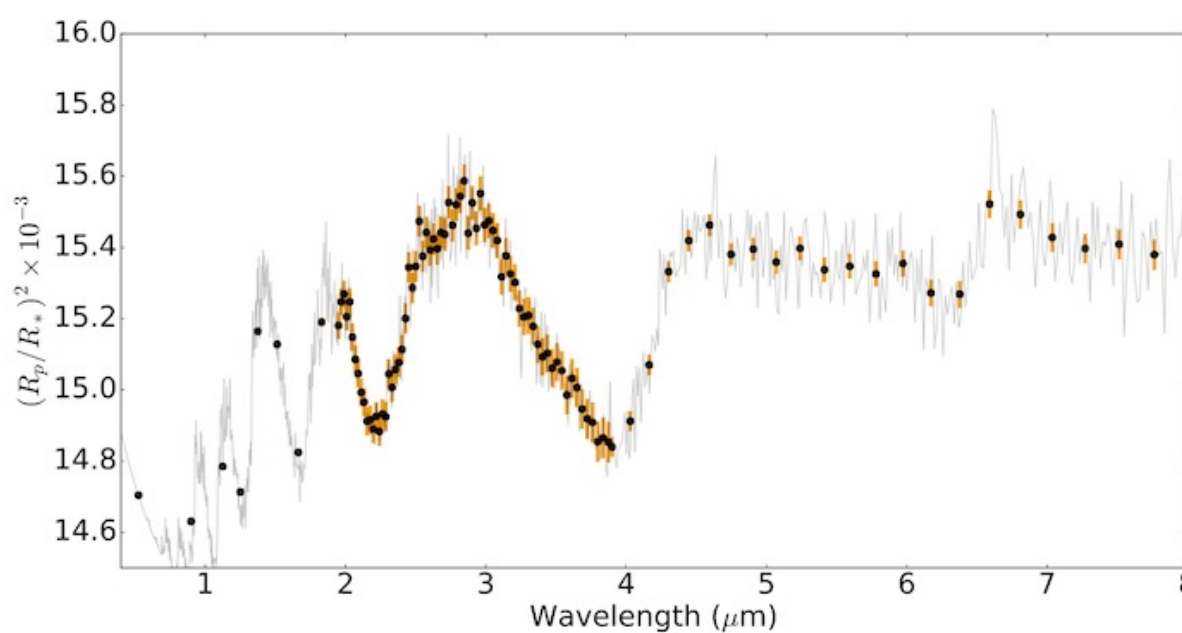
ASTROAI

Enabling Next Generation Astrophysics

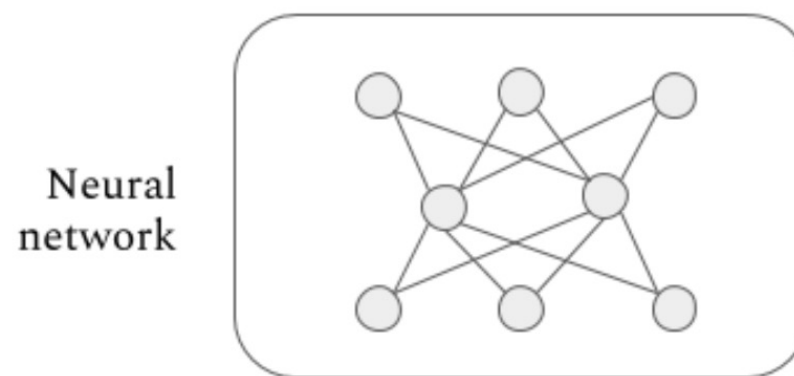


Mayeul Aubin Carol Cuesta-Lázaro

Normalising Flows

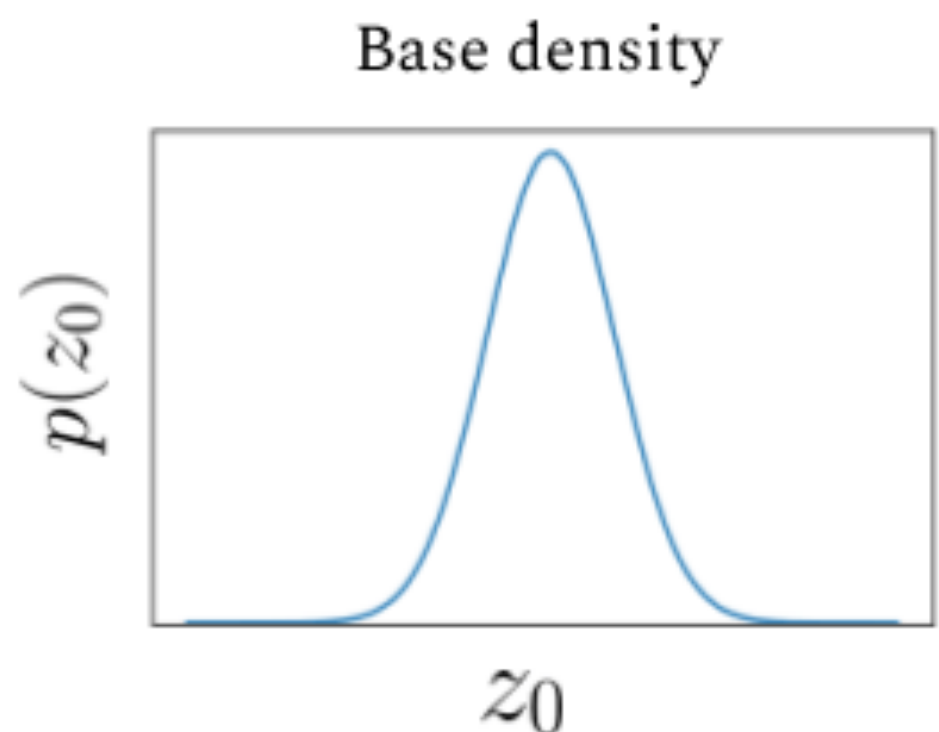


x ↓ Input vector



Neural network

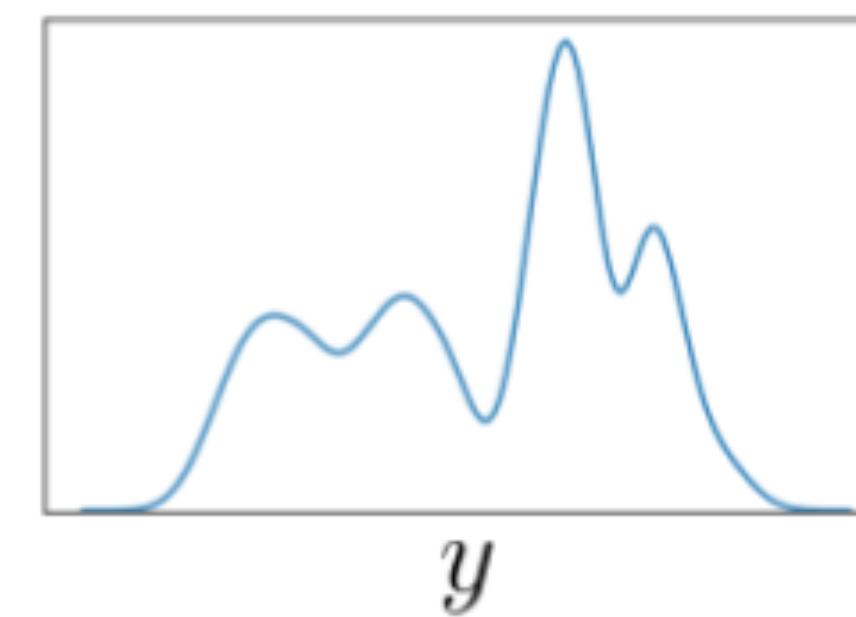
$h_\omega(x) = \theta$ ↓ Parameter vector



Base density

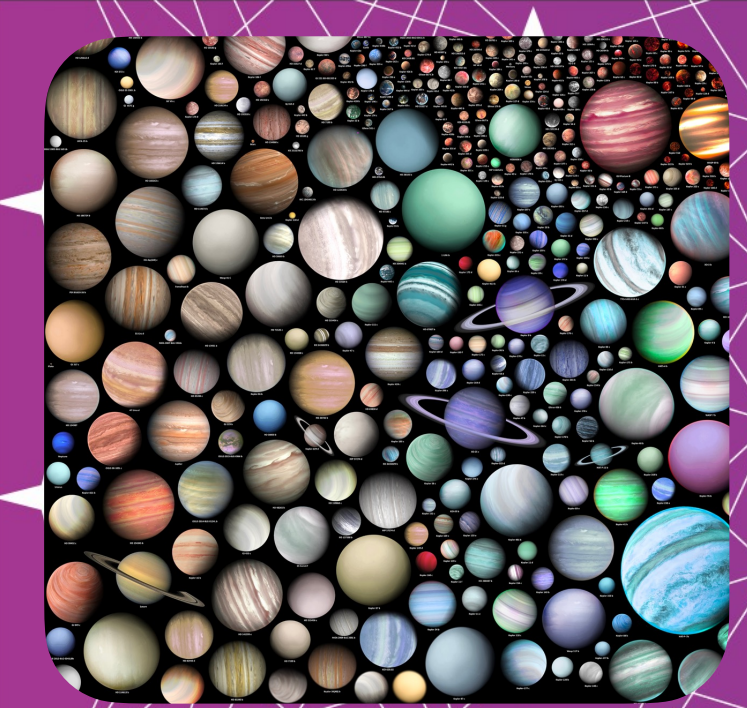
$f_{\theta_1} \circ \dots \circ f_{\theta_N}$
← Normalizing Flow

$\hat{p}(y|h_\omega(x))$



Transformed density

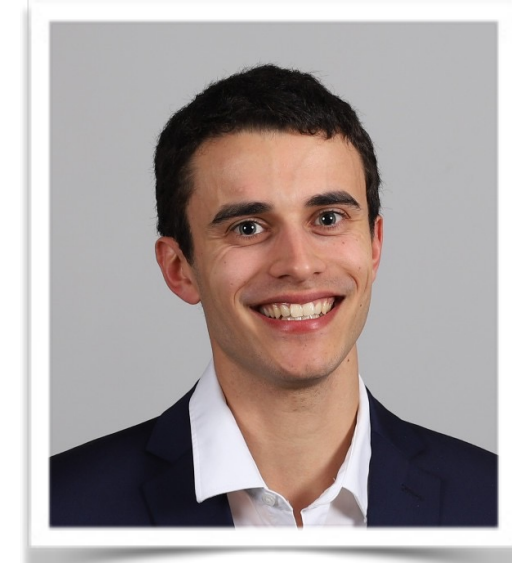




ASTROAI

Enabling Next Generation Astrophysics

The 2023 Ariel Data Challenge: Scientists invite AI experts to help study exoplanets



Mayeul Aubin

Leader Board

Rank	Name	Score
1	Mayeul_Aubin	679
2	gators	666
3	Les3Stagios	650
4	asweet	618
5	caokyhan	615
6	hieucao	610
7	dungpt	602
8	aescalantelopez	596
9	MALTO	595
10	brian_jonestown_massacre	586
11	inosen_infinity	582



1st of 293 teams!

Simulation-based Inference for Exoplanet Atmospheric Retrieval: Insights from winning the Ariel Data Challenge 2023 using Normalizing Flows

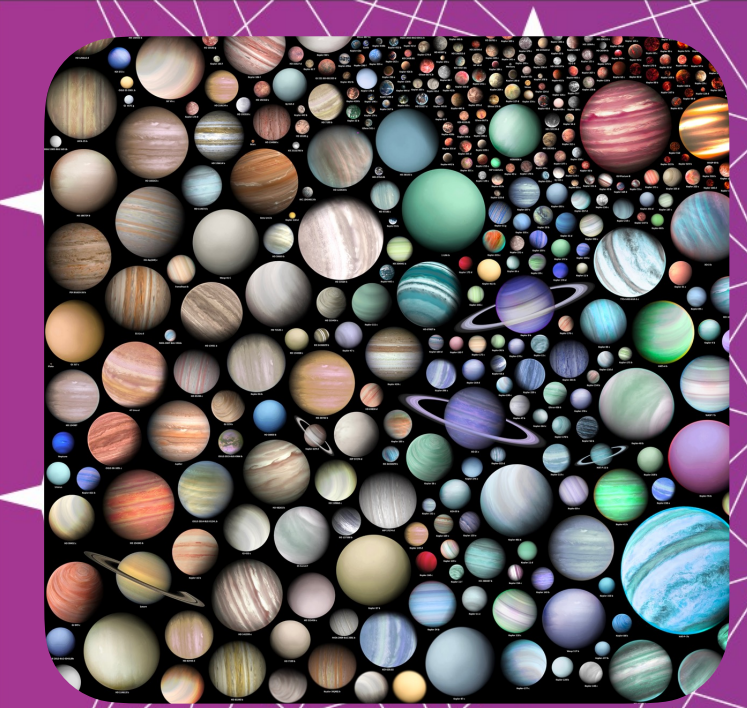
Mayeul Aubin^{1,2*}, Carolina Cuesta-Lazaro^{3,4}, Ethan Tregidga^{1,5}, Javier Viaña⁶, Cecilia Garraffo^{1,7}, Iouli E. Gordon⁸, Mercedes López-Morales⁸, Robert J. Hargreaves⁸, Vladimir Yu. Makhnev⁸, Jeremy J. Drake⁷, Douglas P. Finkbeiner³, and Phillip Cargile⁹



Cecilia Garraffo - CfA



AI Goes MAD², IFT UAM-CSIC, Oct 2024



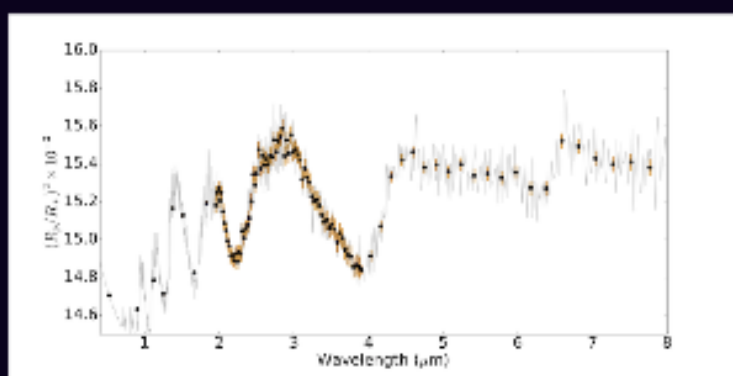
ASTROAI

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Mayeul Aubin

Input Spectrum



1D base distrib

1D target posterior

Independent NF

Independent NF

Independent NF

R_p

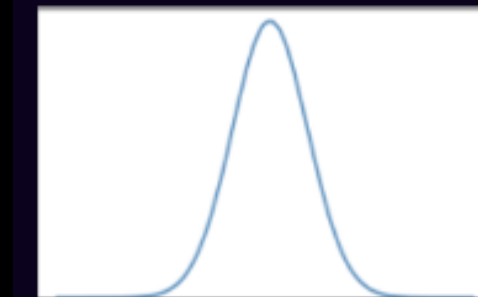
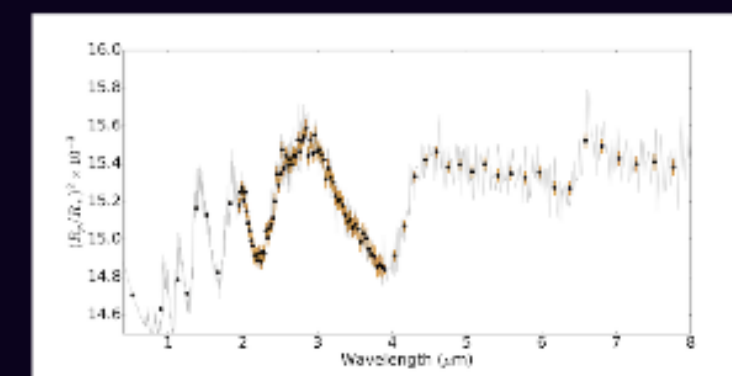
T_p

NH_3

R_p
 T_p
 H_2O
 CO_2
 CO
 CH_4
 NH_3

A set of independent Normalising Flows

Input Spectrum



7D base distrib

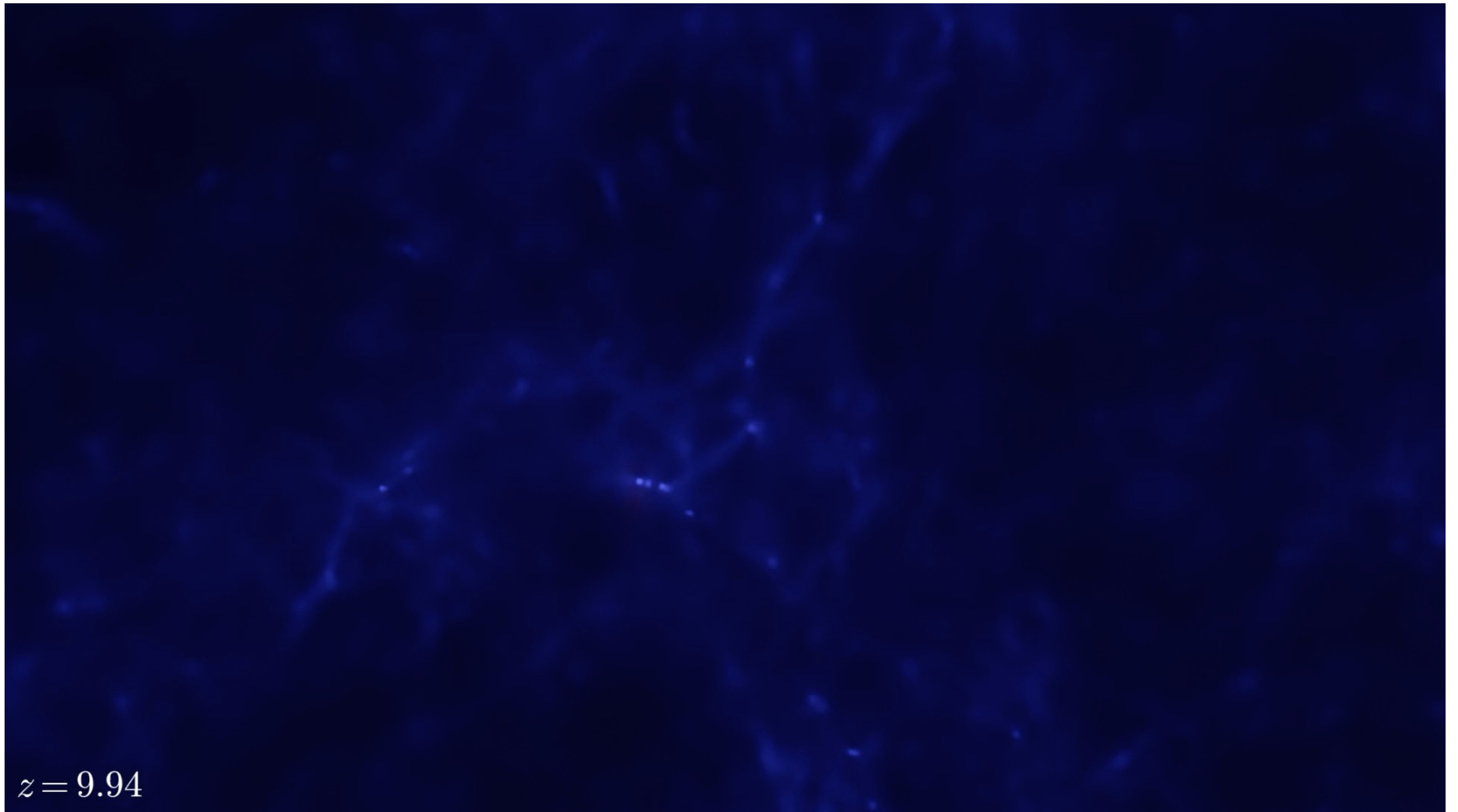
Complete NF

R_p
 T_p
 H_2O
 CO_2
 CO
 CH_4
 NH_3

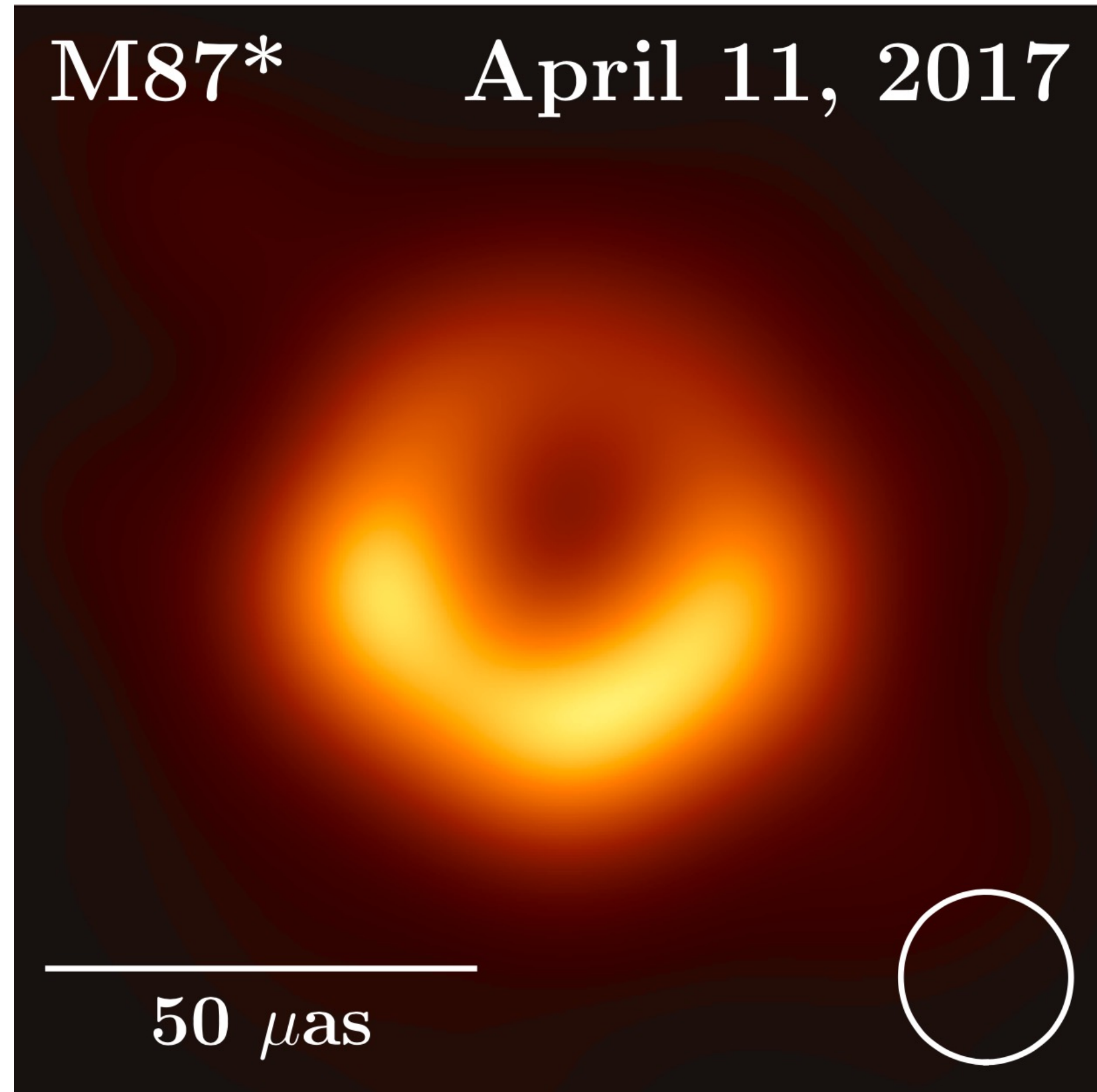
7D target posterior

One complete Normalising Flow

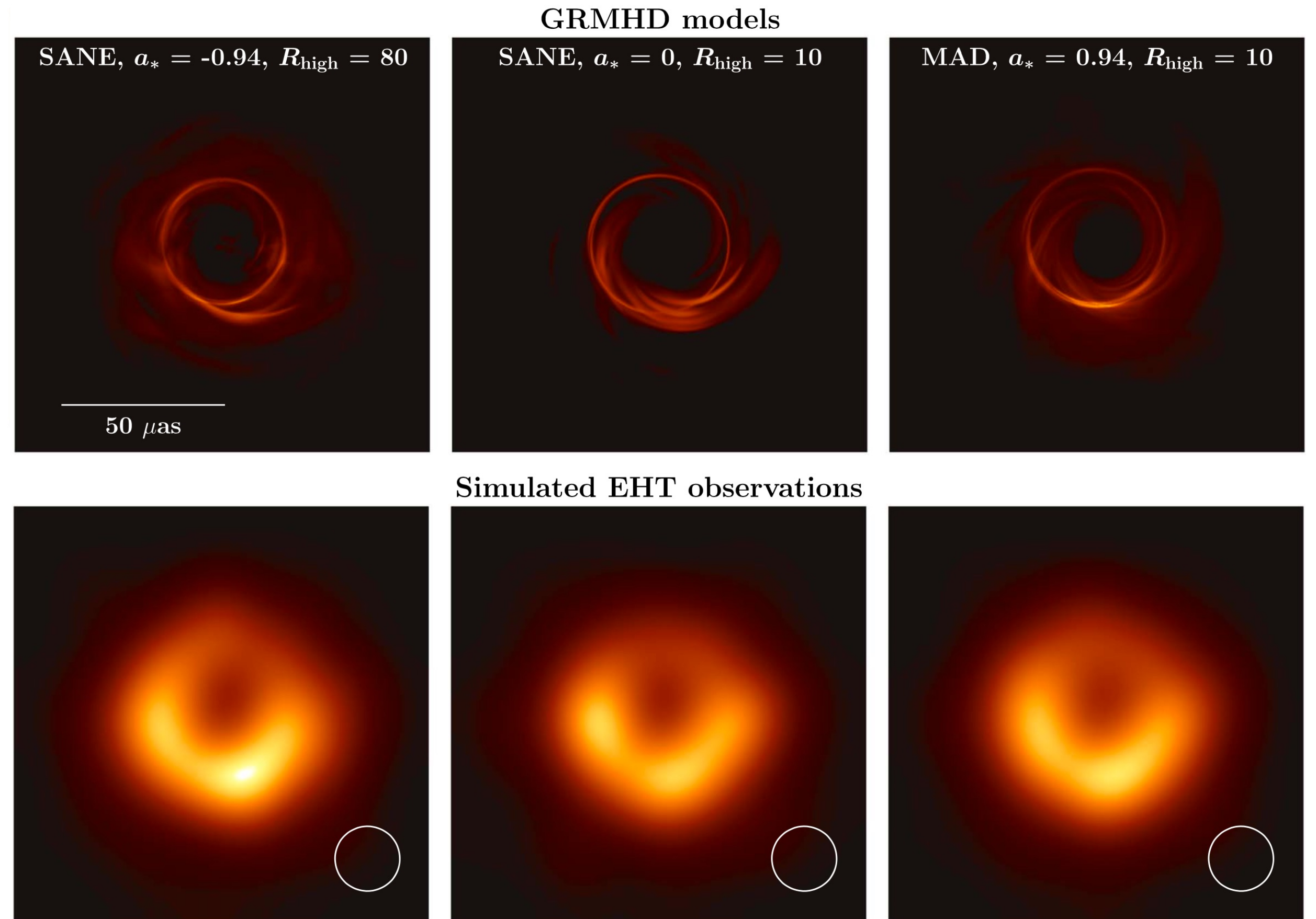
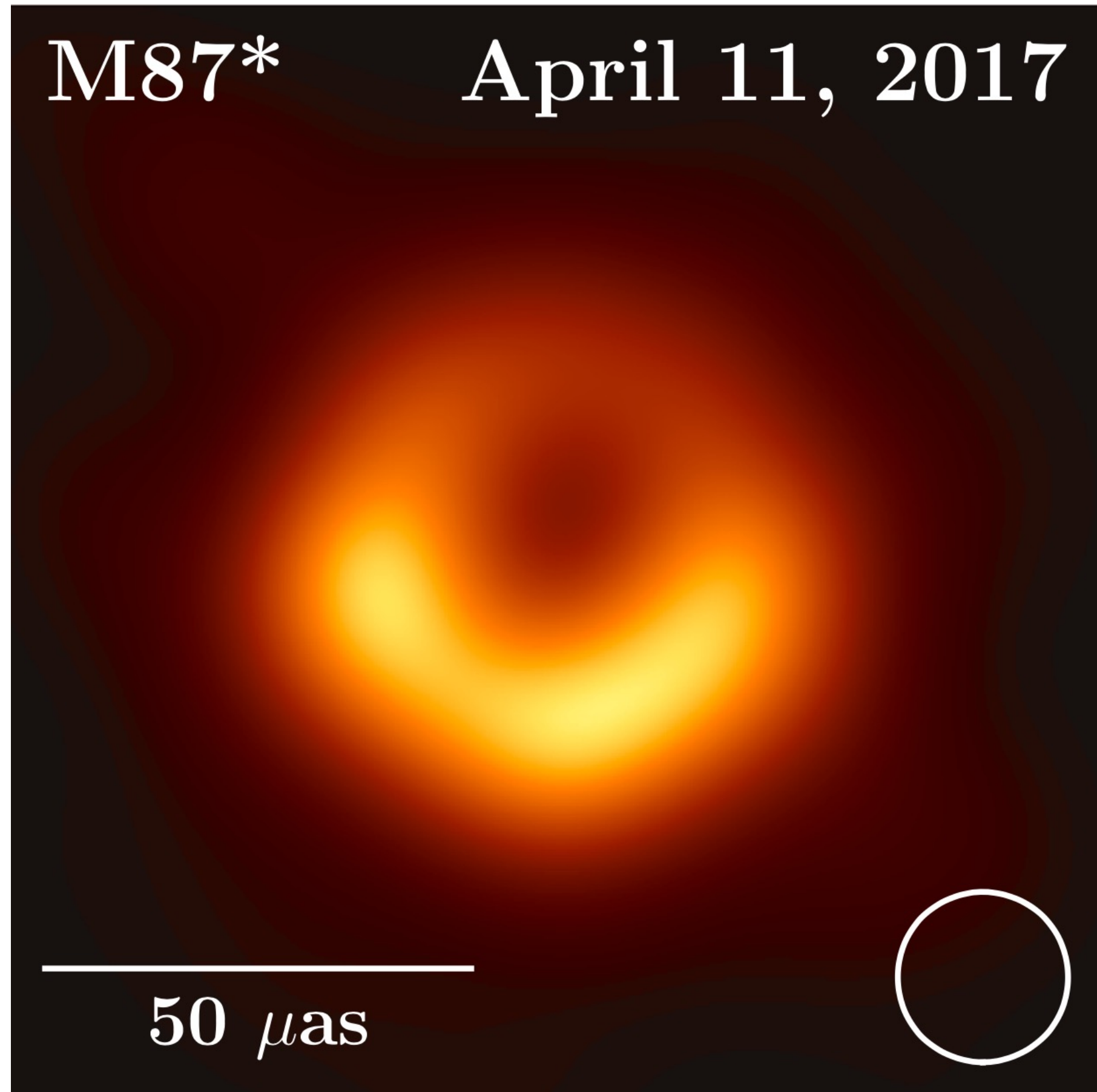
AI Simulations

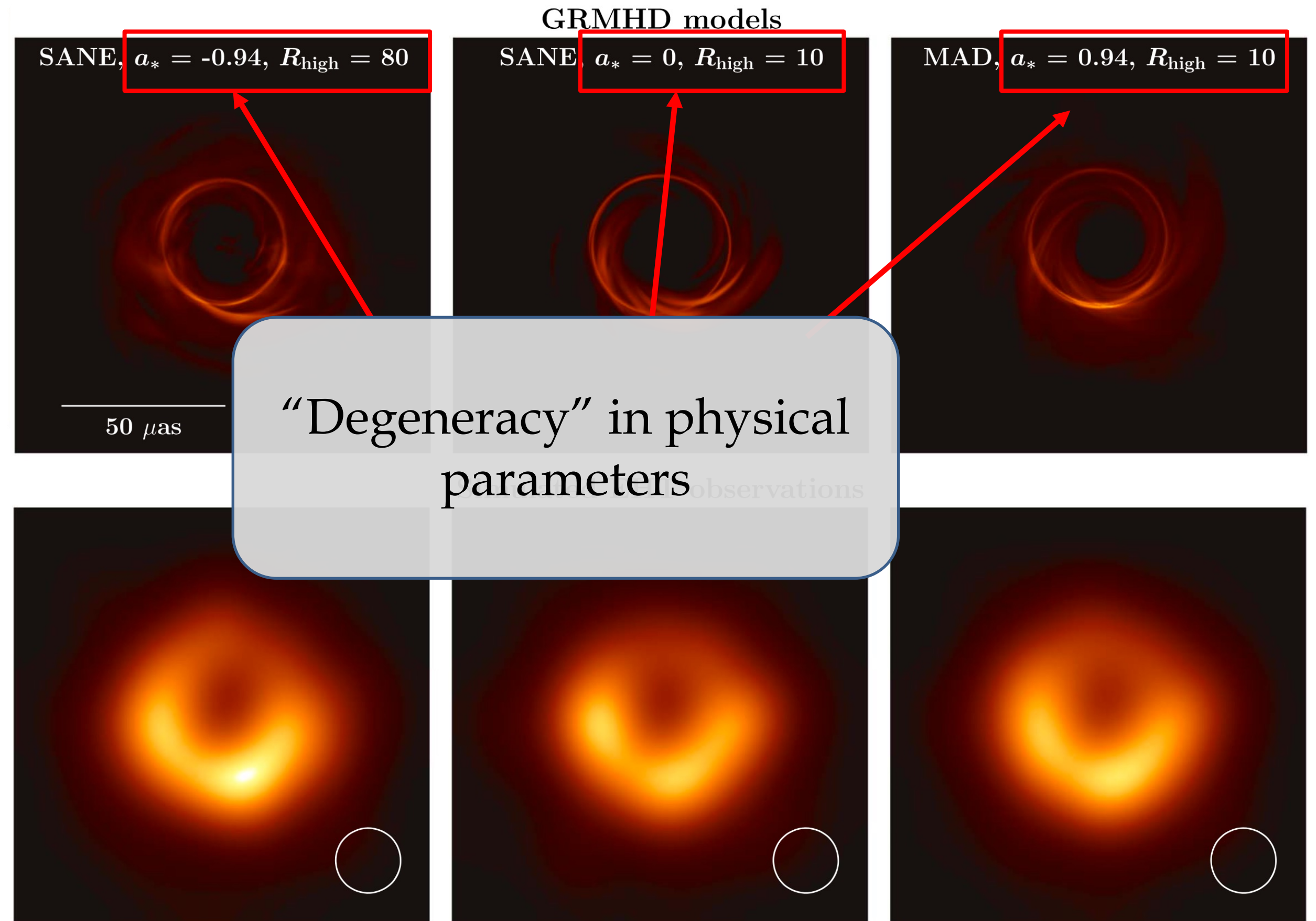
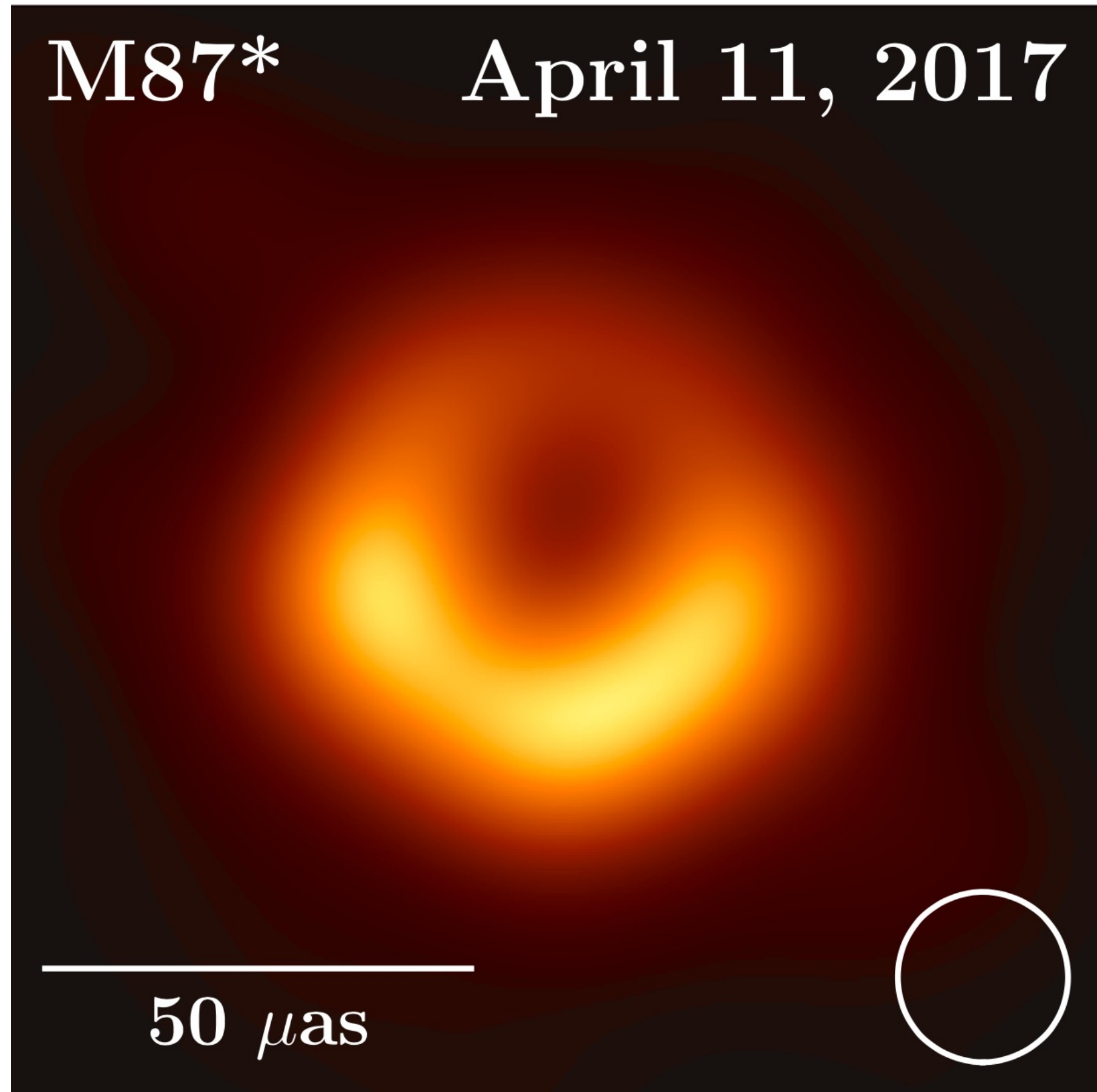


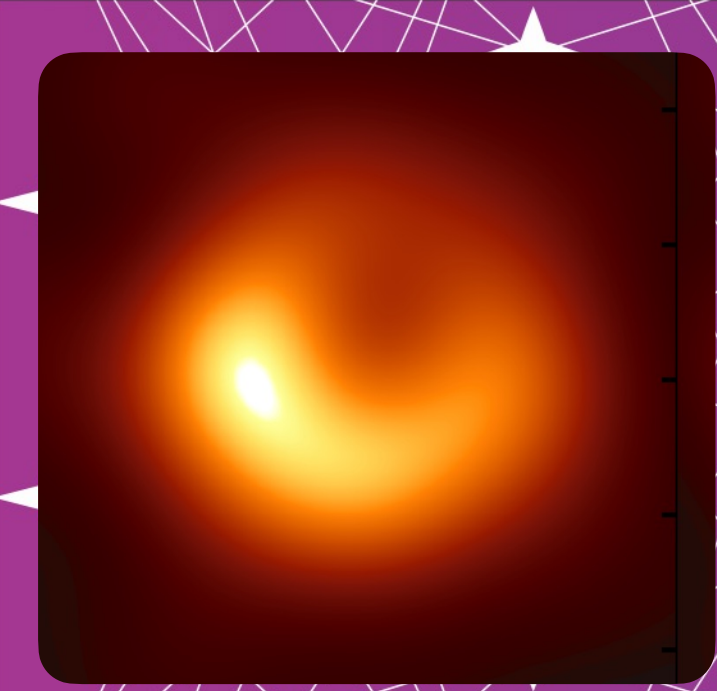
Effects of supermassive black holes feedback from a CAMELS-SIMBA cosmological simulation
Francisco Villaescusa-Navarro, CCA Flatiron Institute



Event Horizon Telescope Collaboration 2019

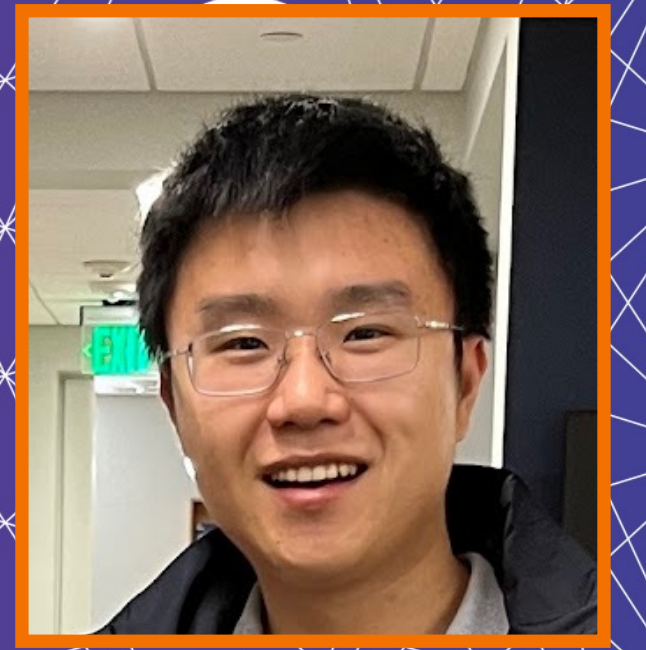






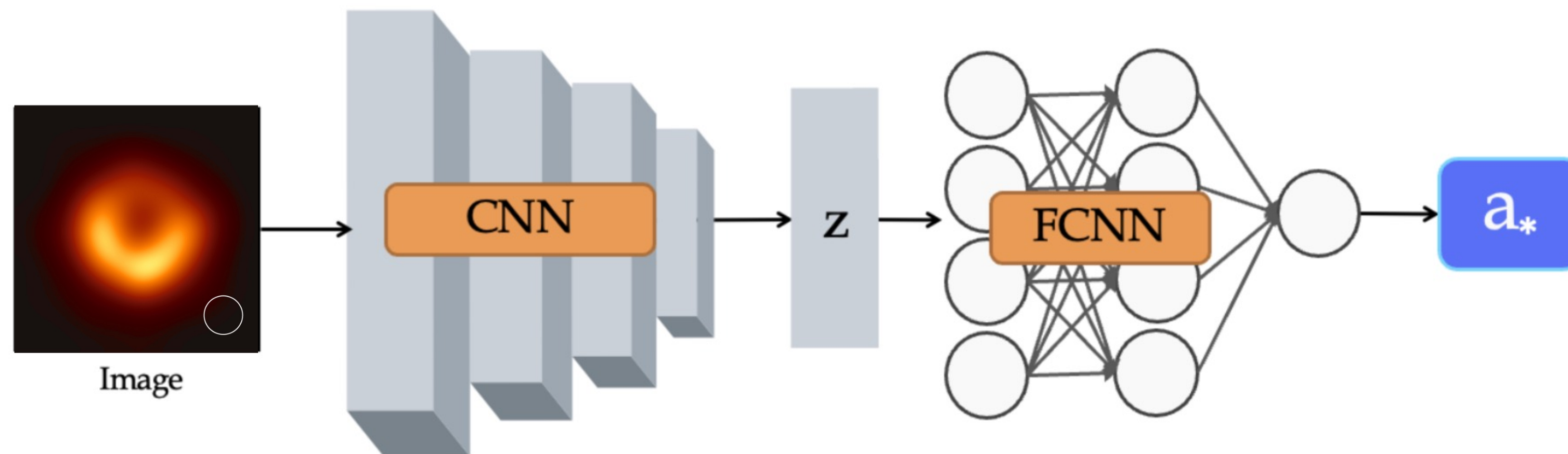
ASTROAI

Enabling Next Generation Astrophysics

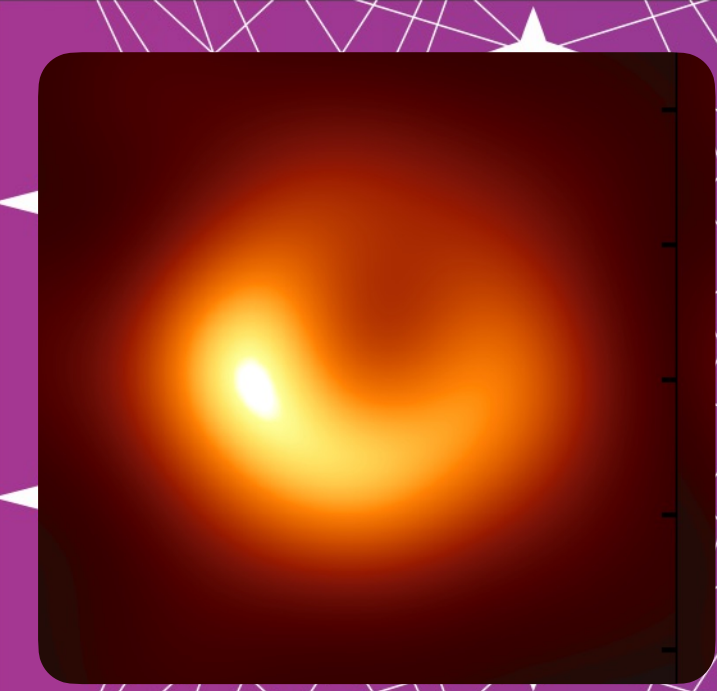


Tao Tsui

Black Hole Characterization from EHT images



Tsui et al. in Press



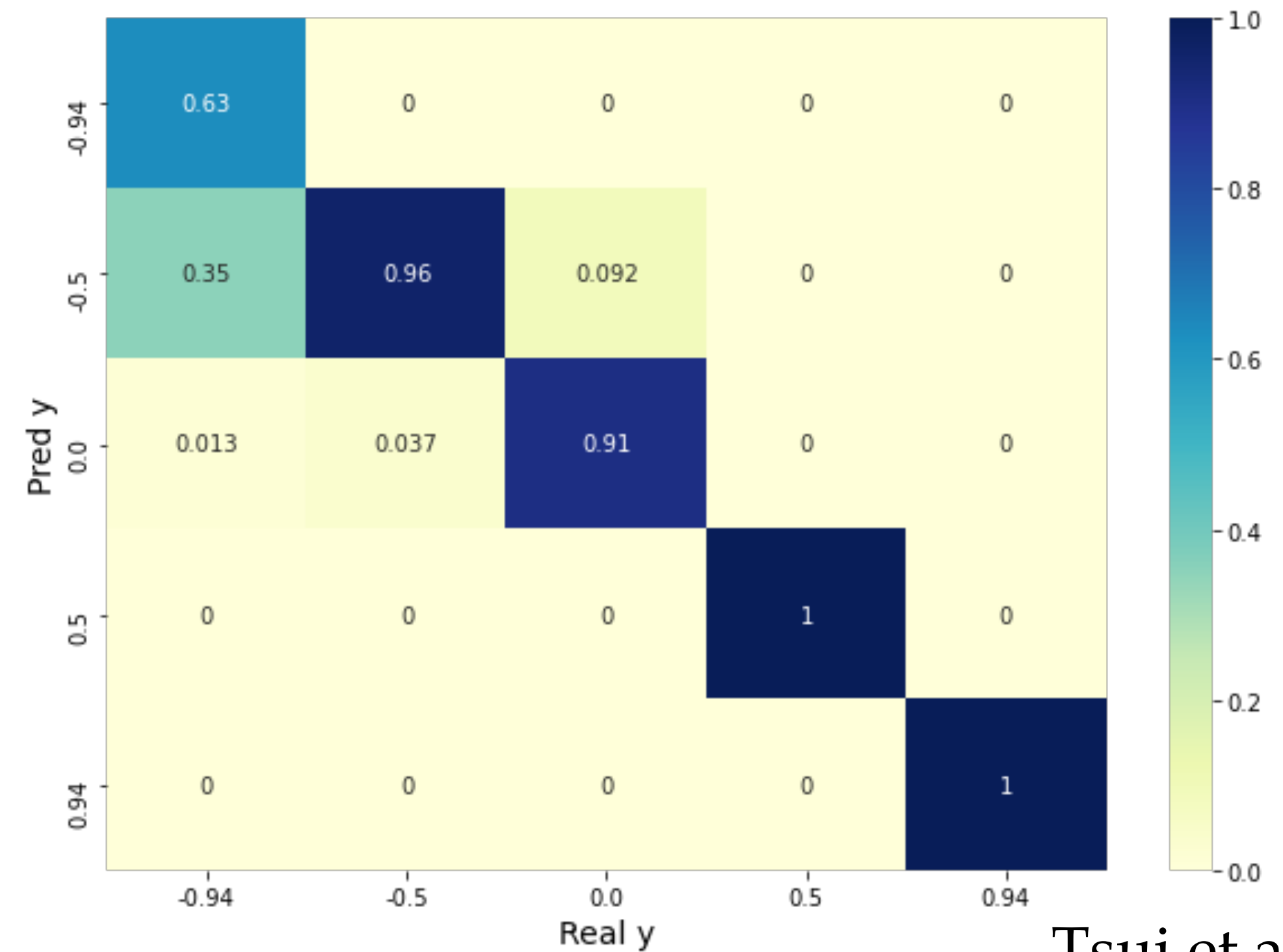
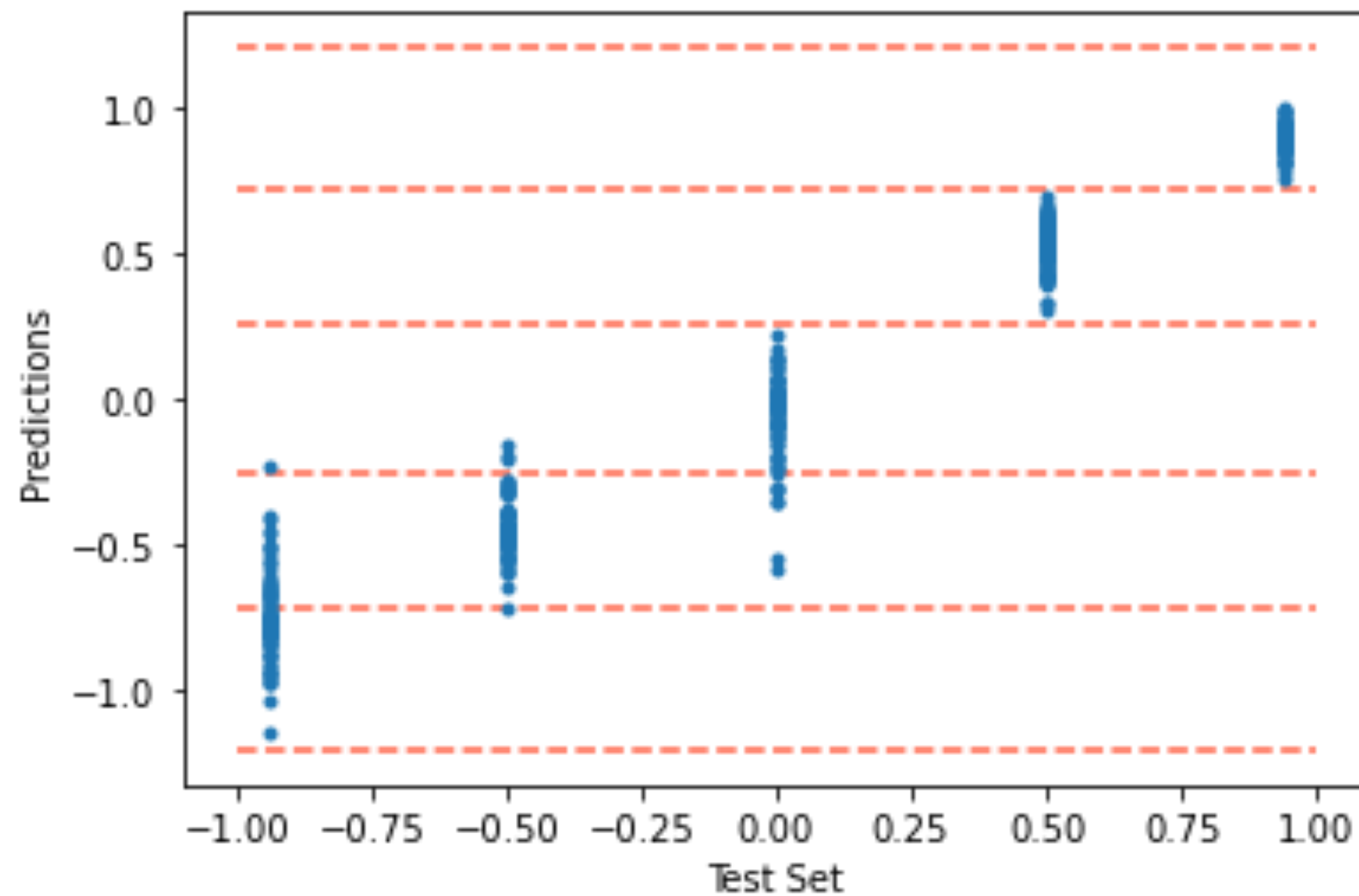
ASTROAI

Enabling Next Generation Astrophysics

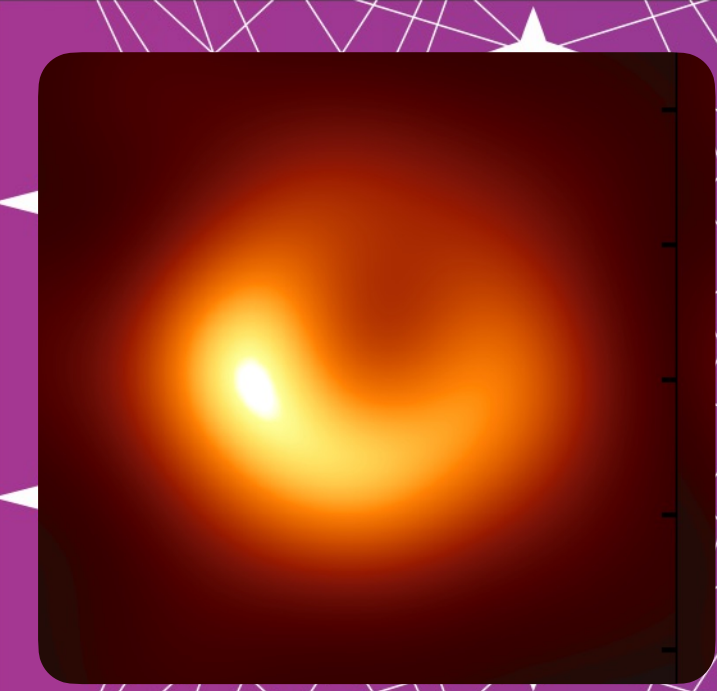


Tao Tsui

Black Hole Characterization from EHT images



Tsui et al. in Press



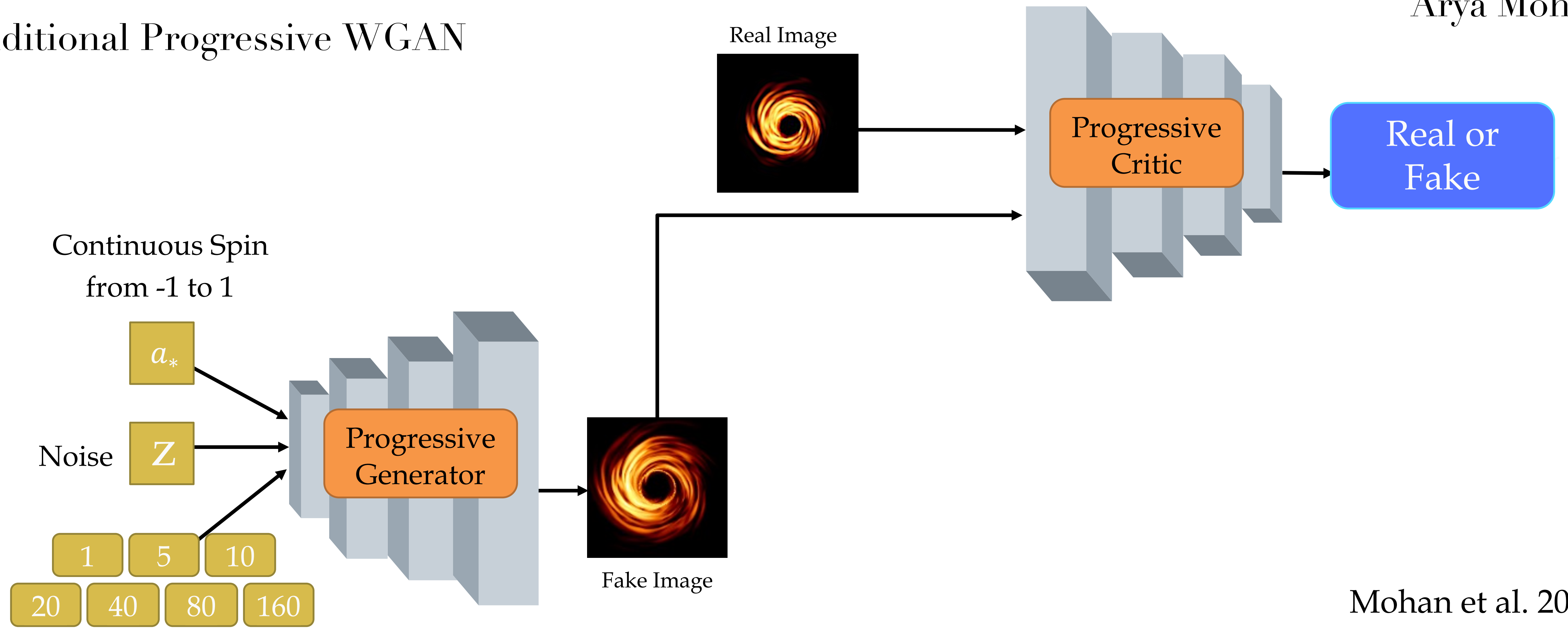
ASTROAI

Enabling Next Generation Astrophysics

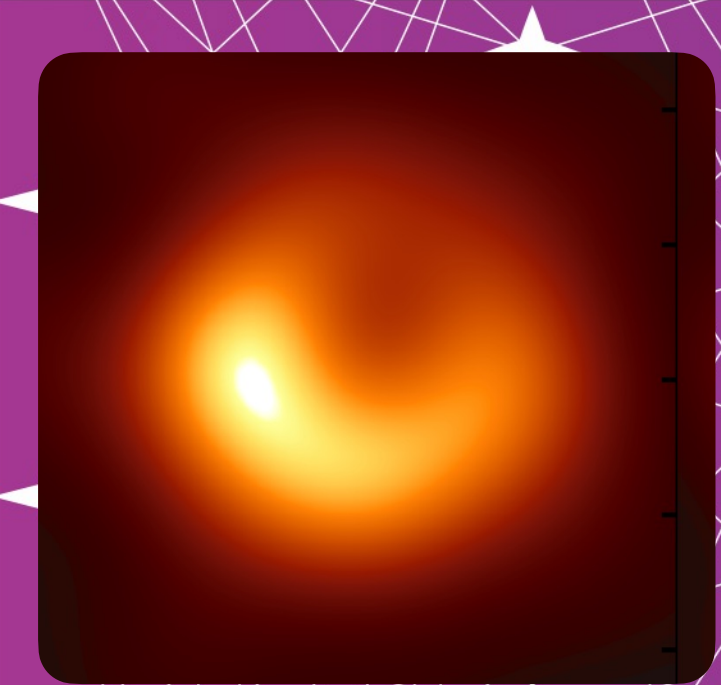


Arya Mohan

Conditional Progressive WGAN



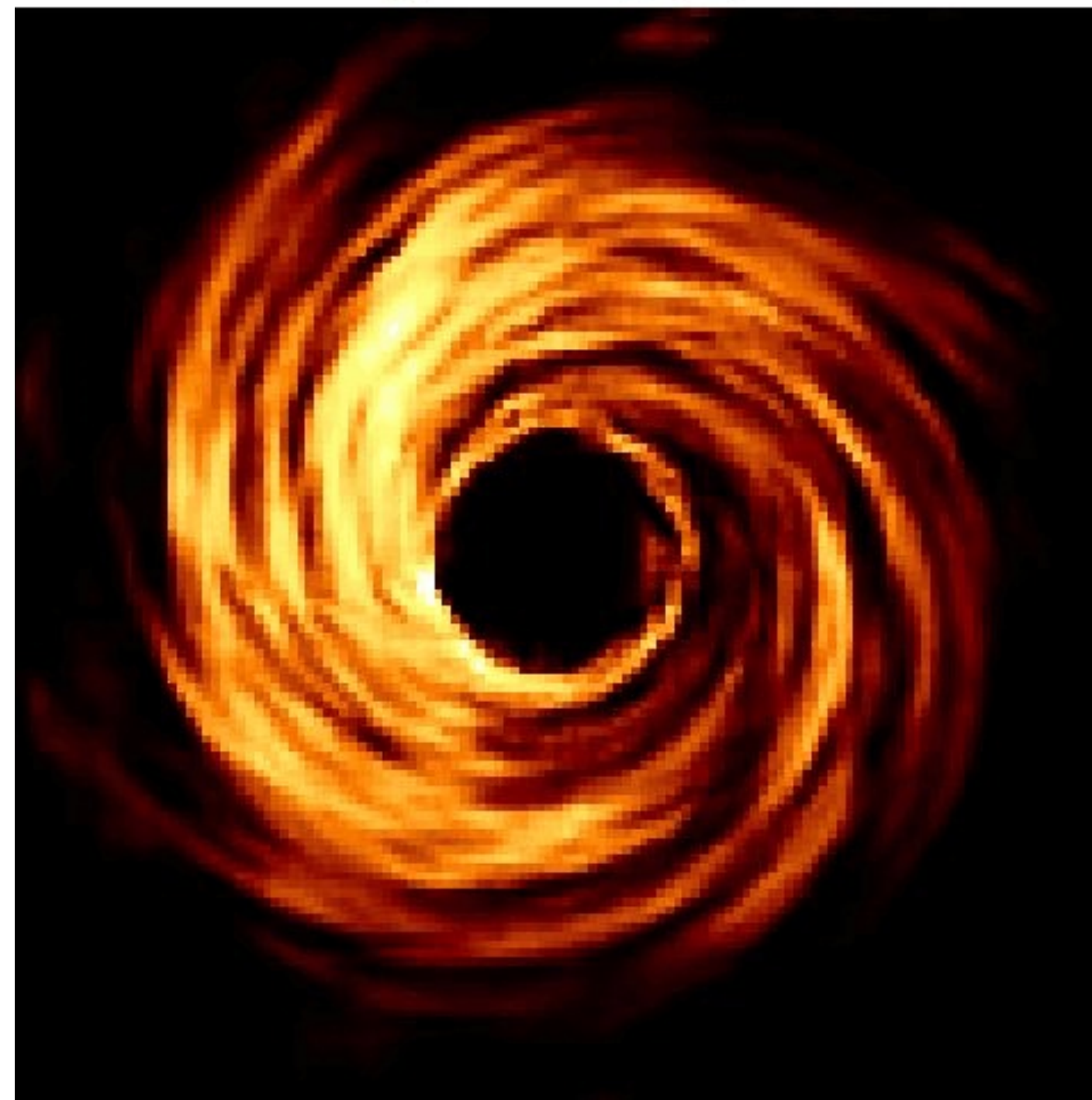
Mohan et al. 2023



ASTROAI

Enabling Next Generation Astrophysics

$a = -0.4$

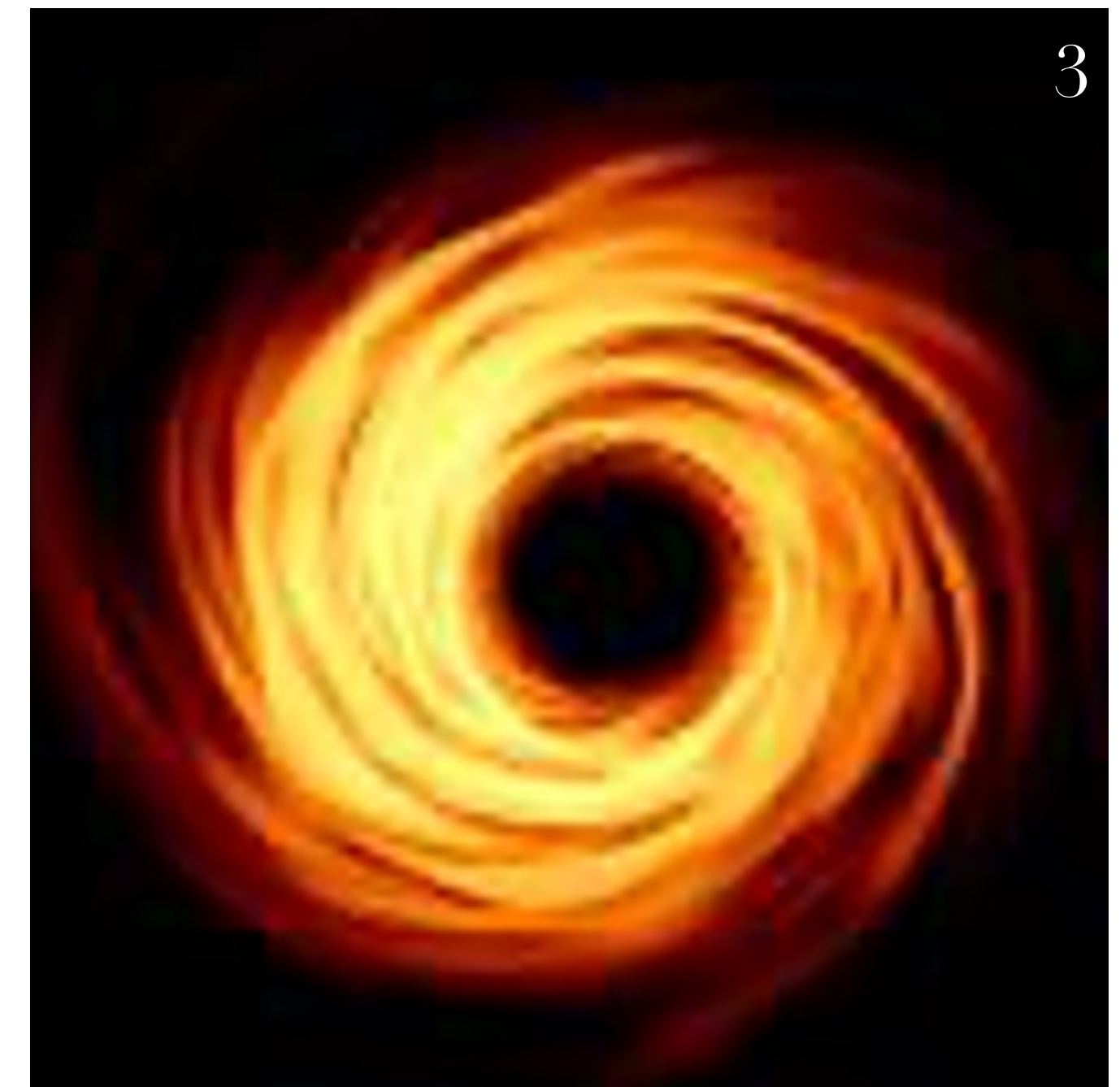
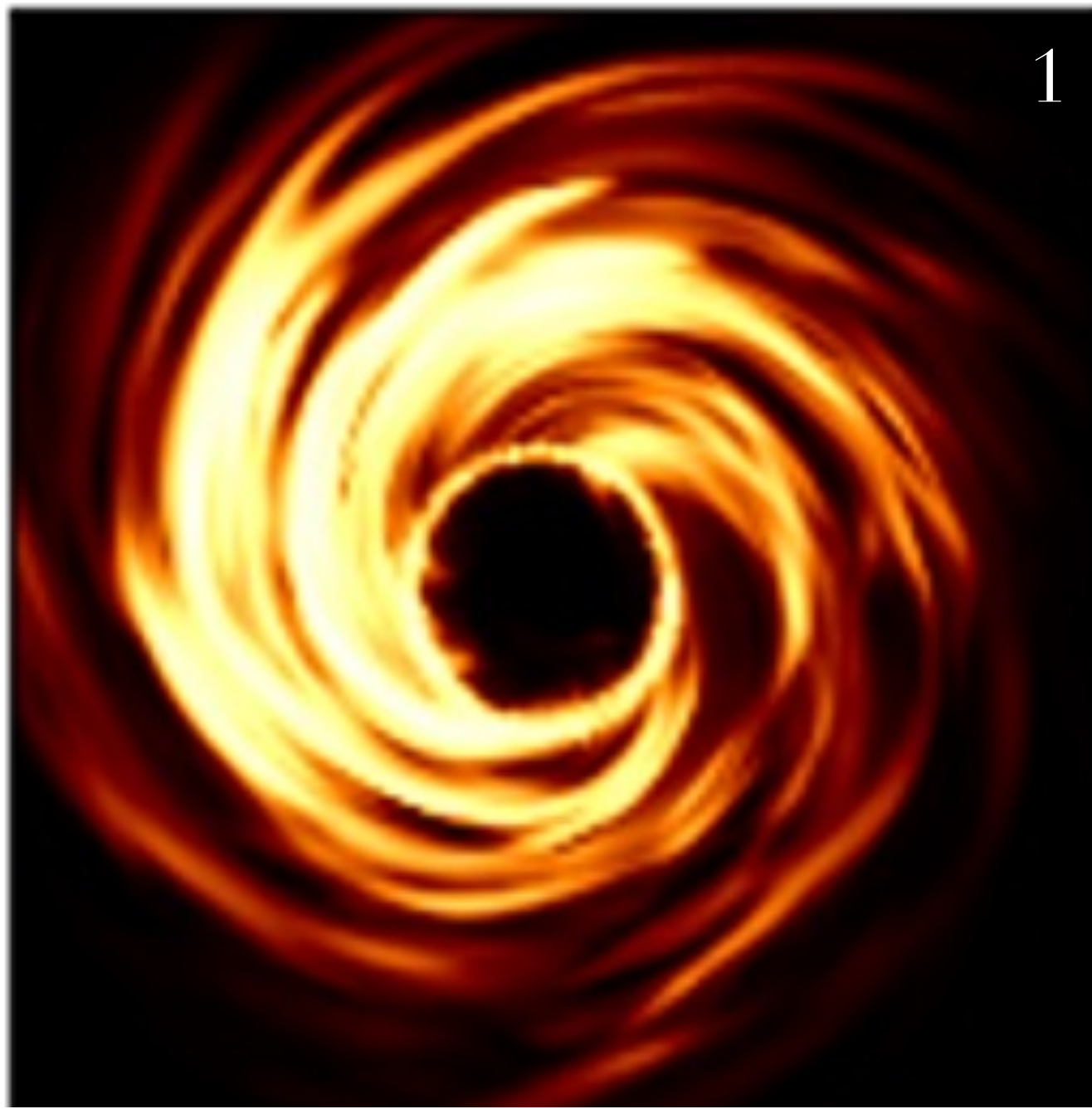


Mohan et al. 2023

ASTROAI

Enabling Next Generation Astrophysics

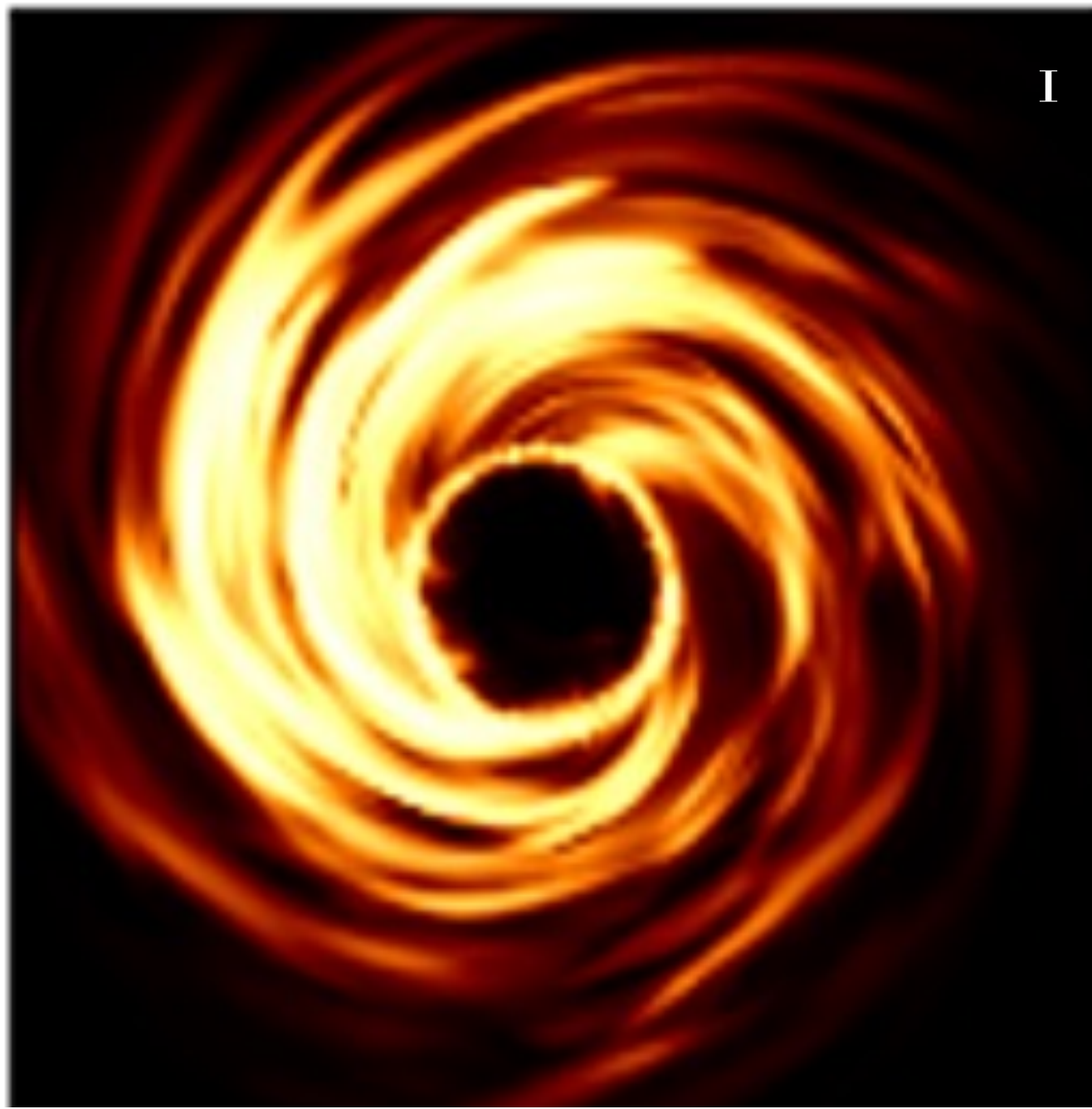
Supermassive BHs



ASTROAI

Enabling Next Generation Astrophysics

Supermassive BHs



GRMHD



GenAI



GRMHD

Generative *AI* for *Astrophysics*

Diffusion Models



DALL-E generated

Diffusion Models for Astrophysics

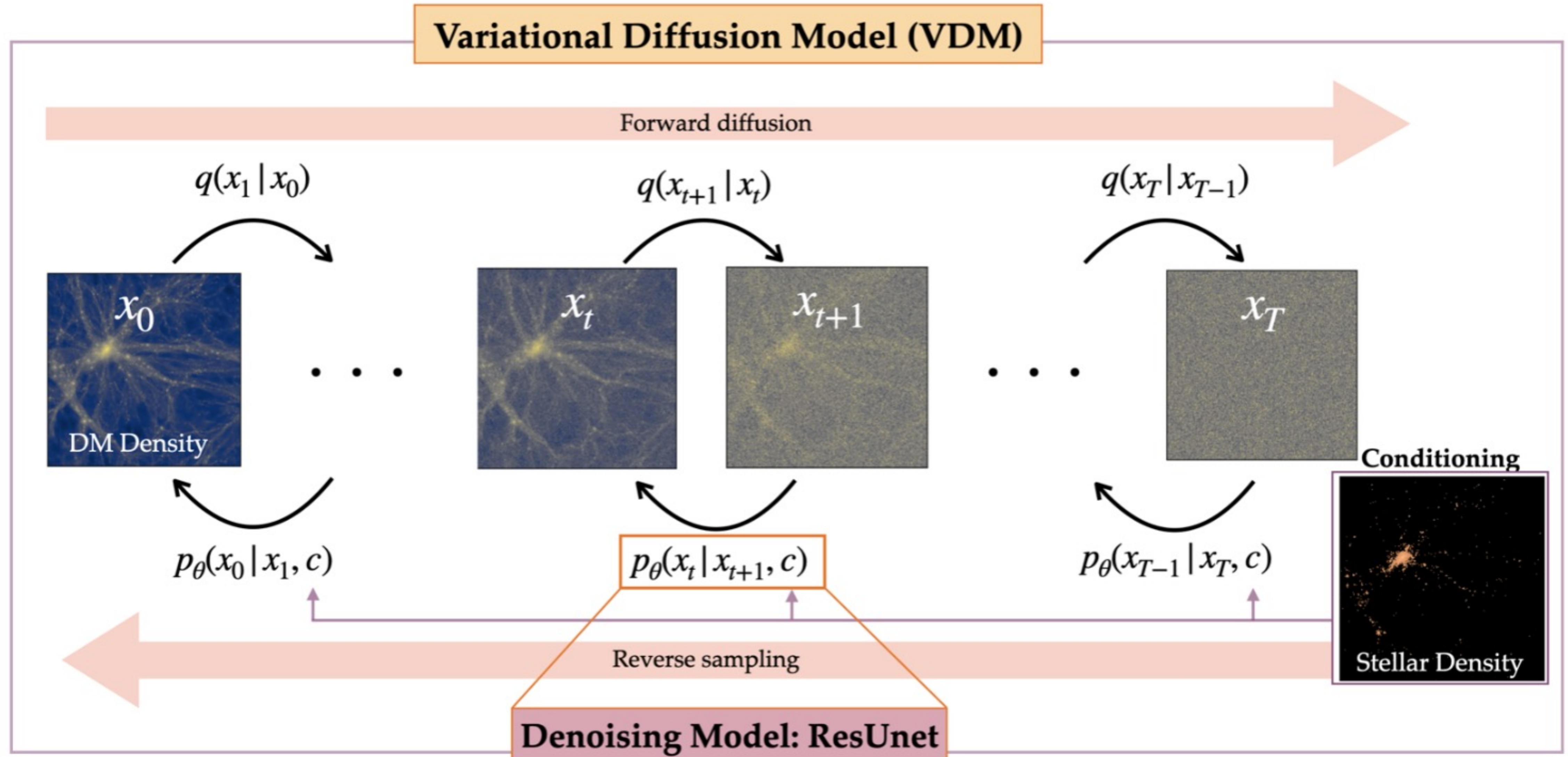
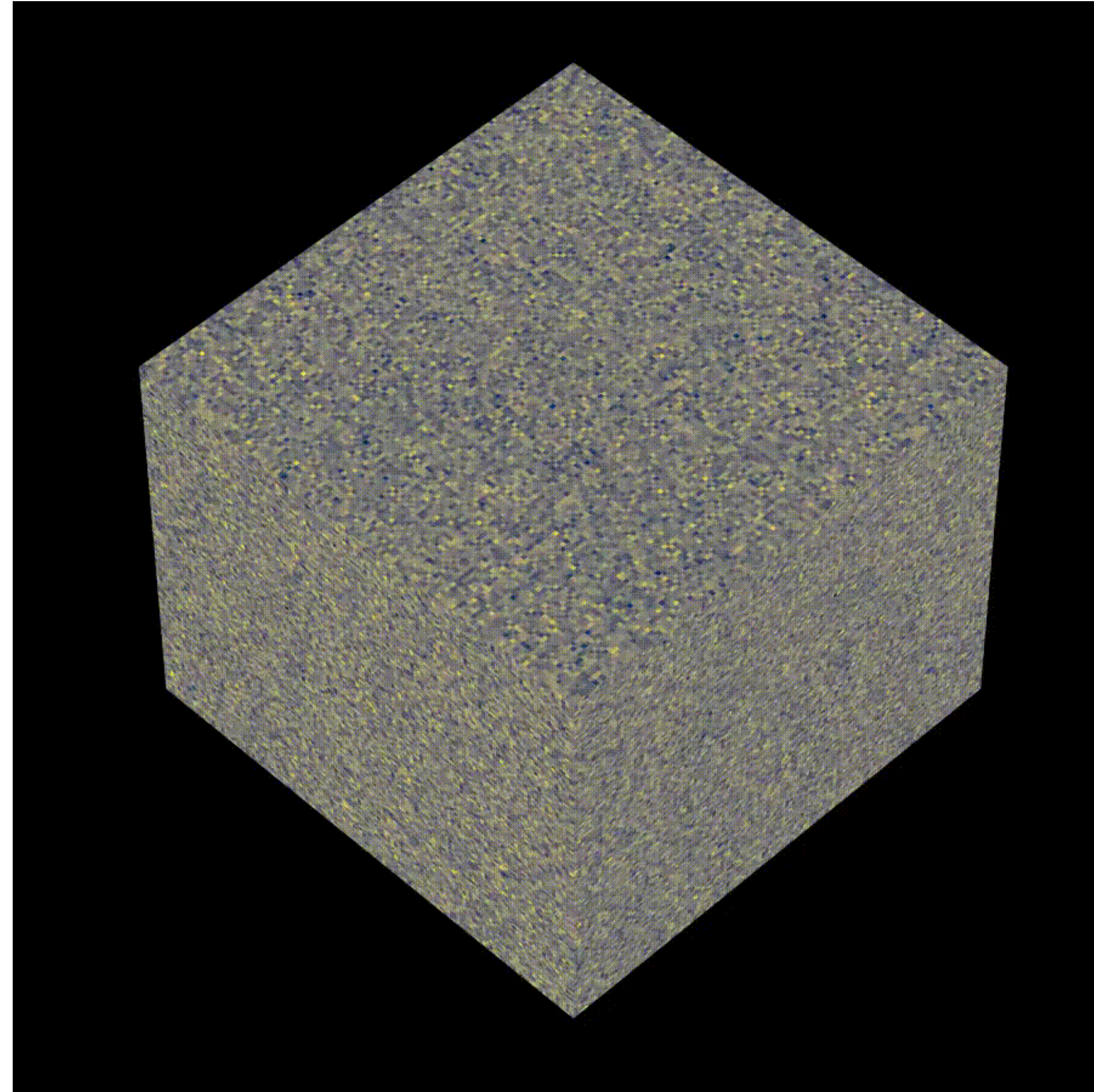


Fig: Core Francisco Park

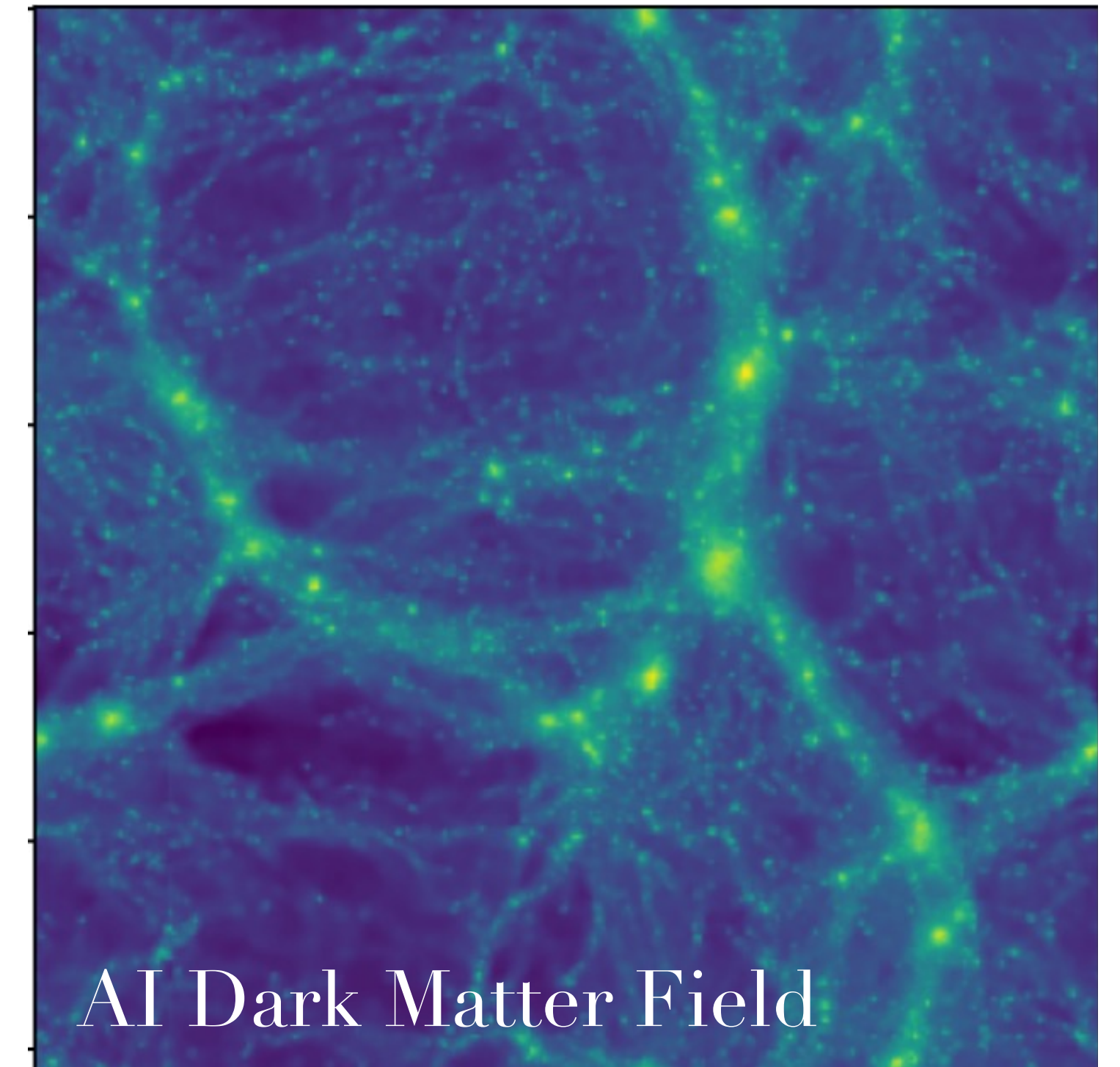
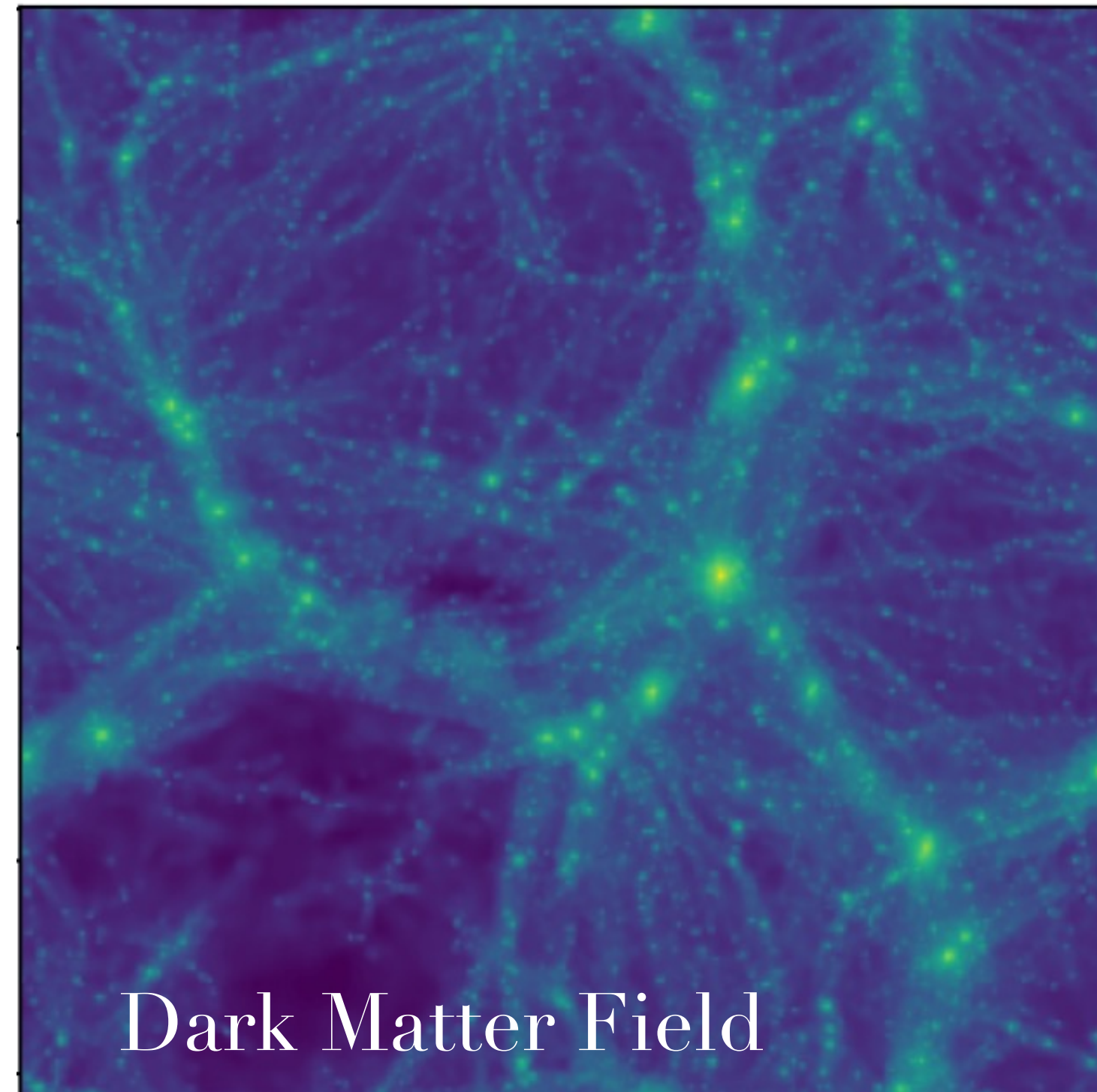
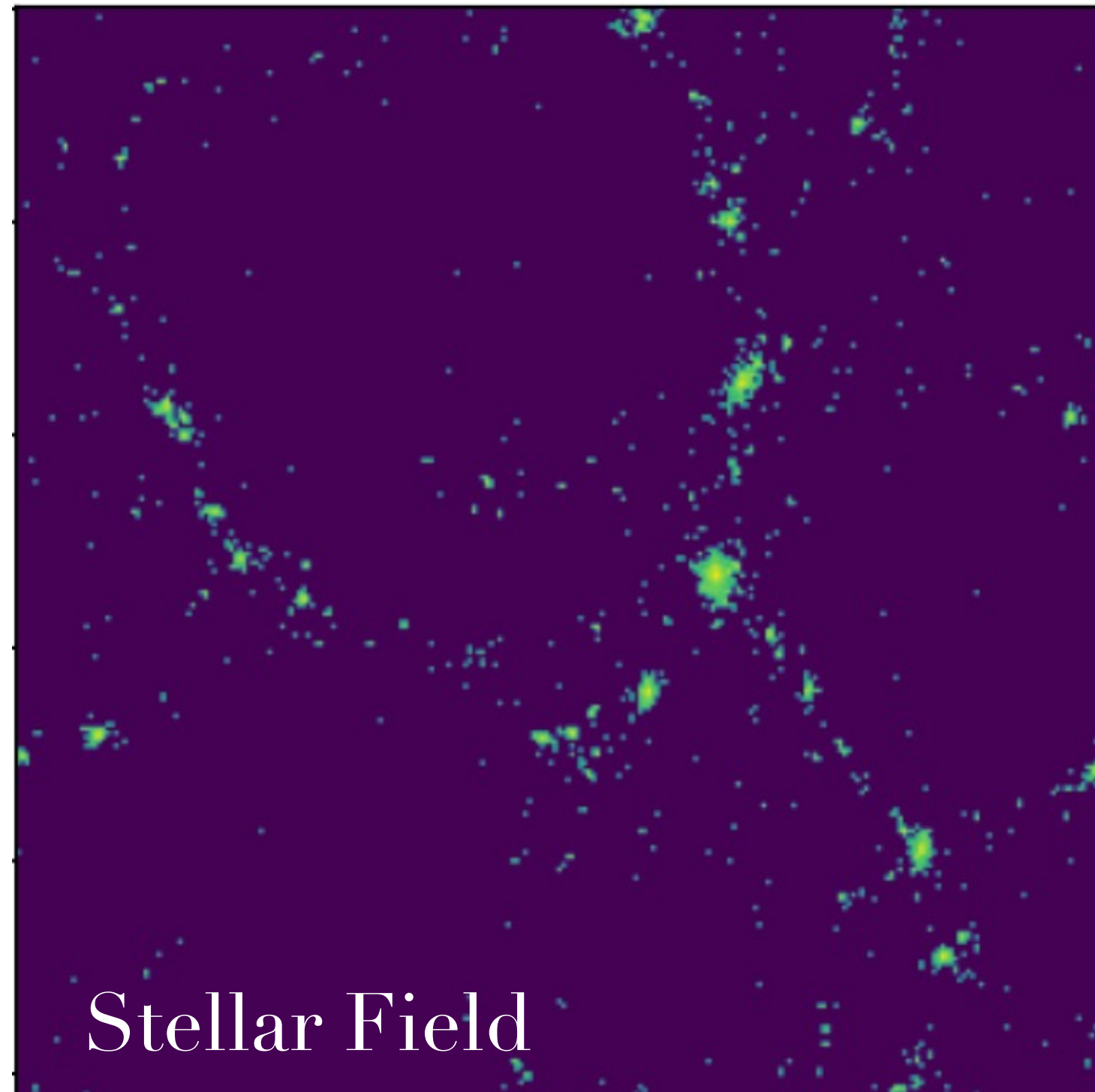
Diffusion Models for Astrophysics



ASTROAI

Enabling Next Generation Astrophysics

Dark Matter Field Simulations

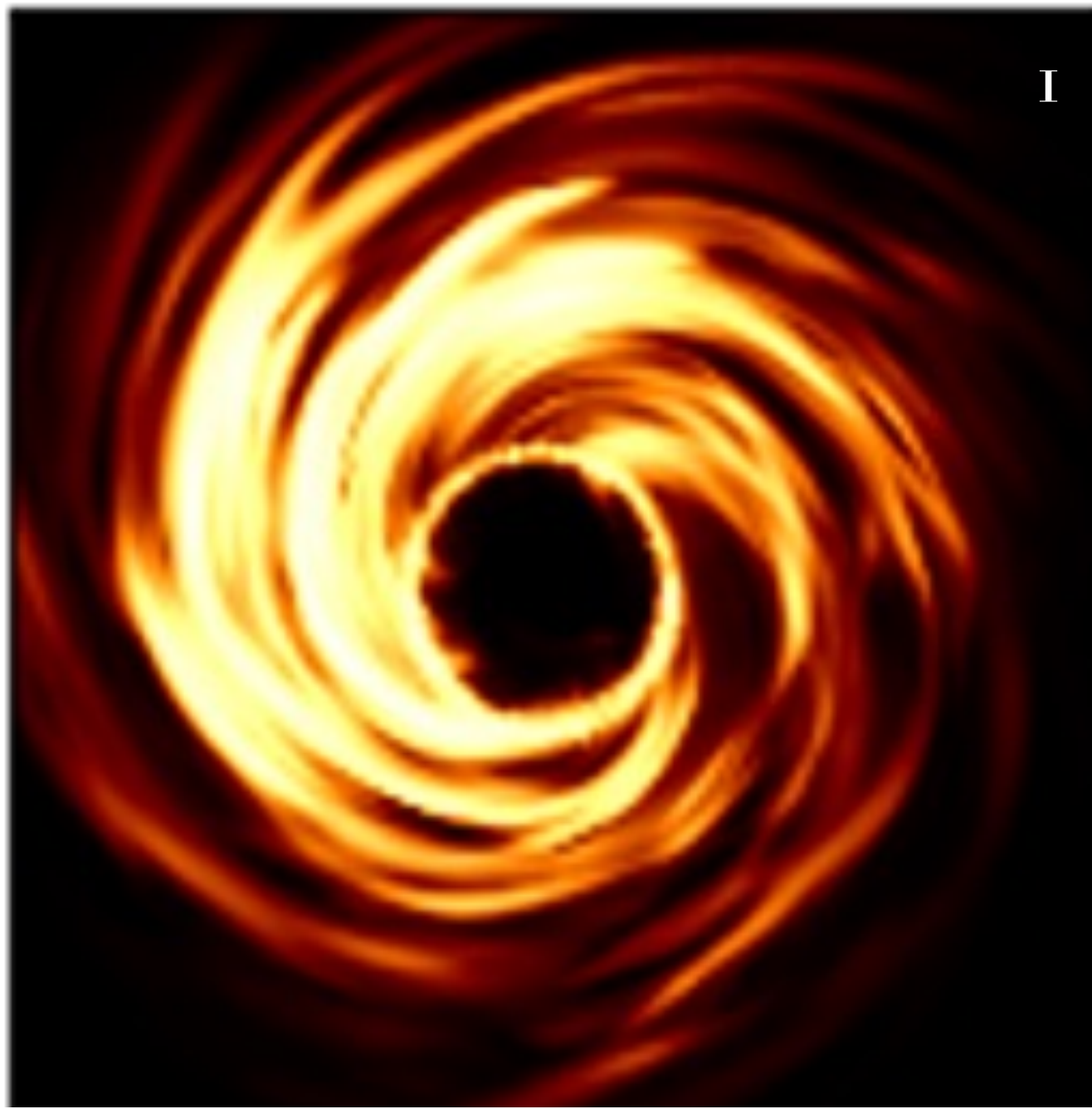


V. Ono, C. F. Park, Y. Ni, C. Cuesta-Lázaro, F. Villaescusa-Navarro 2024

ASTROAI

Enabling Next Generation Astrophysics

Supermassive BHs



GRMHD



GenAI



GRMHD

ASTROAI

Stellar
Spectra

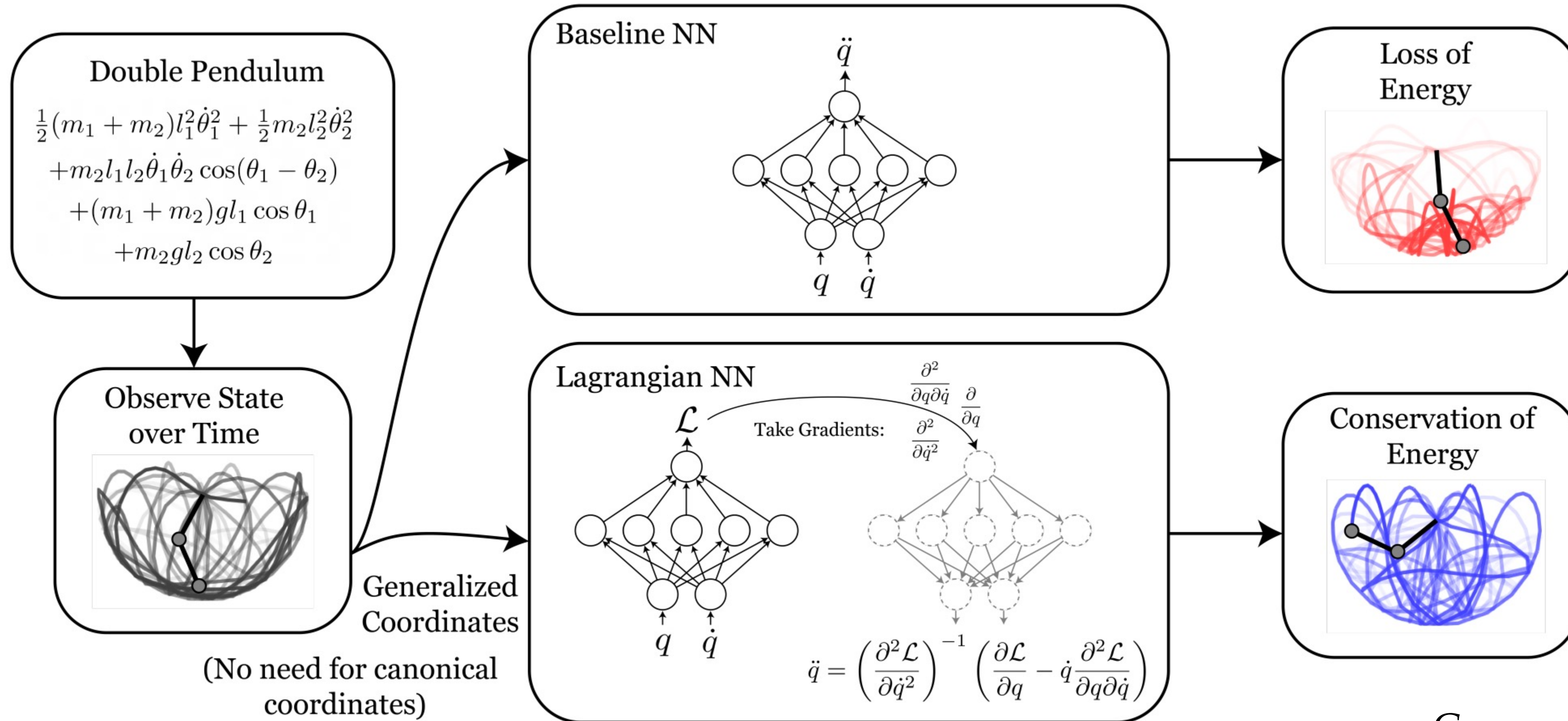


What does realistic mean?



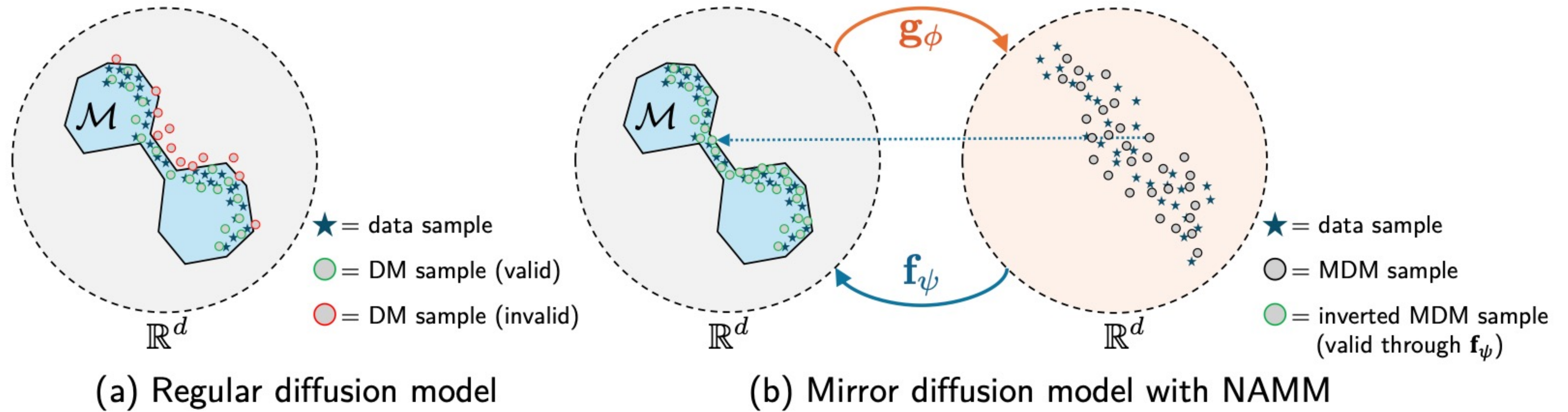
Towards Physical AI Simulations

Lagrangian Neural Networks



Cranmer et al. 2020

Constrained Diffusion Models



Berthy Feng, Ricardo Baptista and Katie Bouman NeurIPS 2024

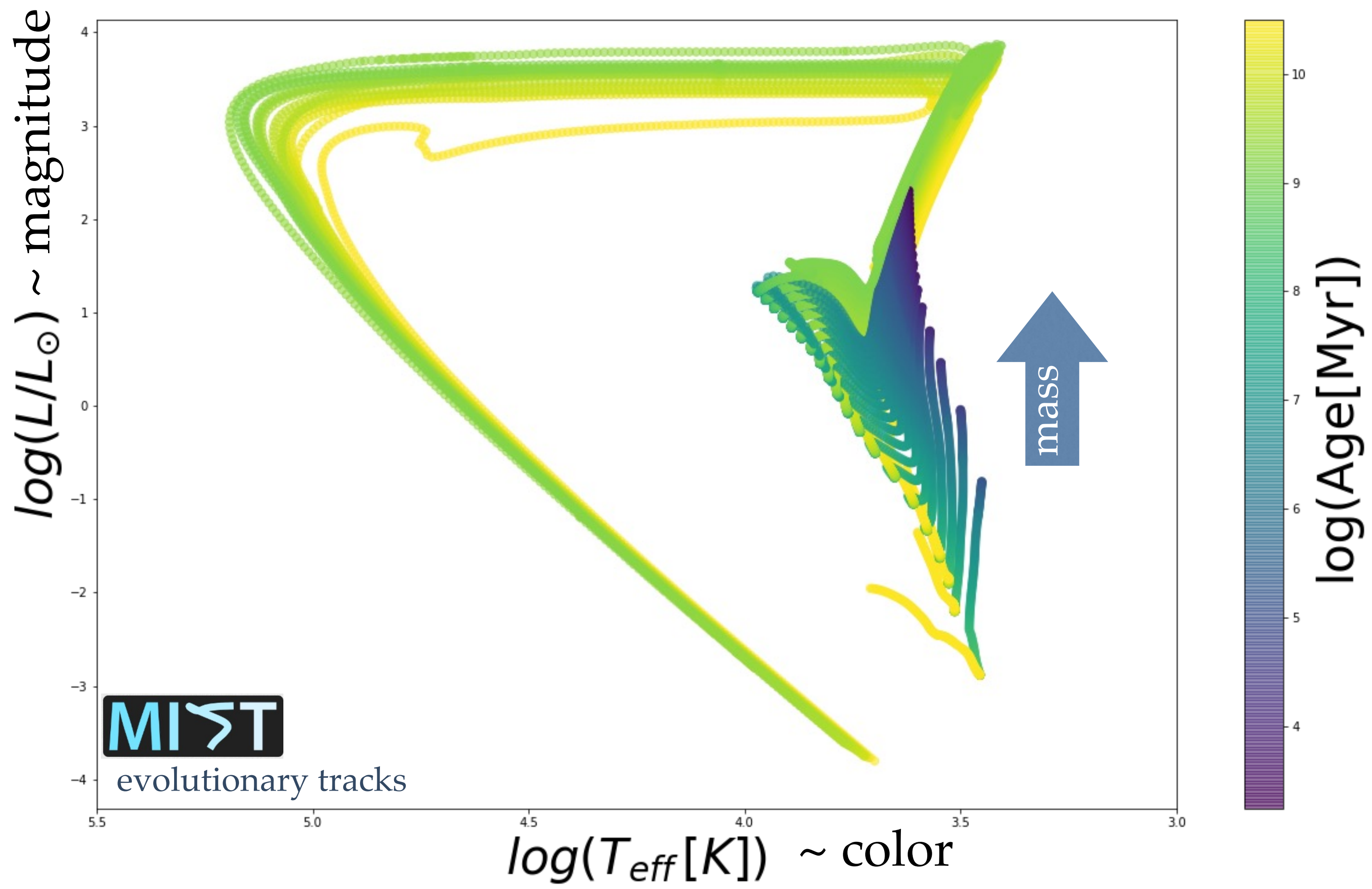
Can we get the best of both worlds?

From Simulations to Observations: Transfer Learning

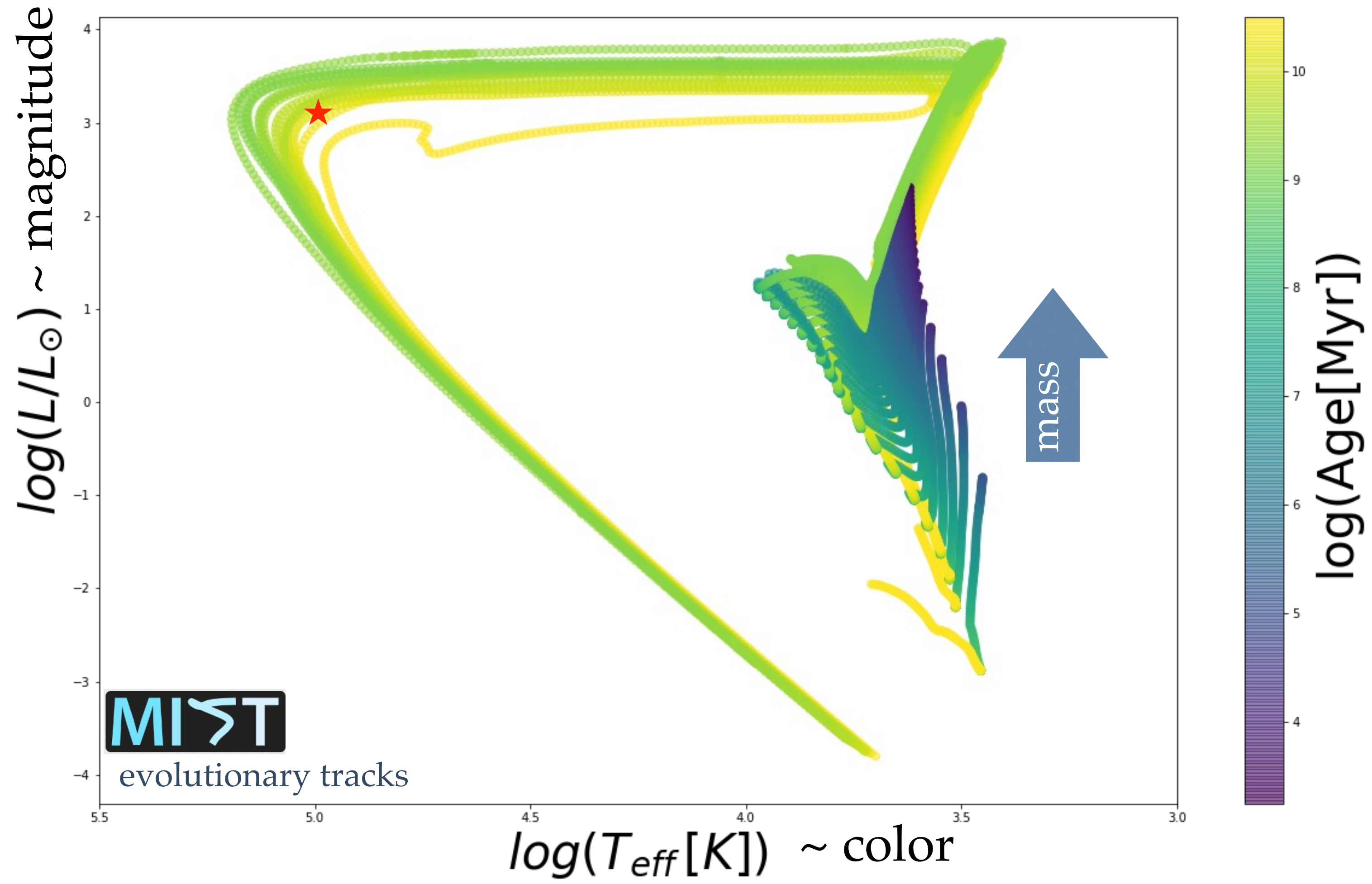
Automatic Stellar Characterization for Gaia



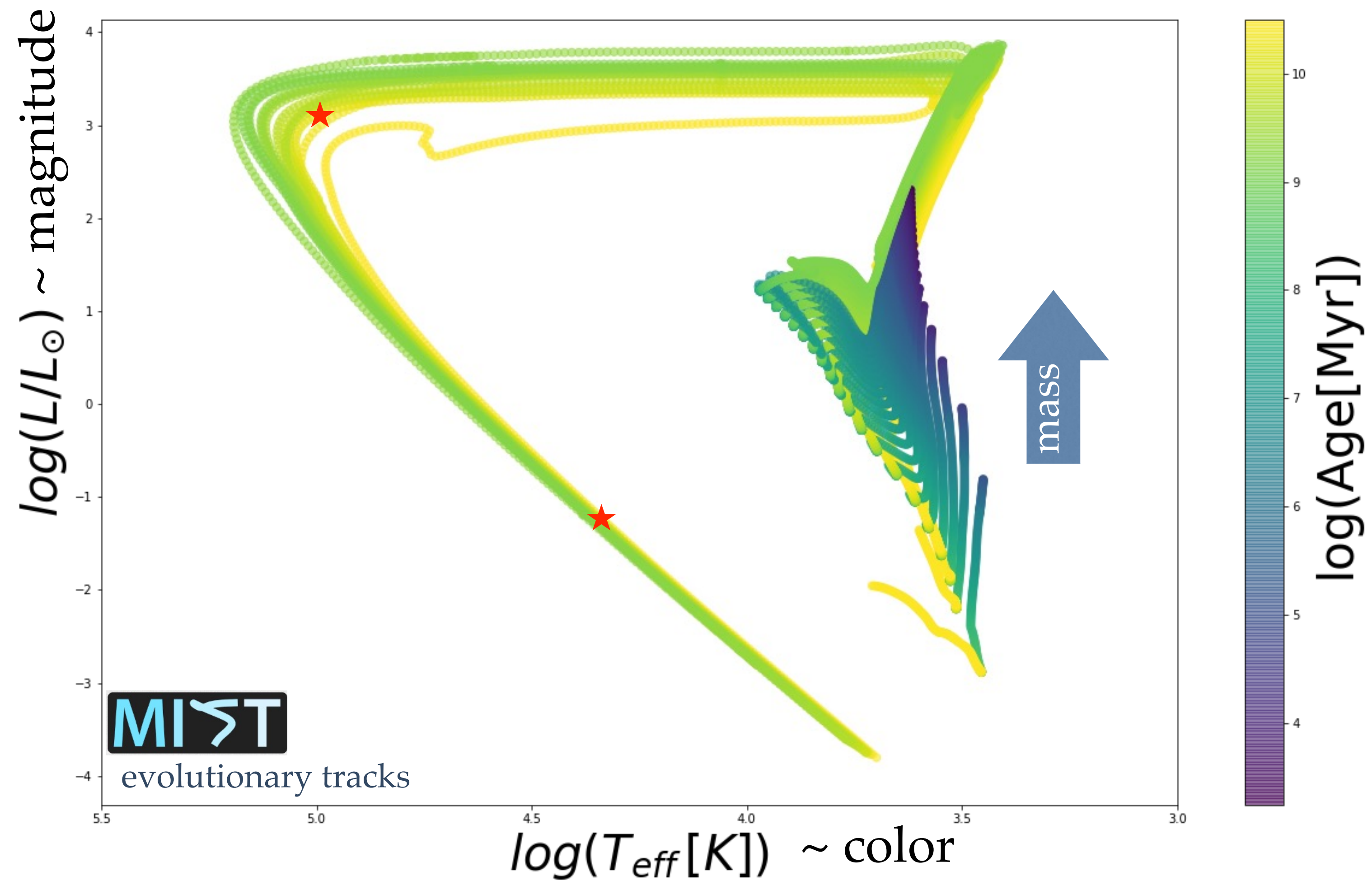
ESA



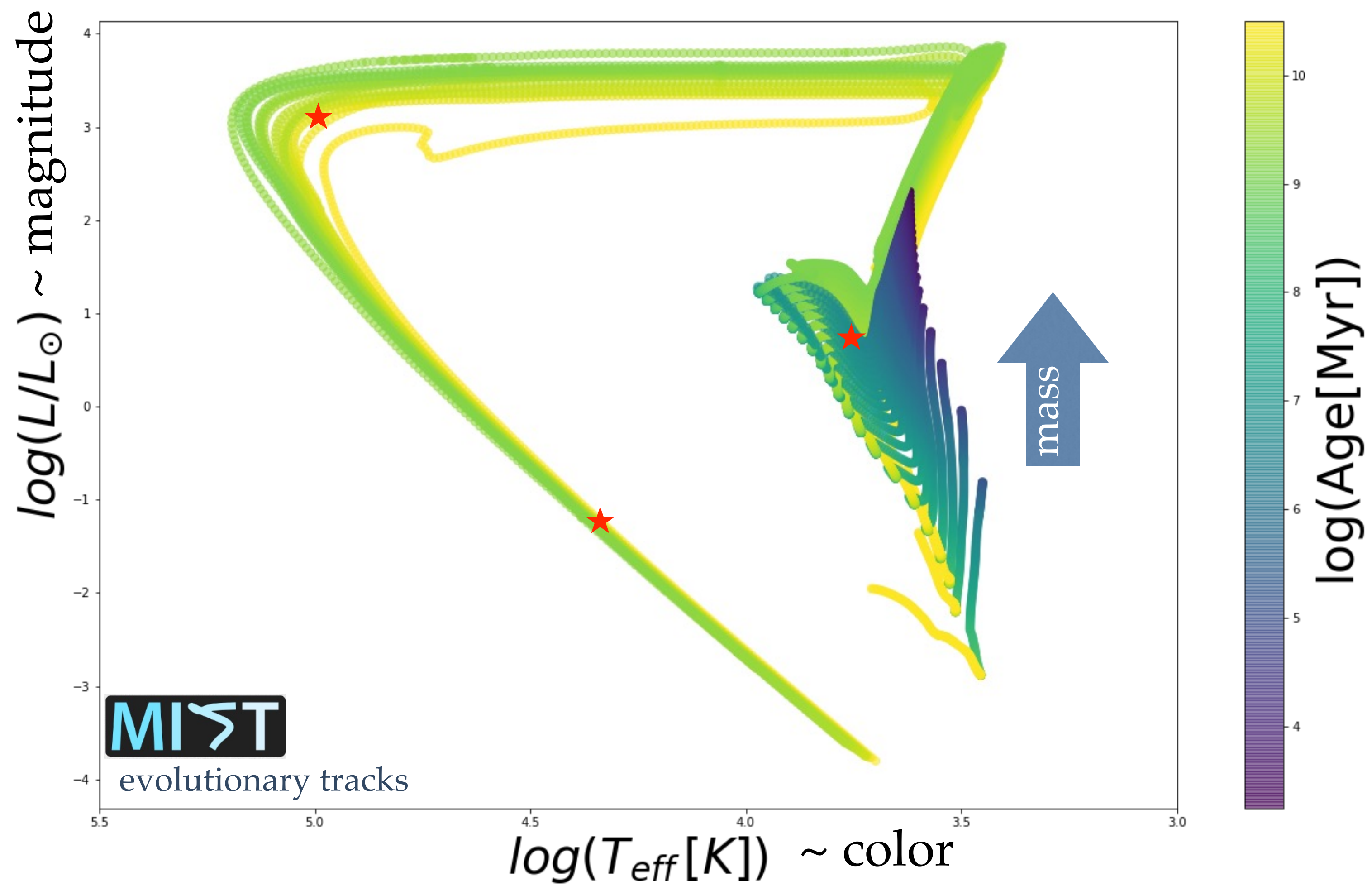
❖ Non-linearity



- ❖ Non-linearity
- ❖ Confidence variations

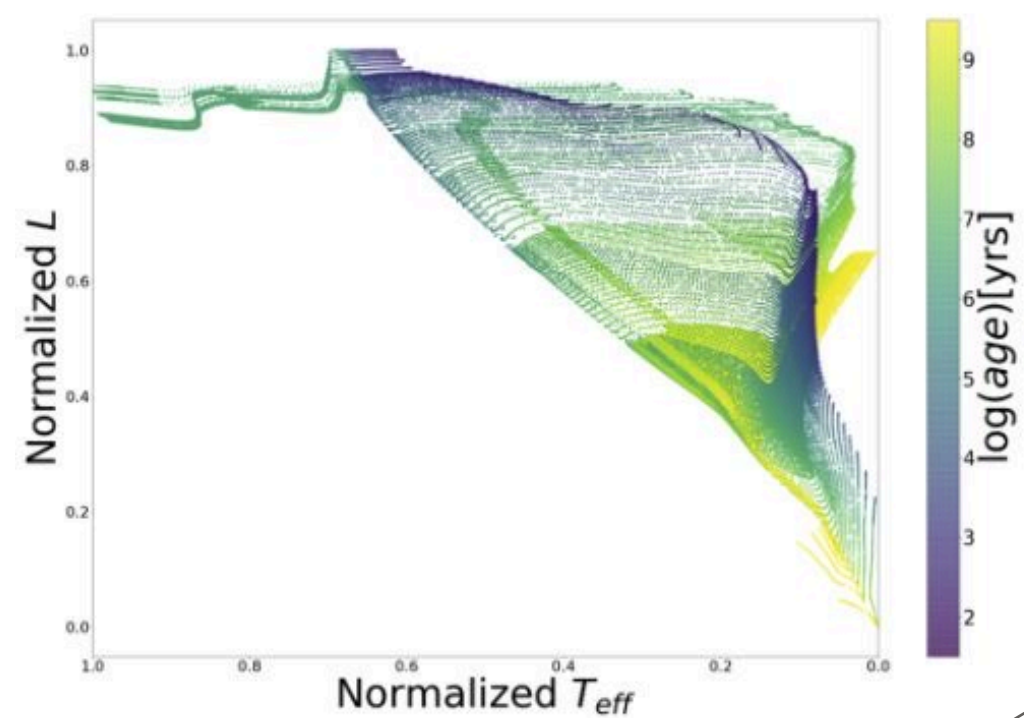


- ❖ Degeneracies
- ❖ Non-linearity
- ❖ Confidence variations

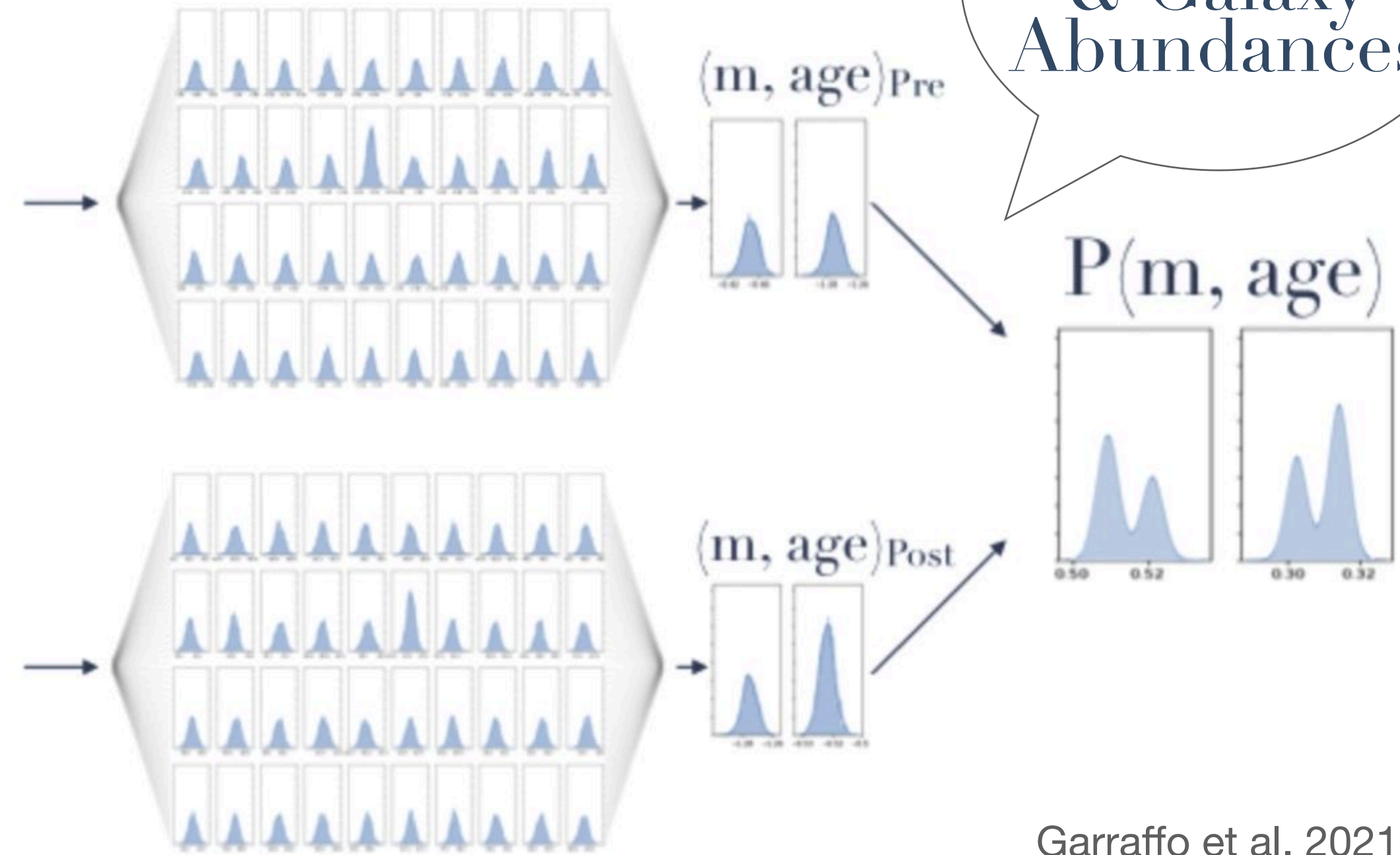
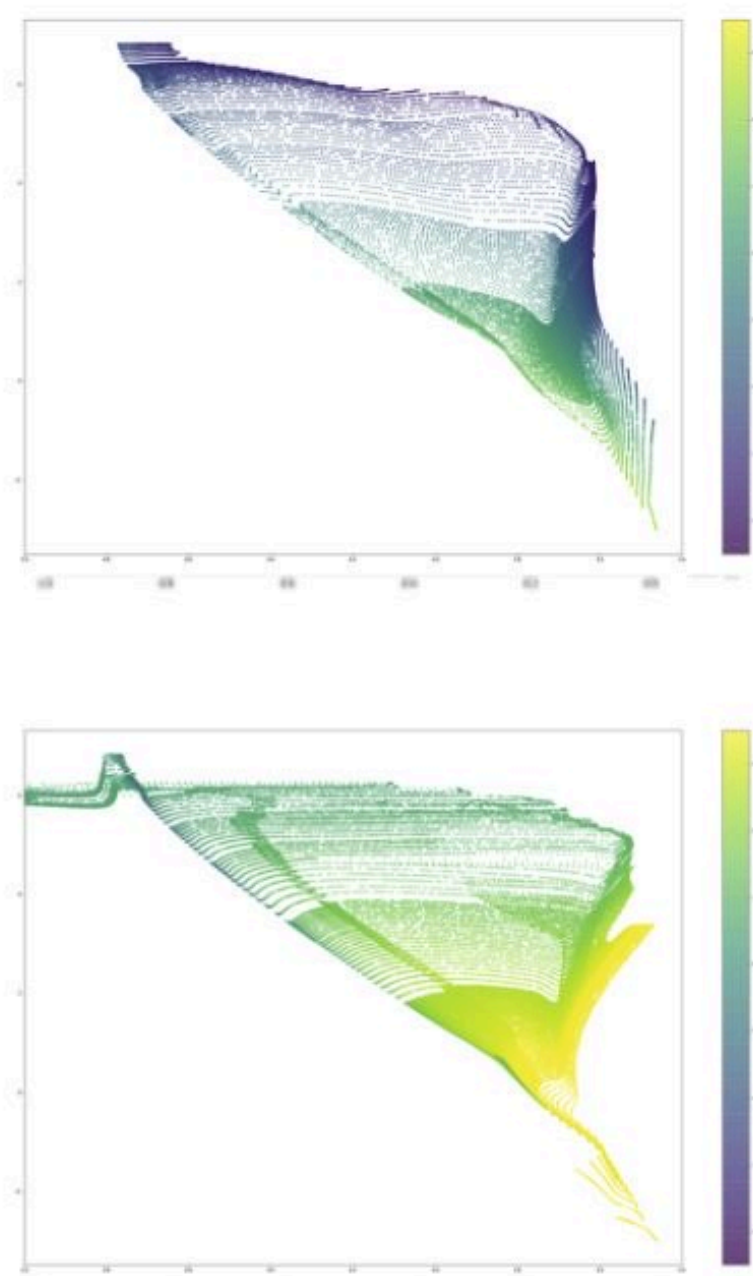


- ❖ Degeneracies ✓
- ❖ Non-linearity ✓
- ❖ Confidence variations ✓

L
T_{eff}

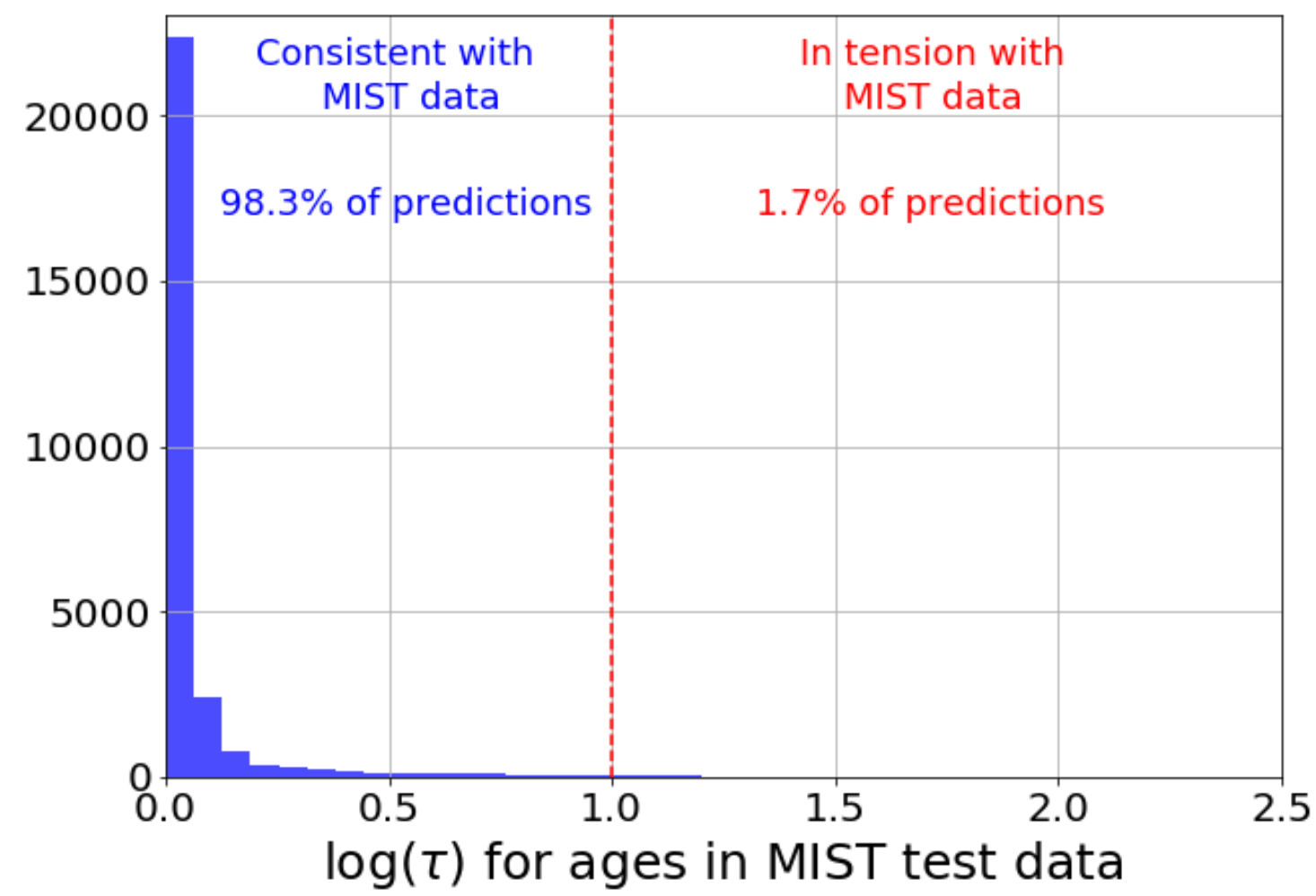
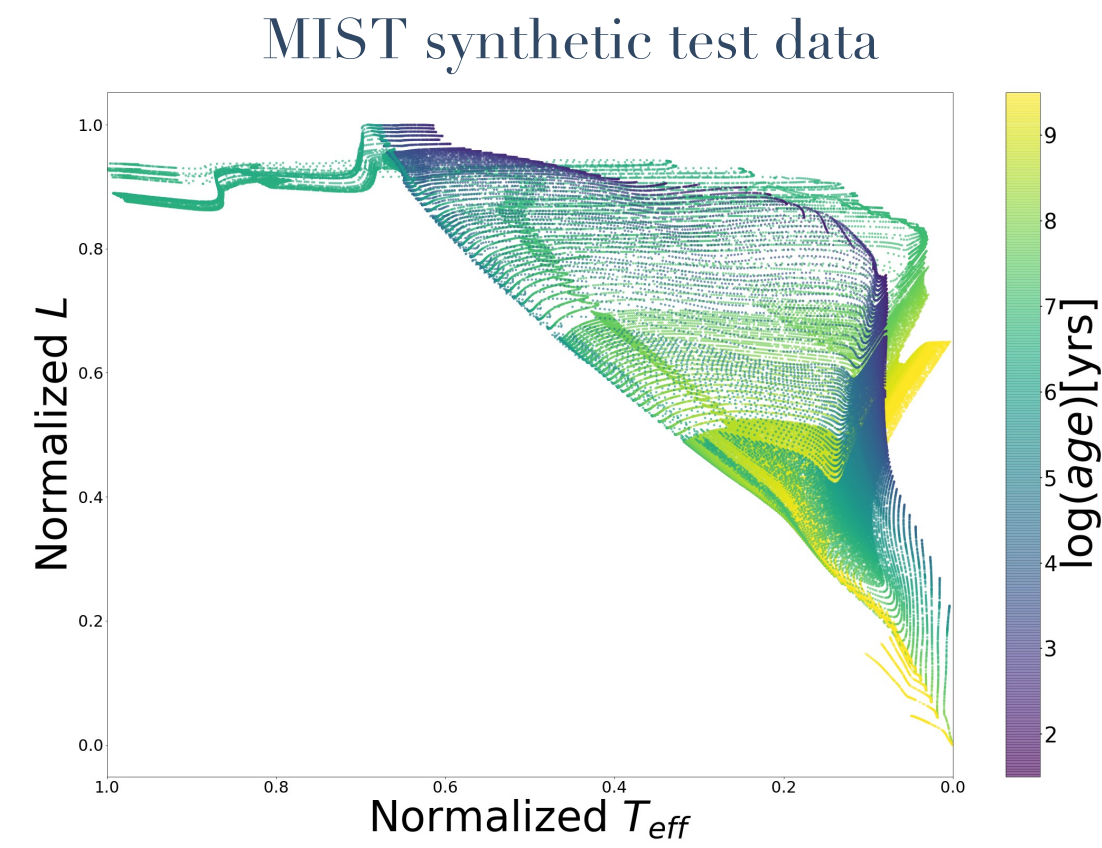


Split at
ZAMS



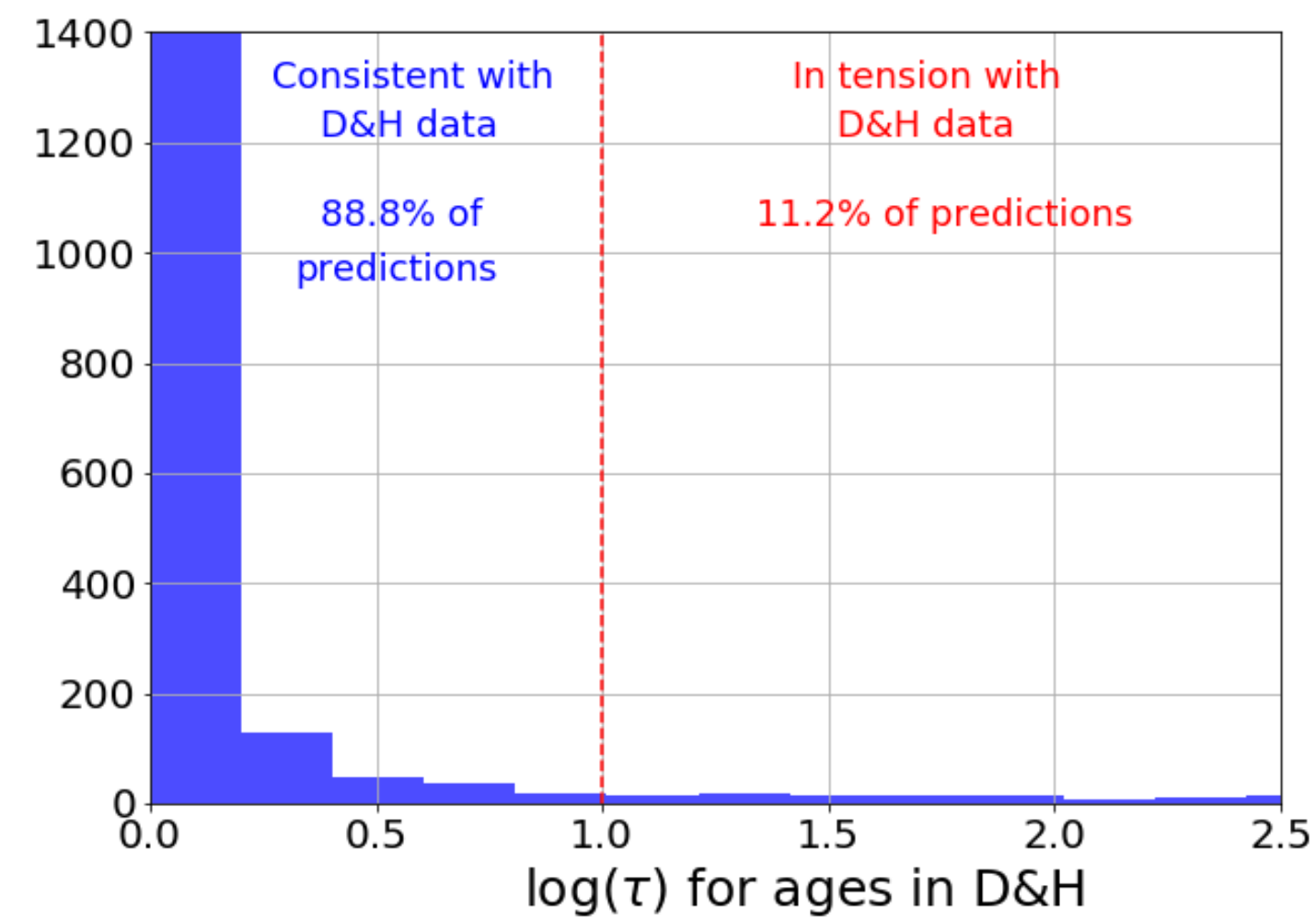
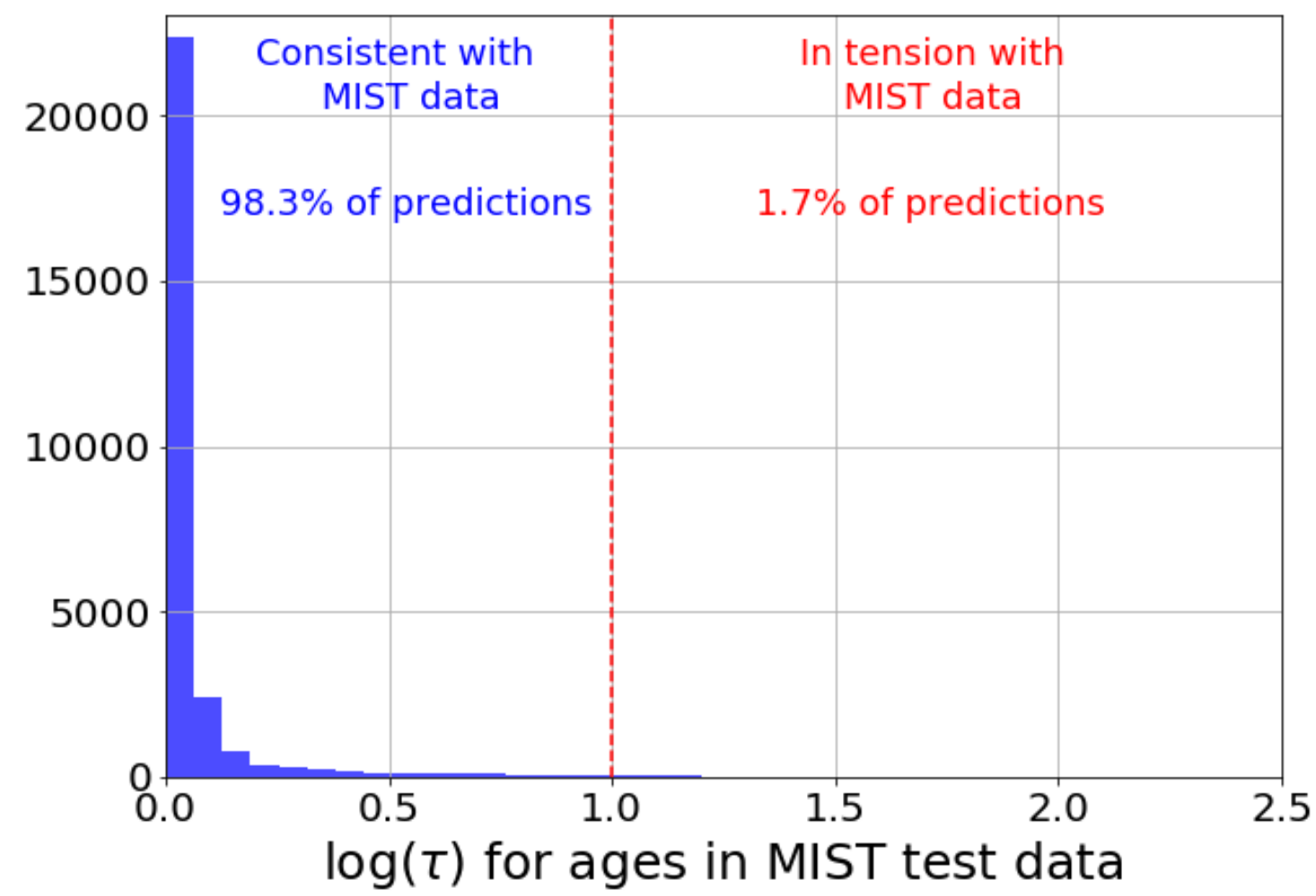
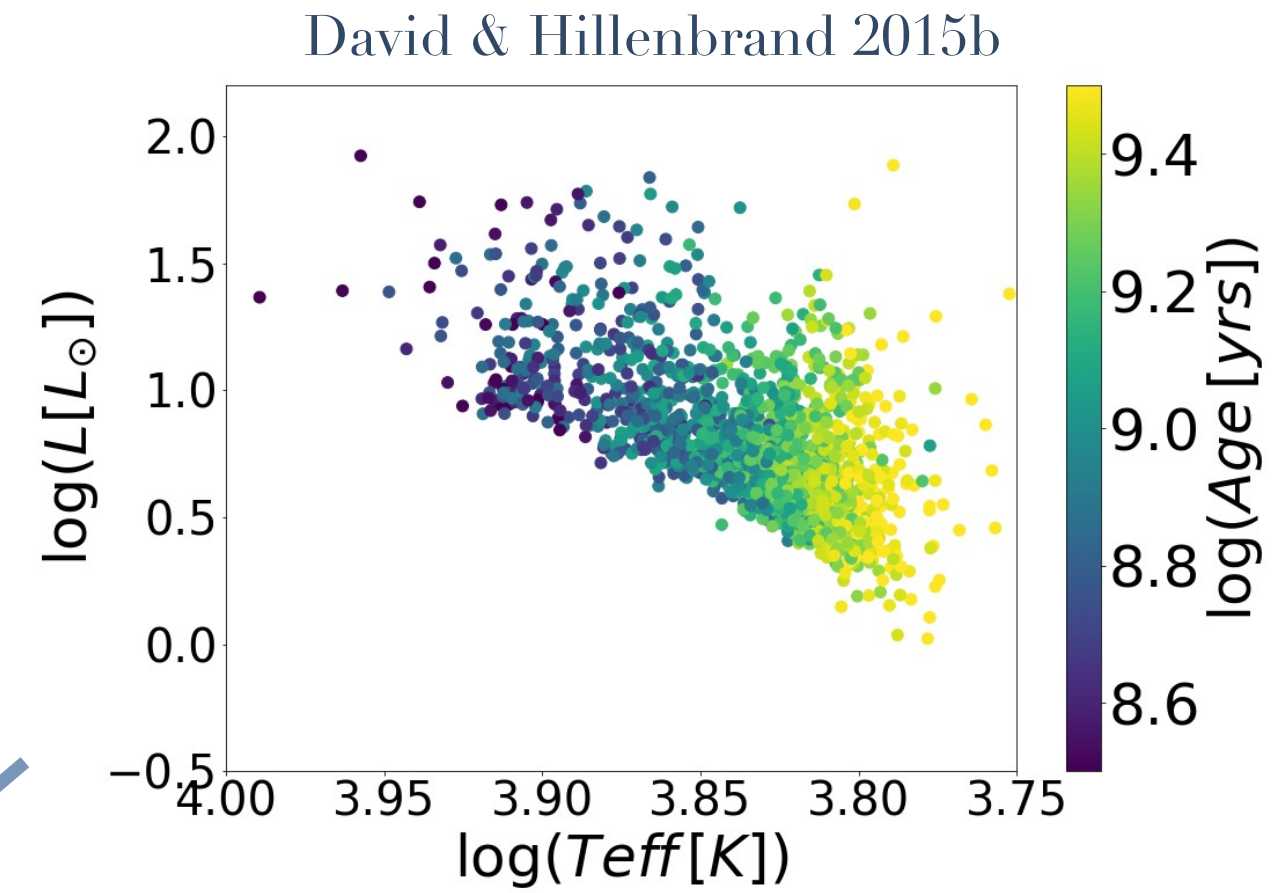
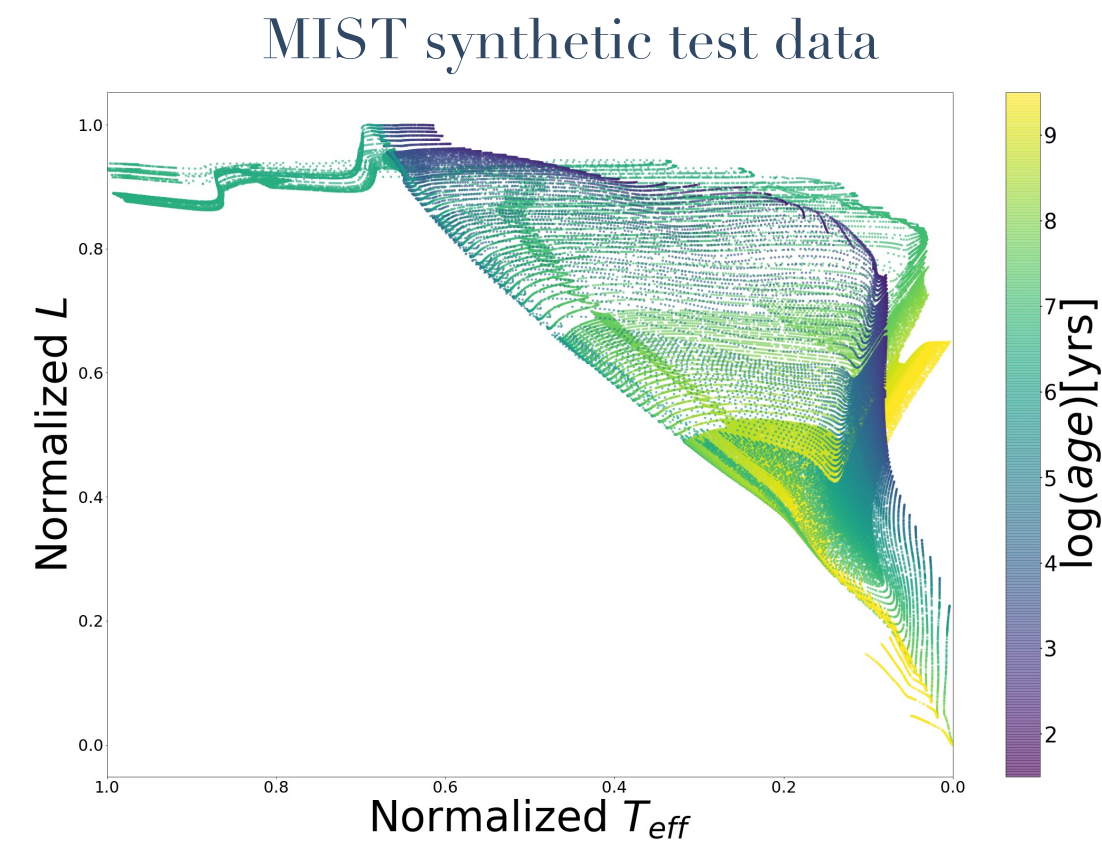
Garraffo et al. 2021

Quantifying performance on test *MIST* synthetic data and on observed data



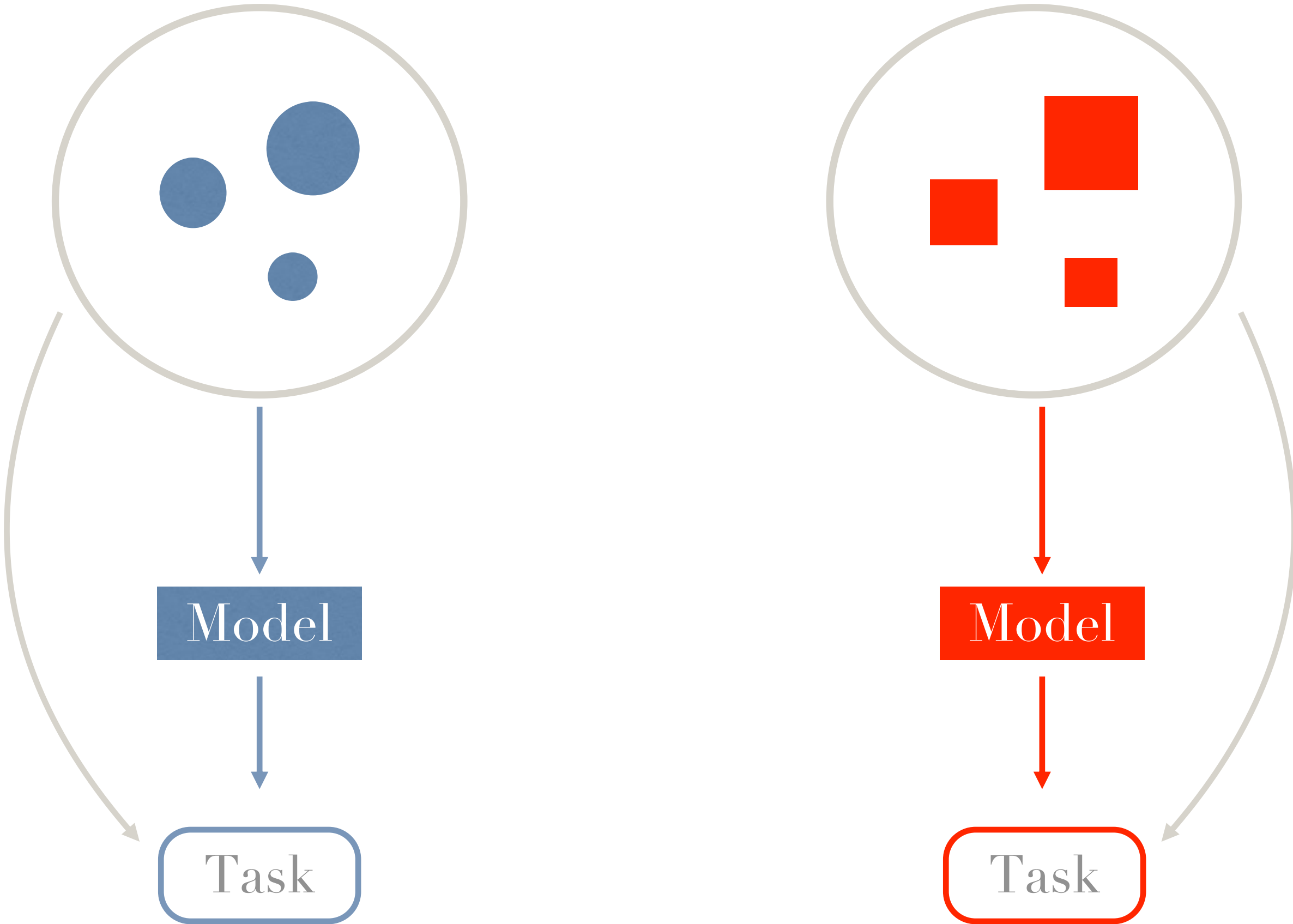
Garraffo et al. 2021

Quantifying performance on test *MIST* synthetic data and on observed data



Garraffo et al. 2021

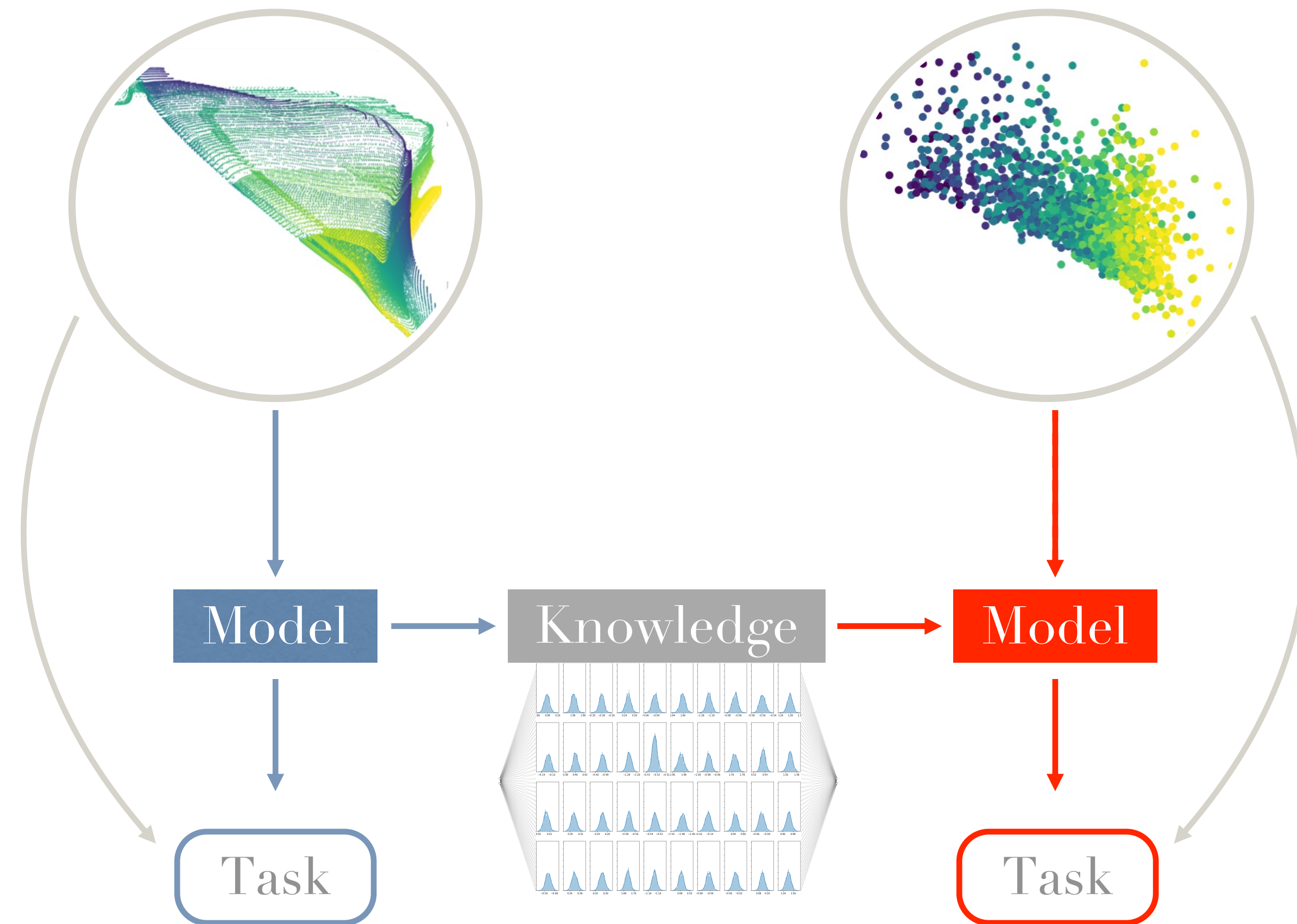
Traditional Machine Learning



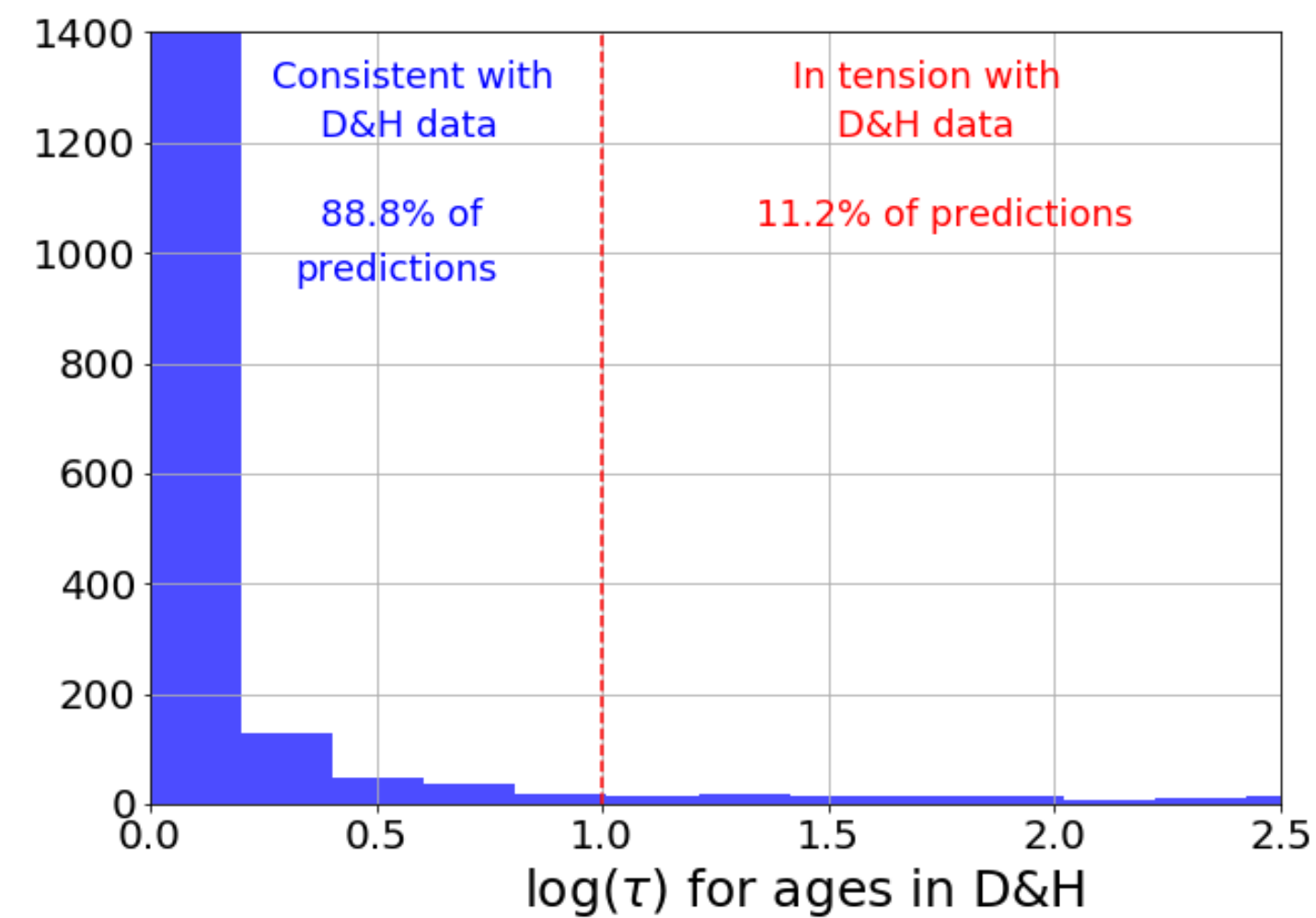
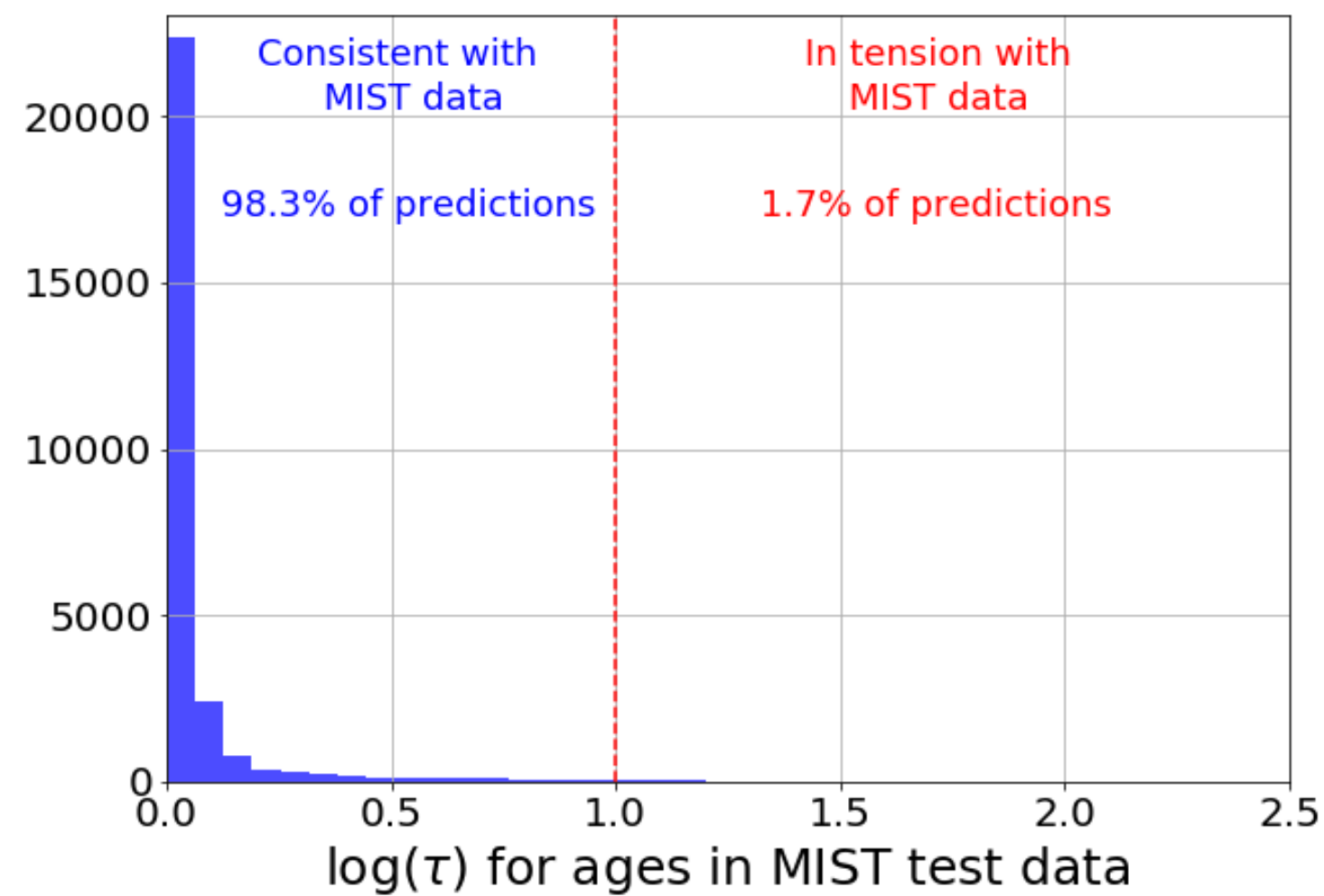
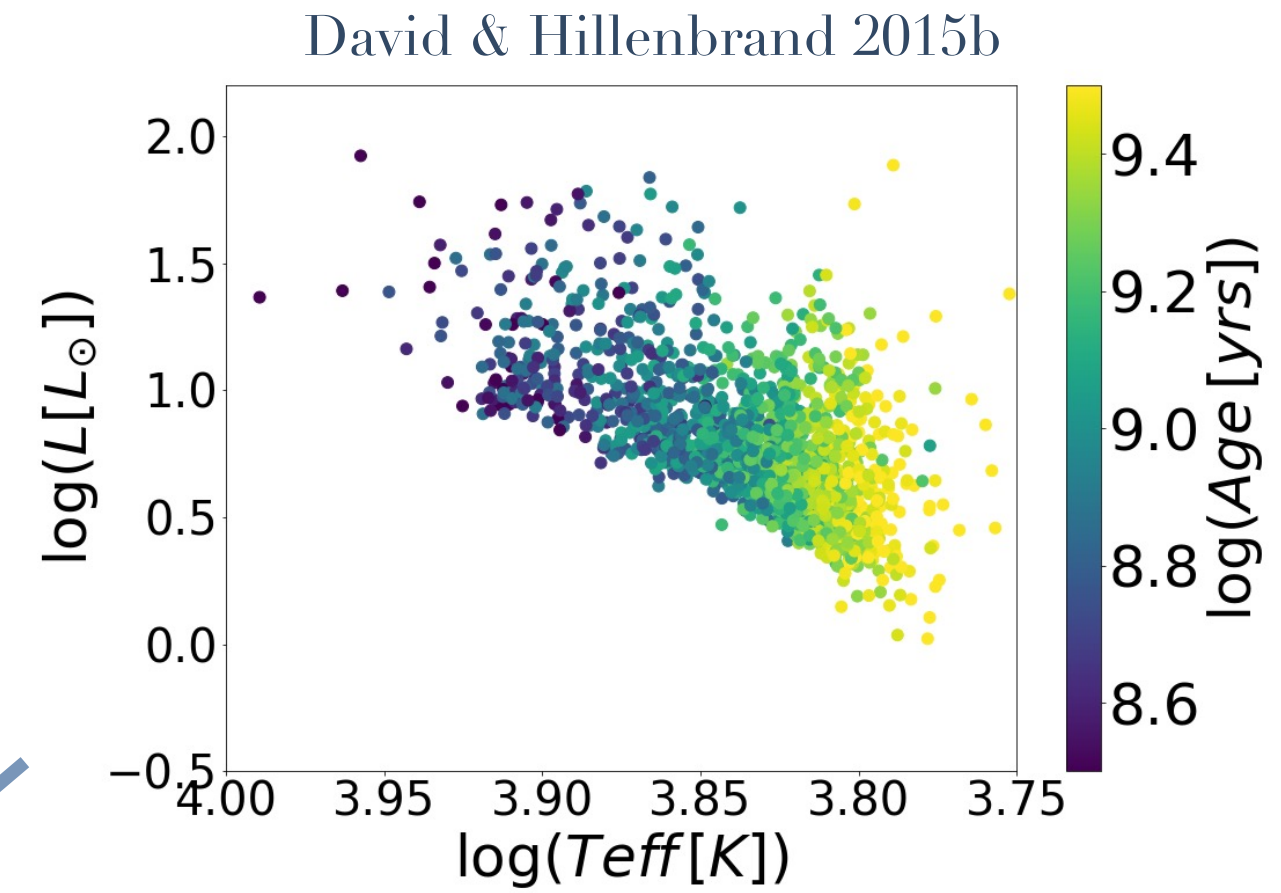
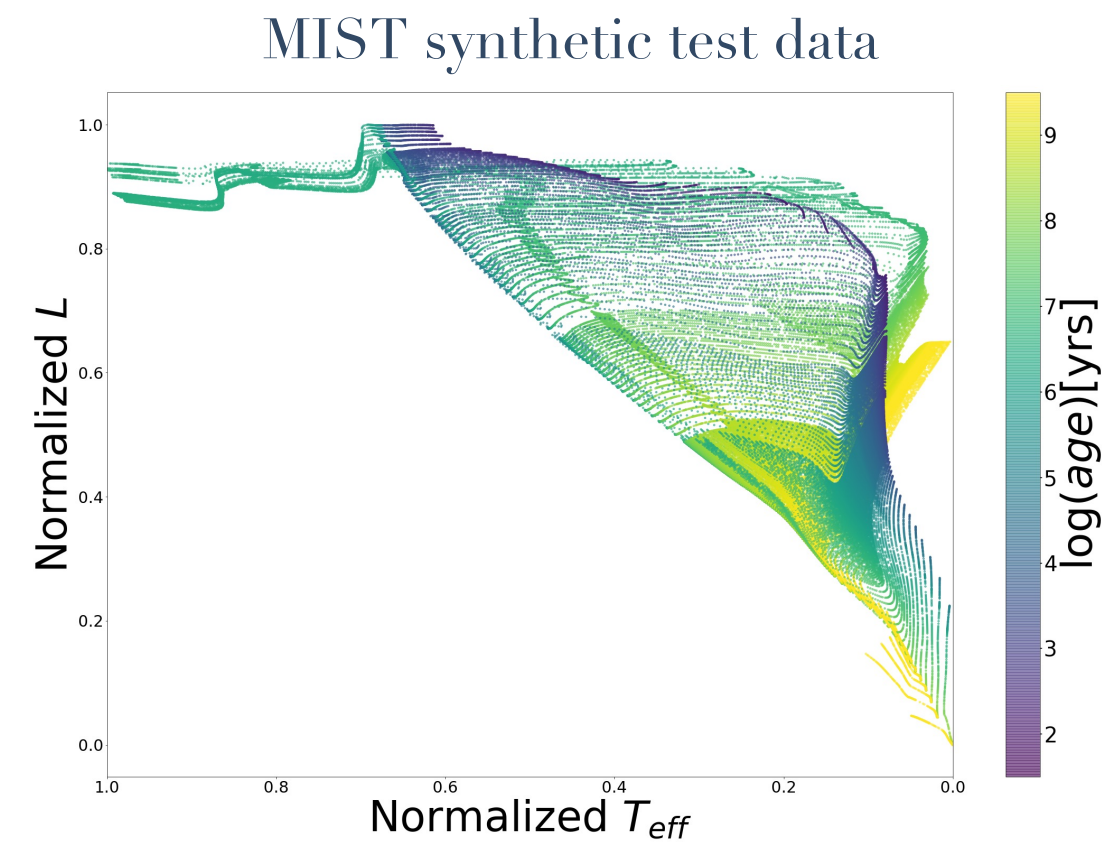
Transfer Learning

MIST Synthetic data

D&H observed data



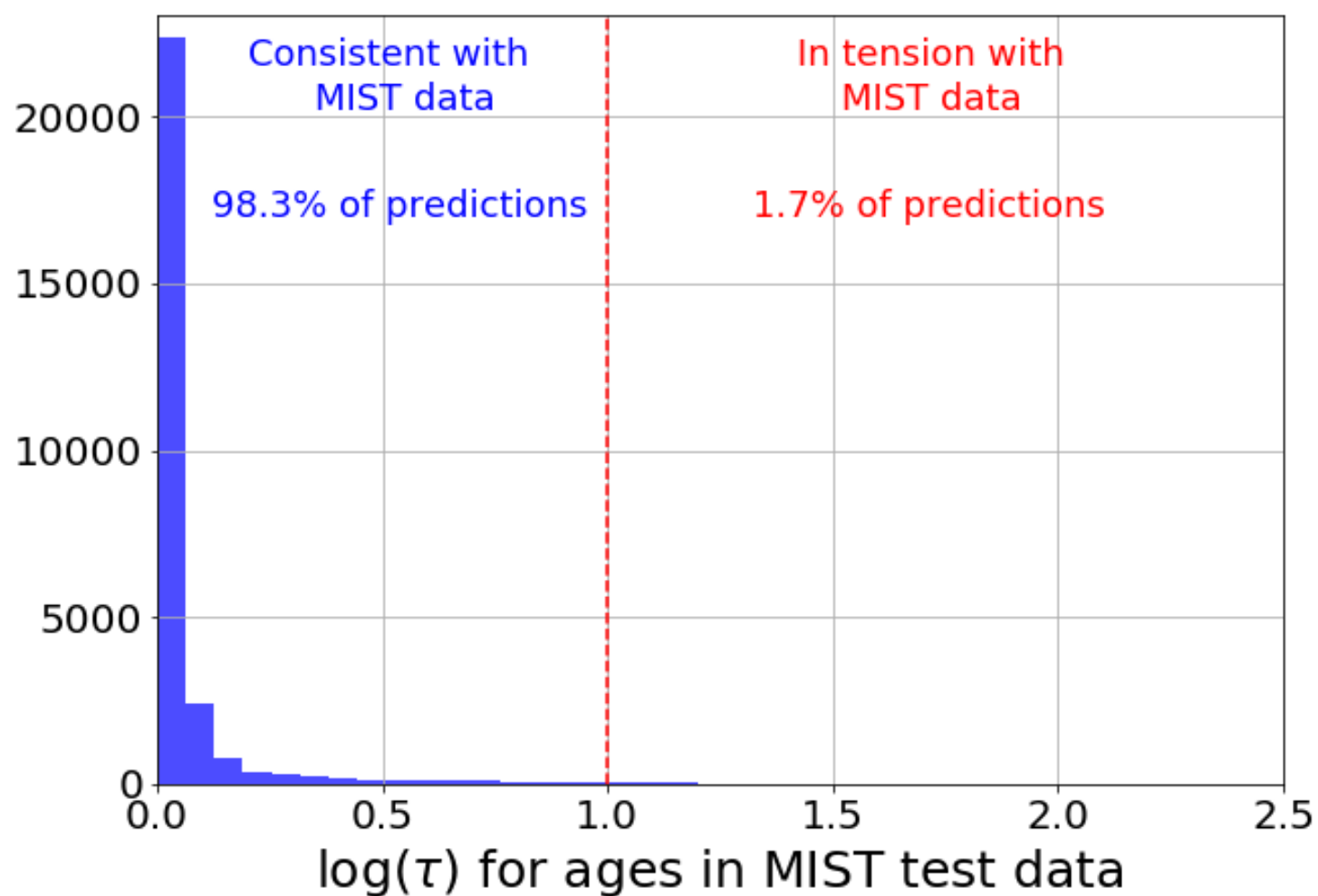
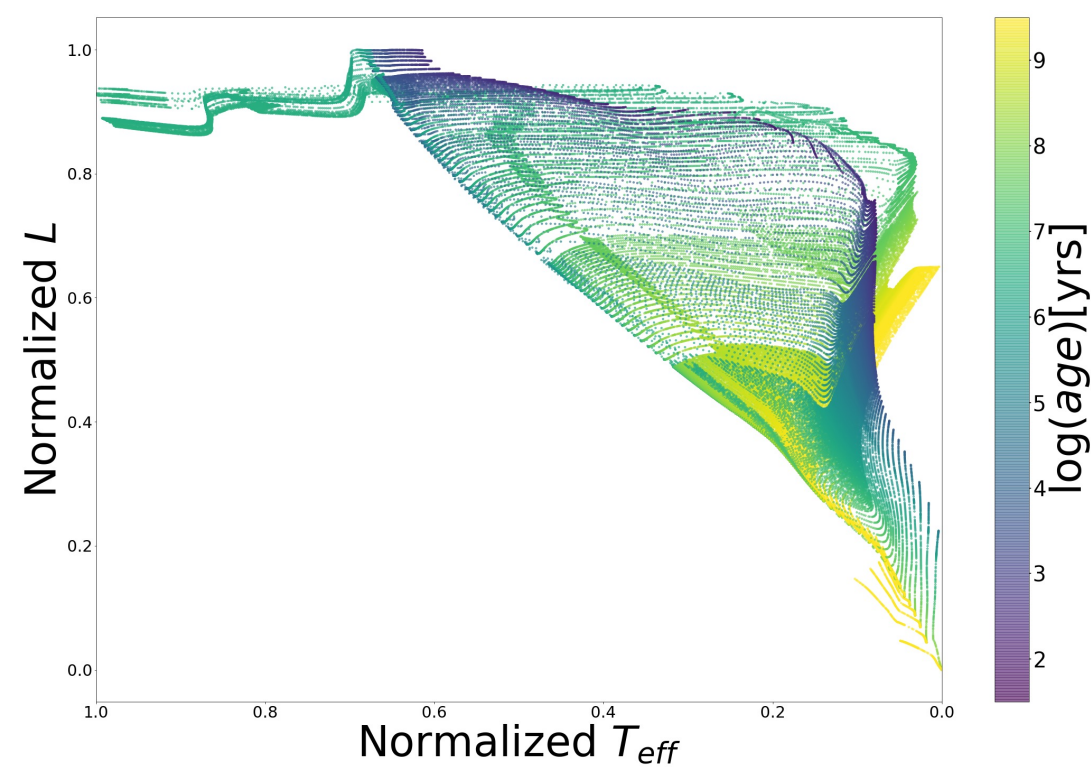
Quantifying performance on test *MIST* synthetic data and on observed data



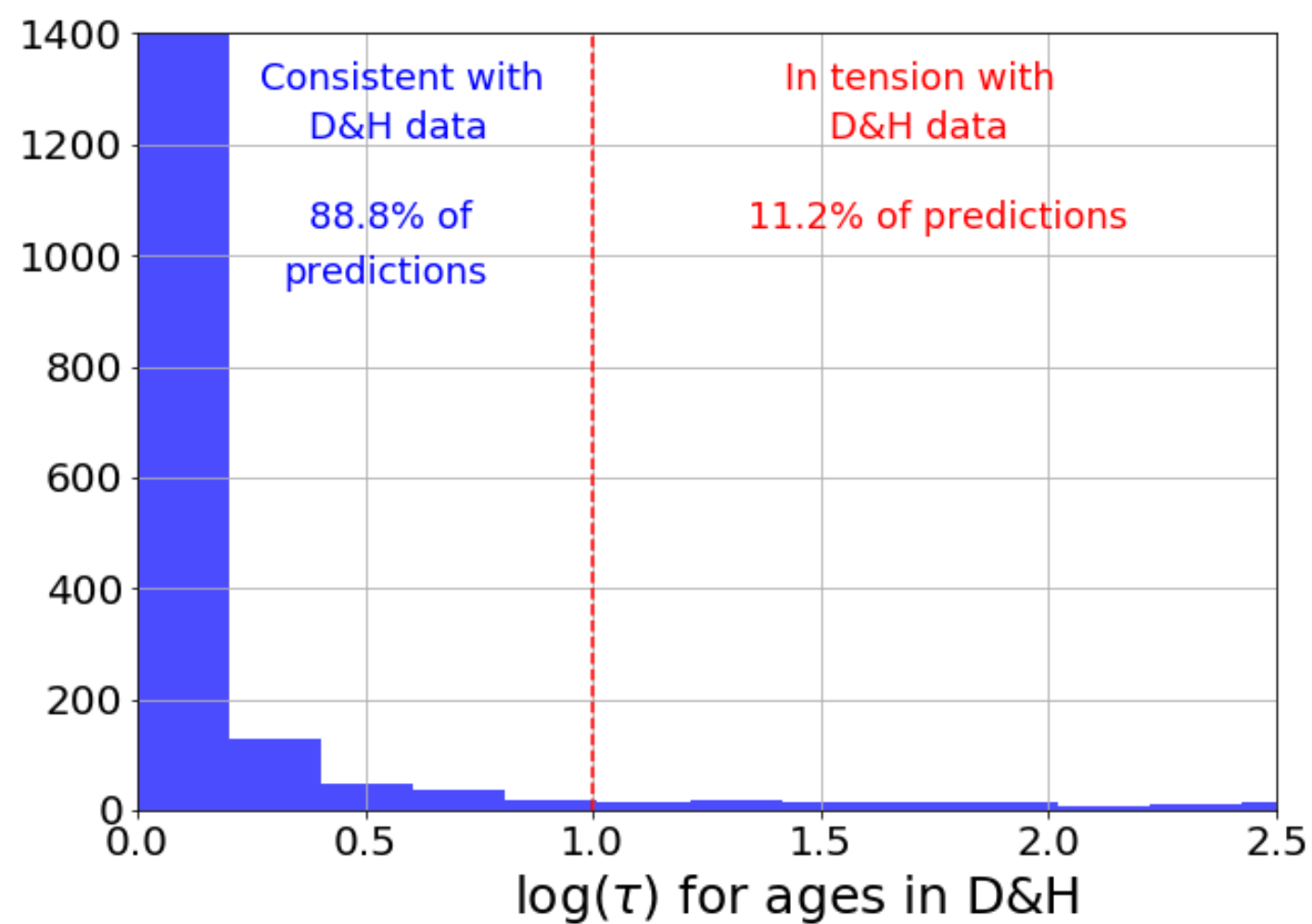
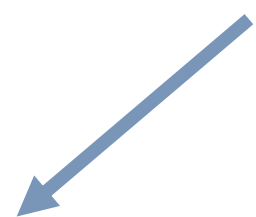
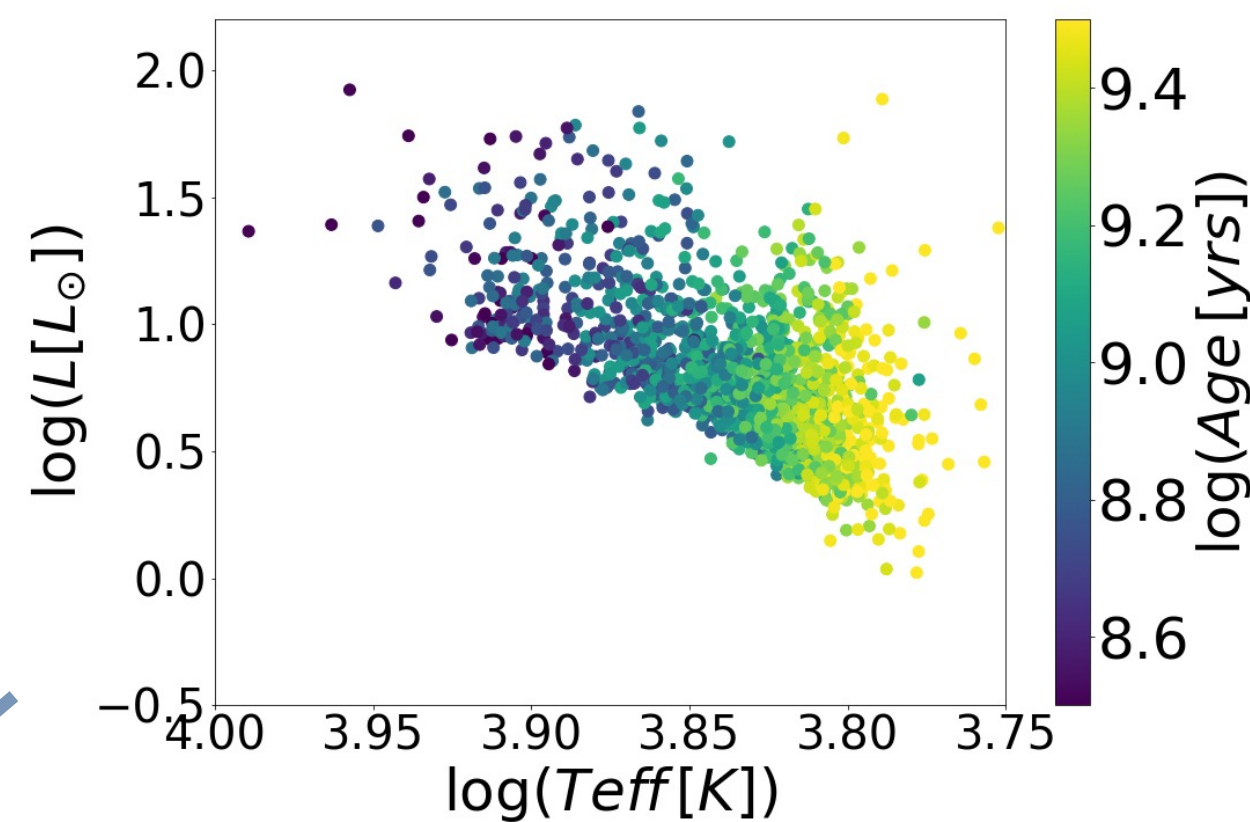
Garraffo et al. 2021

Quantifying performance on test *MIST* synthetic data and on observed data

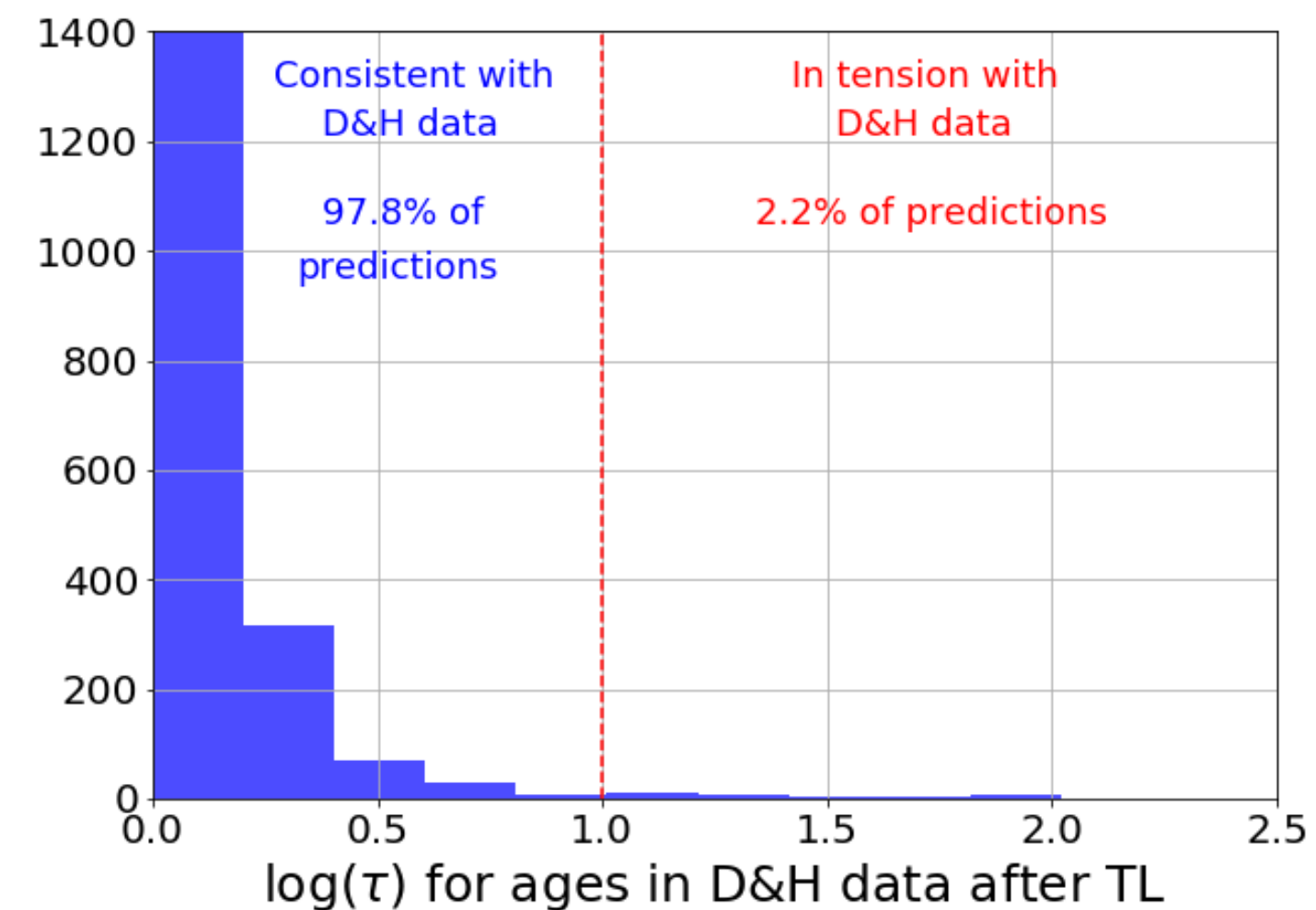
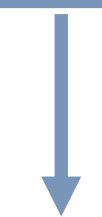
MIST synthetic test data



David & Hillenbrand 2015b



Using Transfer Learning



Garraffo et al. 2021

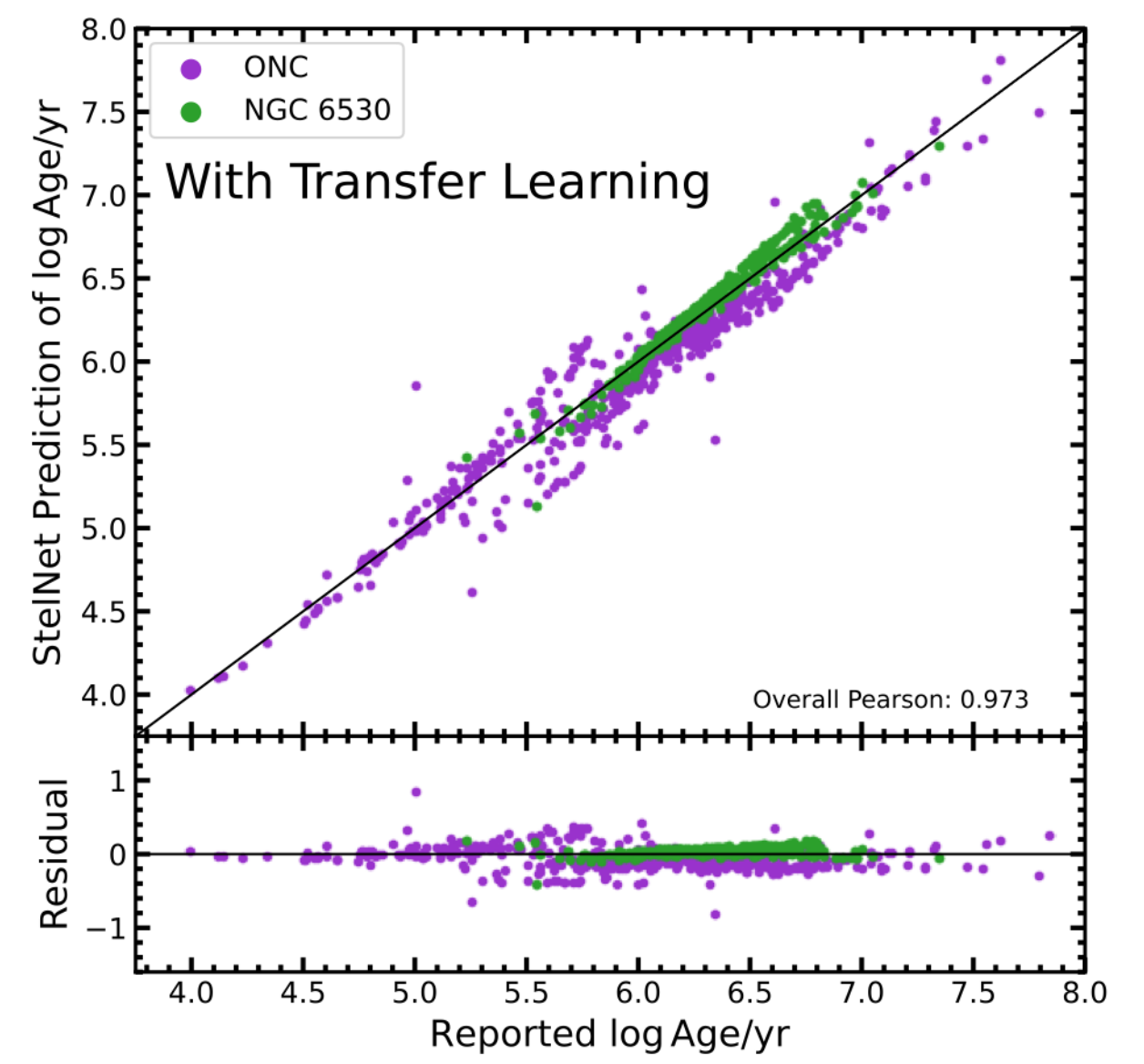
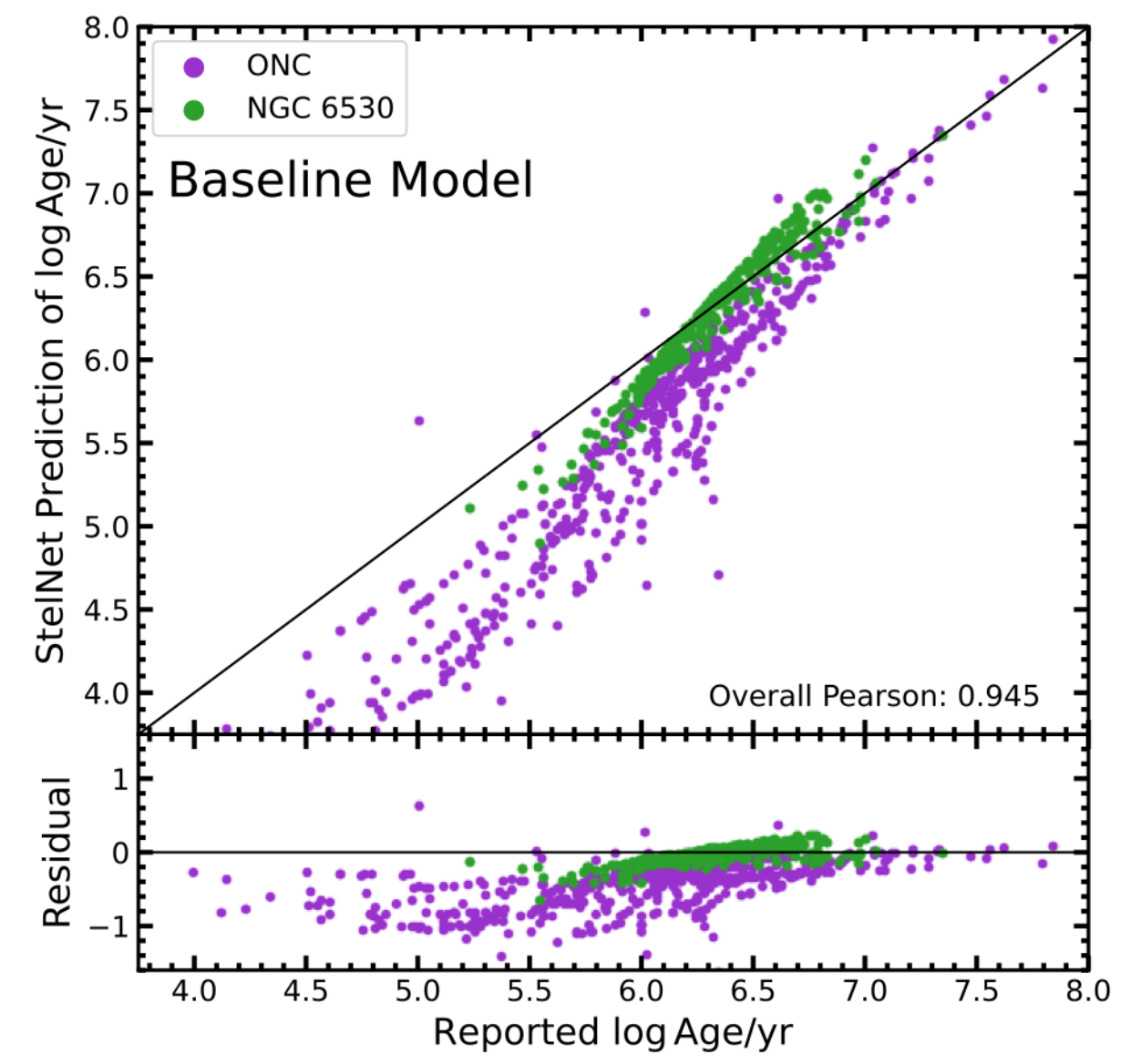
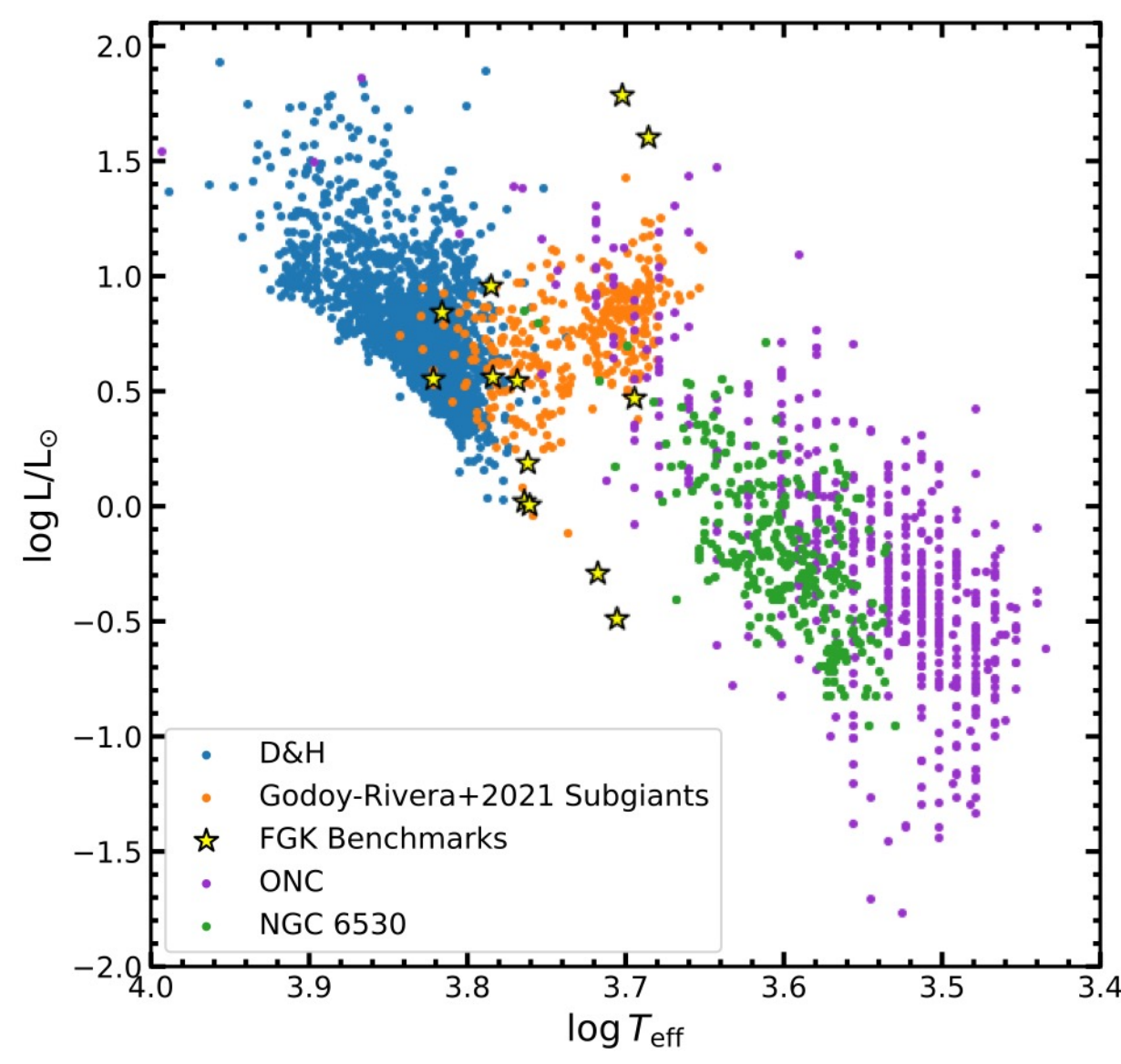


ASTROAI

Enabling Next Generation Astrophysics

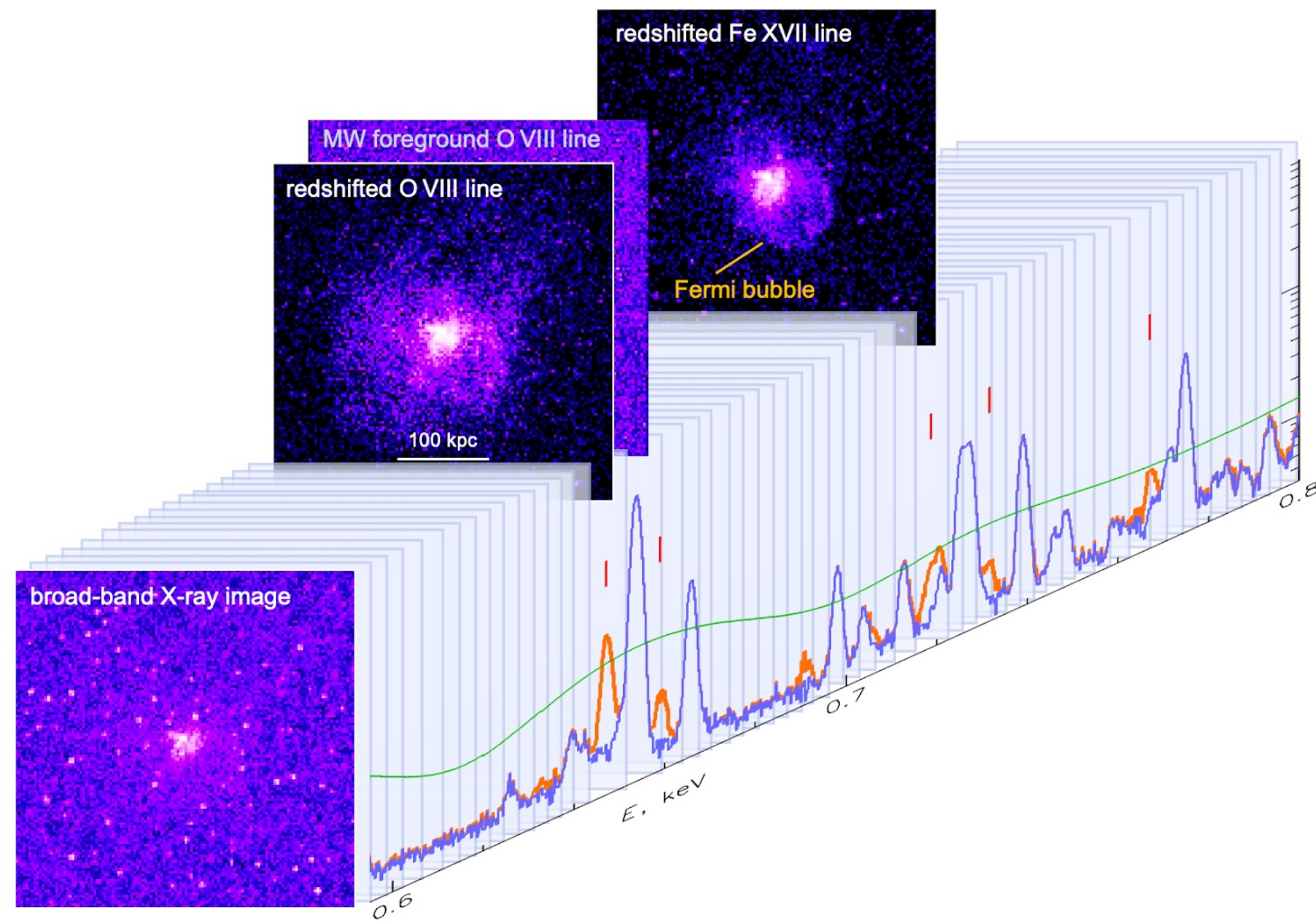


Anya Phillips



Phillips et al. in prep

Domain Adaptation

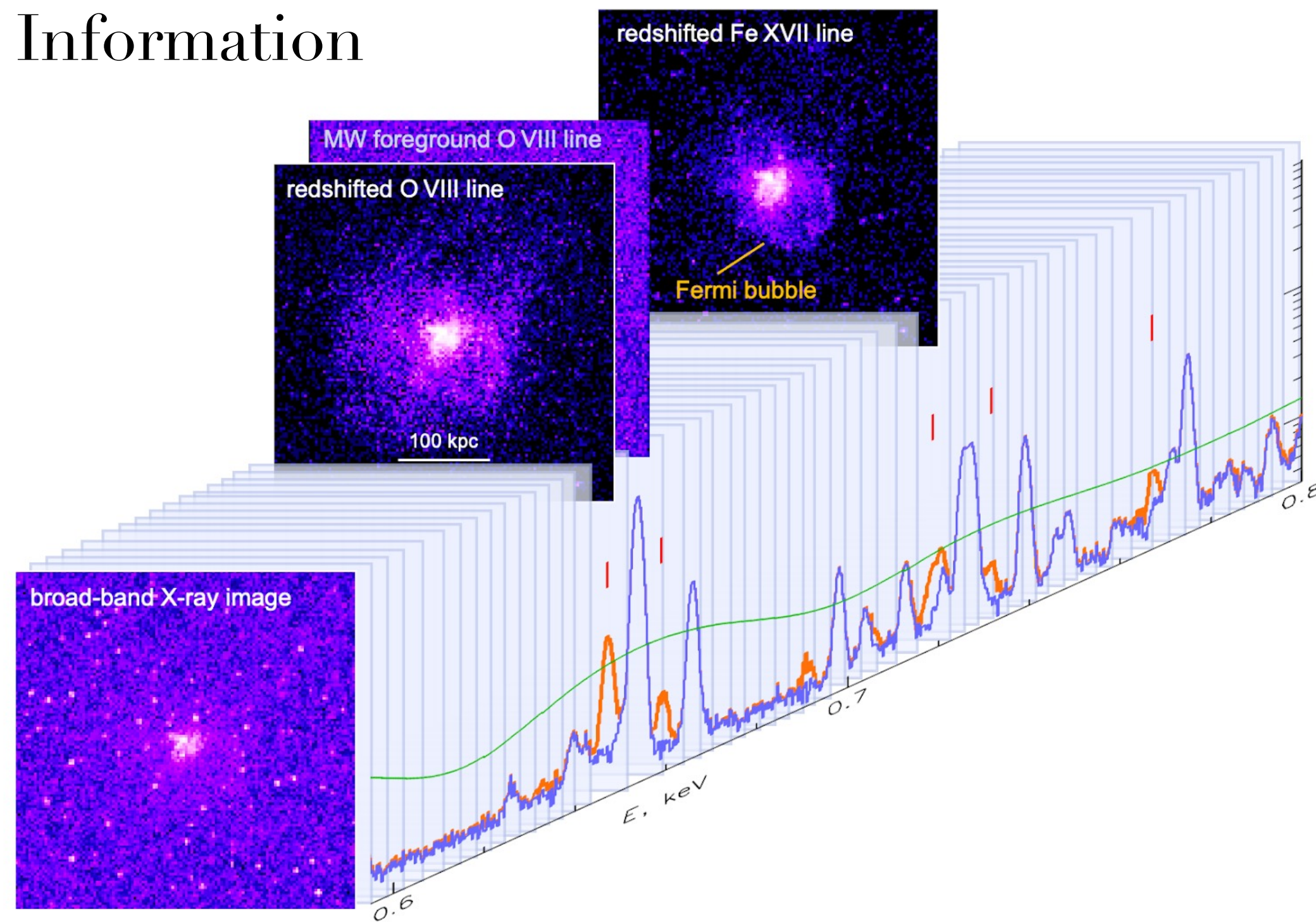




Remote Sensing for Climate Science

Same data and task:

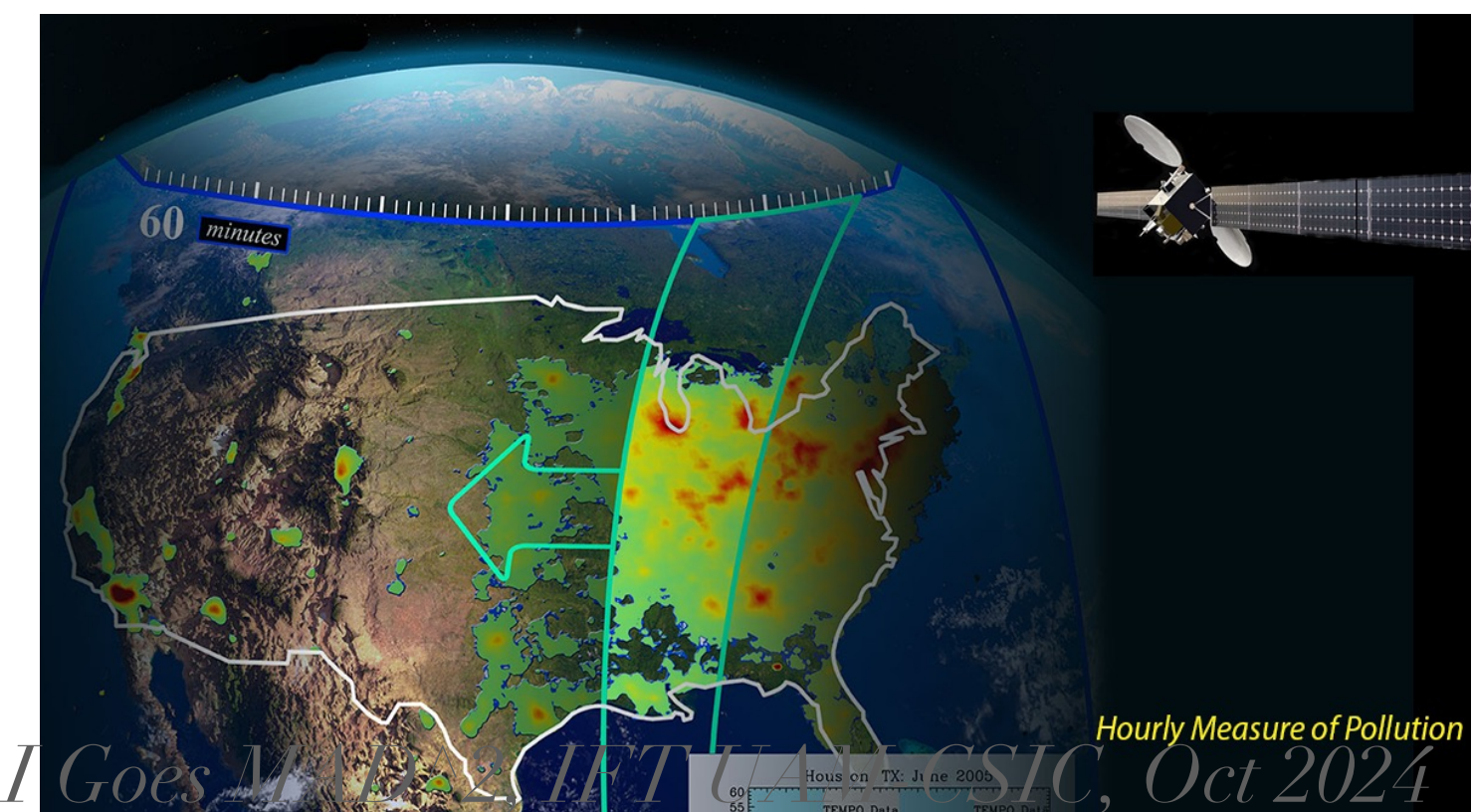
- Hyperspectral Data
- Extract Physical Information



MethaneSAT



TEMPO





Our Partners



MethaneSAT



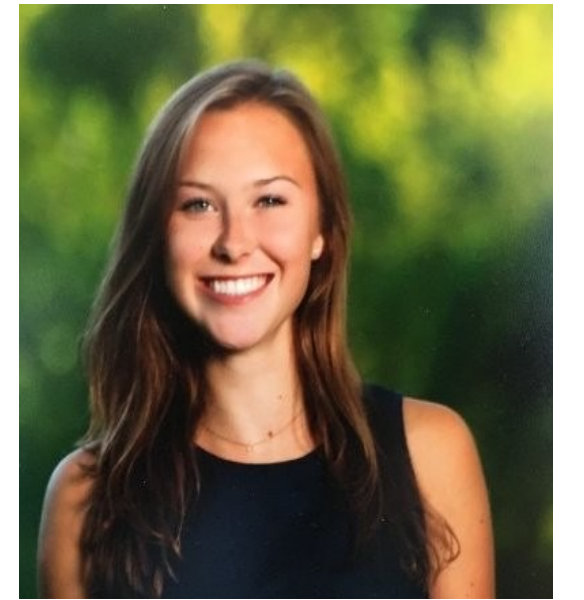
Maya Nasr

EAI's MethaneSAT Lead



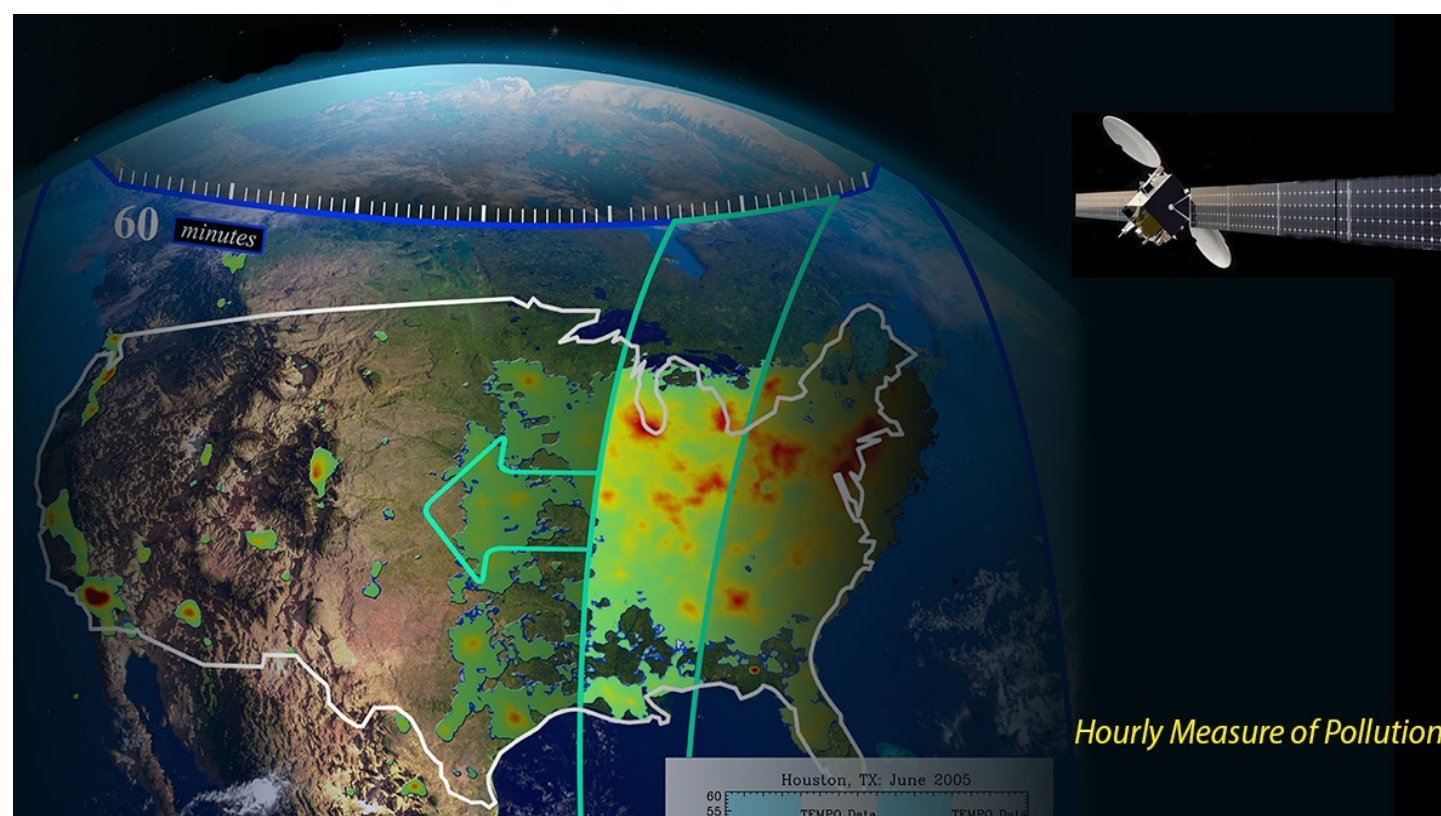
Steven Wofsy

Data Processing PI



Eleanor Walker

Postdoctoral Fellow



TEMPO



Caroline Nowlan

EAI's TEMPO Lead



Xiong Liu

TEMPO's Deputy PI



Gonzalo Gonzalez

Scientist

Thank you!



The Team



Cecilia Garraffo
Director



Douglas Finkbeiner
Project Scientist



Core Park
PhD Student



Manuel Perez
Carrasco
Software Lead



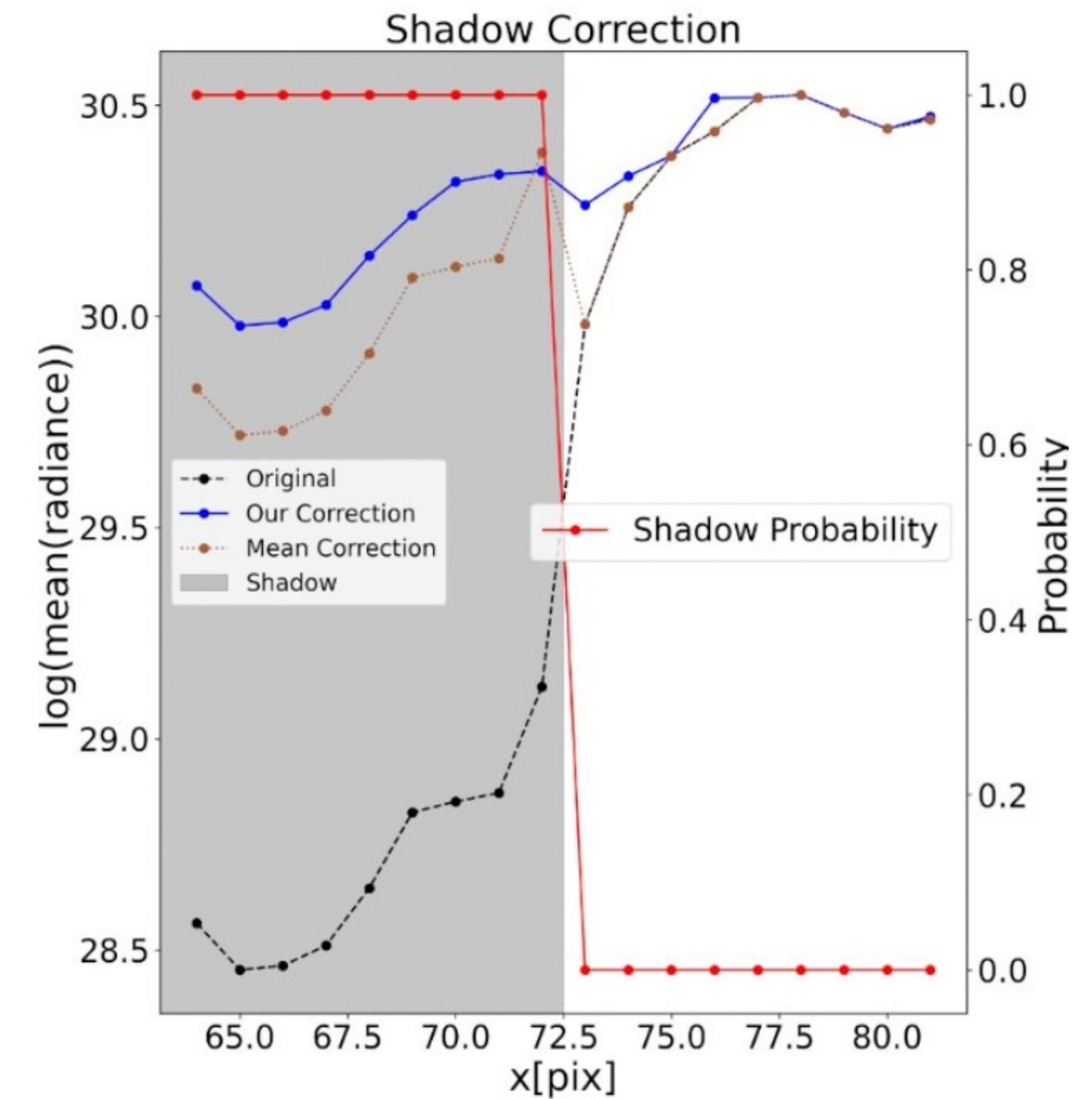
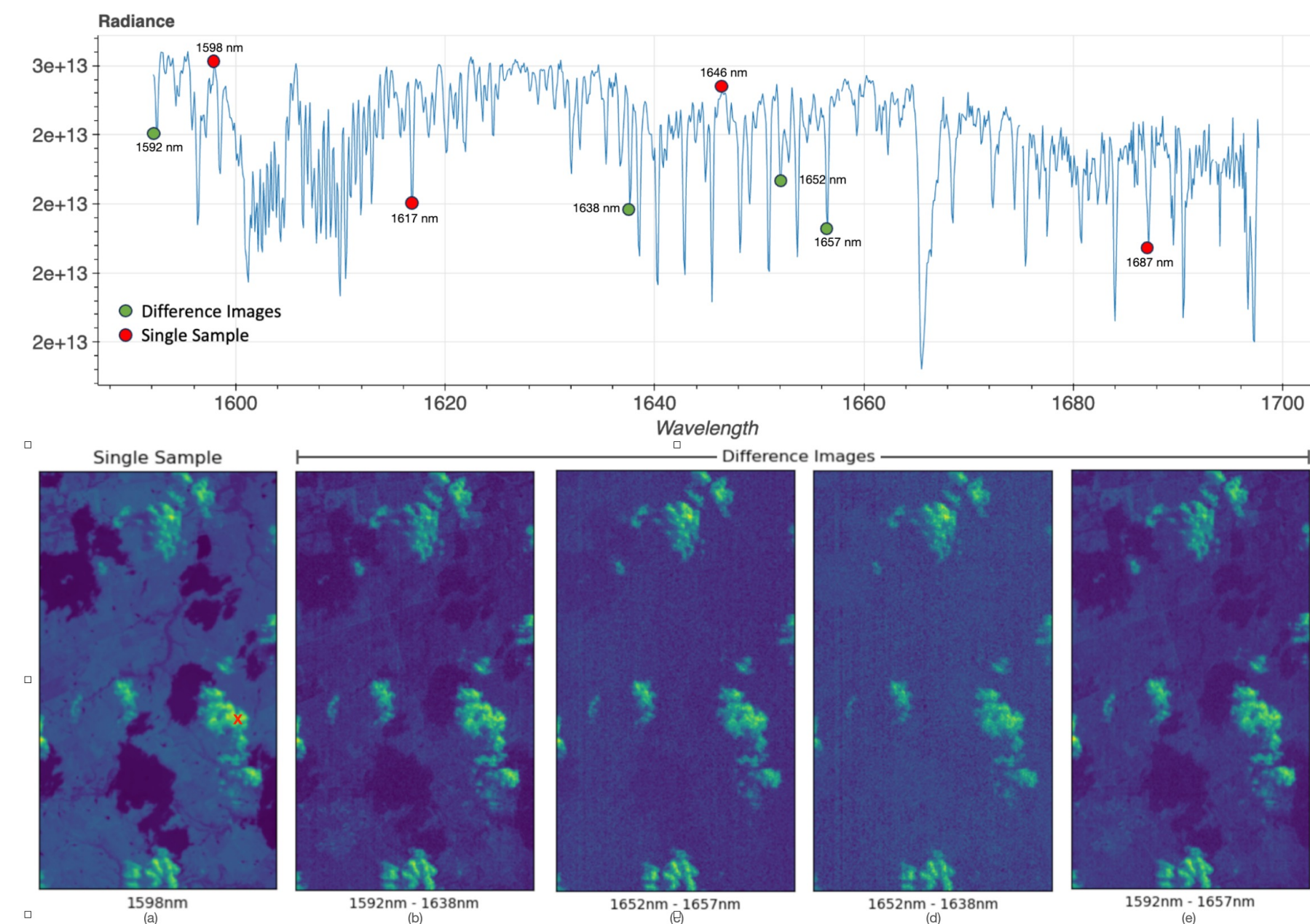
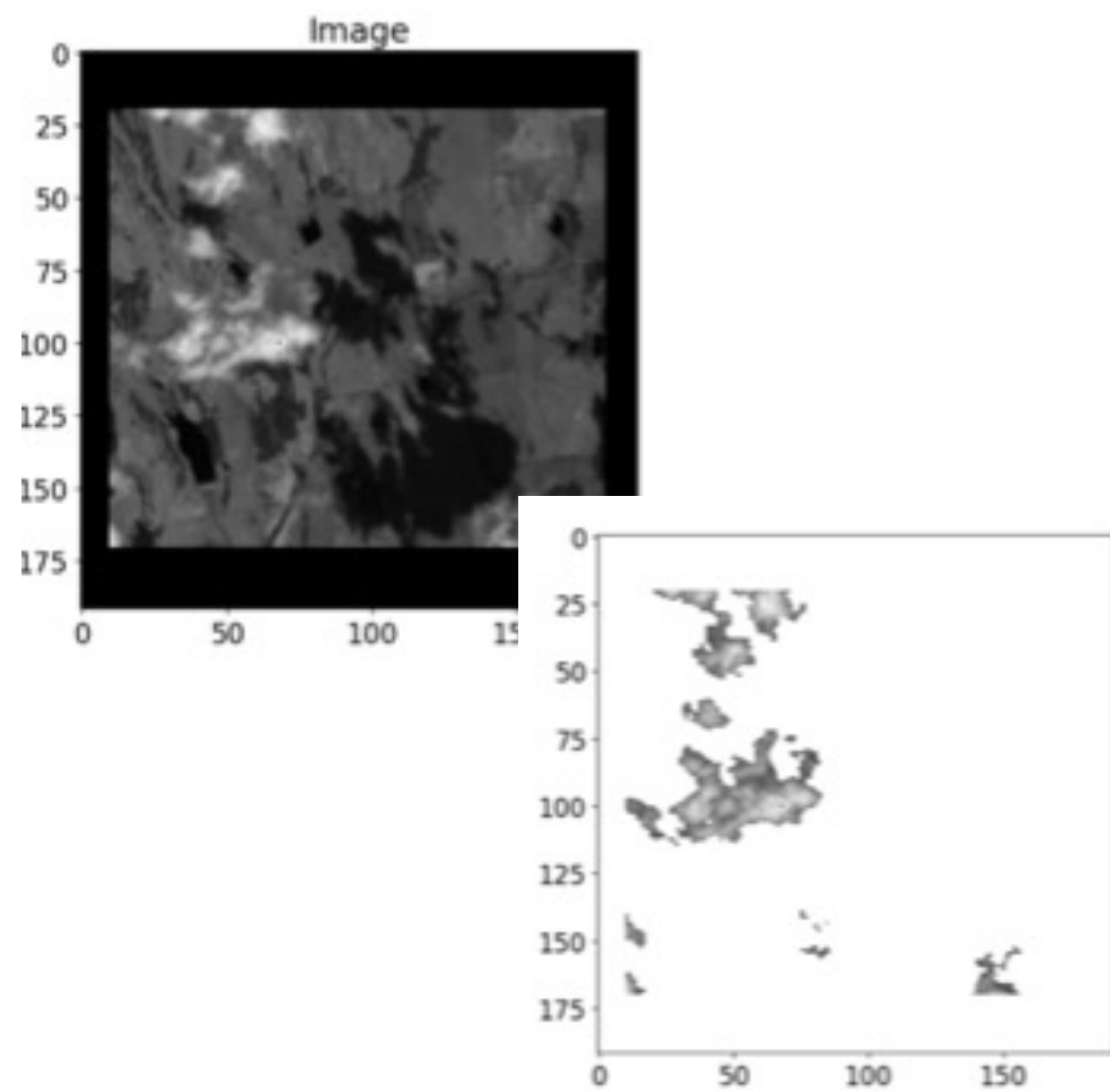
Caroline Nowlan
TEMPO Lead



Maya Nasr
MethaneSAT Lead



MethaneSAT: Enhanced Cloud Filtering / Correction



1. MethaneSAT Cloud Filtering Pipeline uses only the image information that let to significant data loss

2. We built an AI model that uses spectral information we enhanced the performance of cloud detection and filtering to 97%

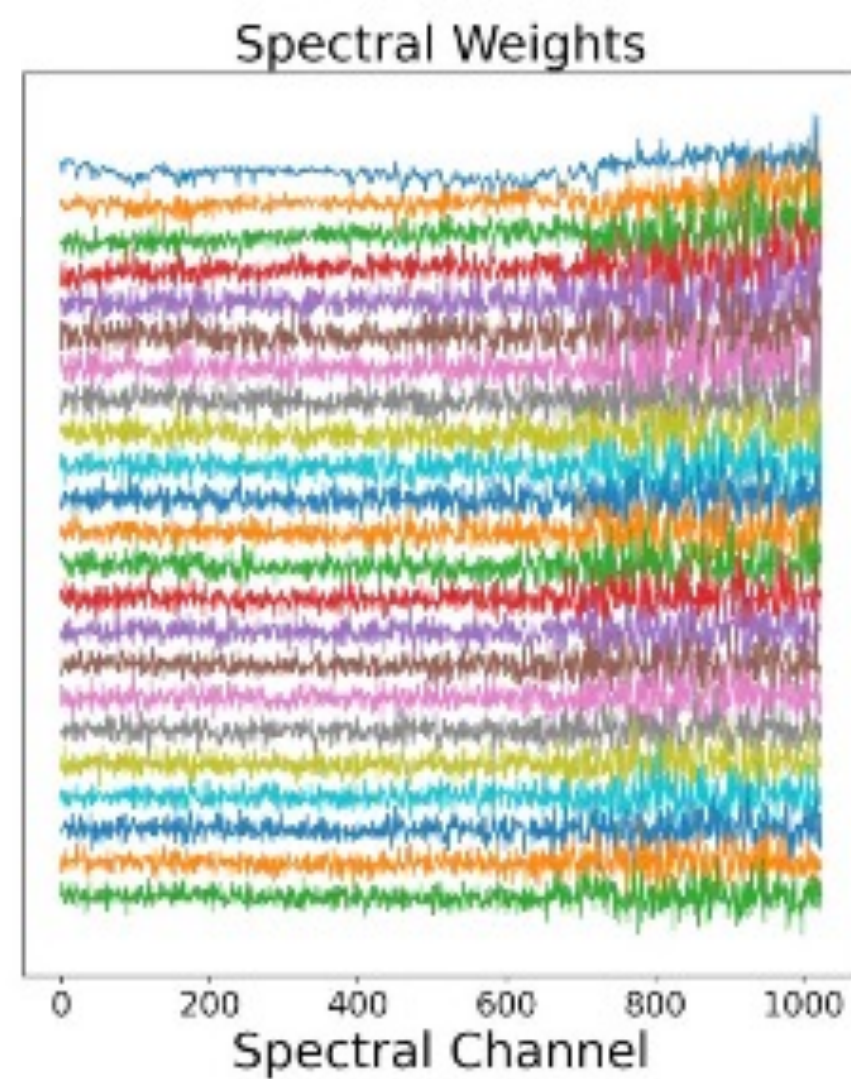
3. We trained an AI model to remove the effect of shadows from the spectra itself, making all the data useable!



MethaneSAT: Enhanced Plume Detection

In Partnership with Google, we are building an AI model to enhance plume detection by using the full spectral information from MethaneSAT data together with Geospatial Data from Google Earth.

MethaneSAT

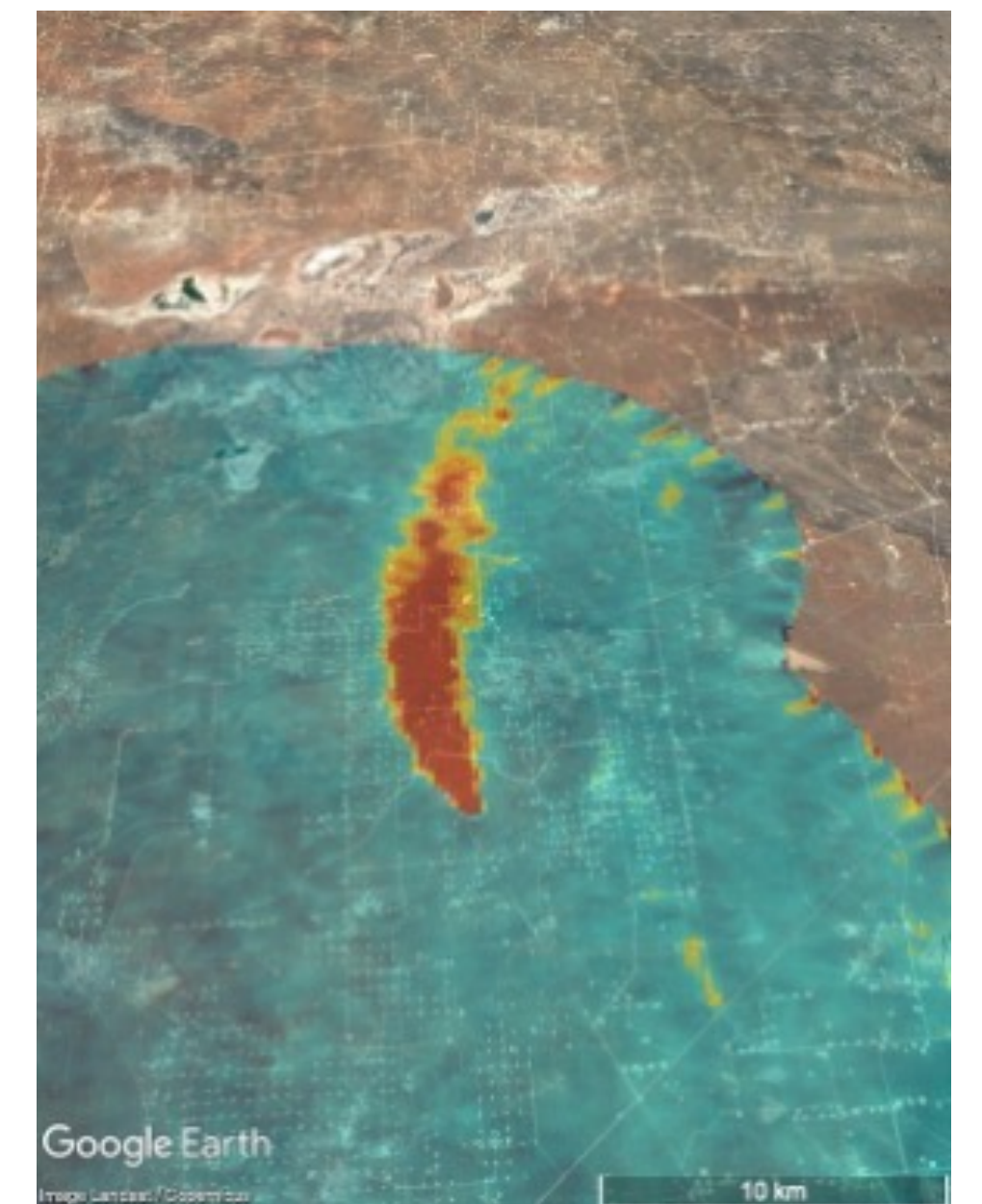


+



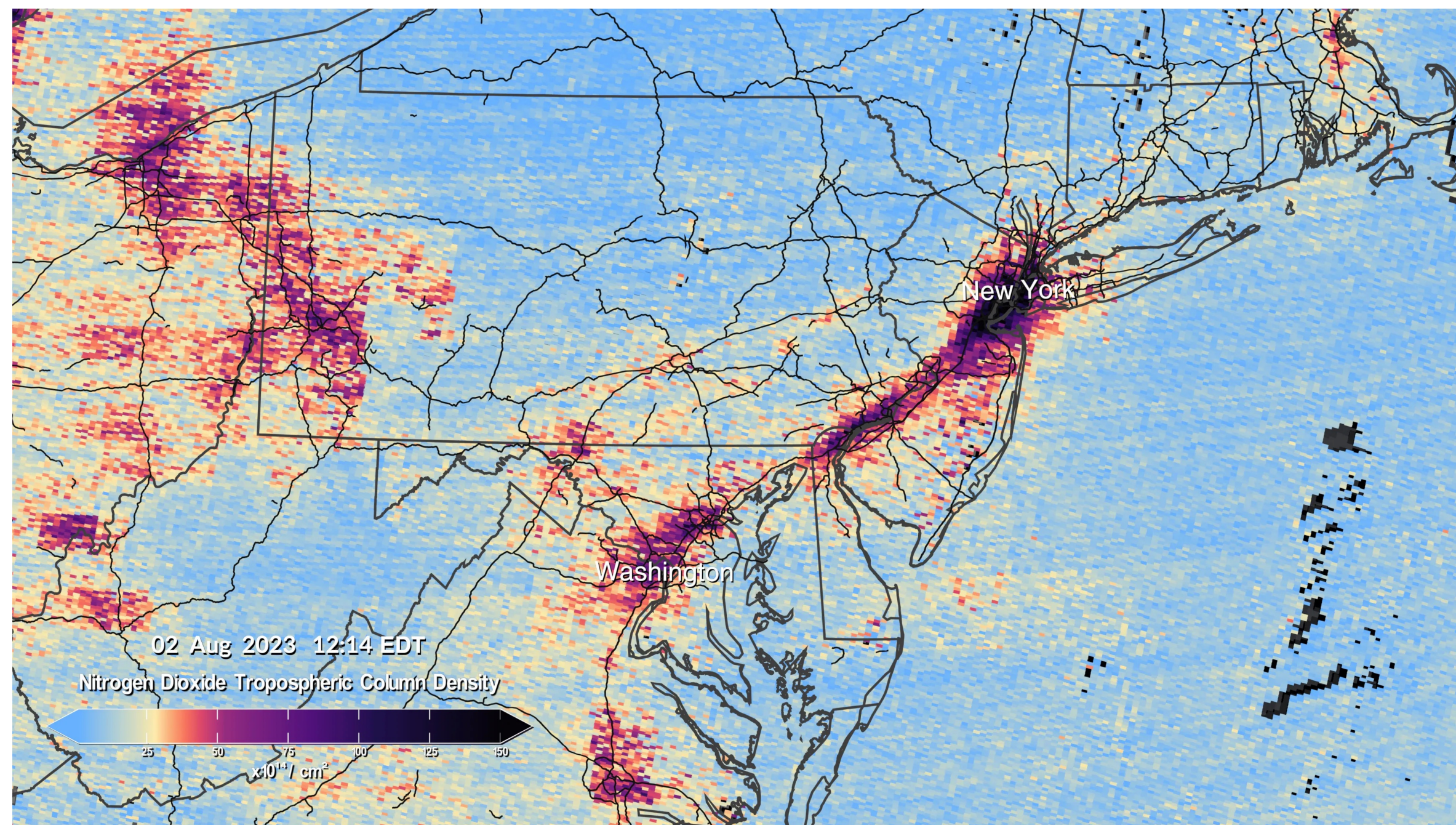
=

Reliable Plume Detection





TEMPO: Resolving the Altitude of Pollutants



Nitrogen dioxide (NO_2) plays a central role in air quality and atmospheric chemistry, and has direct detrimental effects on human health when concentrated near the surface of Earth.

TEMPO is able to successfully retrieve the total column density of pollutants, such as nitrogen dioxide (NO_2), but not its vertical distribution.

We are building a multimodal AI model to integrate TEMPO data with other data (GEOS-CF, EPA Air Quality System, and aircraft profiles like STAQ) to resolve the vertical distribution of pollutants, like NO_2 to assess the air quality where it has human health impact

TEMPO nitrogen dioxide over part of the East Coast on August 2, 2023 at 12:14 EDT. High levels of NO_2 are seen over major urban regions and the I-95 corridor. High levels of NO_2 over Eastern Pennsylvania and Ohio are due to biomass burning.

Bayesian Inference

Probability as a measure of *believability in an event*

THE PROBABILITY OF "B" BEING TRUE GIVEN THAT "A" IS TRUE

THE PROBABILITY OF "A" BEING TRUE

$$P(A|B) = \frac{P(B|A) P(A)}{P(B)}$$

THE PROBABILITY OF "A" BEING TRUE GIVEN THAT "B" IS TRUE

THE PROBABILITY OF "B" BEING TRUE

The diagram shows the equation $P(A|B) = \frac{P(B|A) P(A)}{P(B)}$ with arrows pointing from descriptive text to each part of the equation. An arrow points from the top text to $P(B|A)$, from the top-right text to $P(A)$, from the bottom-left text to $P(A|B)$, and from the bottom-right text to $P(B)$.

A.I. Wiki

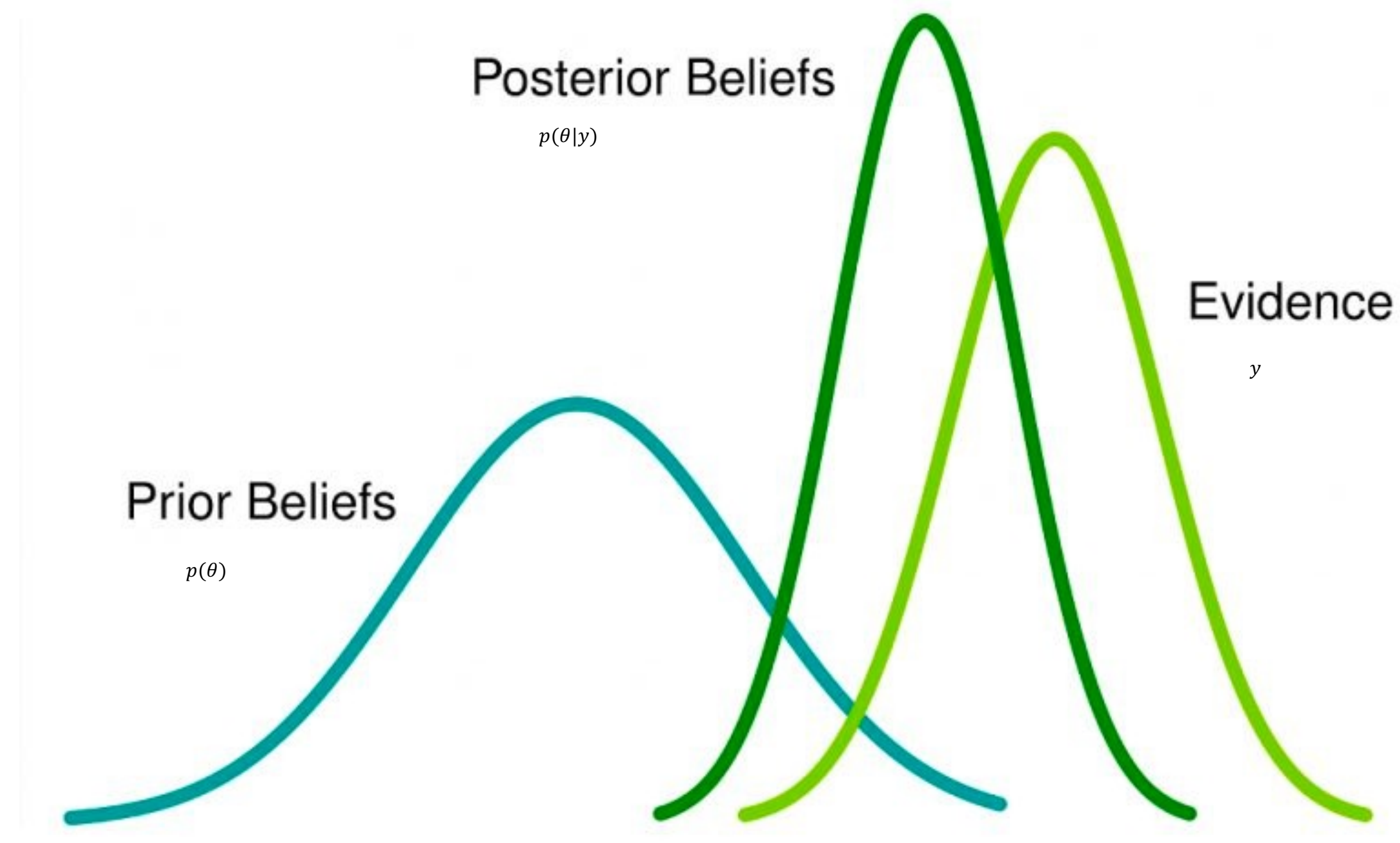
$$p(\theta|y) \propto p(y|\theta)p(\theta)$$

Weights & biases

Data

Bayesian Inference

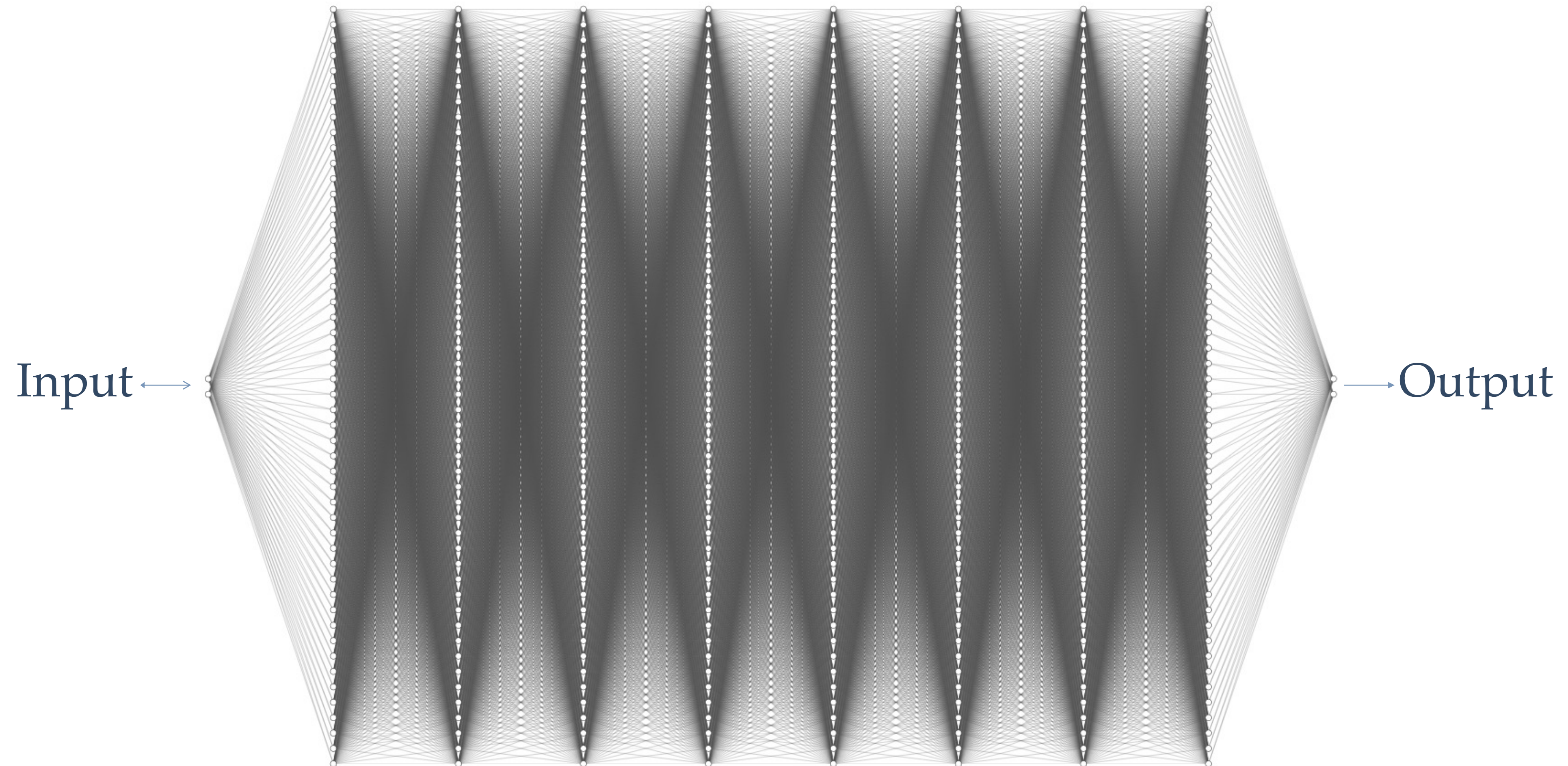
$$p(\theta|y) \propto p(y|\theta)p(\theta)$$



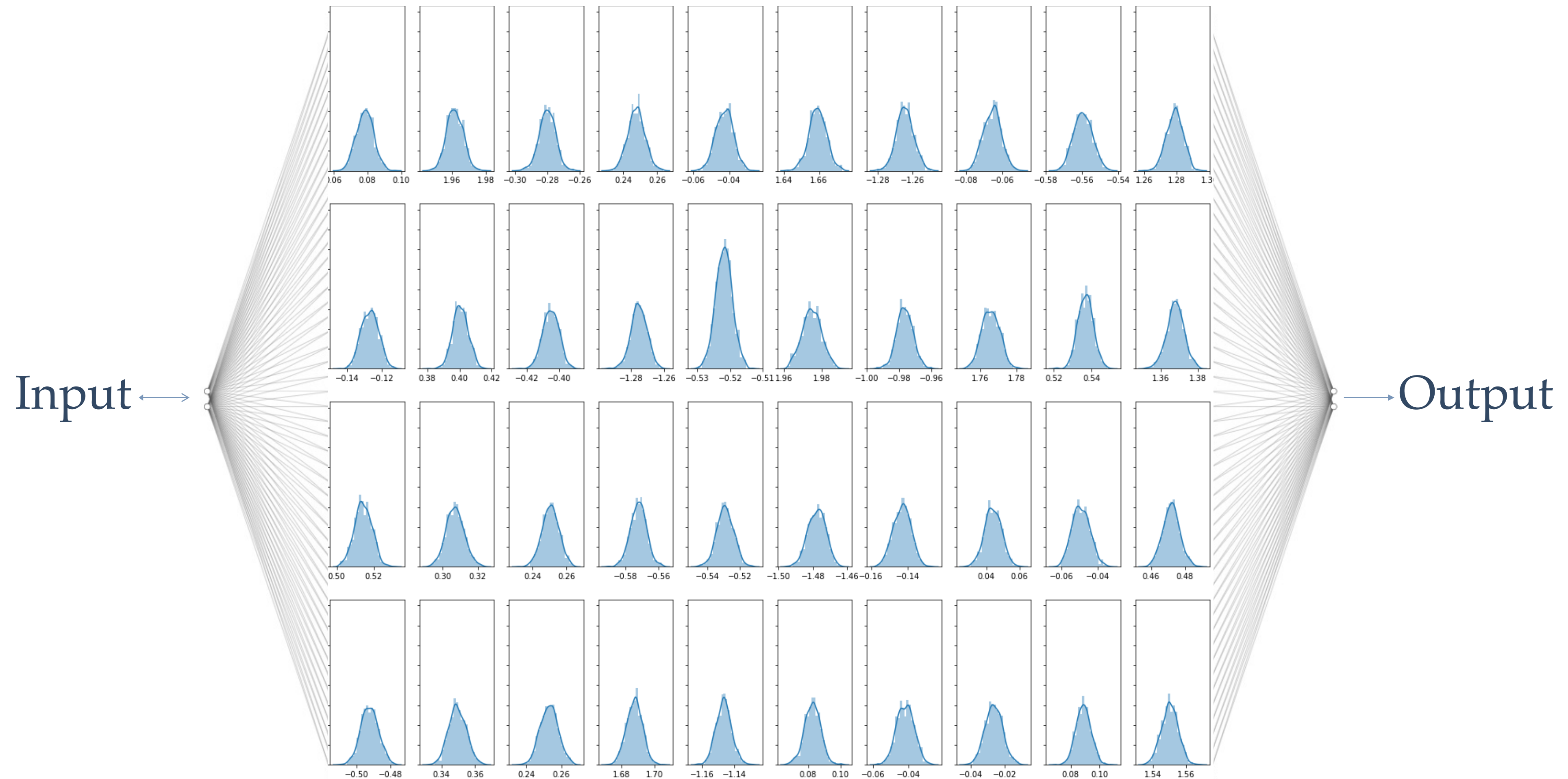
“When the facts change, I change my mind. What do you do, sir? “

John Maynard Keynes

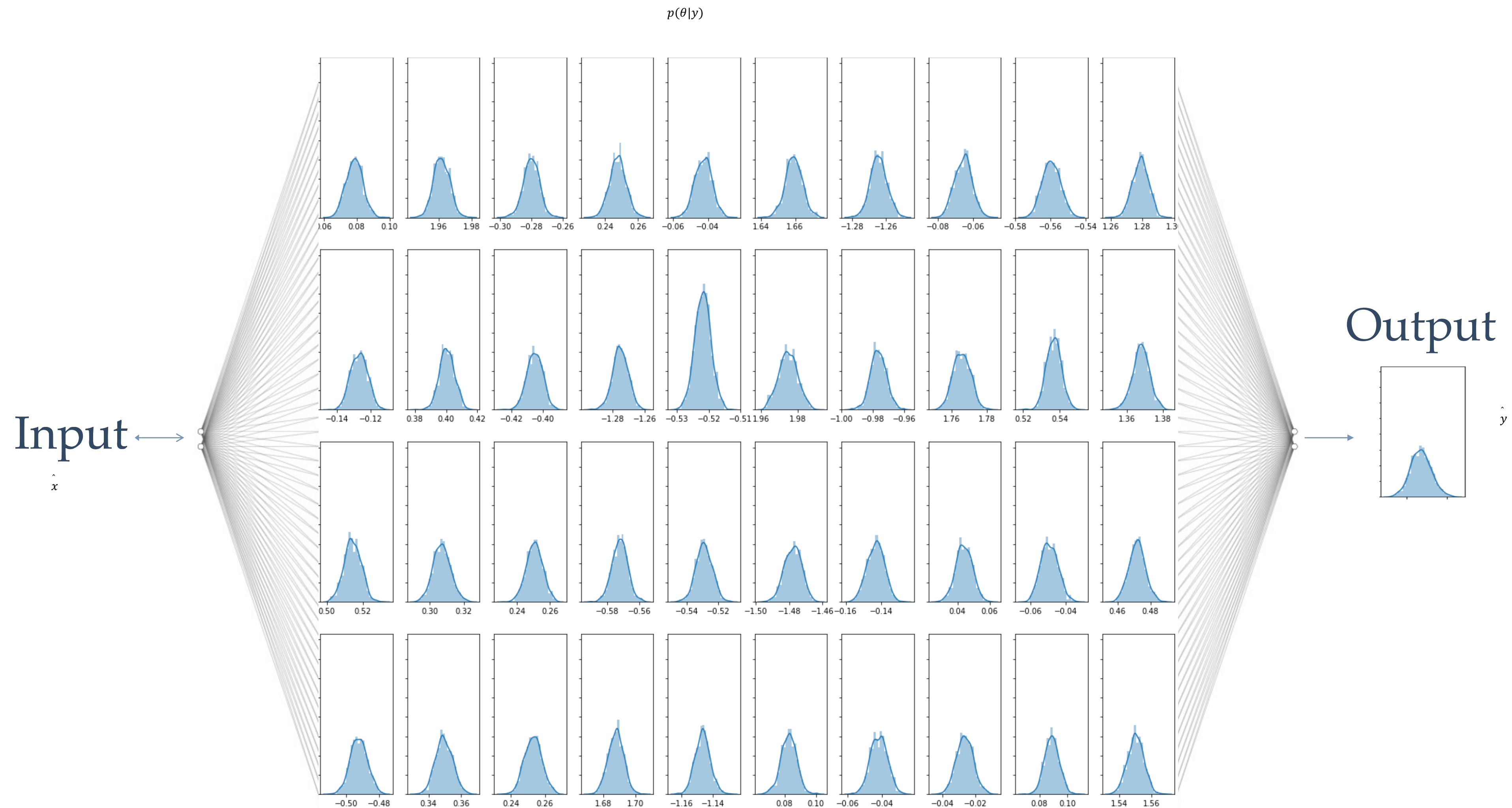
Bayesian Neural Networks



Bayesian Neural Networks



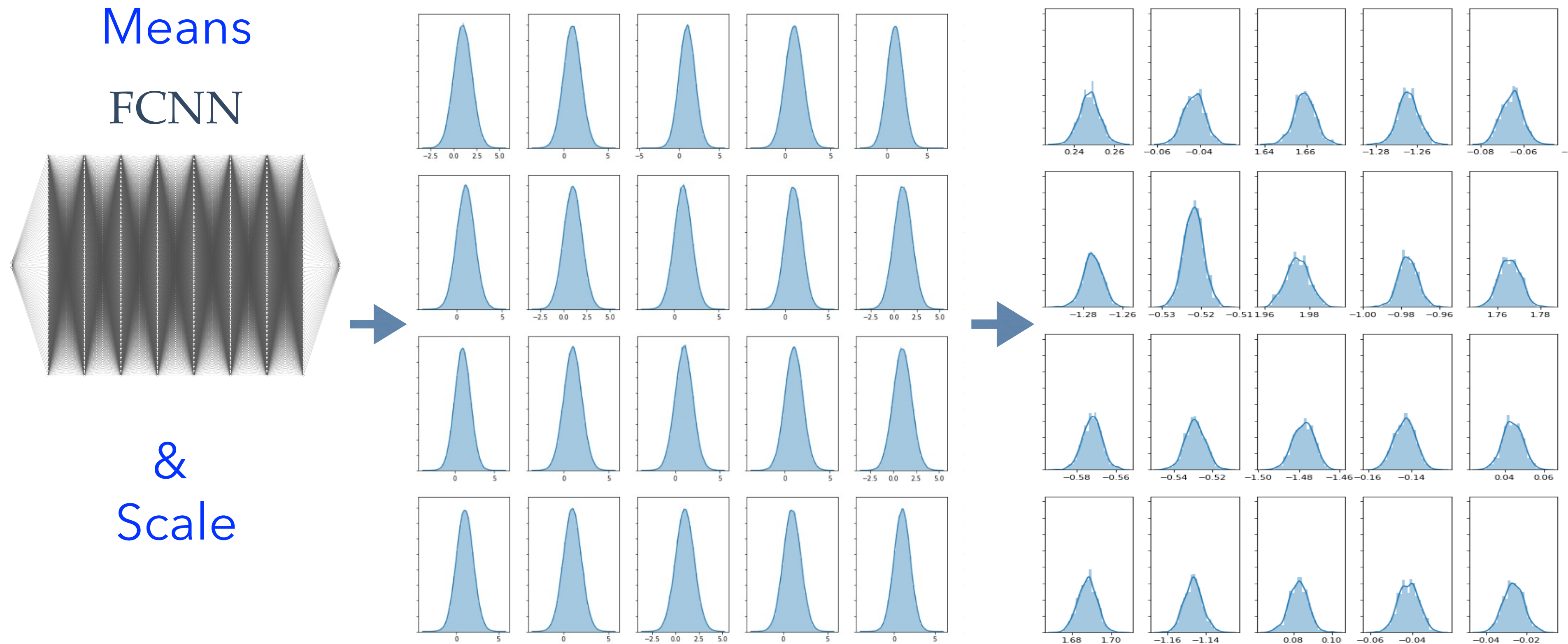
Bayesian Neural Networks



BI for NN calculates the posterior distribution of the weights given the training data

Bayesian Neural Networks

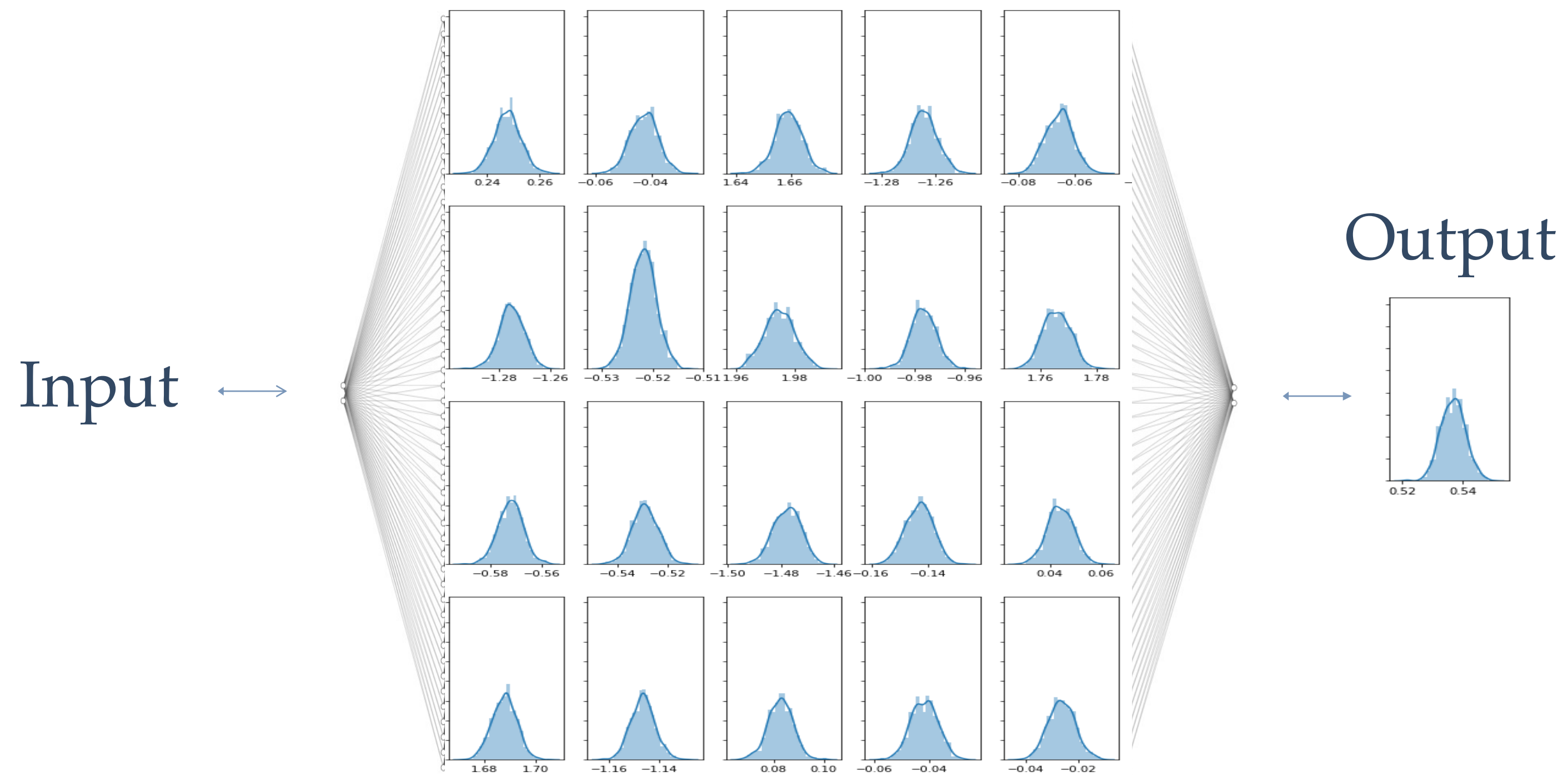
Priors $p(\theta)$ \longleftrightarrow $\frac{p(\theta)p(y|\theta)}{p(y)} = p(\theta|y)$
intractable



Bayesian Neural Networks

MCMC: **Eventually** accurate

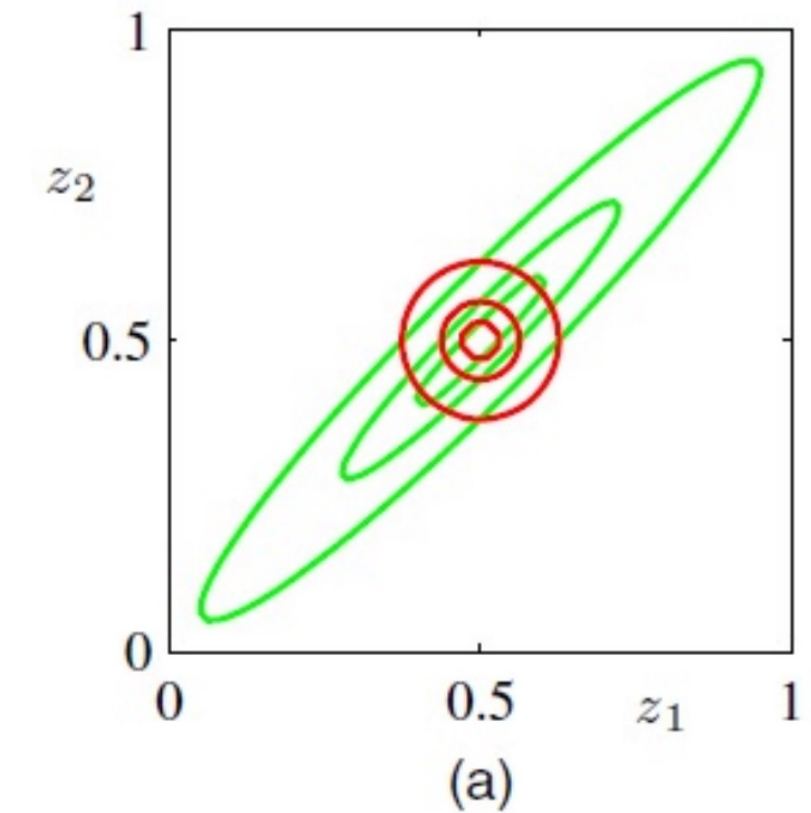
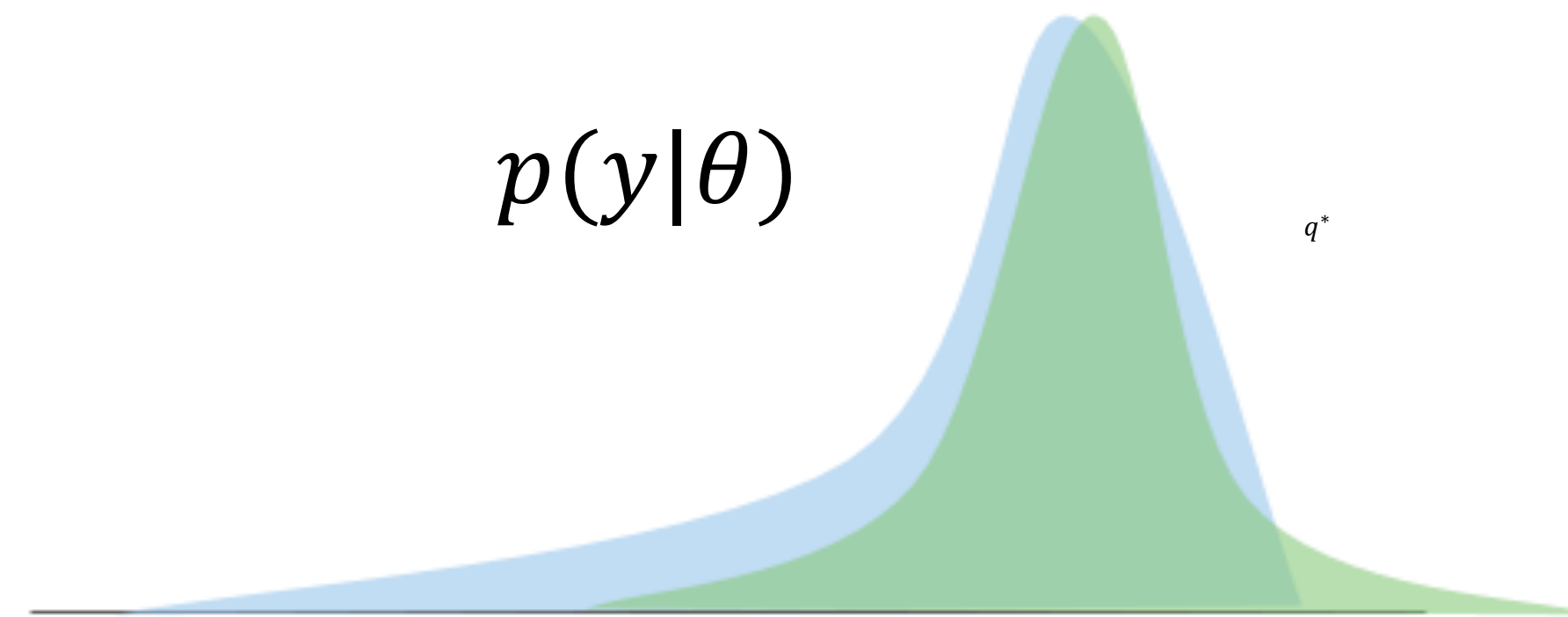
$$p(\theta) \times p(y|\theta) \propto p(\theta|y)$$



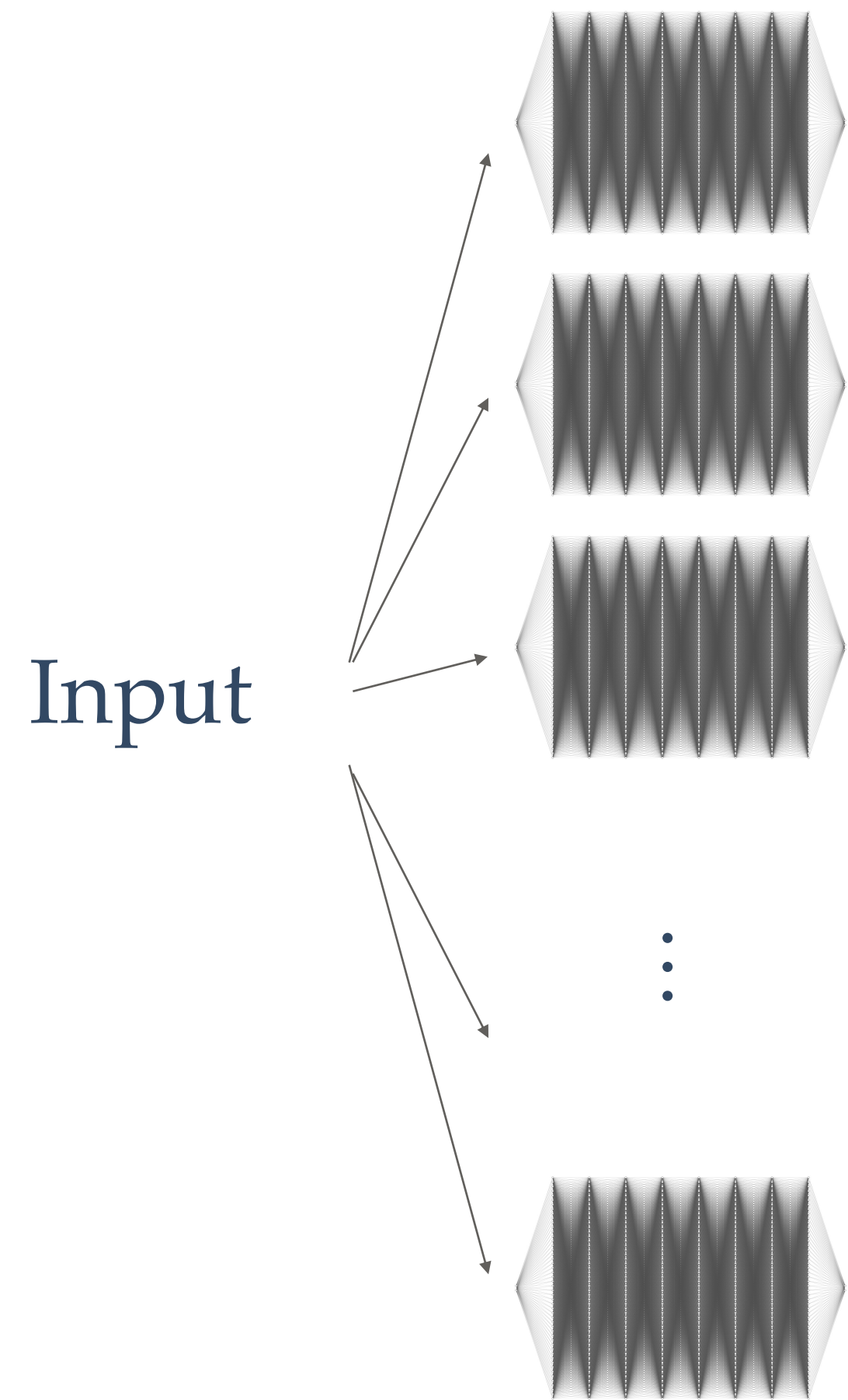
Approximate Bayesian Inference: Variational Bayes

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{\int p(y, \theta)d\theta} \approx q^*$$

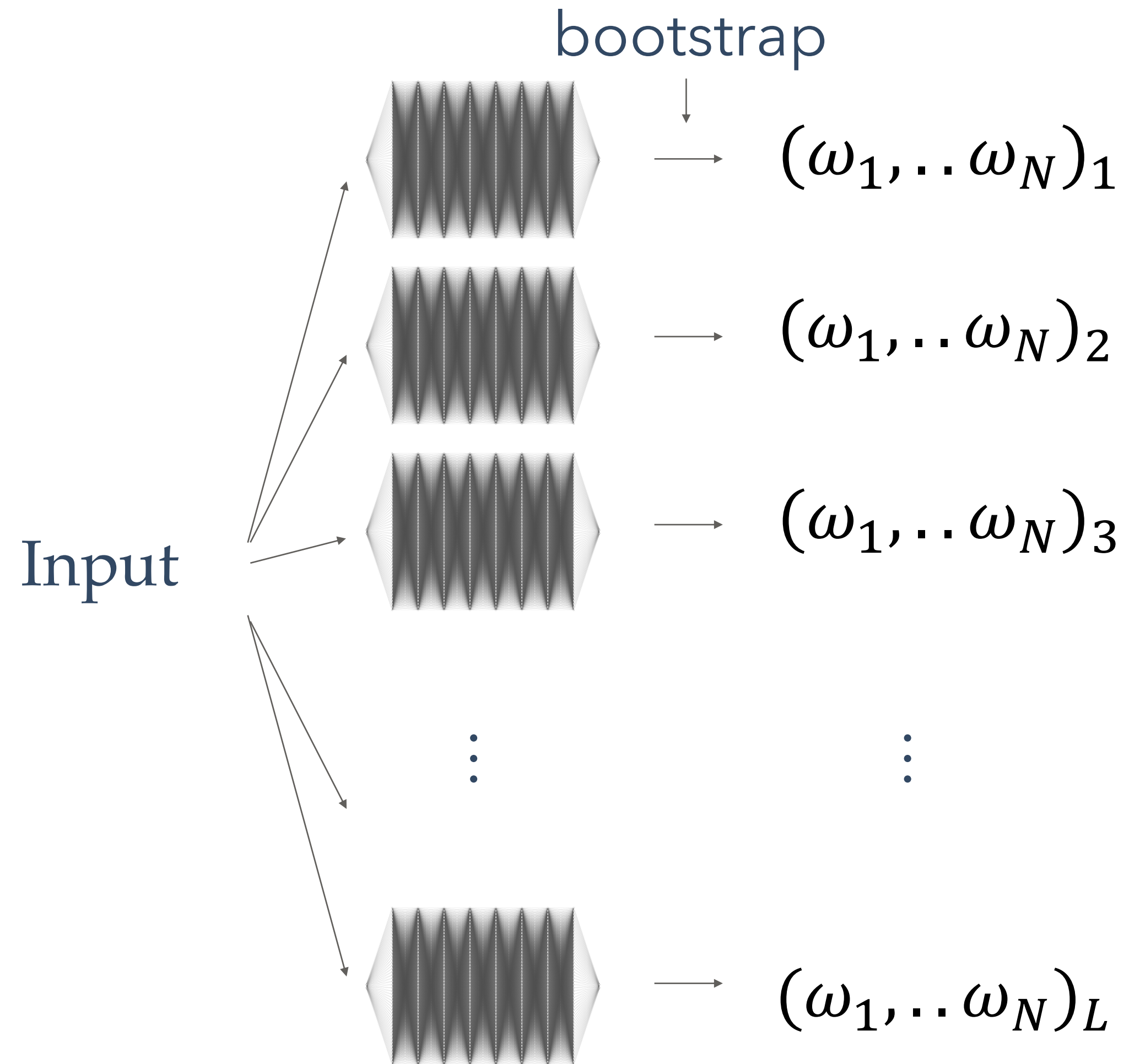
Optimization approach \rightarrow Q a family of “nice” distributions



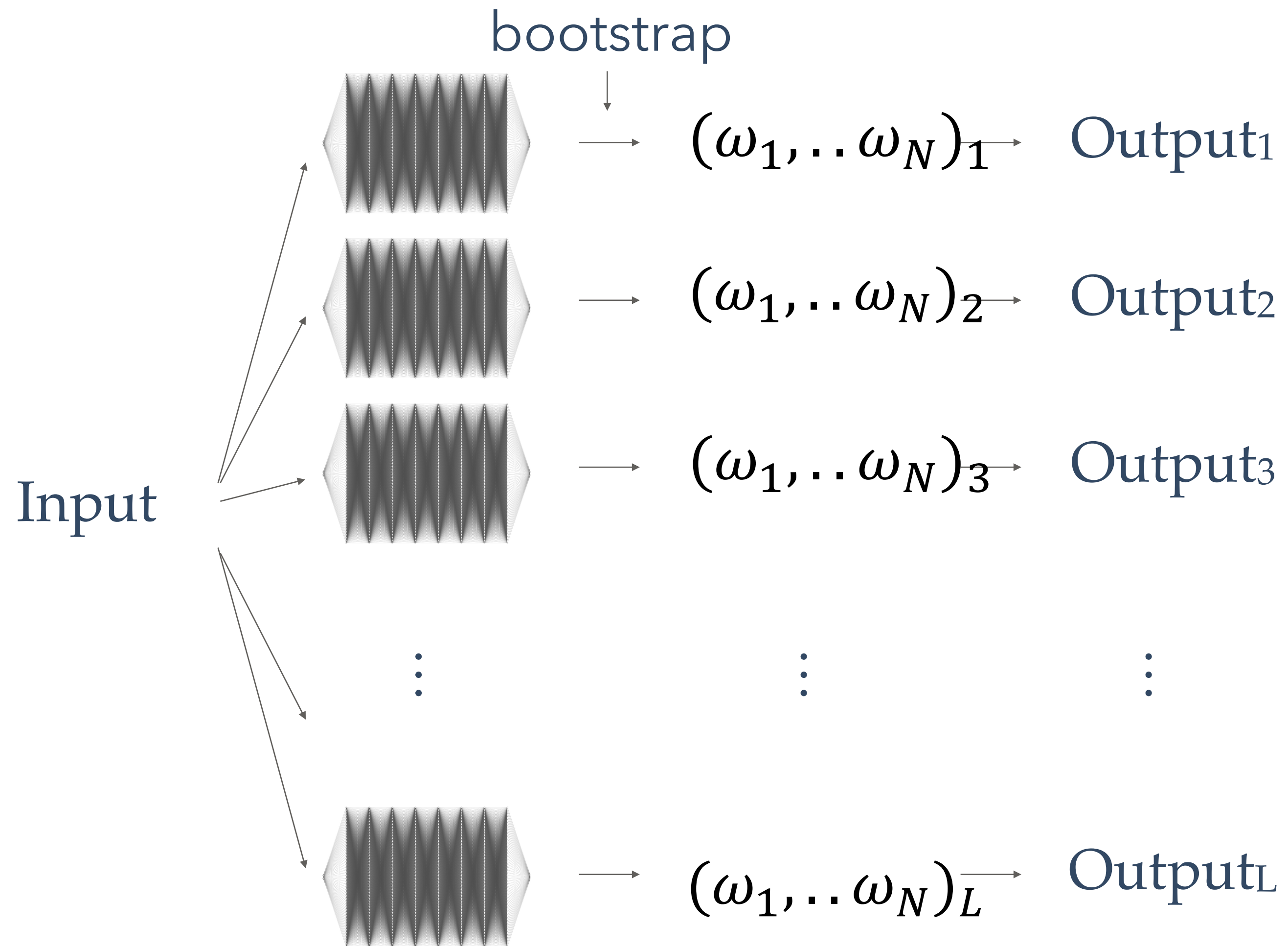
Bootstrap: L models



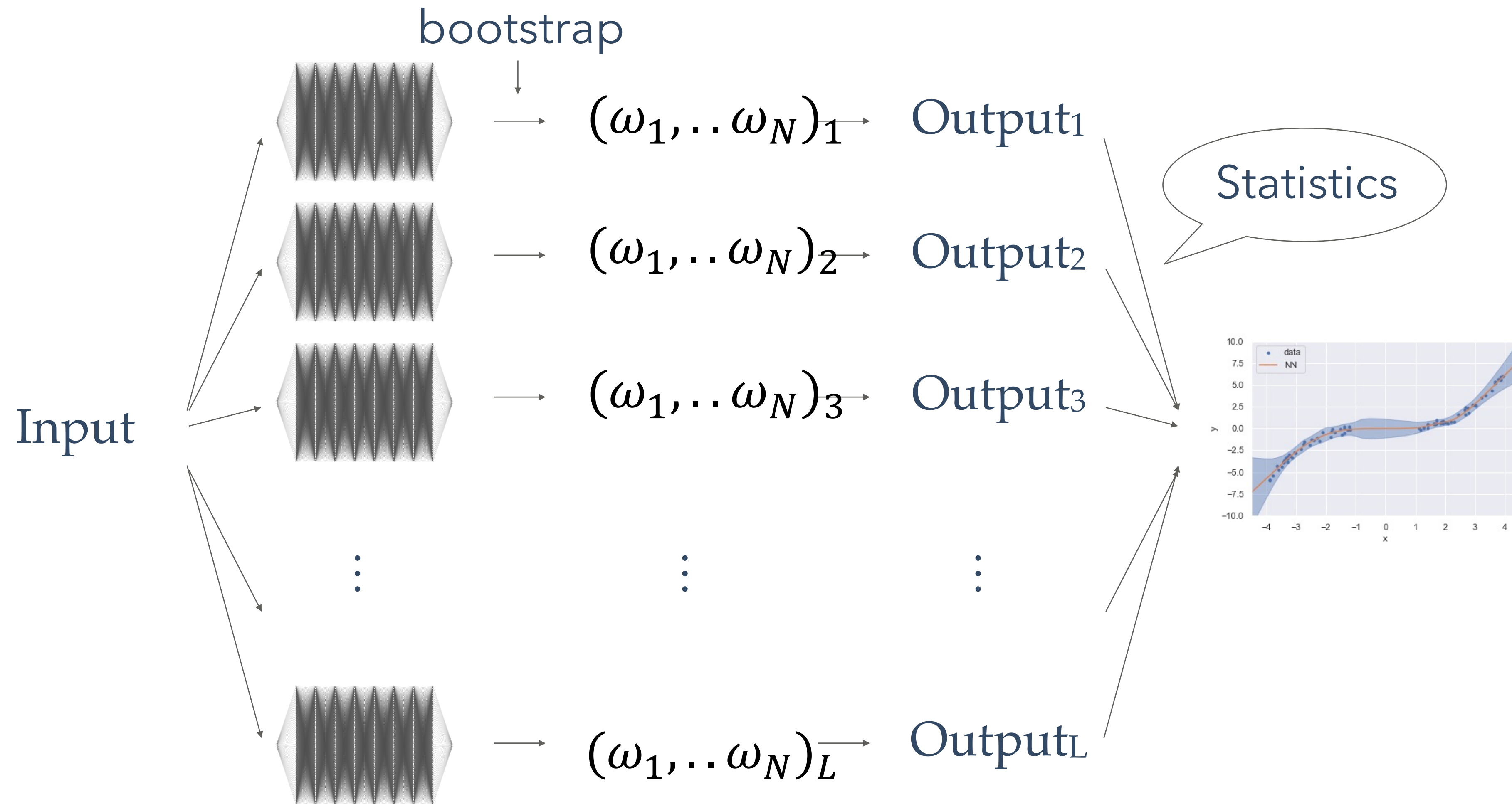
Bootstrap: L models



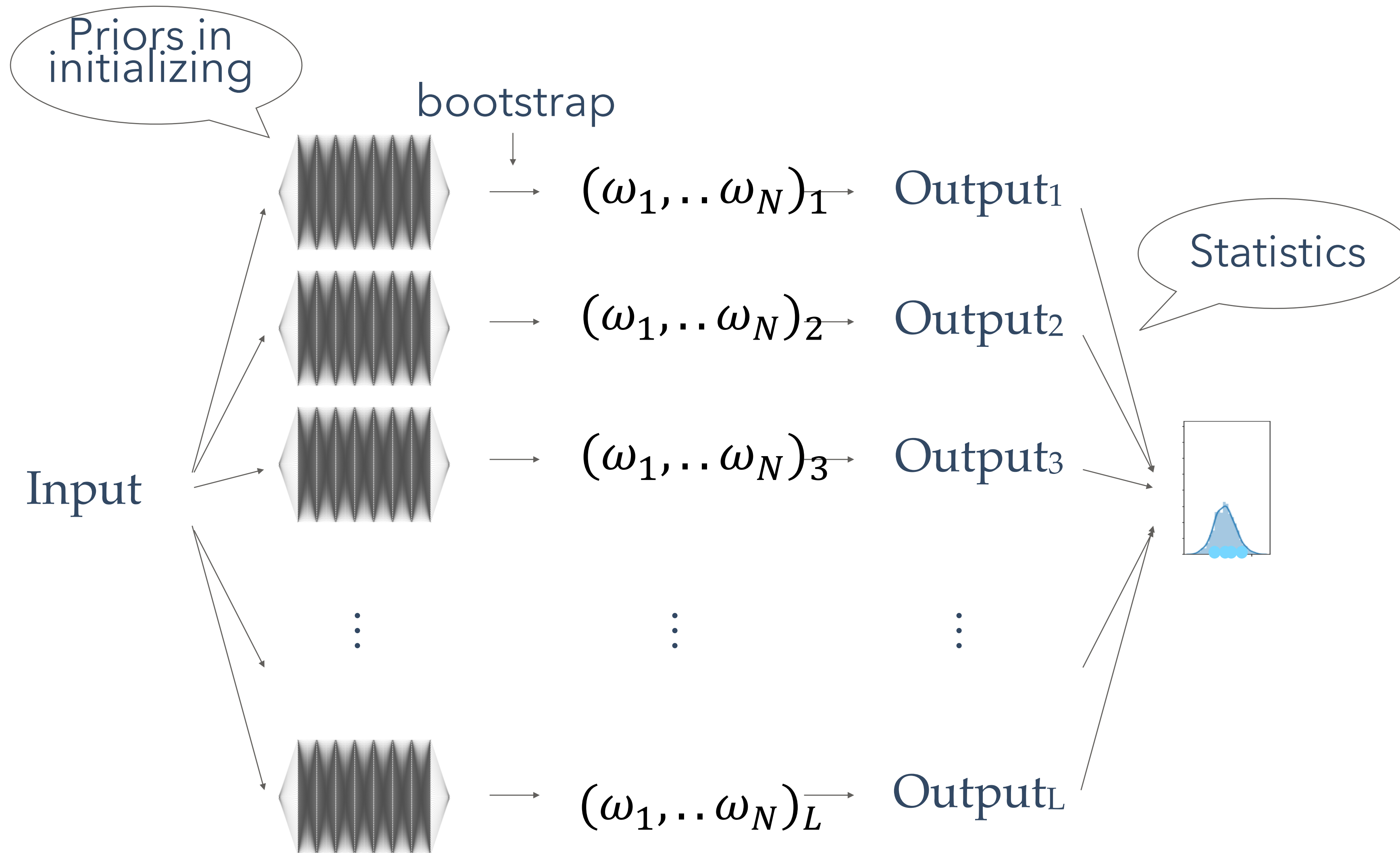
Bootstrap: L models



Bootstrap: L models

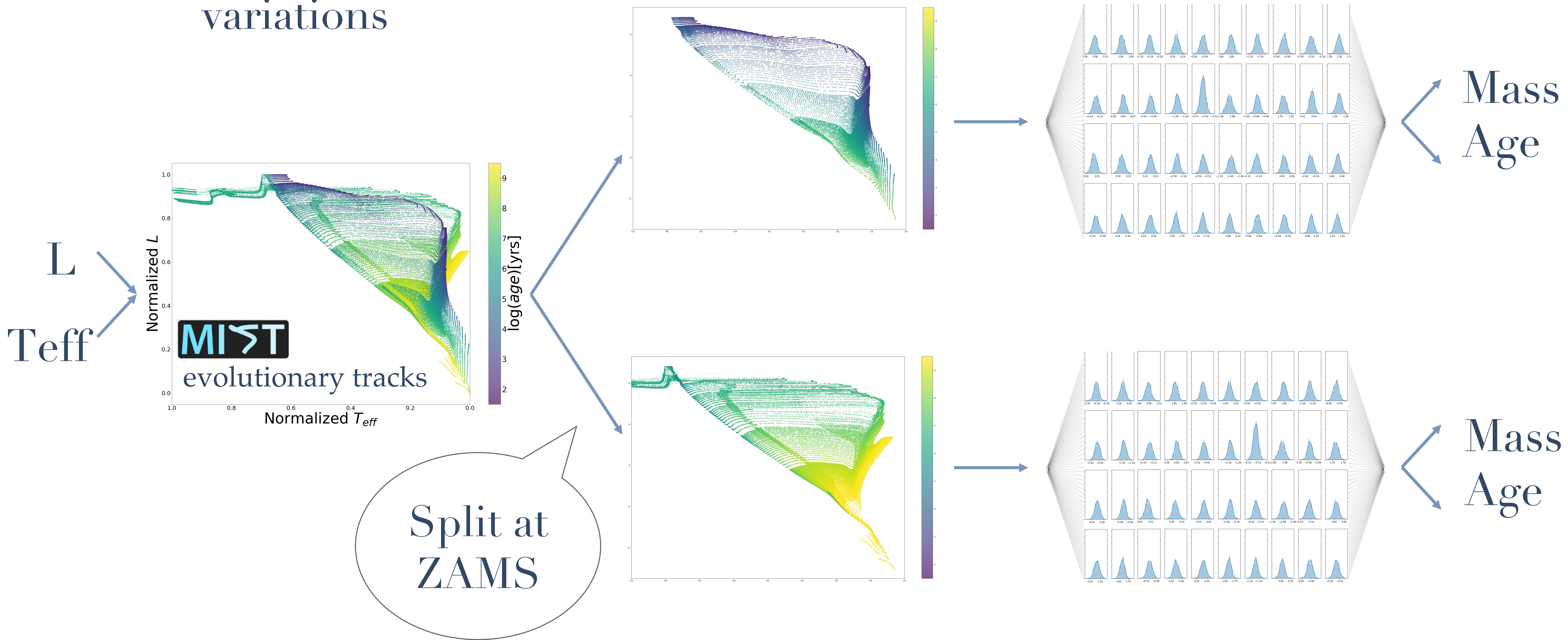


Bootstrap: L models



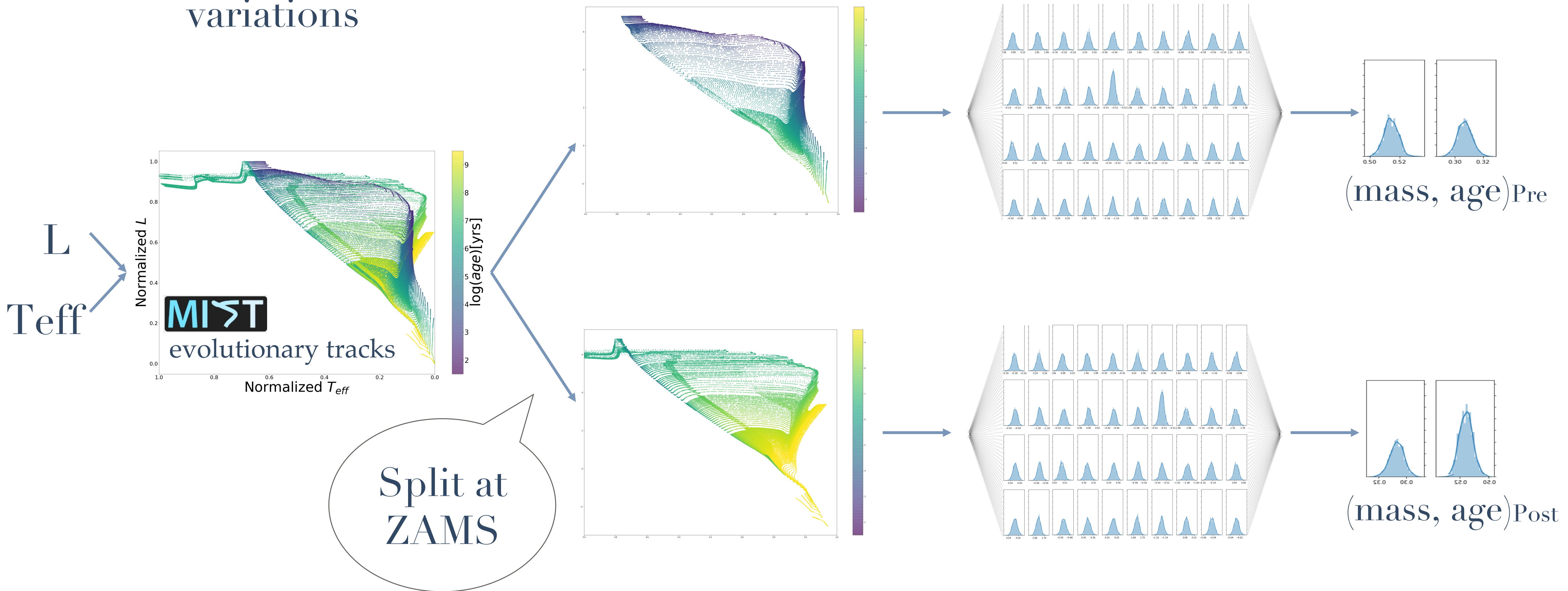
StelNet: A Hierarchical Neural Network for Inference in Stellar Characterization

- ❖ Degeneracies ✓
- ❖ Non-linearity ✓
- ❖ Confidence variations



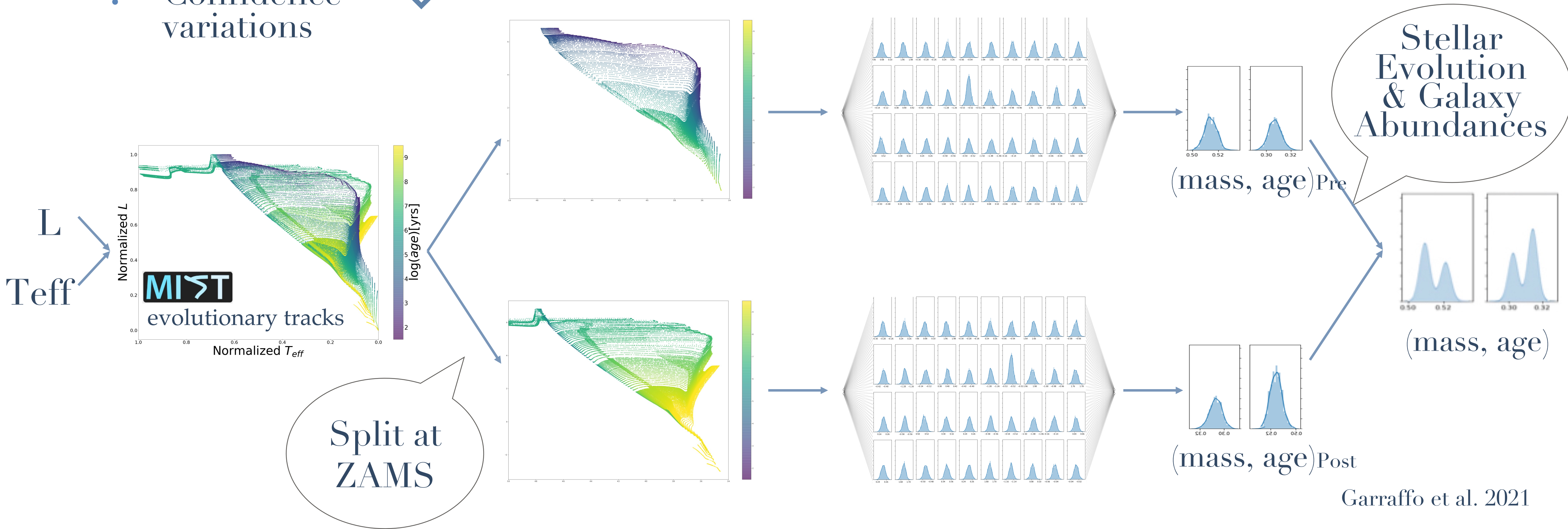
StelNet: A Hierarchical Neural Network for Inference in Stellar Characterization

- ❖ Degeneracies ✓
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- ❖ Confidence variations ✓



StelNet: A Hierarchical Neural Network for Inference in Stellar Characterization

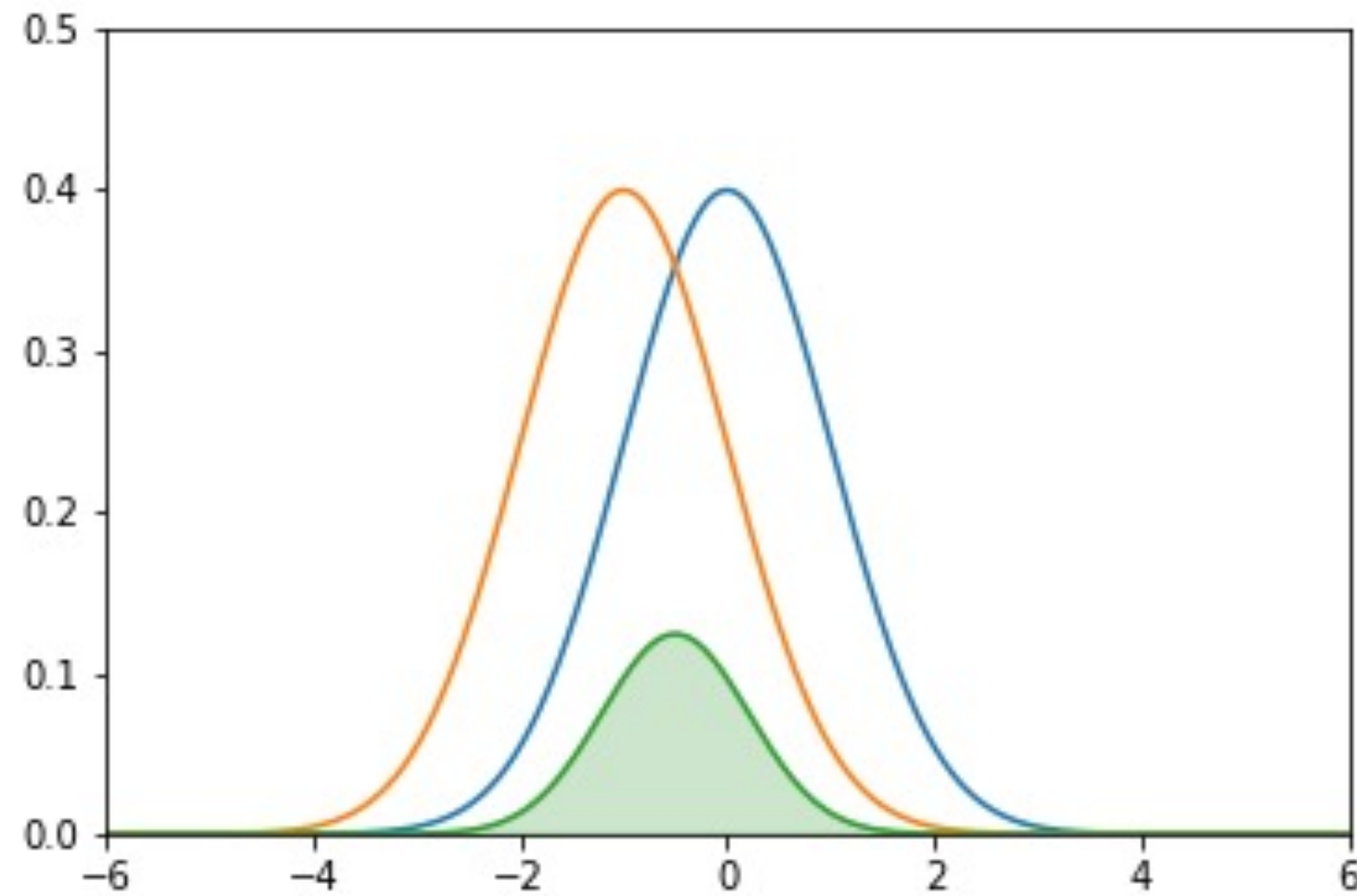
- ❖ Degeneracies ✓
- ❖ Non-linearity ✓
- ❖ Confidence variations ✓



Garraffo et al. 2021

StelNet: A Hierarchical Neural Network for Inference in Stellar Characterization

Comparing distributions



$$\int \bar{P}_A \bar{P}_B dx = \bar{\varepsilon} |_{\max A = \max B} \quad \text{Bayesian Evidence}$$

$$\int \bar{P}_A \bar{P}_B dx = \varepsilon < \bar{\varepsilon}$$

$$\tau = \frac{\bar{\varepsilon} |_{\max A = \max B}}{\varepsilon} \quad \text{Tension}$$

A large tension means that the null hypothesis ($\max A = \max B$) is unlikely

Jeffrey's scale:

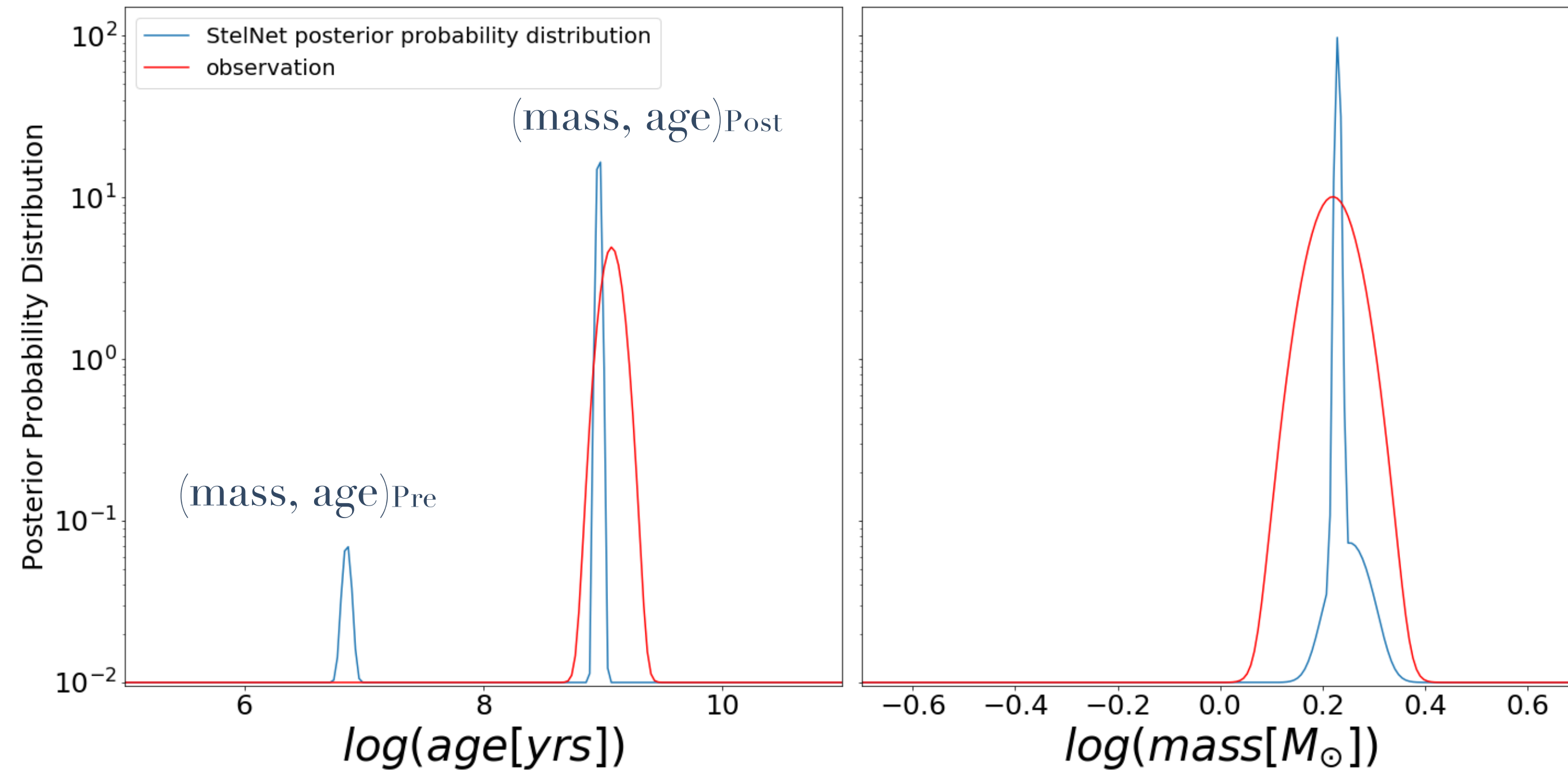
$\log \tau < 1$
not significant

$1 < \log \tau < 2.5$
substantial

$\log \tau > 5$
highly significant

StelNet: A Hierarchical Neural Network for Inference in Stellar Characterization

Quantifying performance



τ : Tension

Jeffrey's scale:

$$\log \tau < 1$$

not significant ✓

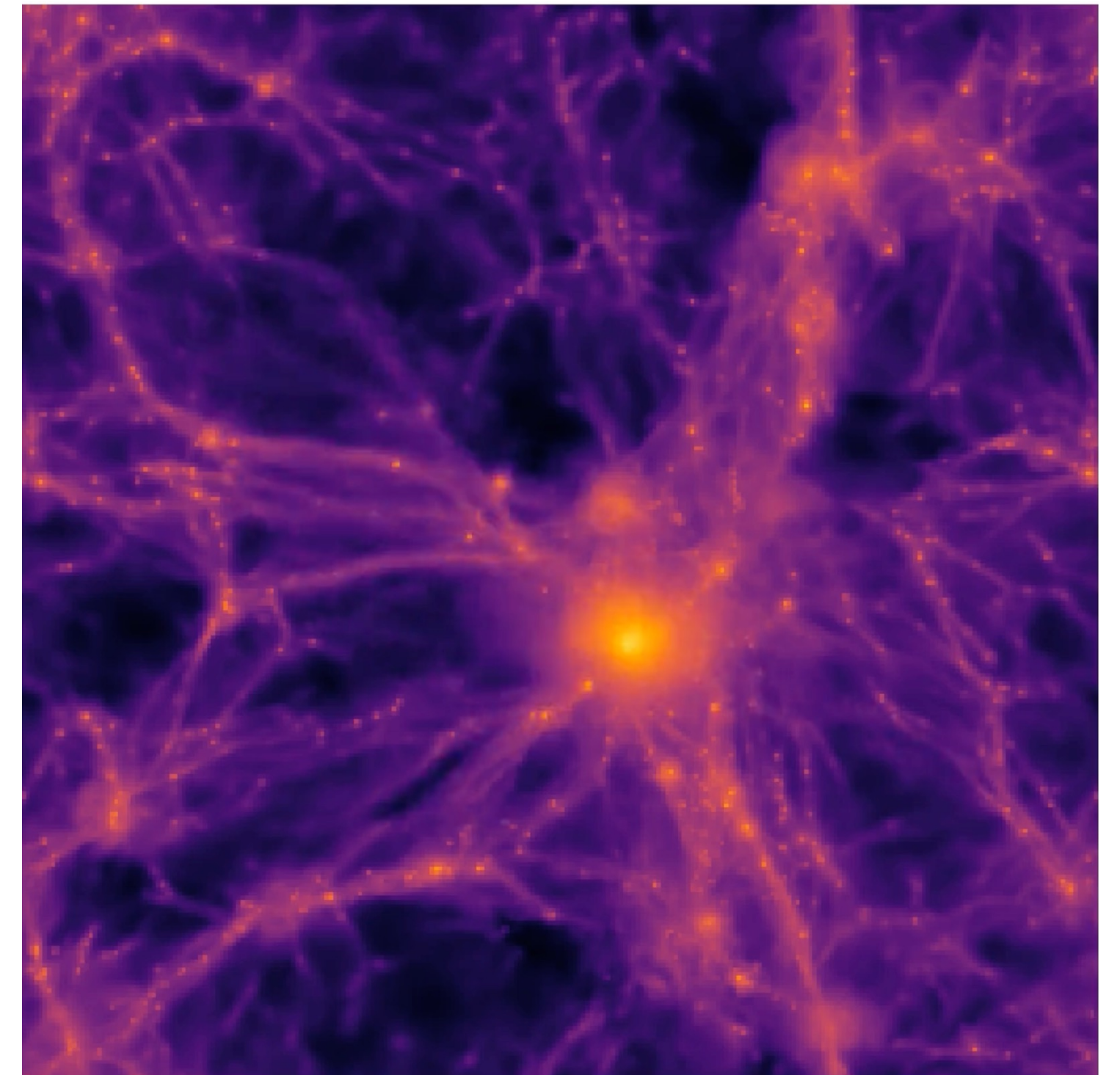
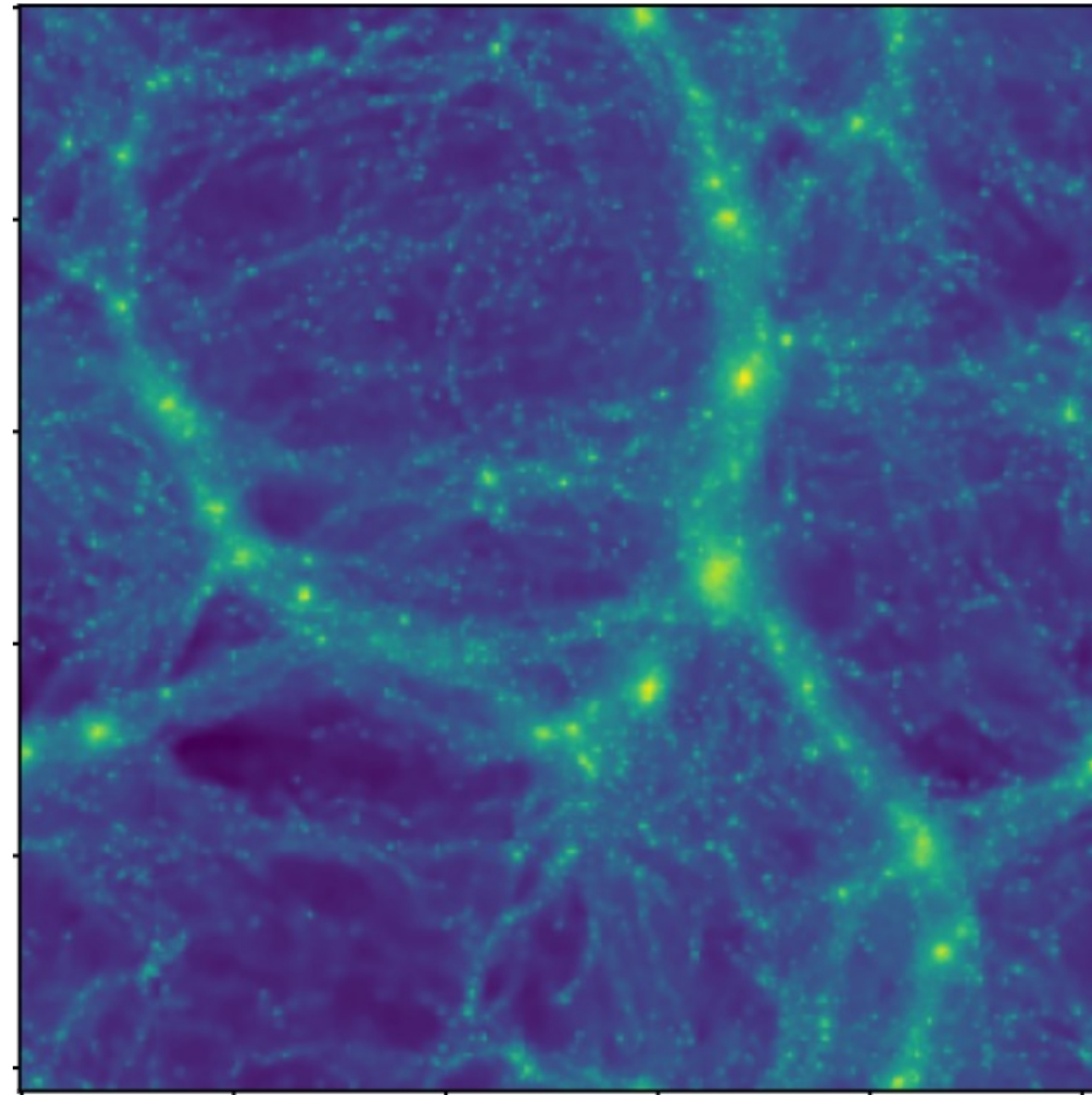
$$1 < \log \tau < 2.5$$

substantial

$$\log \tau > 5$$

highly significant

What does realistic mean?



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AI for Astronomy

Probabilistic

Physical

Interpretable

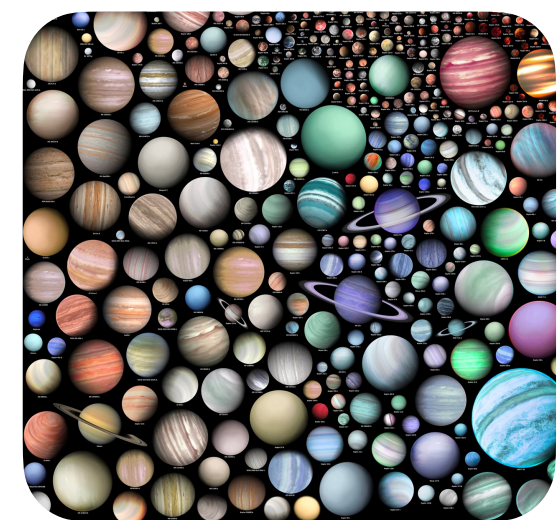
Robust

Multimodal

Multi-Scale

Generative

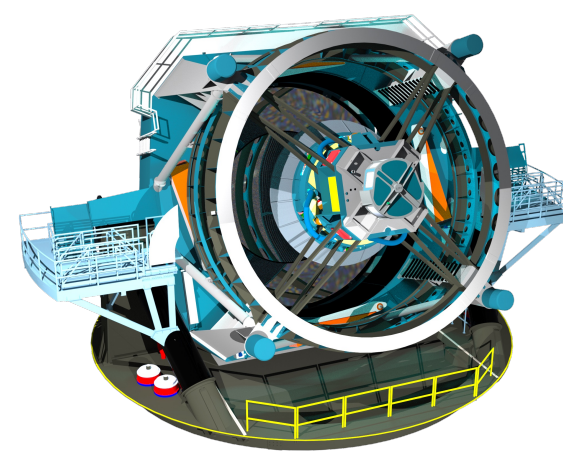
Open Source



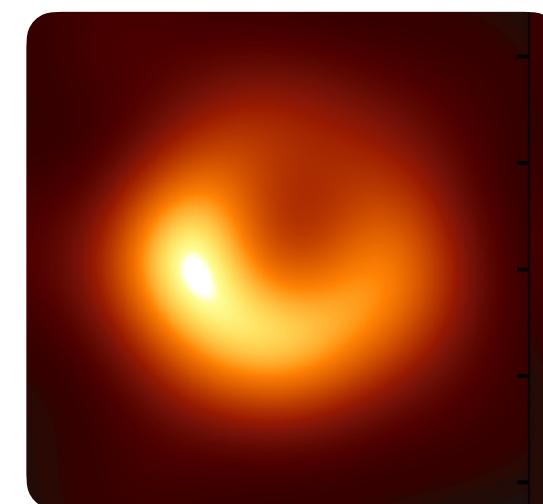
Biomarkers



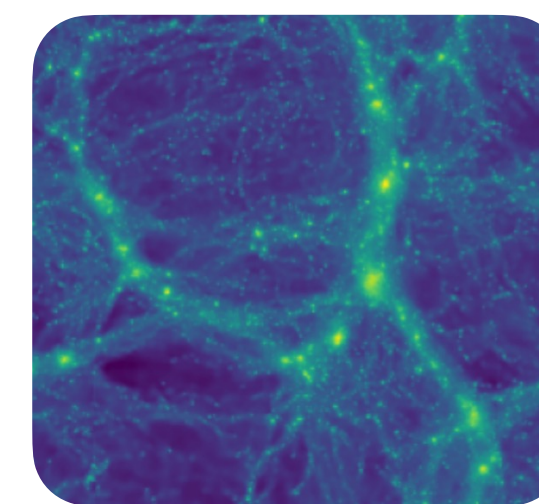
Stars



Dynamic Sky



Black Holes



Cosmology



LLMs for Astronomy



GravAI

ASTROAI

Enabling Next Generation Astrophysics

A bit of (modern!) History

November 2022

13 Members

4 Projects



Cecilia Garraffo



Rafael Martinez



Varshini Reddy



Thaddaeus Kiker



Farah Fauth



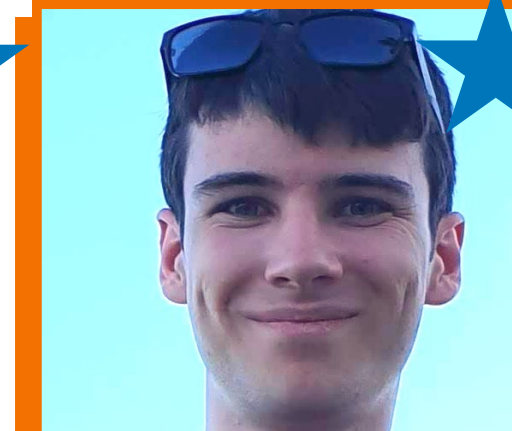
James Steiner



Floor Broekgaarden



Justina Yang



Ethan Tregigda



Leticia Schettino



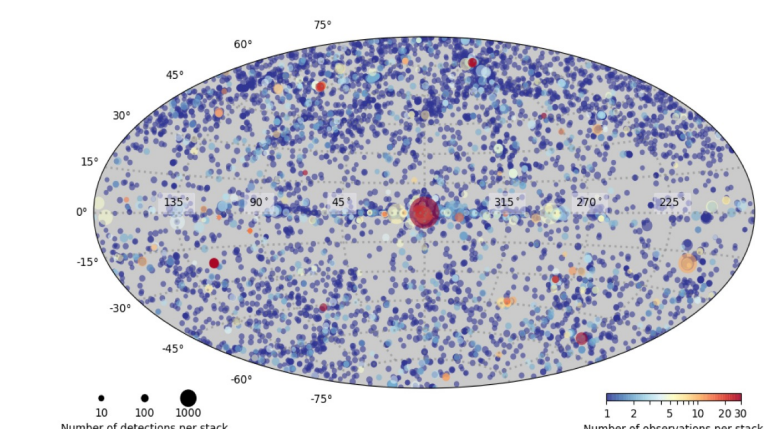
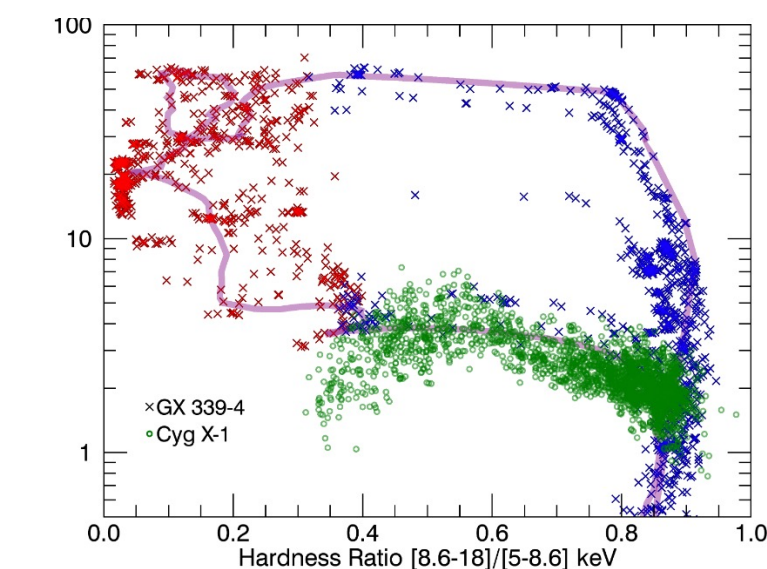
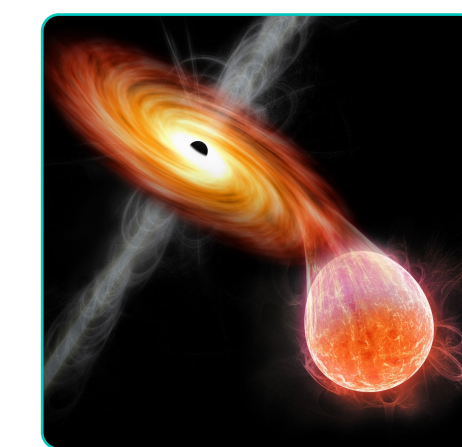
Augusto Chantad



Arya Mohan



Ben Ricketts



Source: CSC Website

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January

5 Partners

19 Members

10 Projects



Nov Jan

ASTROAI

Enabling Next Generation Astrophysics

January

April

5 Partners

18 Partners

19 Members

36 Members

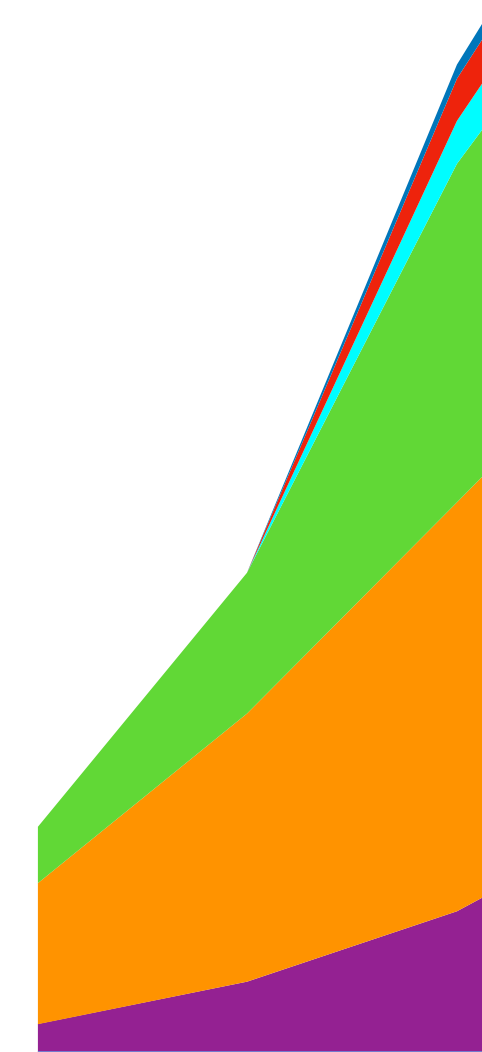
10 Projects

29 Projects

5 Invited talks

3 Papers

1 Internship Program

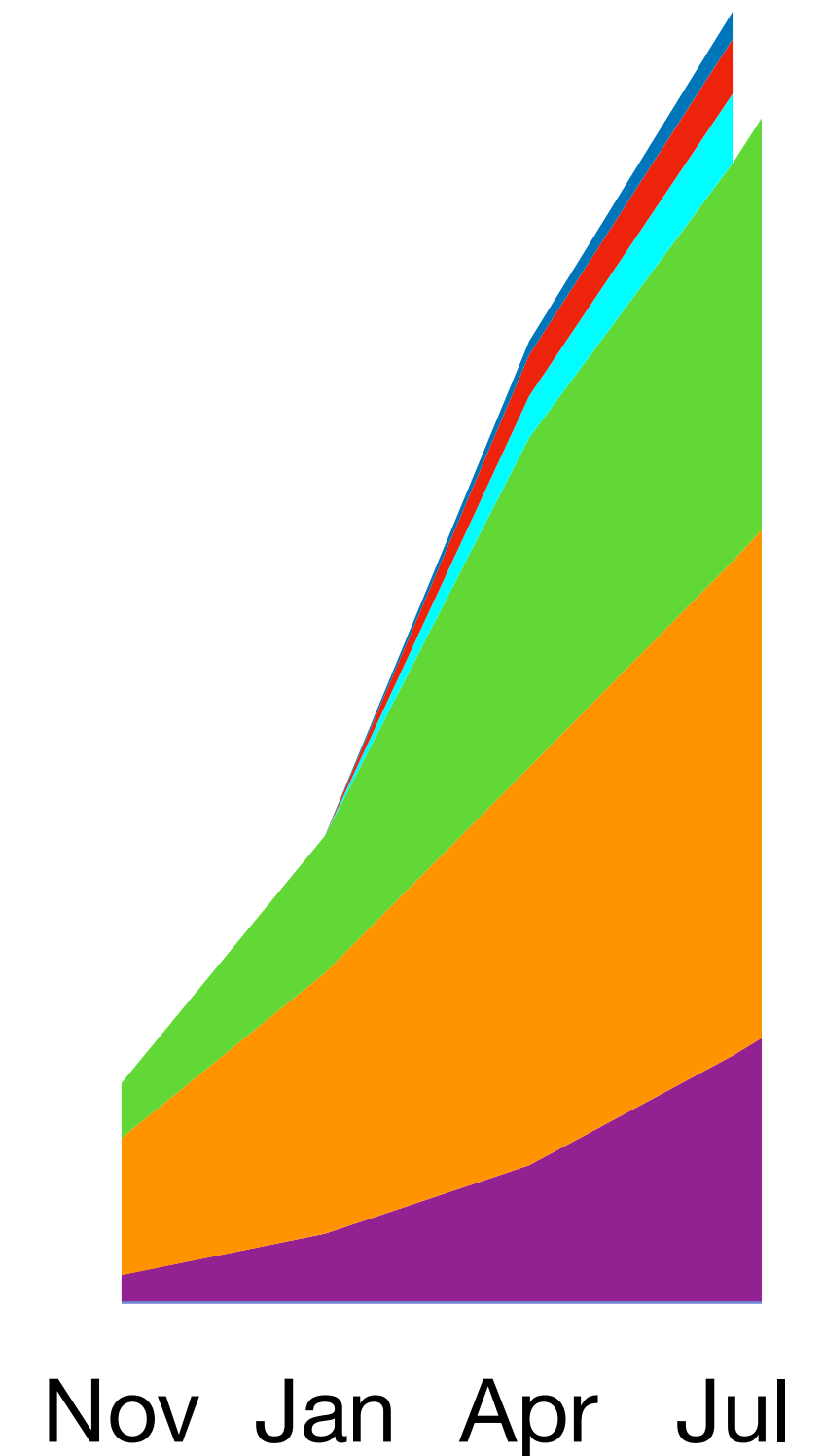


Nov Jan Apr

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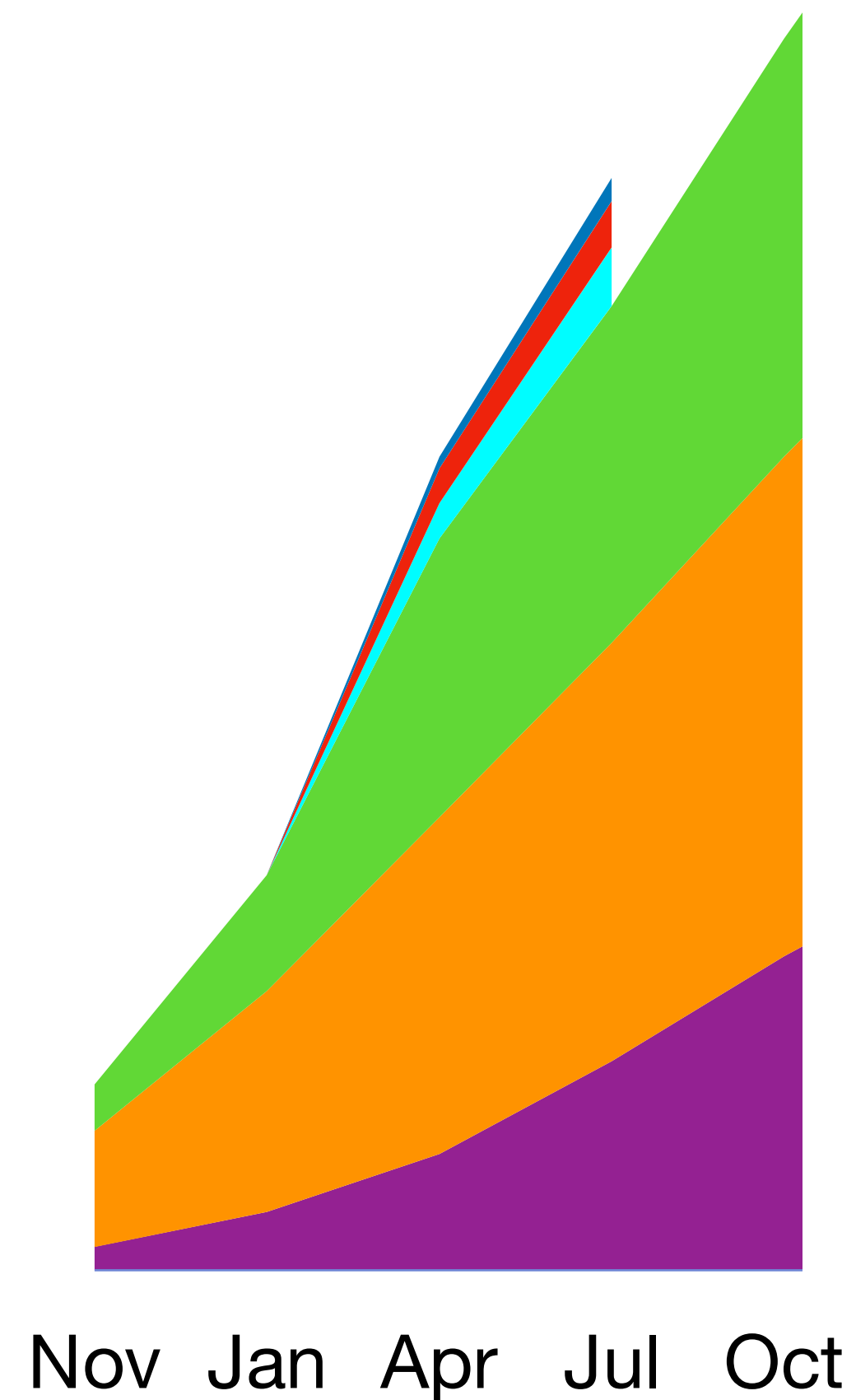
January	April	July
5 Partners	18 Partners	27 Partners
19 Members	36 Members	43 Members
10 Projects	29 Projects	31 Projects
	5 Invited talks	7 Invited talks
	3 Papers	6 Papers
	1 Internship Program	1 Internship Programs
		2 Small funds
		1 Position



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Enabling Next Generation Astrophysics

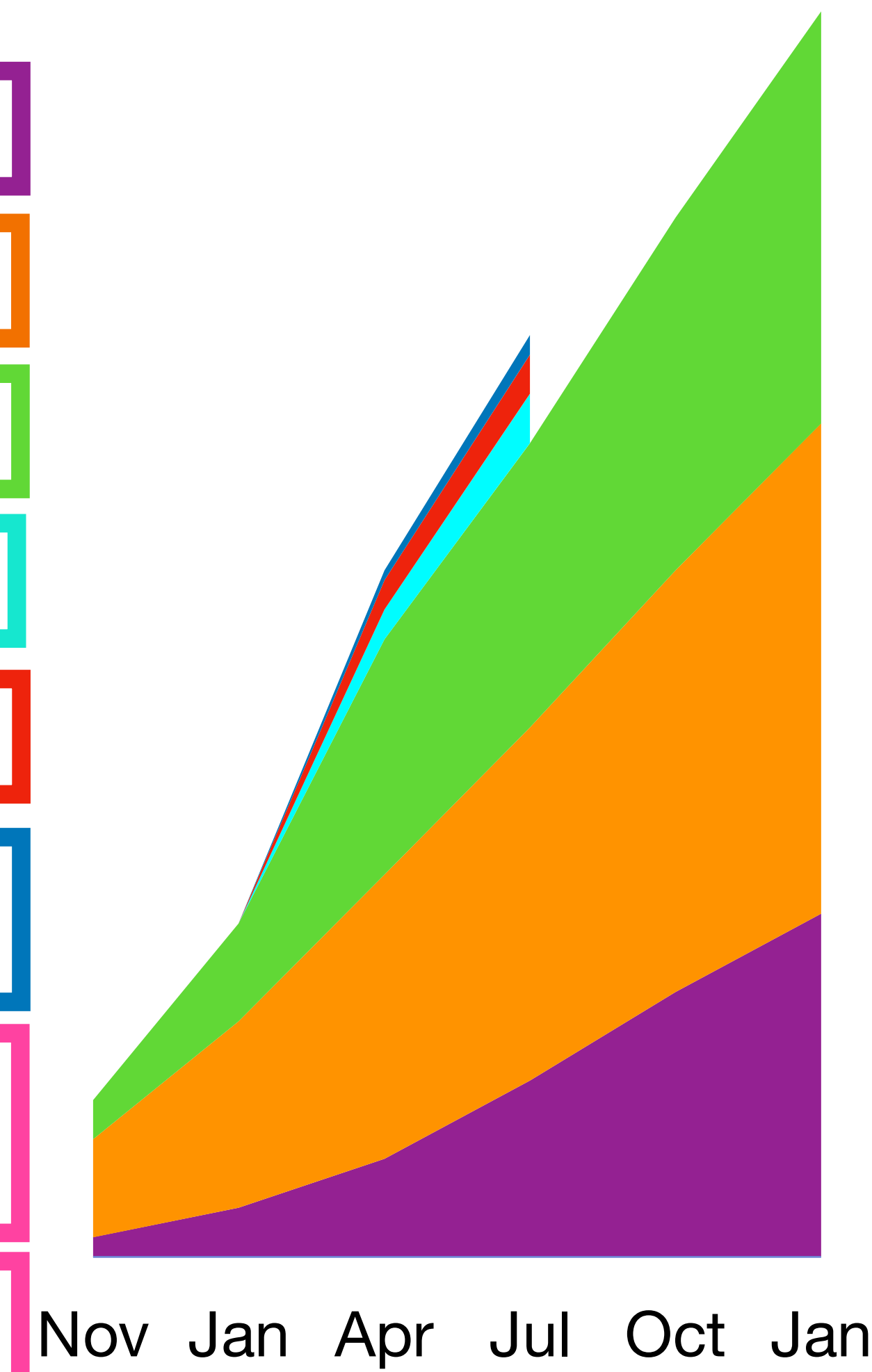
January	April	July	October
5 Partners	18 Partners	27 Partners	32 Partners
19 Members	36 Members	43 Members	45 Members
10 Projects	29 Projects	31 Projects	37 Projects
	5 Invited talks	7 Invited talks	18 Invited talks
	3 Papers	6 Papers	10 Papers
	1 Internship Program	1 Internship Programs	2 Internship Programs
		2 Small funds	5 Small funds and B&P fund
		1 Position	1 Position



ASTROAI

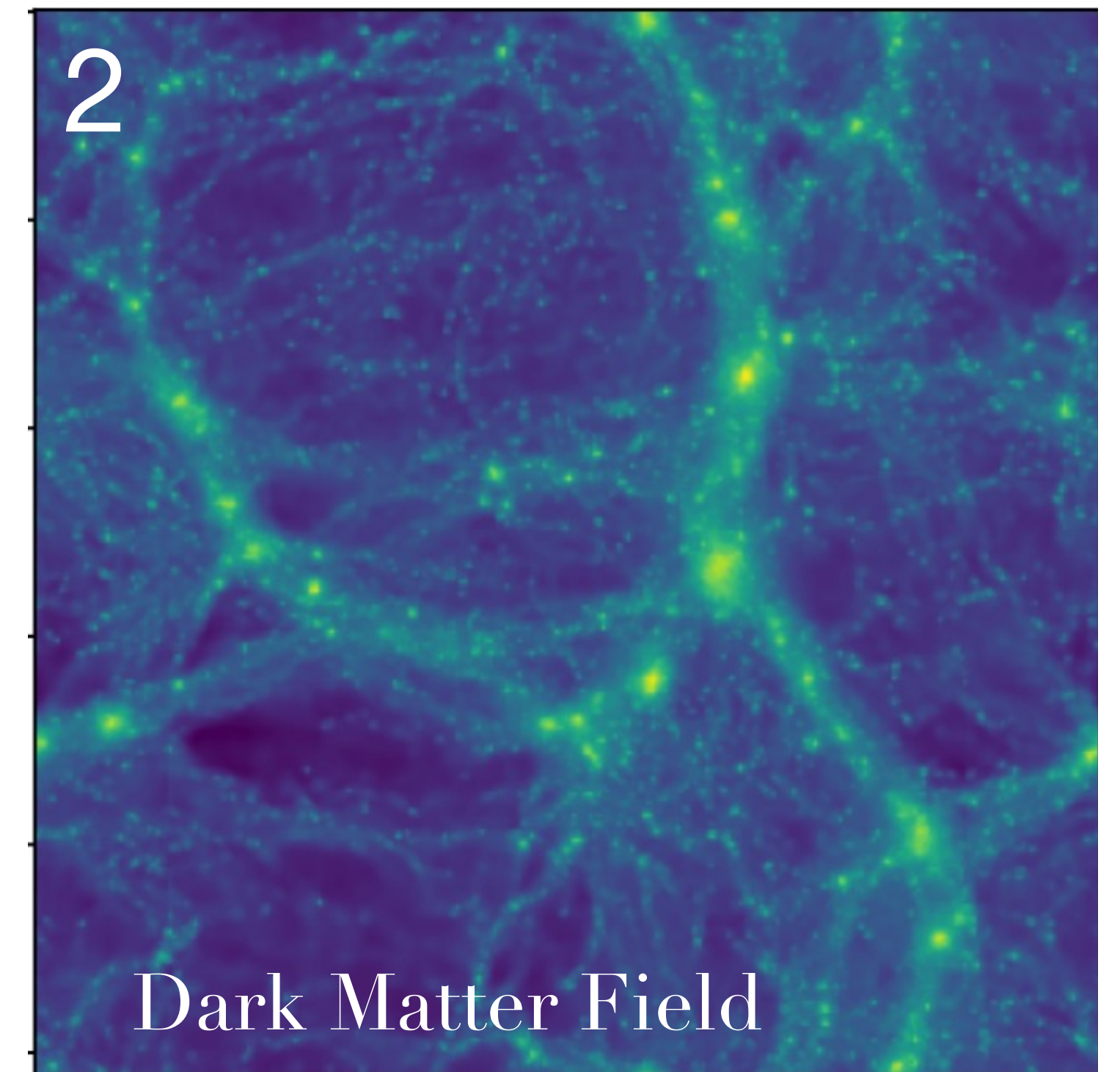
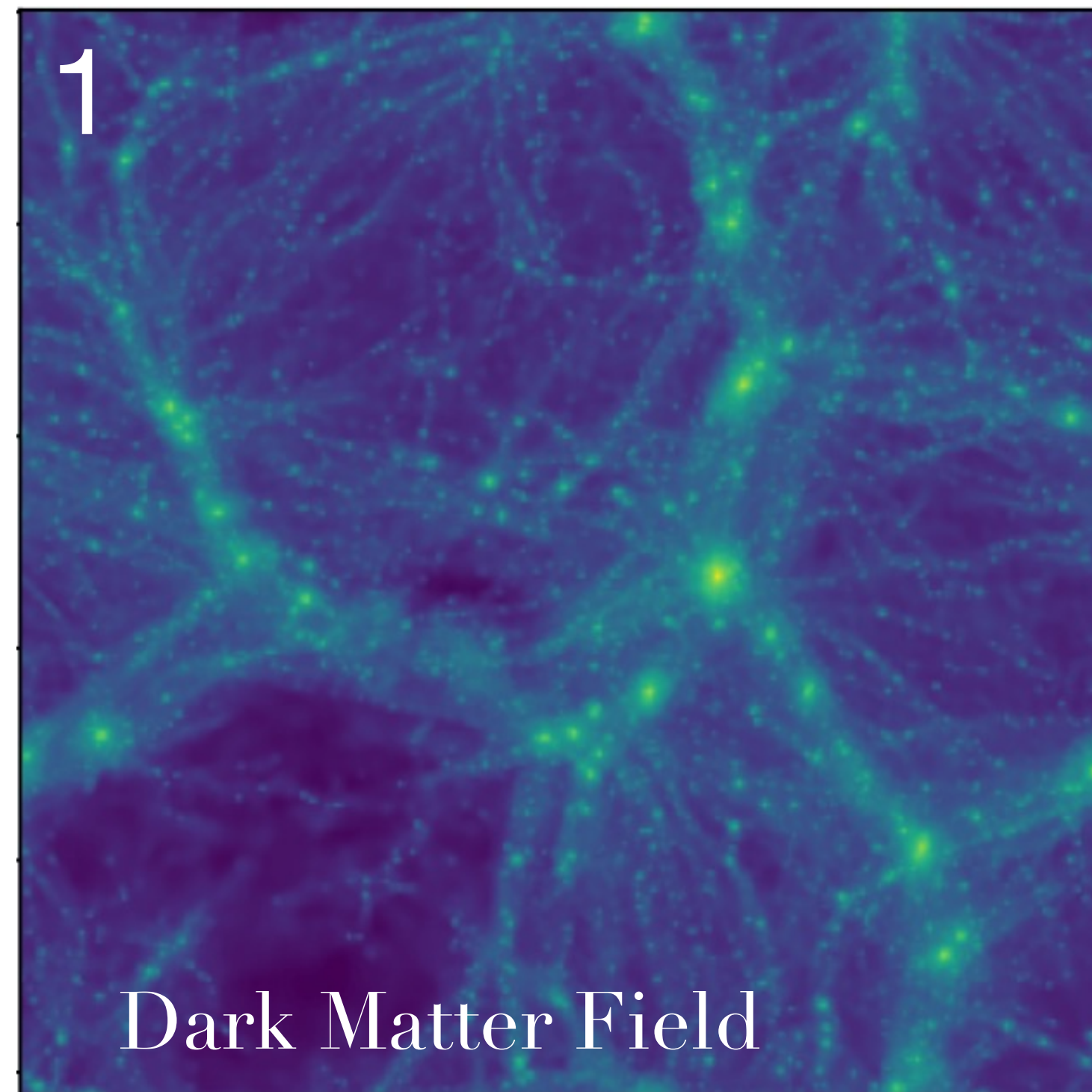
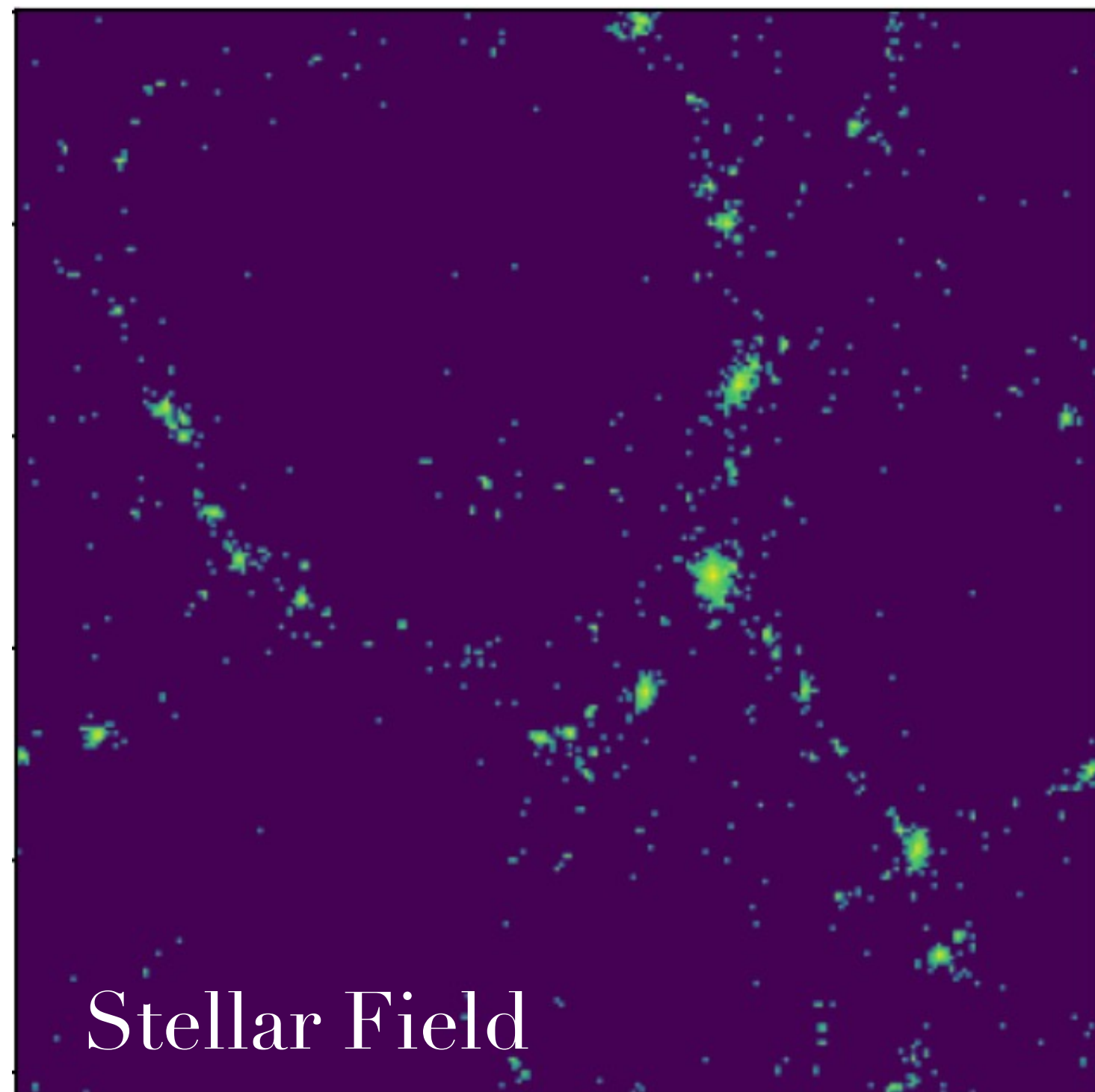
Enabling Next Generation Astrophysics

January	April	July	October	January
5 Partners	18 Partners	27 Partners	32 Partners	>35 Partners
19 Members	36 Members	43 Members	45 Members	>50 Members
10 Projects	29 Projects	31 Projects	37 Projects	37 Projects
	5 Invited talks	7 Invited talks	18 Invited talks	>20 Invited talks
	3 Papers	6 Papers	10 Papers	14 Paper
	1 Internship Program	1 Internship Programs	2 Internship Programs	2 Internship program
		2 Small funds	5 Small funds and B&P fund	5 Small funds and B&P fund
		1 Position	1 Position	1 Position



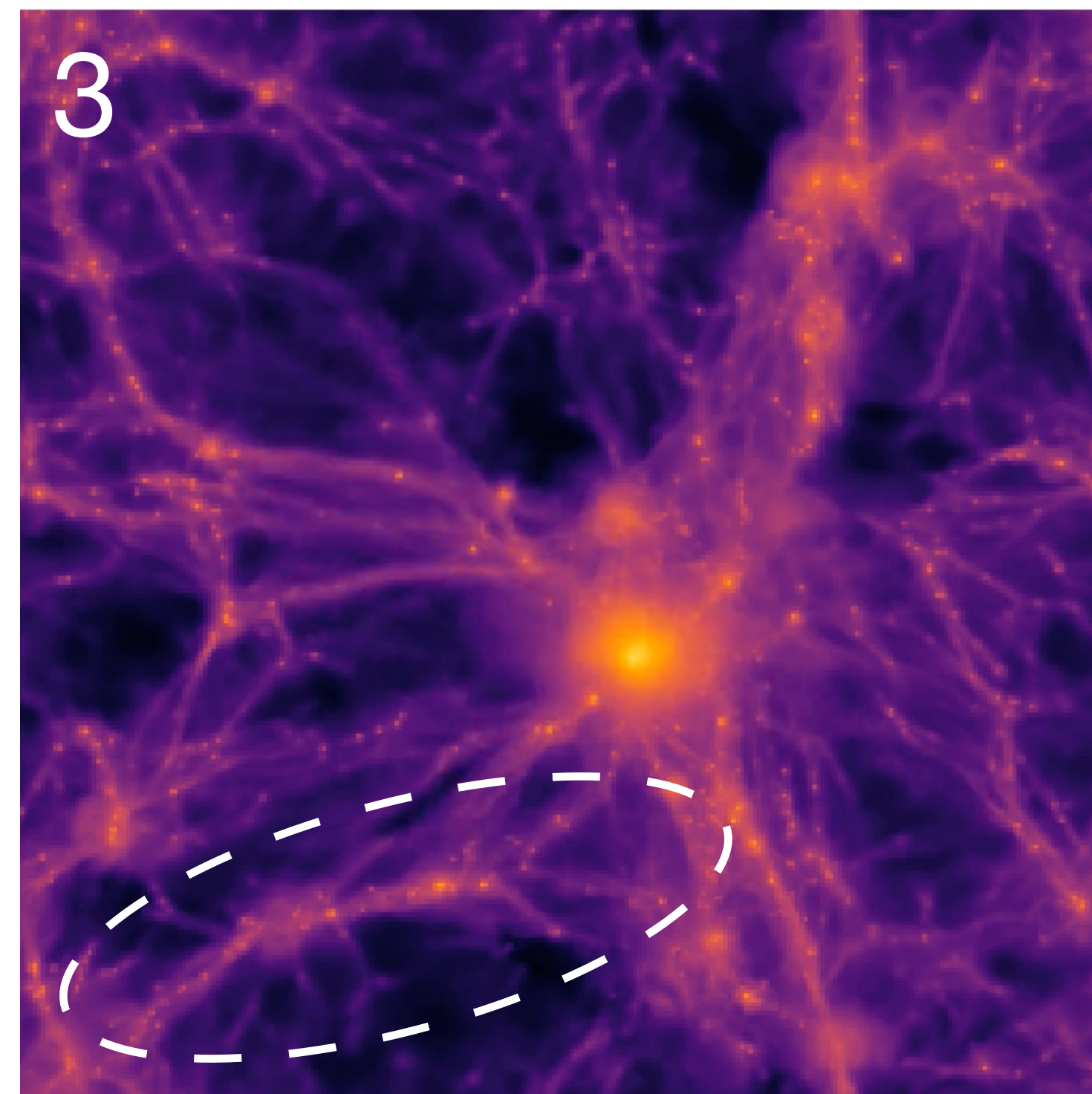
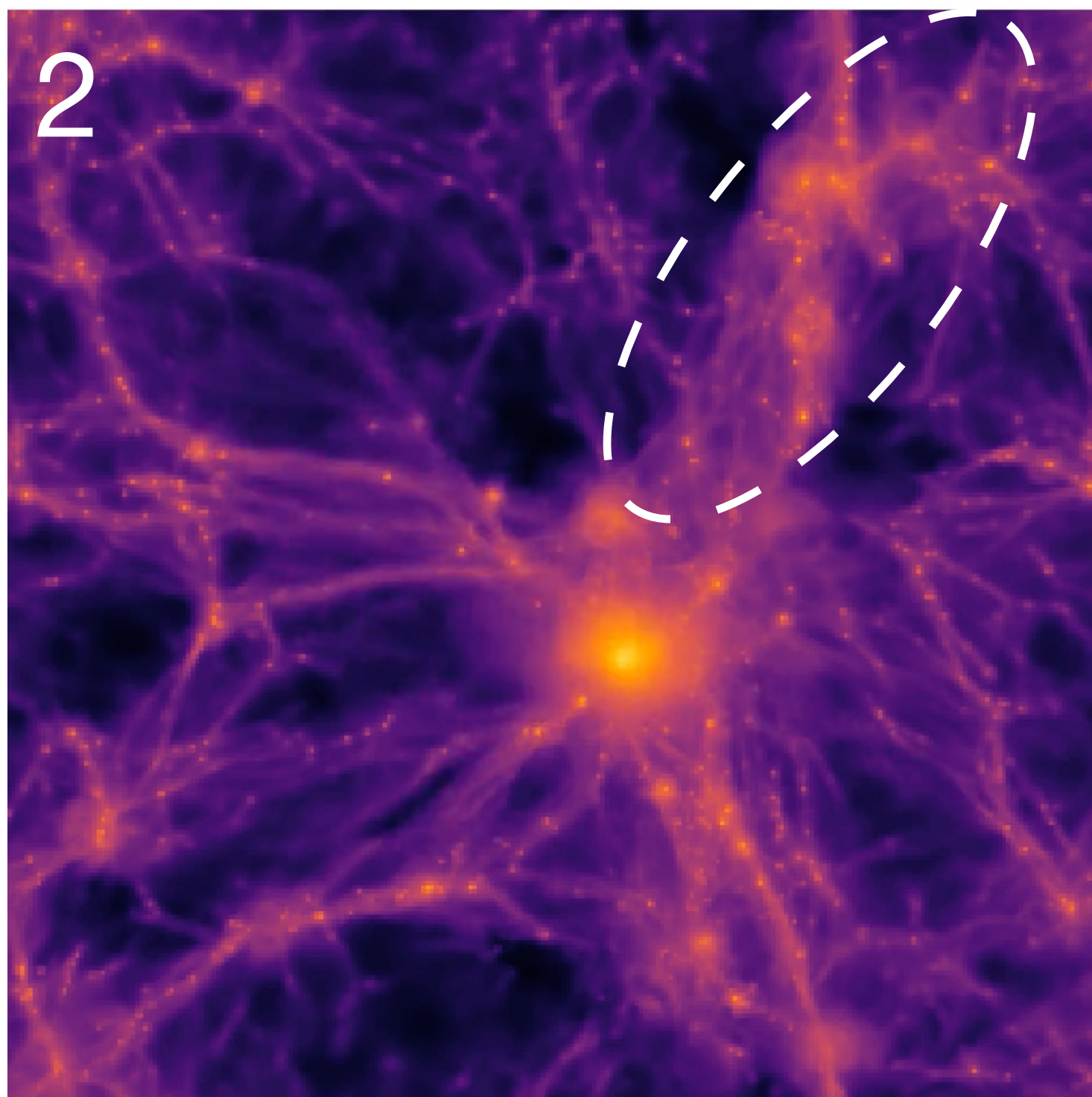
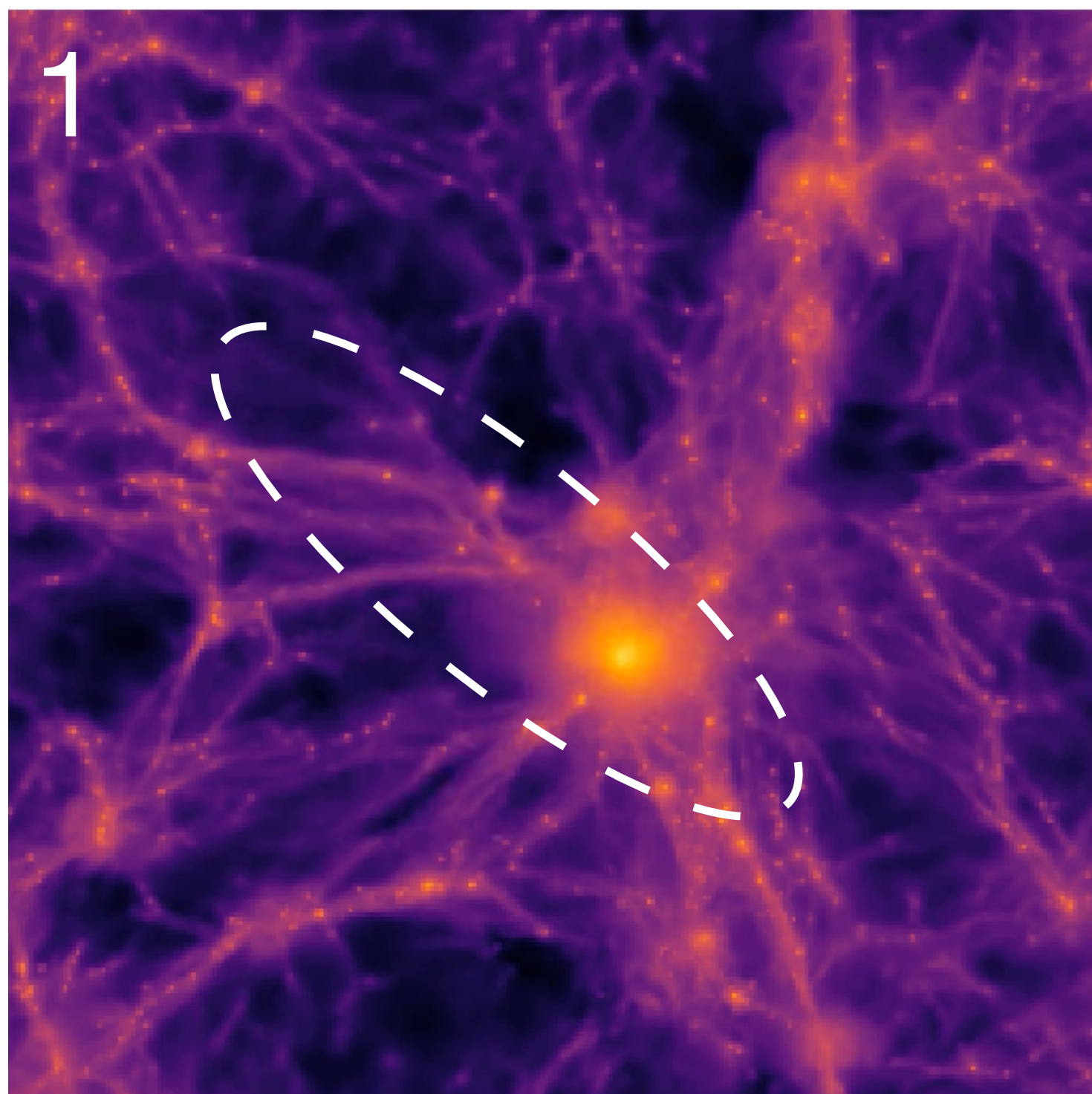
ASTROAI

Dark Matter Field Simulations

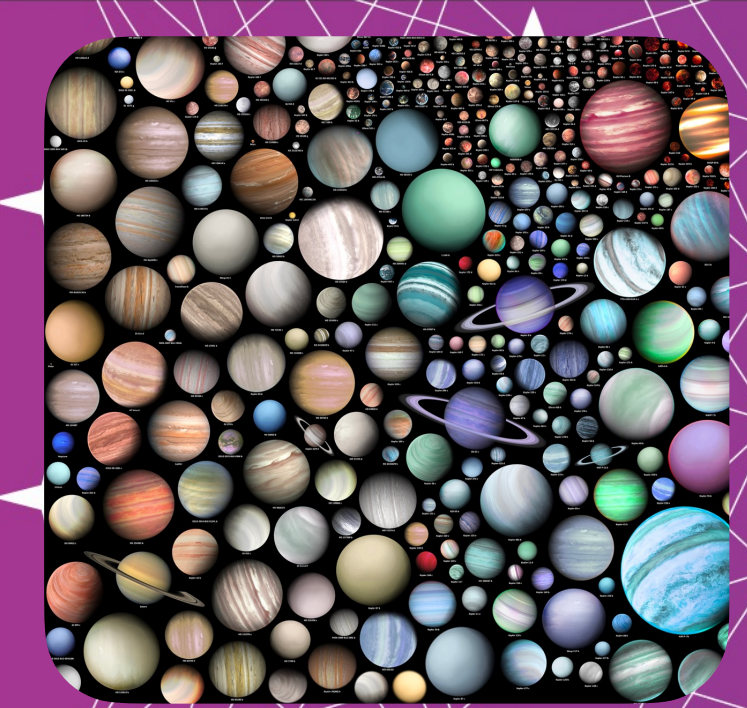


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Galaxy Filament AI-Infill



2. *AI for Instrument Design*



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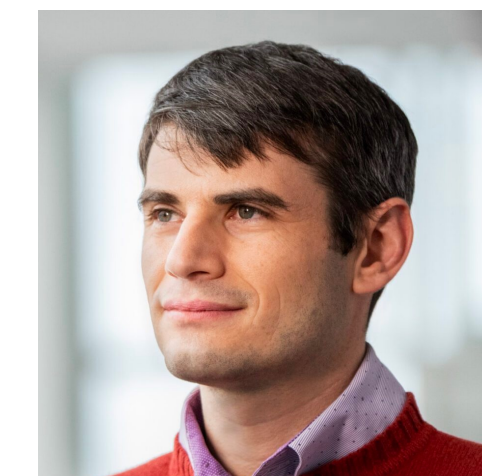
Cecilia Garraffo
Director of AstroAI



Mercedes Lopez-Morales
Exoplanet Atmospheres
World Expert



Bill Freeman, CS
Head of Computer
Vision Institute
MIT
Microsoft

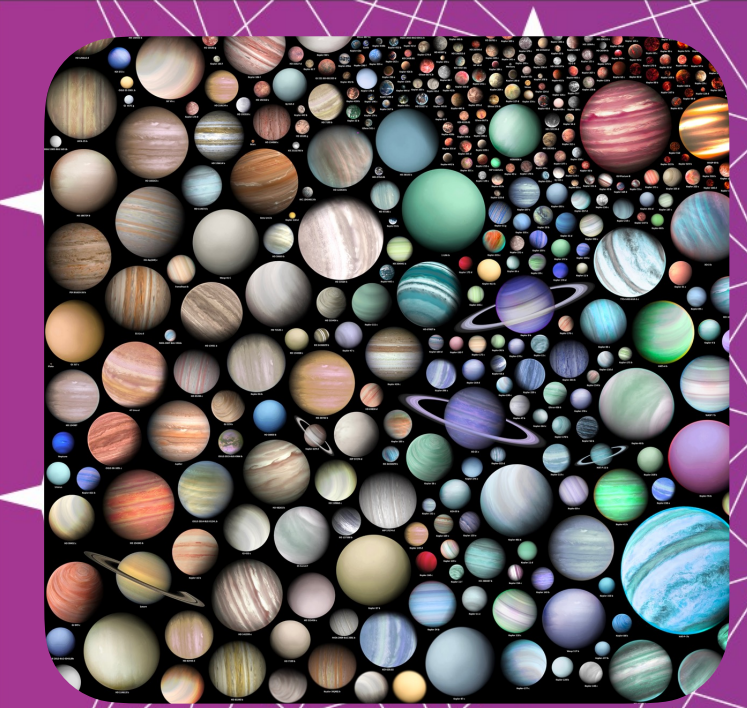


Robin Walters,
Applied Math
Expert on
Equivariant Neural
Networks



Iouli Gordon
Physicist /
Spectroscopist
HEAD of HITRAN

Extend the search with Computer Vision!



ASTROAI

Enabling Next Generation Astrophysics



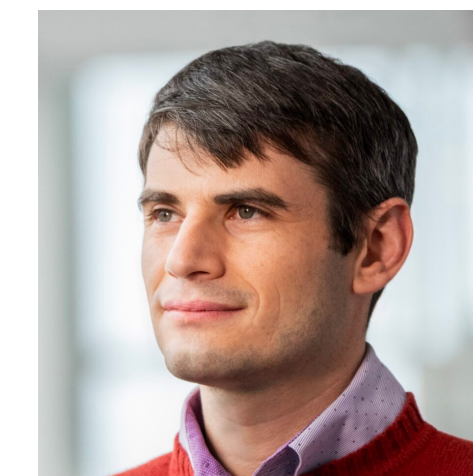
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Vision Institute
MIT
Microsoft



Robin Walters,
Applied Math
Expert on
Equivariant Neural
Networks



Iouli Gordon
Physicist /
Spectroscopist
HEAD of HITRAN

Computer Vision to inform HWO's instrument design

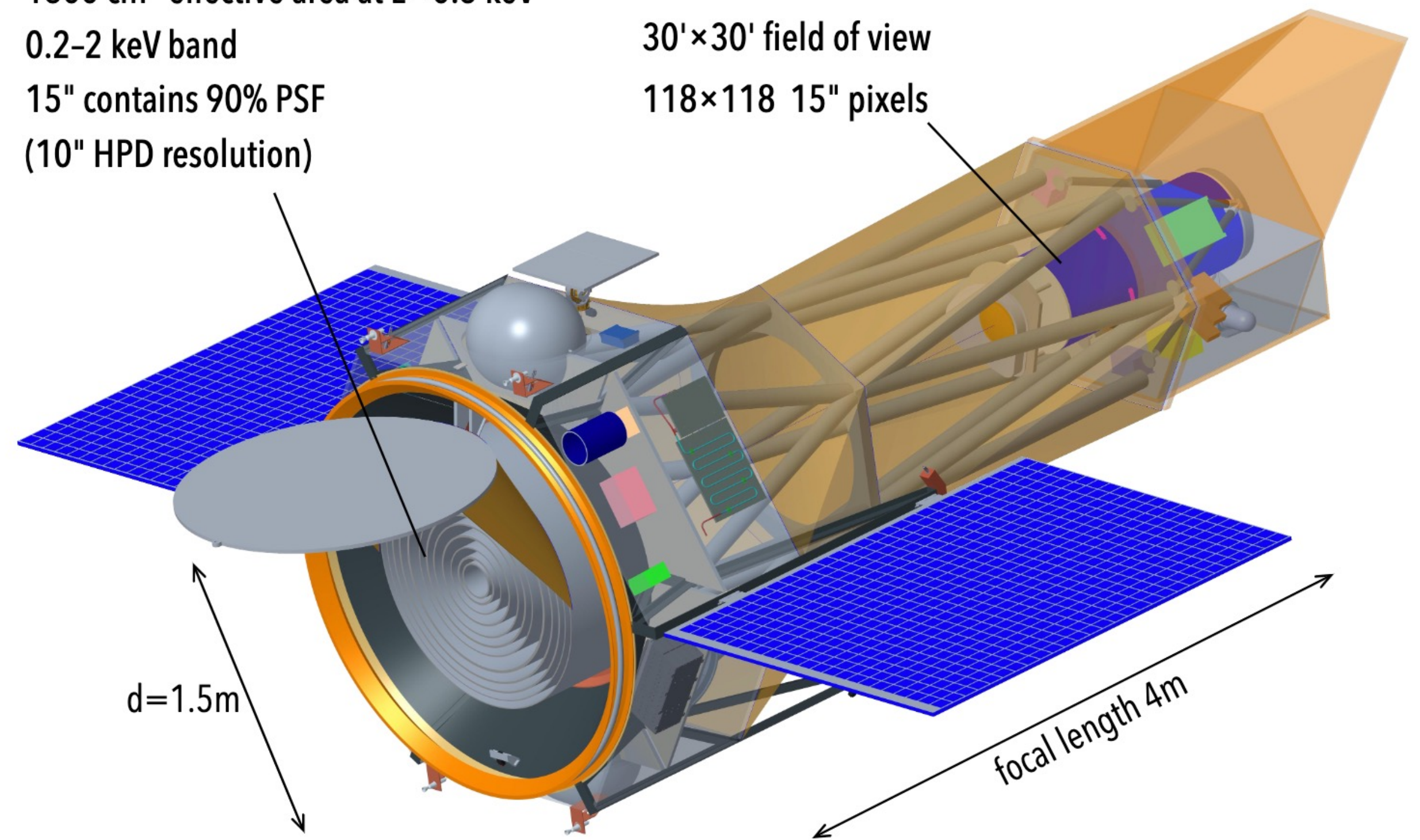
ASTROAI

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Grazing-incidence X-ray mirror:
1600 cm² effective area at E=0.5 keV
0.2–2 keV band
15" contains 90% PSF
(10" HPD resolution)

Imaging spectrometer (IFU):
TES microcalorimeter array, cryocooled
2 eV resolution (central area 1 eV)
30'×30' field of view
118×118 15" pixels



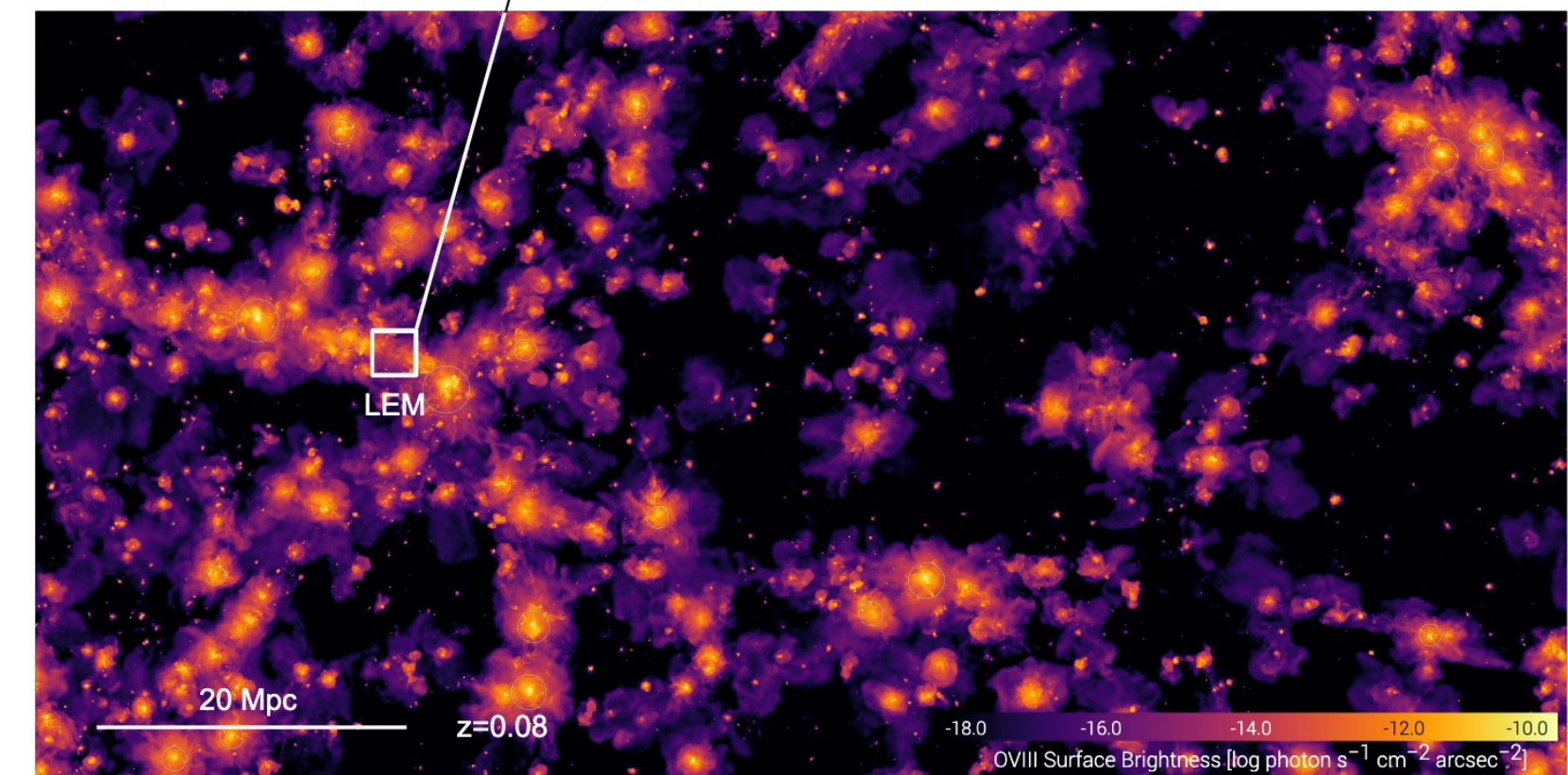
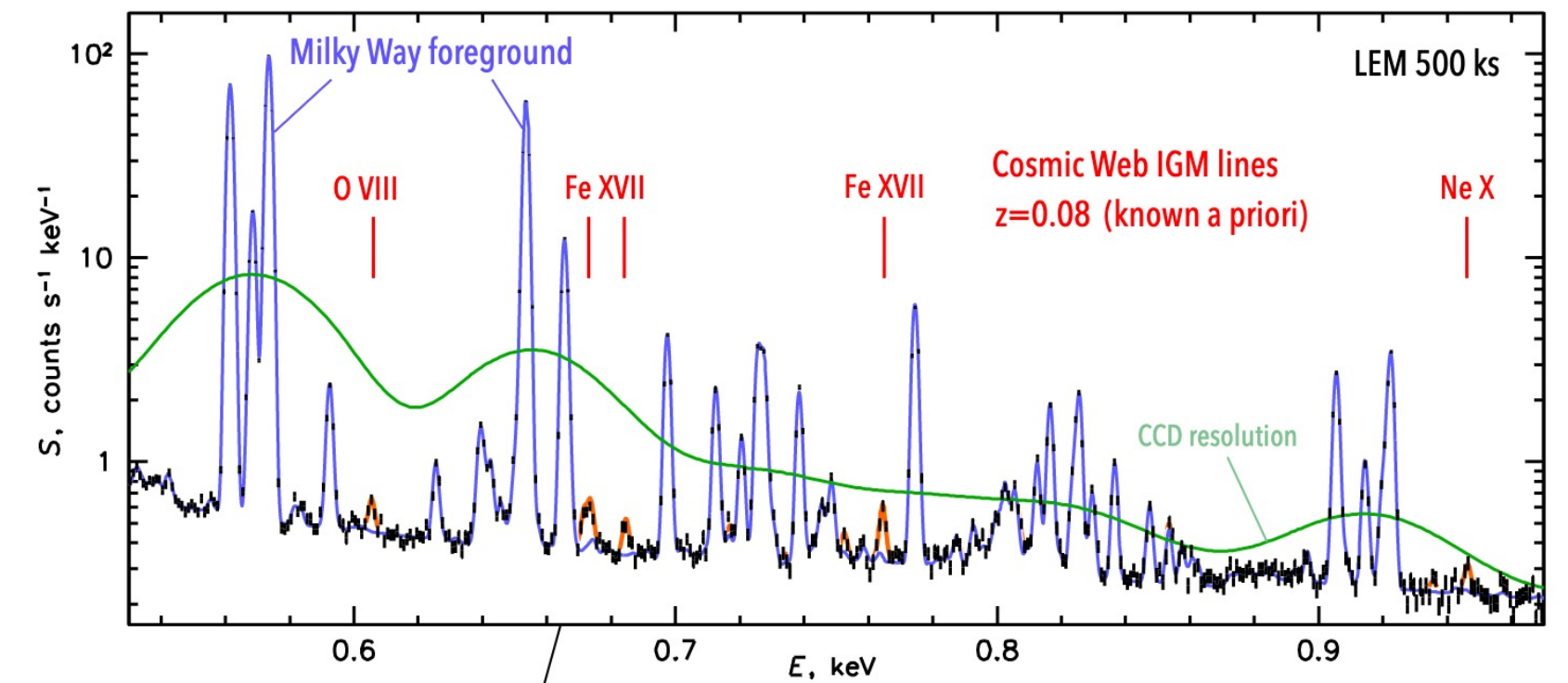
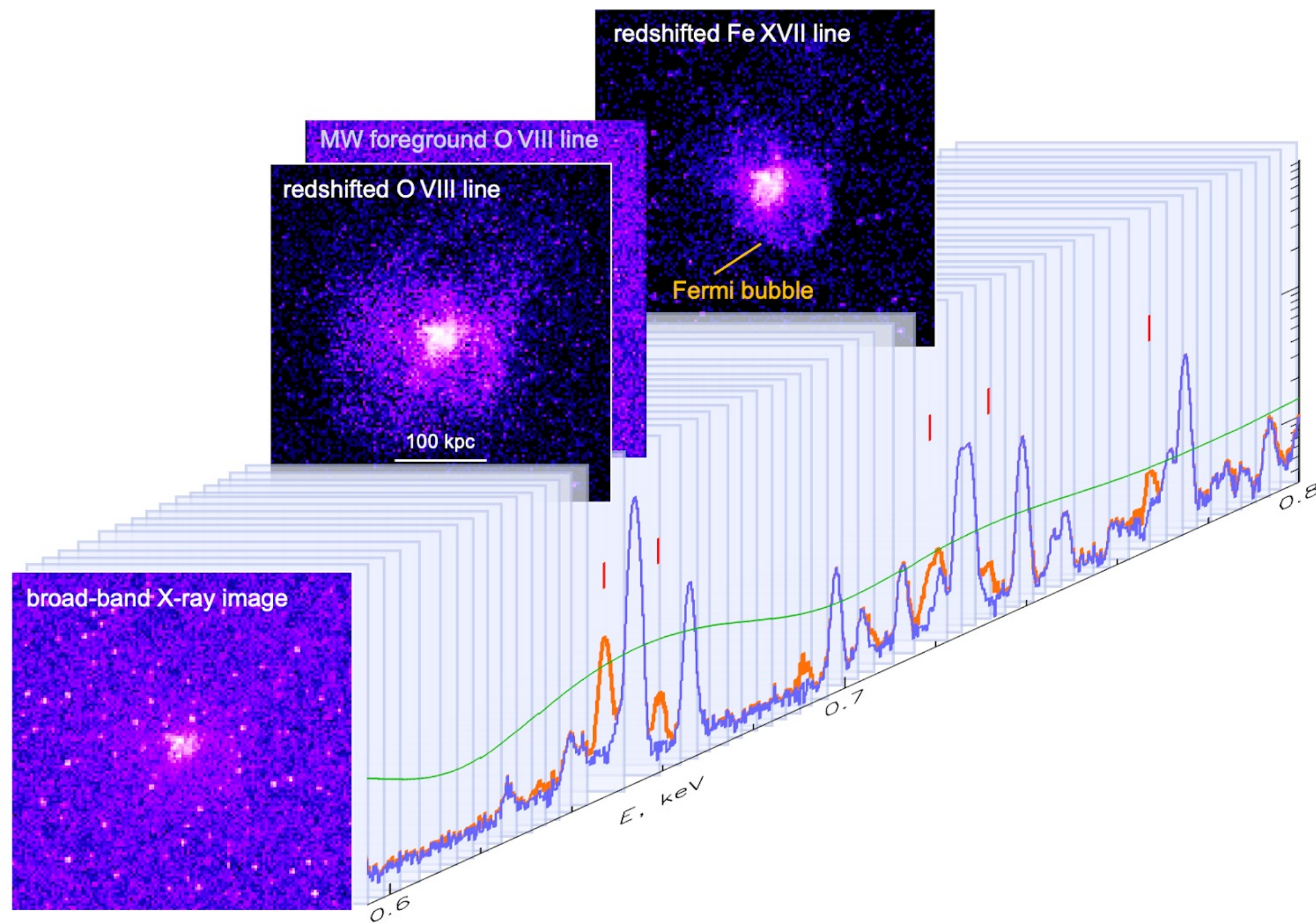
ASTROAI

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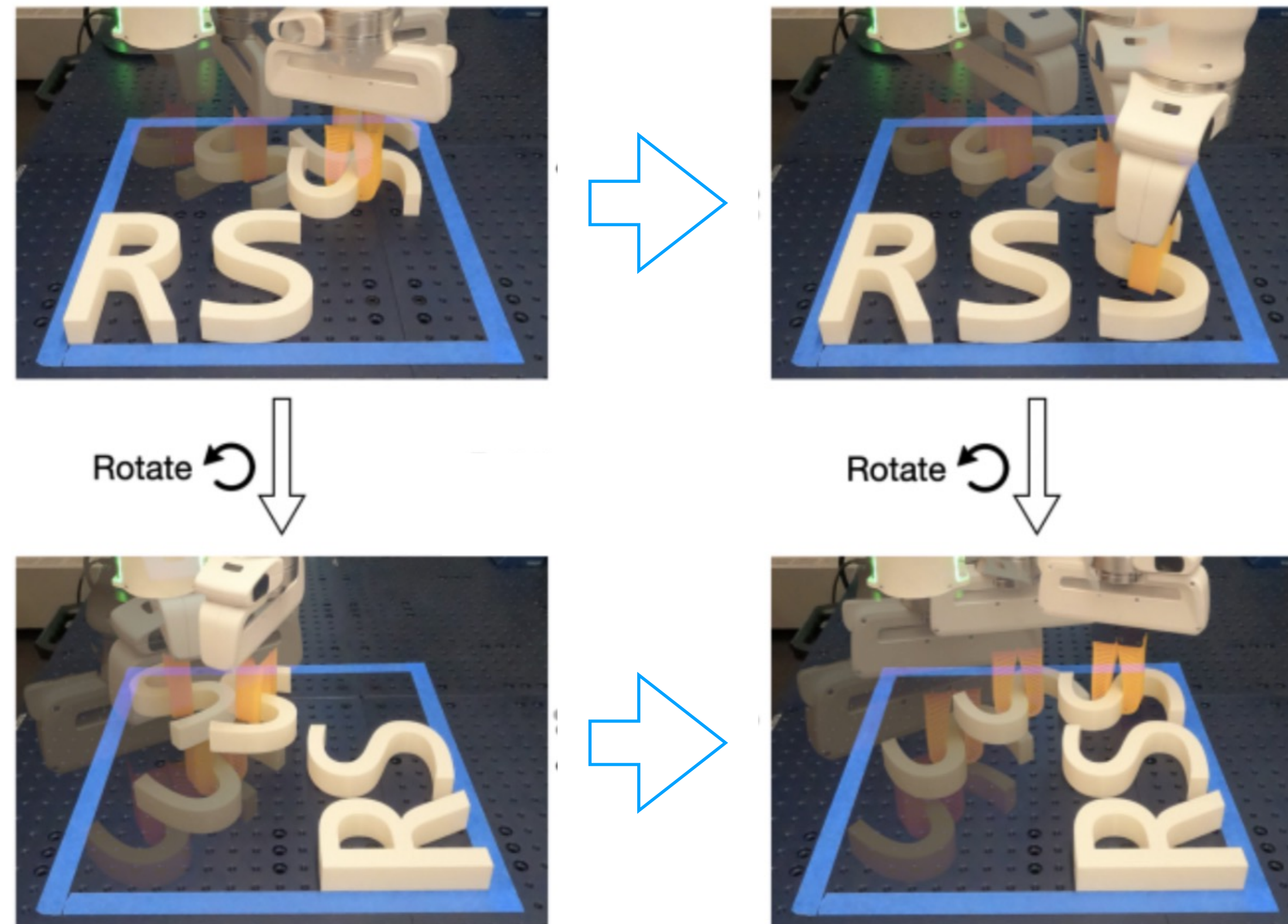


Josh Wing

Automatic Detection of Sources from LEM



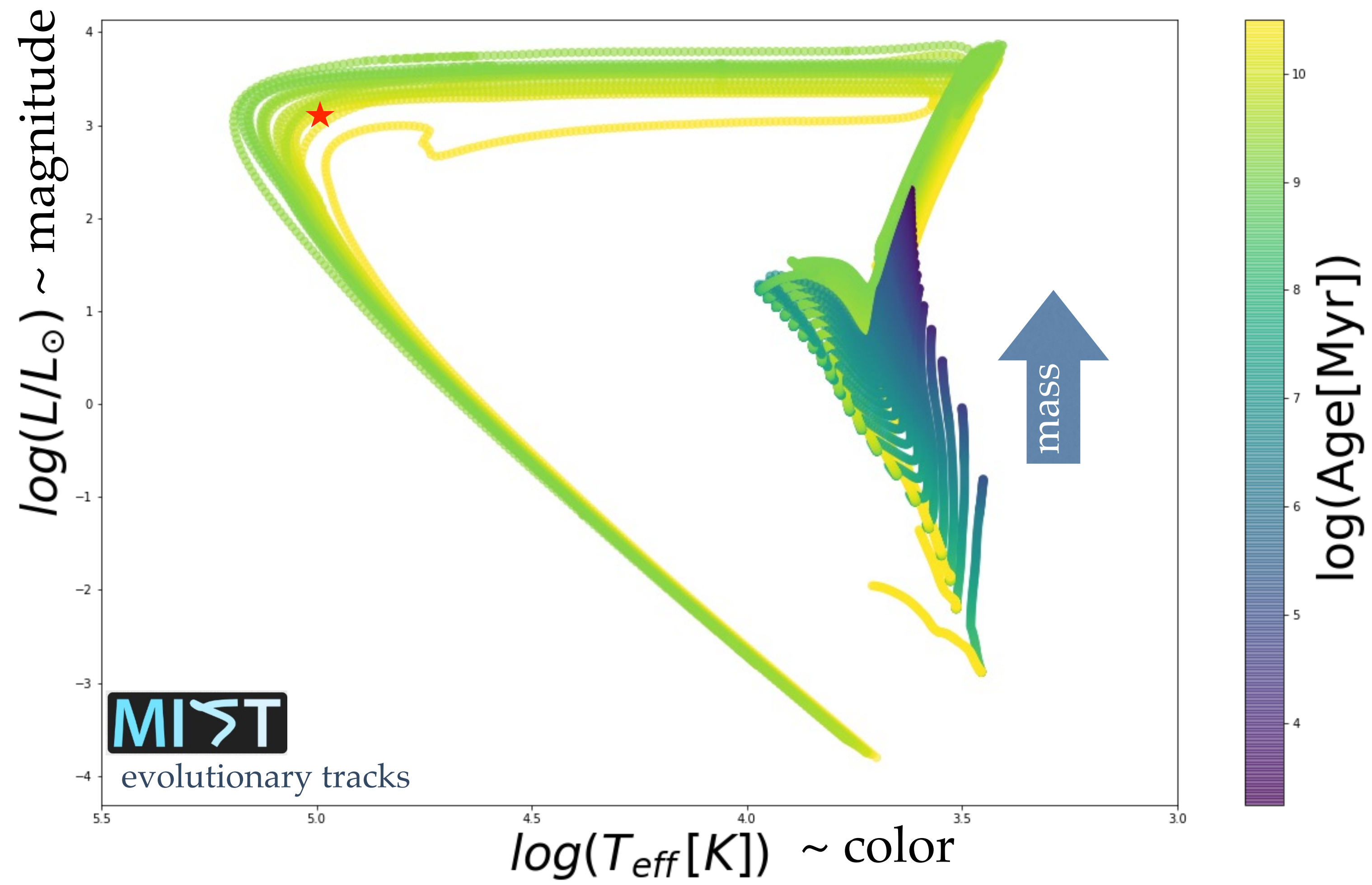
Equivariant Neural Networks



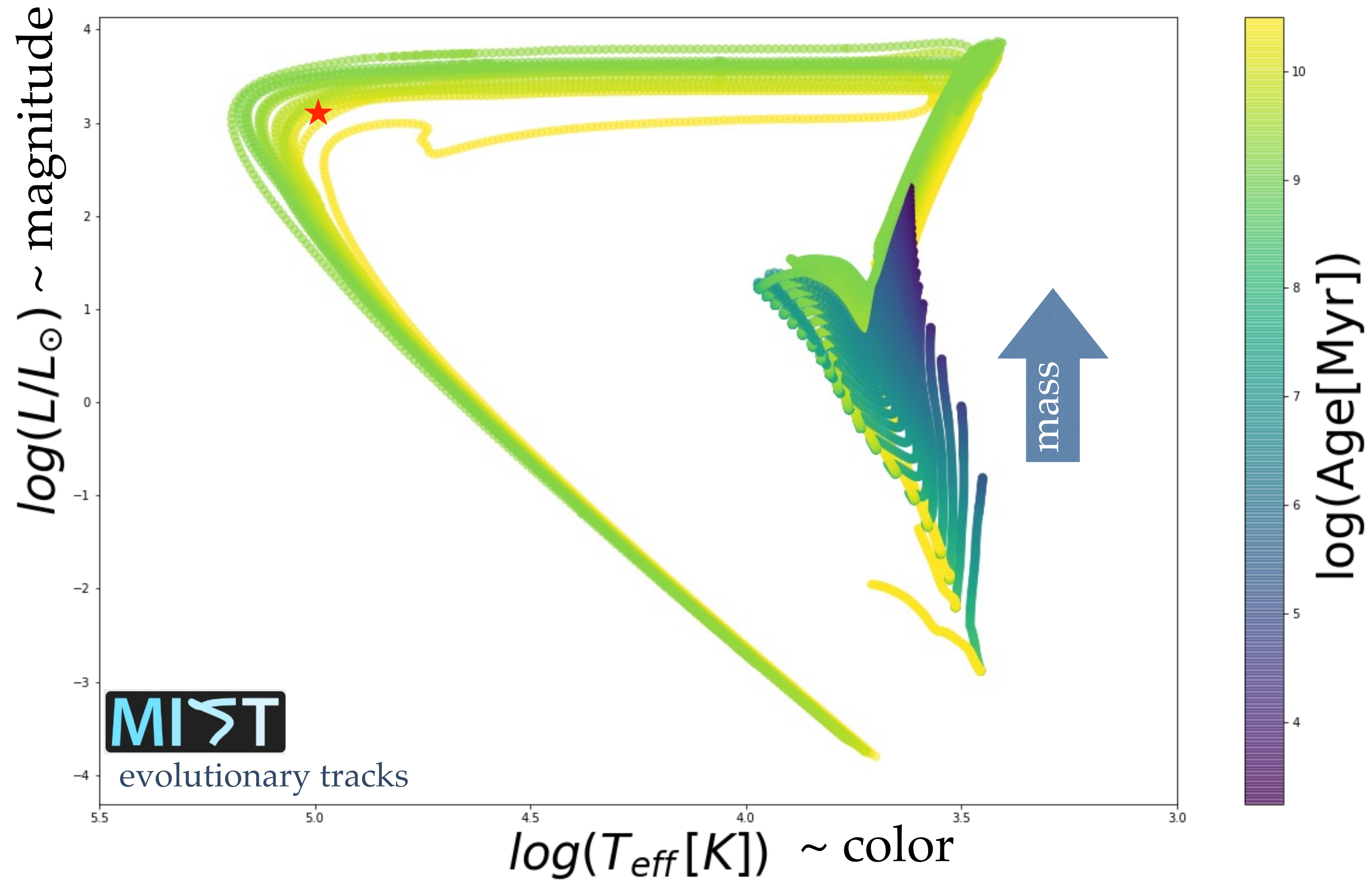
D. Wang, S. Hart, D. Surovik, T. Kelestemur, H. Wang, H. Zhao, J. Wang, R. Walters, R Platt submitted to NeurIPS

*Cecilia Garraffo - CfA
AAS*

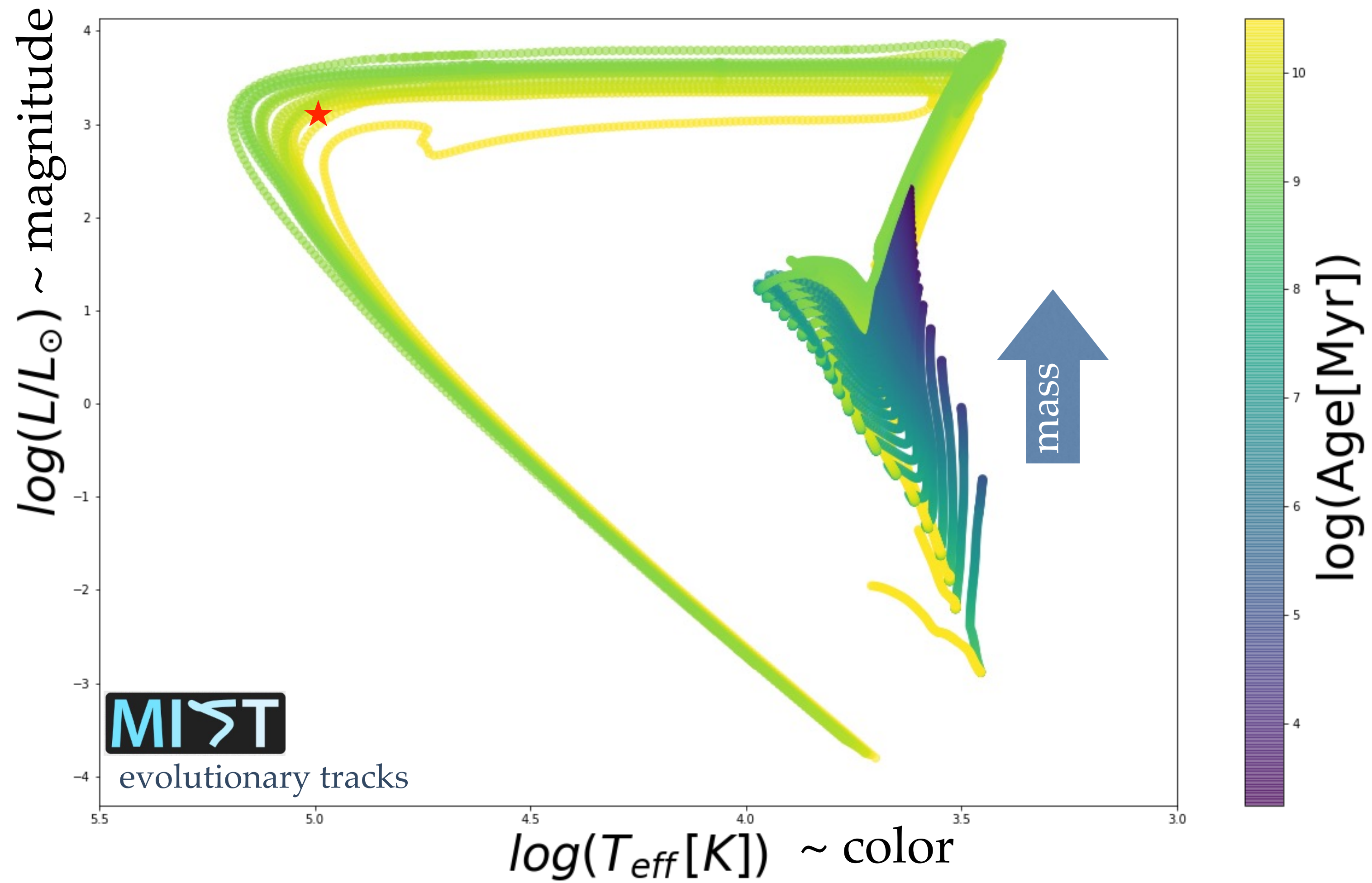
June 11th,



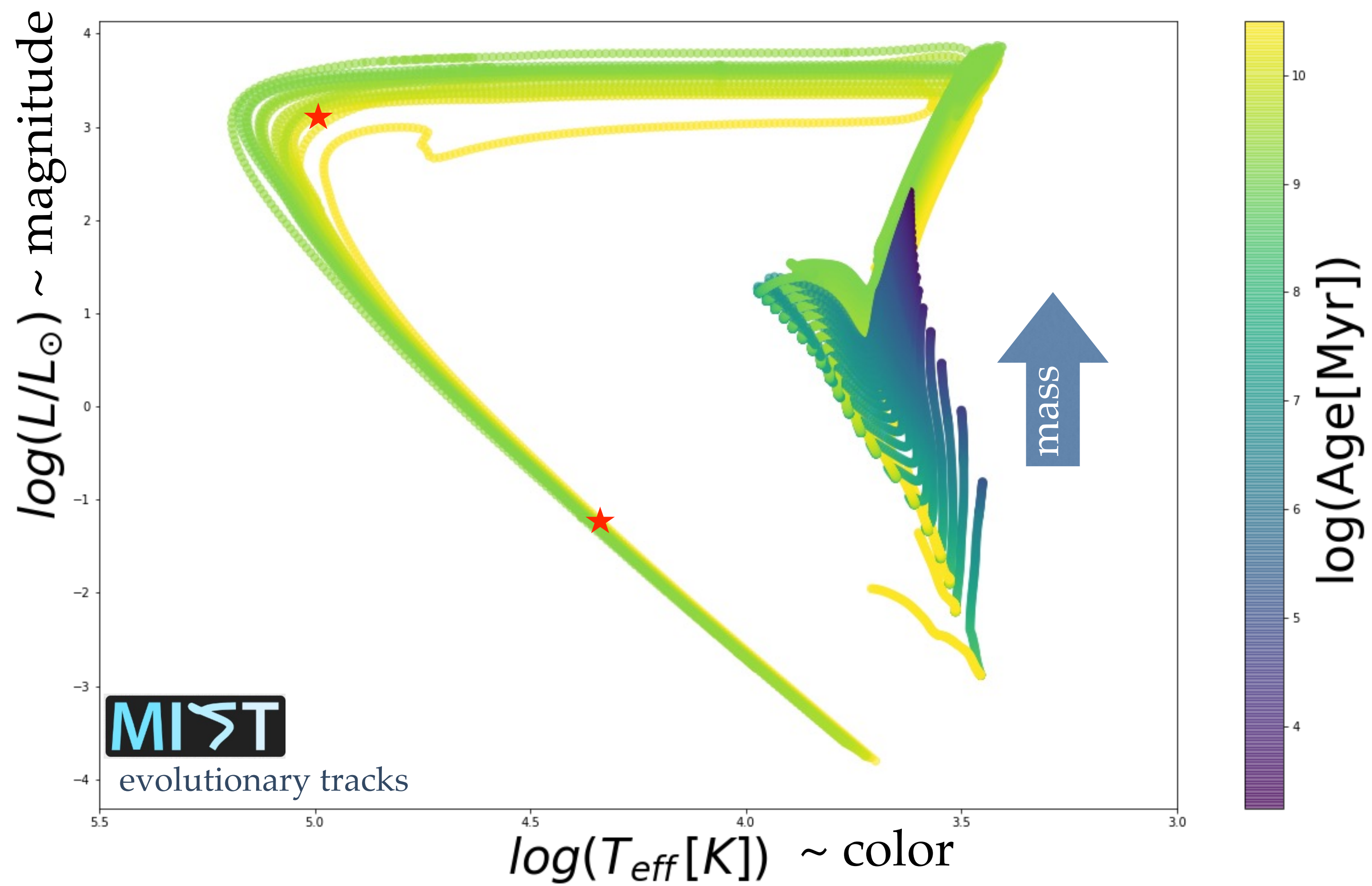
❖ Non-linearity



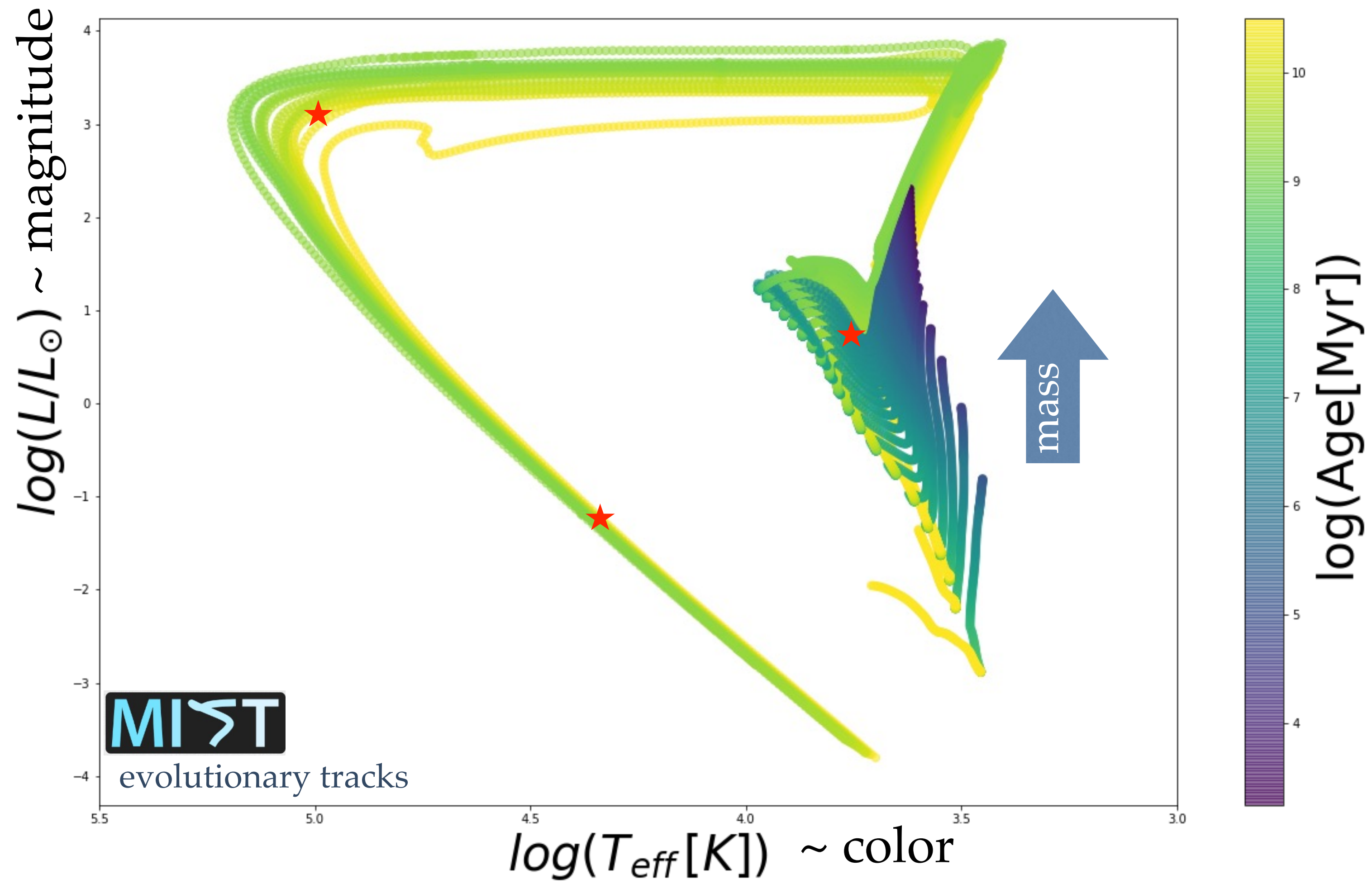
- ❖ Non-linearity
- ❖ Confidence variations



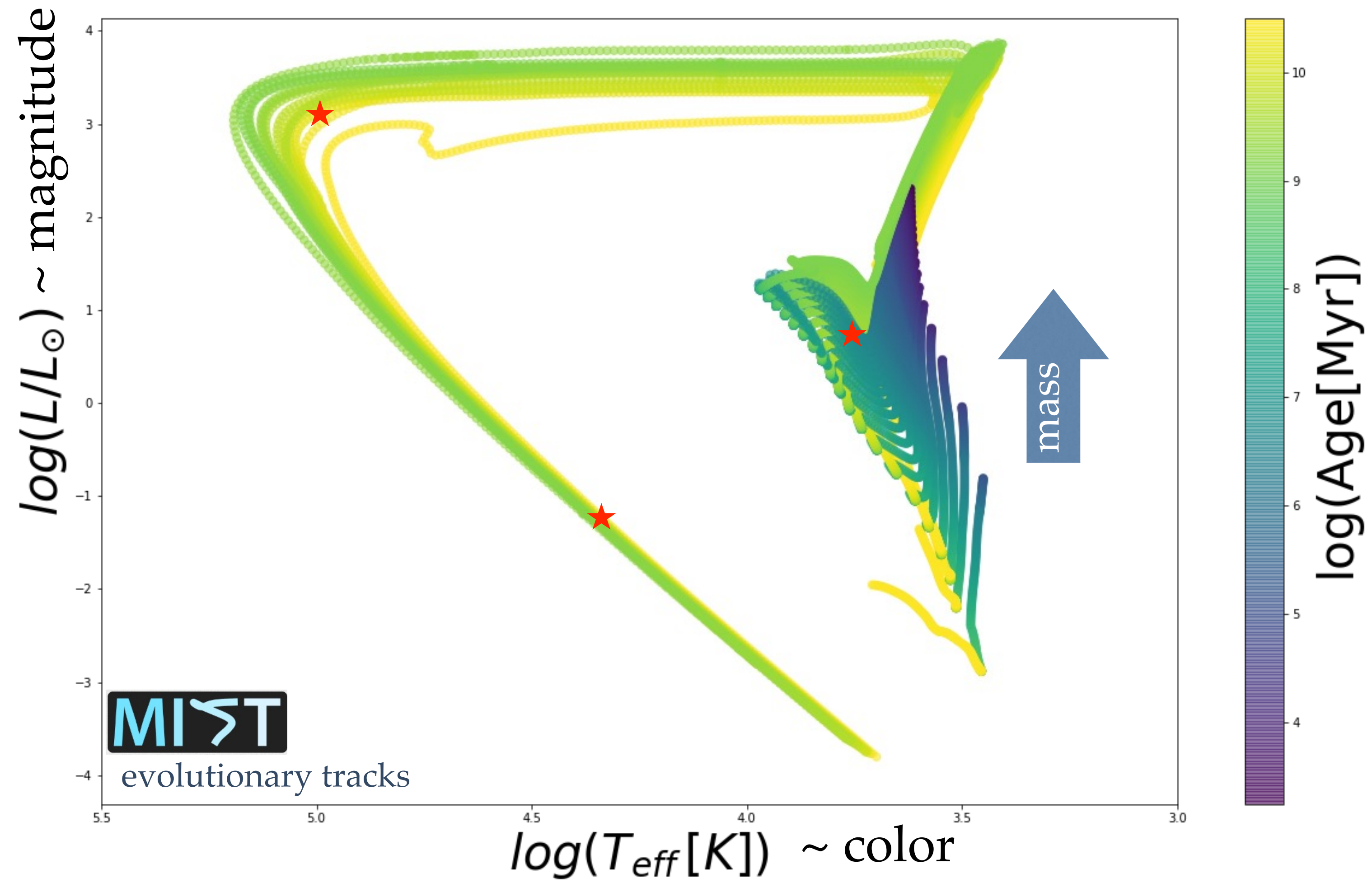
- ❖ Non-linearity
- ❖ Confidence variations



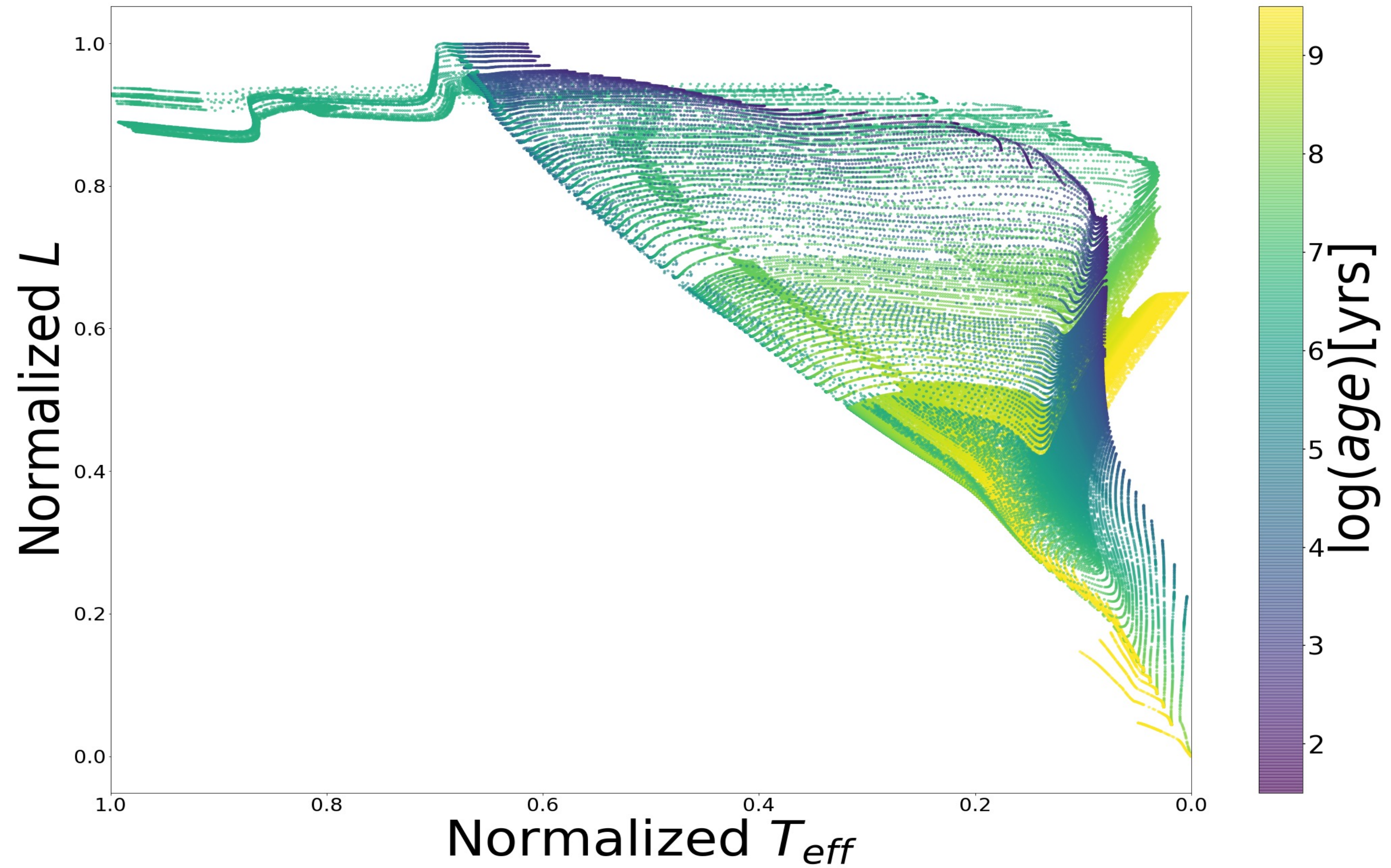
- ❖ Non-linearity
- ❖ Confidence variations



- ❖ Degeneracies
- ❖ Non-linearity
- ❖ Confidence variations



- ✧ Degeneracies
- ✧ Non-linearity
- ✧ Confidence variations

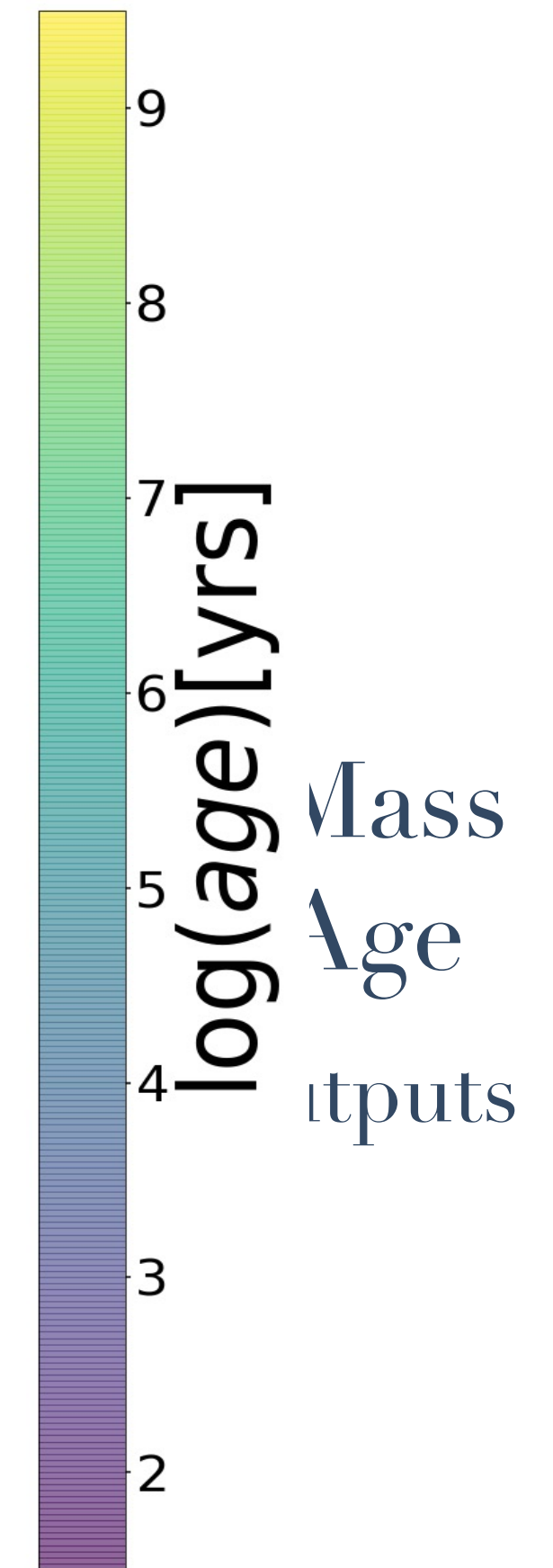
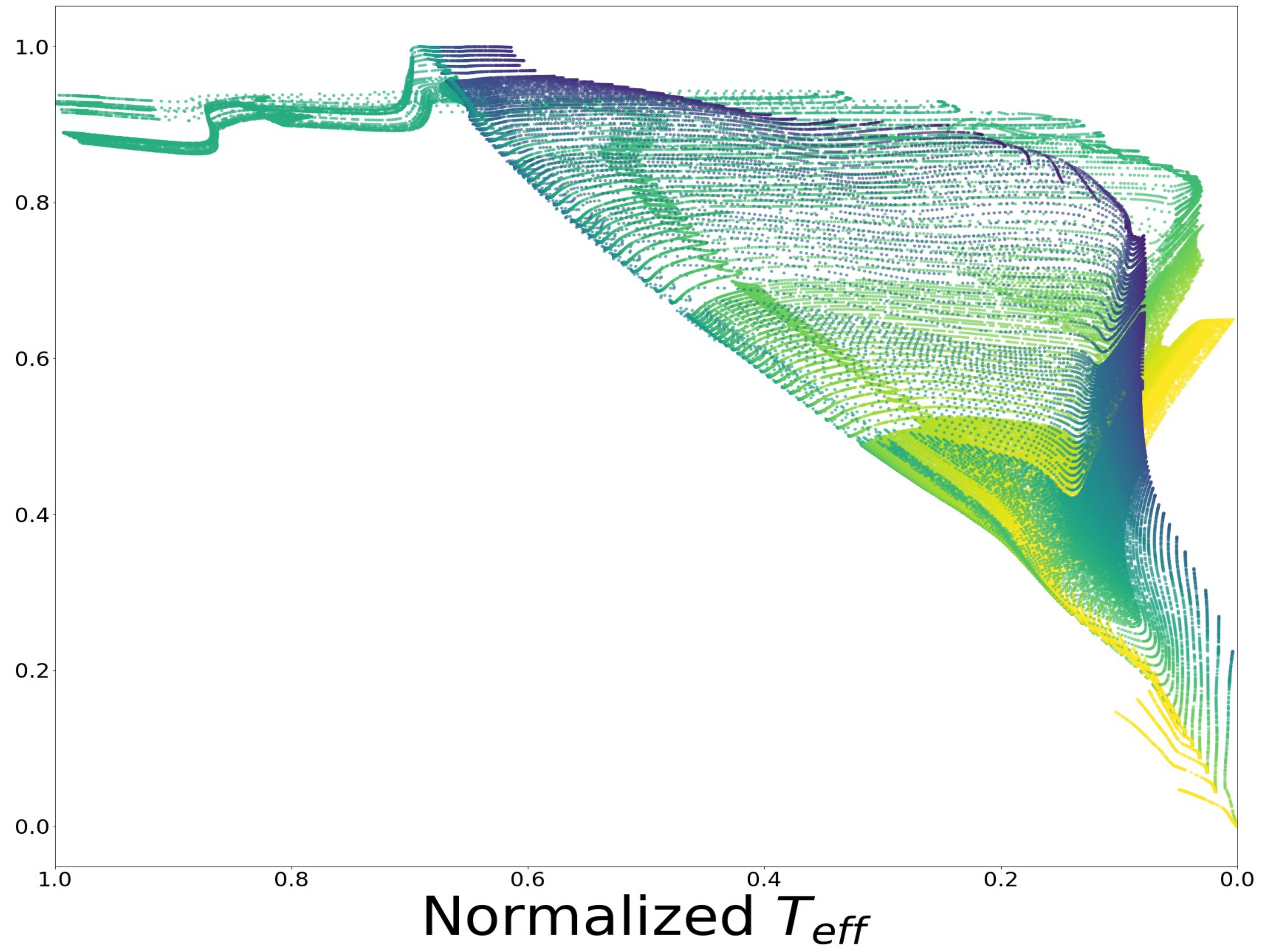


- ✦ Degeneracies
- ✦ Non-linearity
- ✦ Confidence variations



L
T_{eff}
inputs

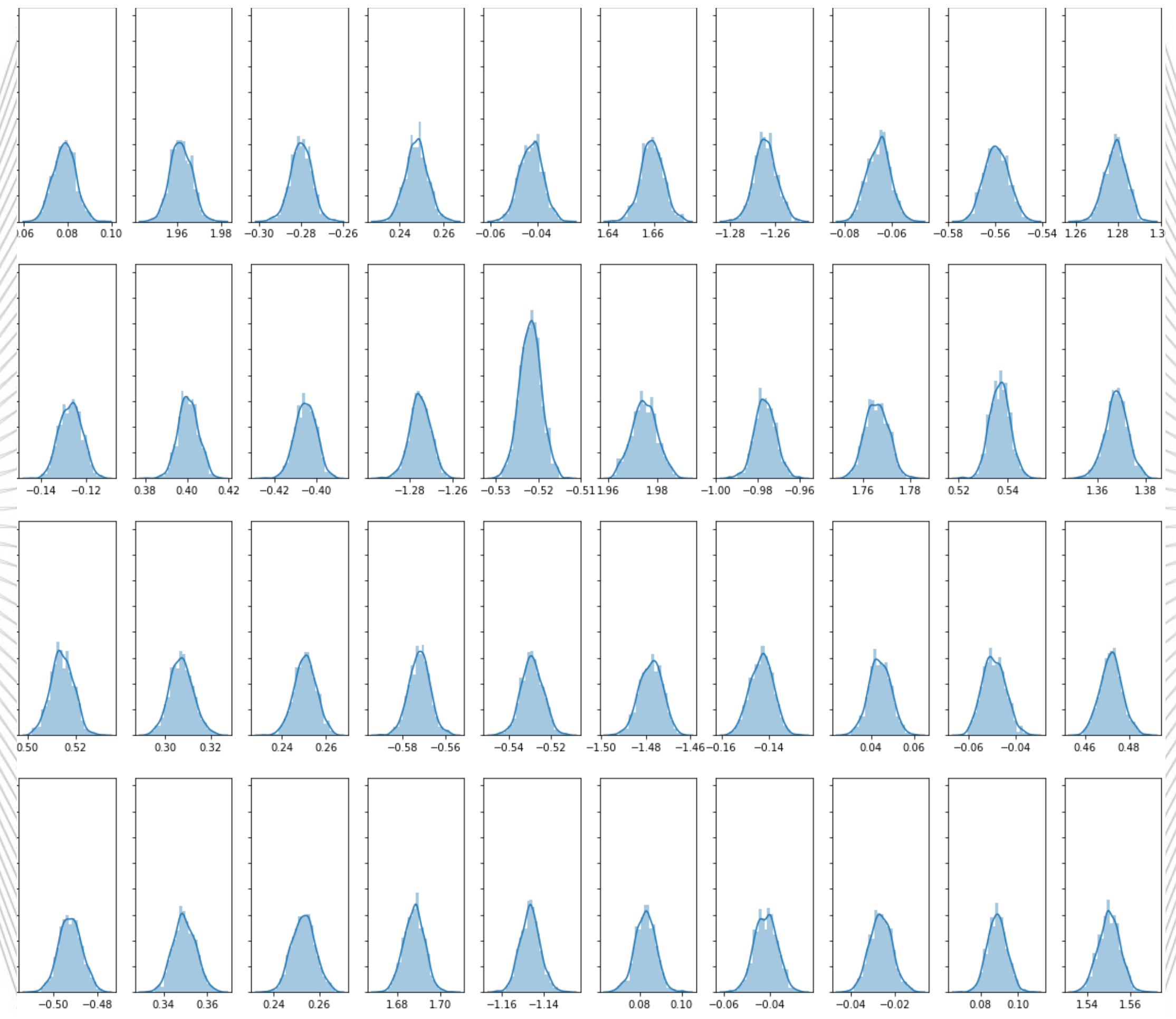
Normalized *L*



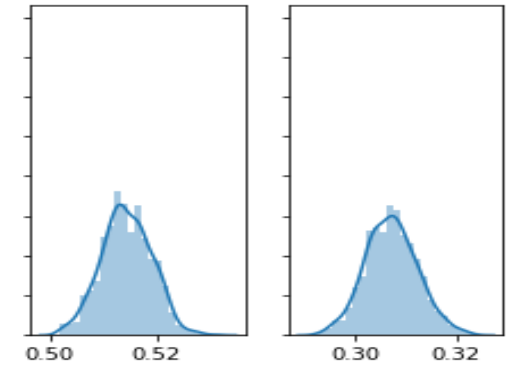
- ✿ Degeneracies
- ✿ Non-linearity
- ✿ Confidence variations



L
Teff



Mass, Age

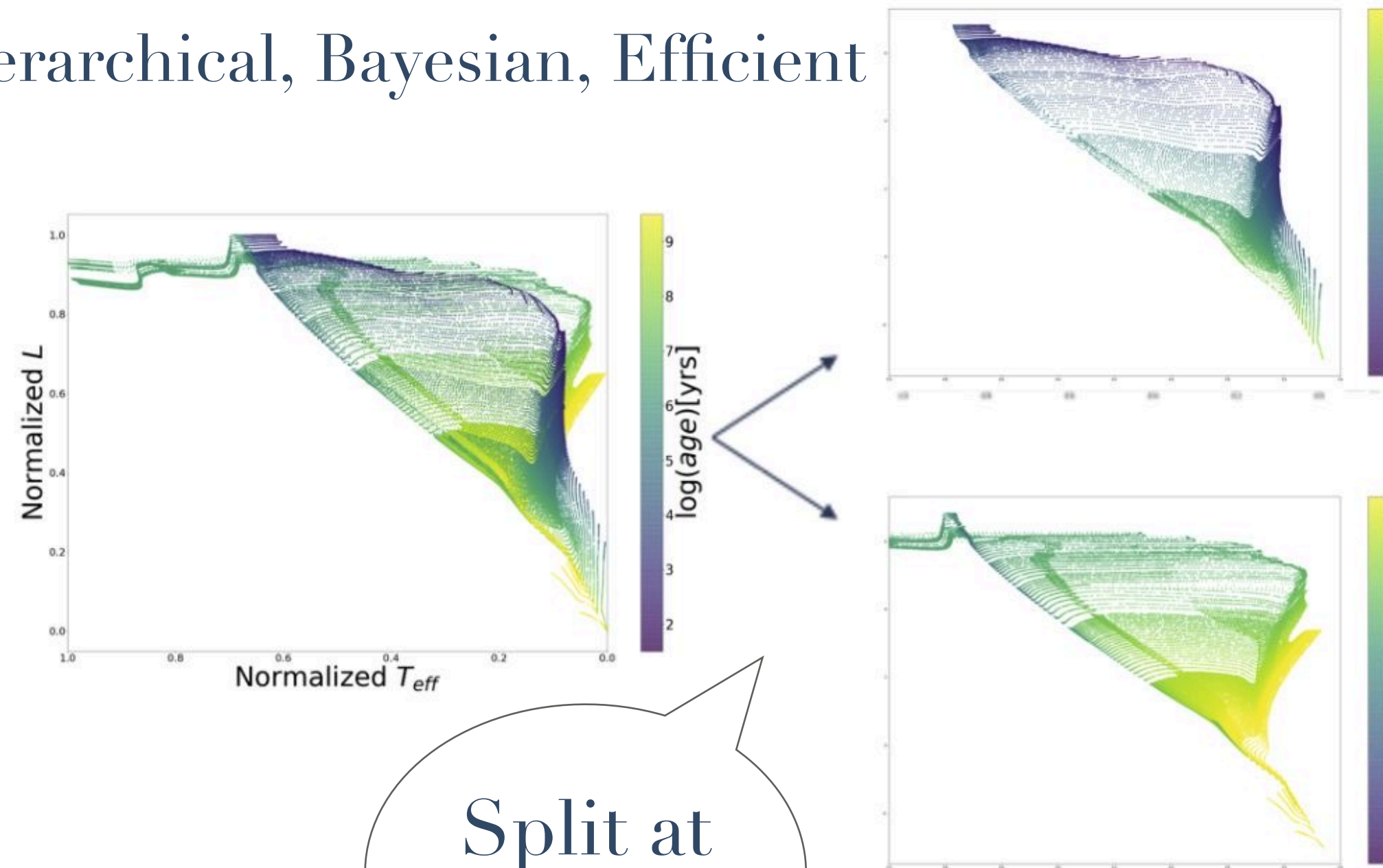


Automatic Stellar Characterization

- ❖ Degeneracies ✓
- ❖ Non-linearity ✓
- ❖ Confidence variations ✓

StelNet: Hierarchical, Bayesian, Efficient

L
T_{eff}



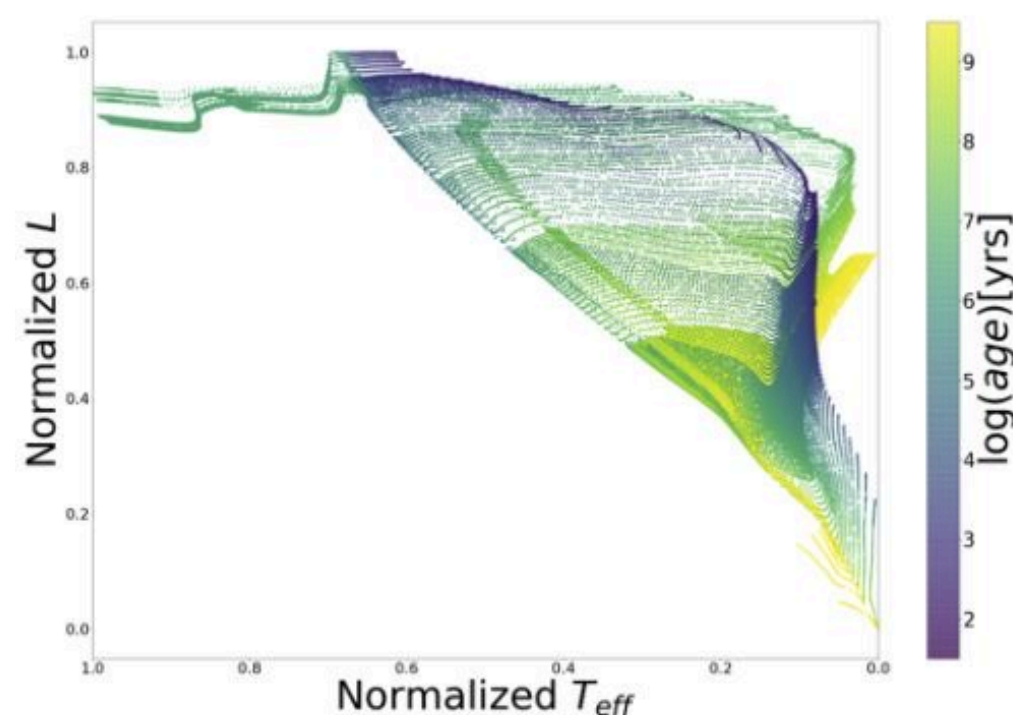
Split at
ZAMS

Automatic Stellar Characterization

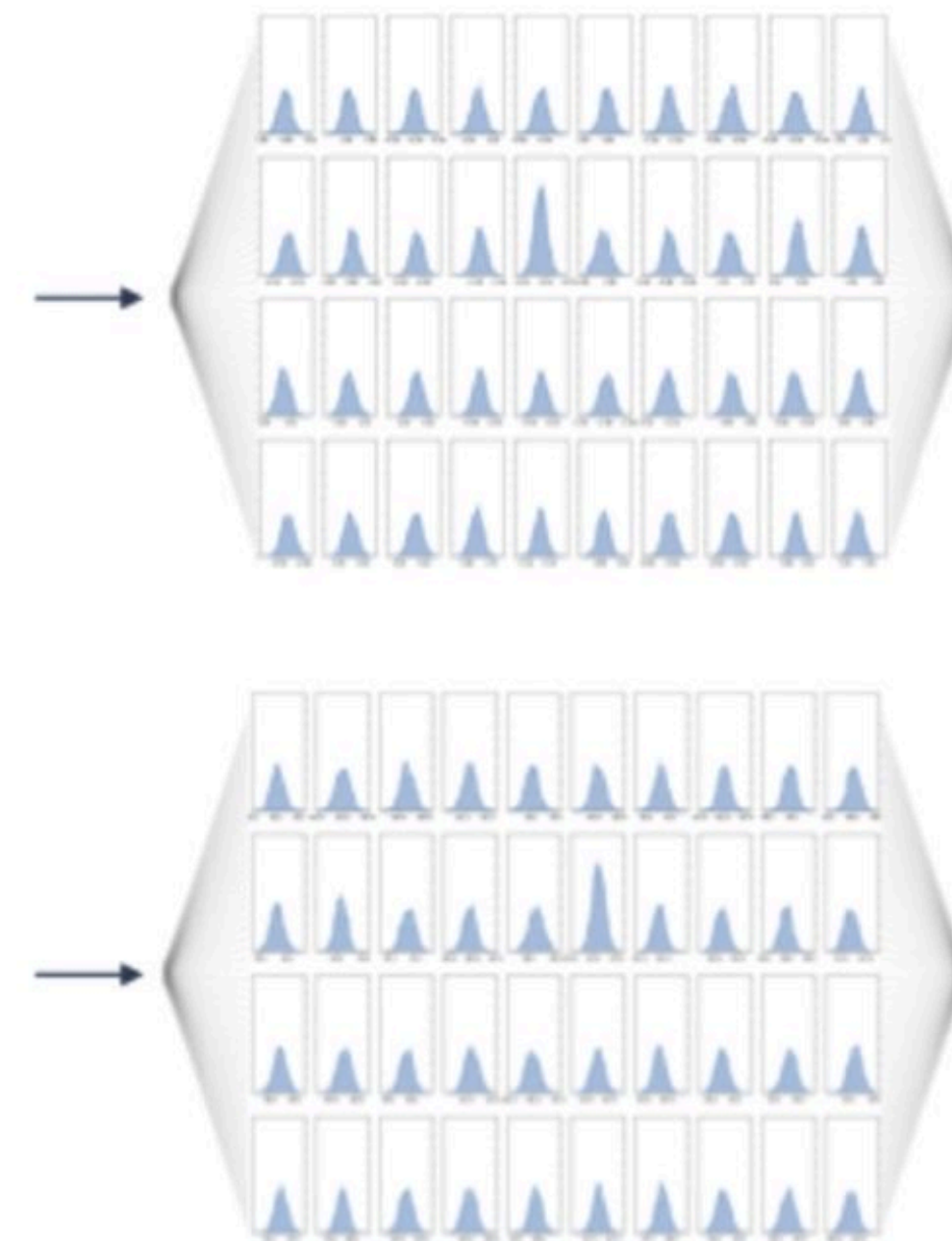
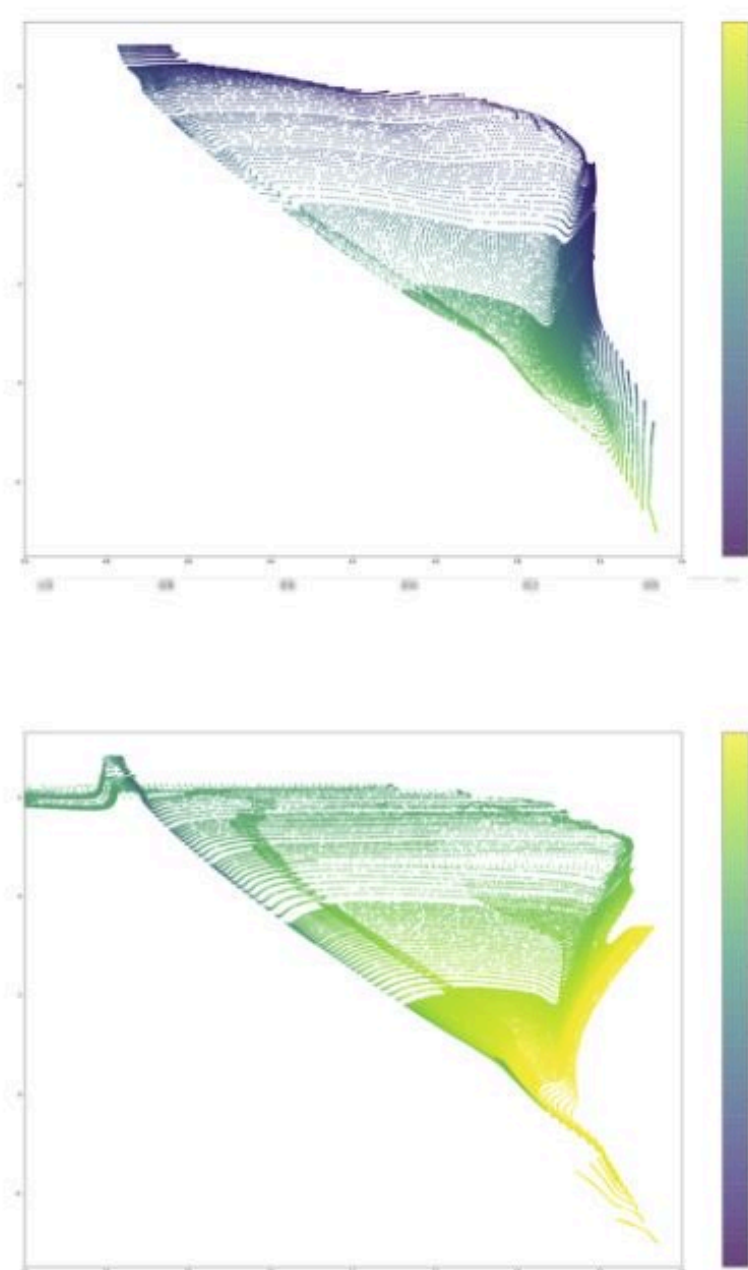
- ✦ Degeneracies ✓
- ✦ Non-linearity ✓
- ✦ Confidence variations ✓

StelNet: Hierarchical, Bayesian, Efficient

L
T_{eff}



Split at ZAMS



(m, age)_{Pre}

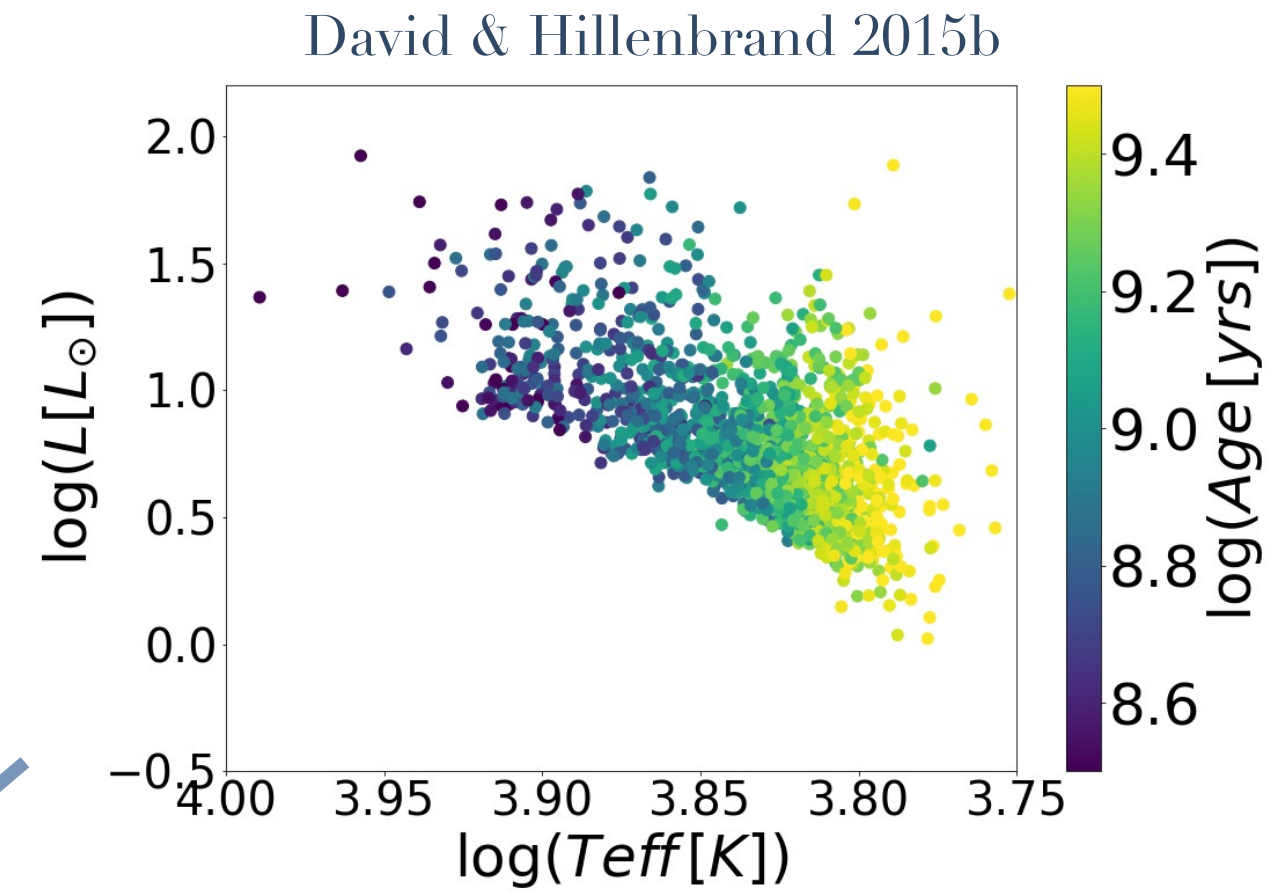
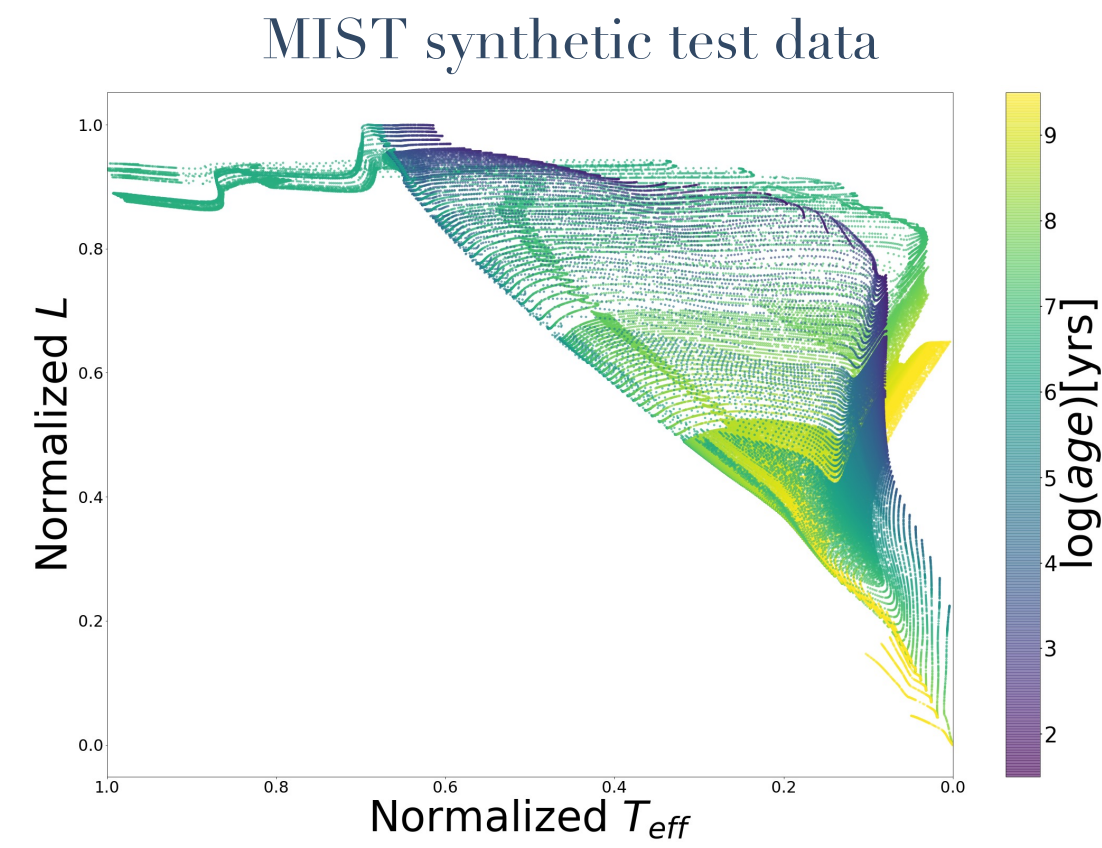
(m, age)_{Post}

Stellar Evolution & Galaxy Abundances

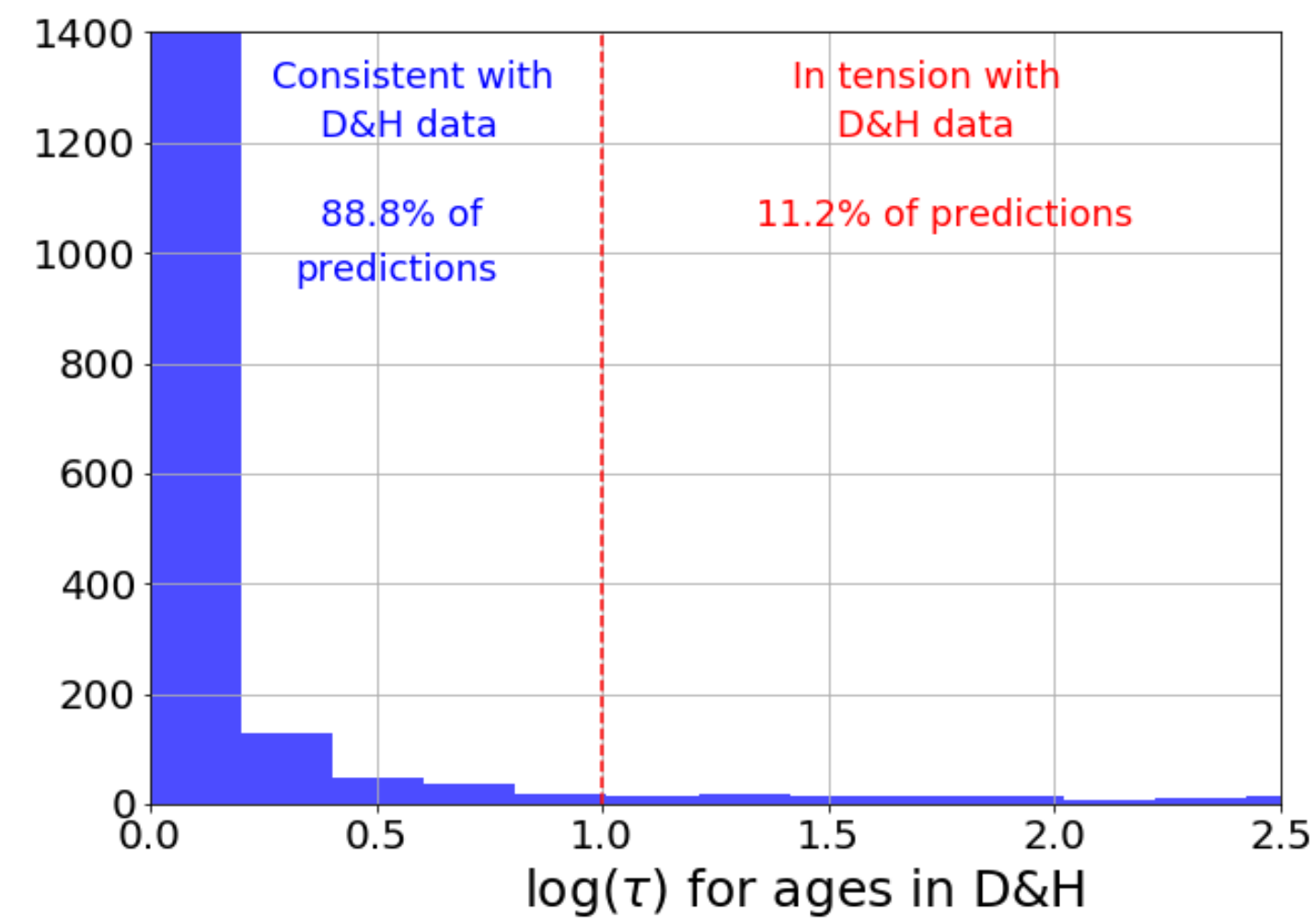
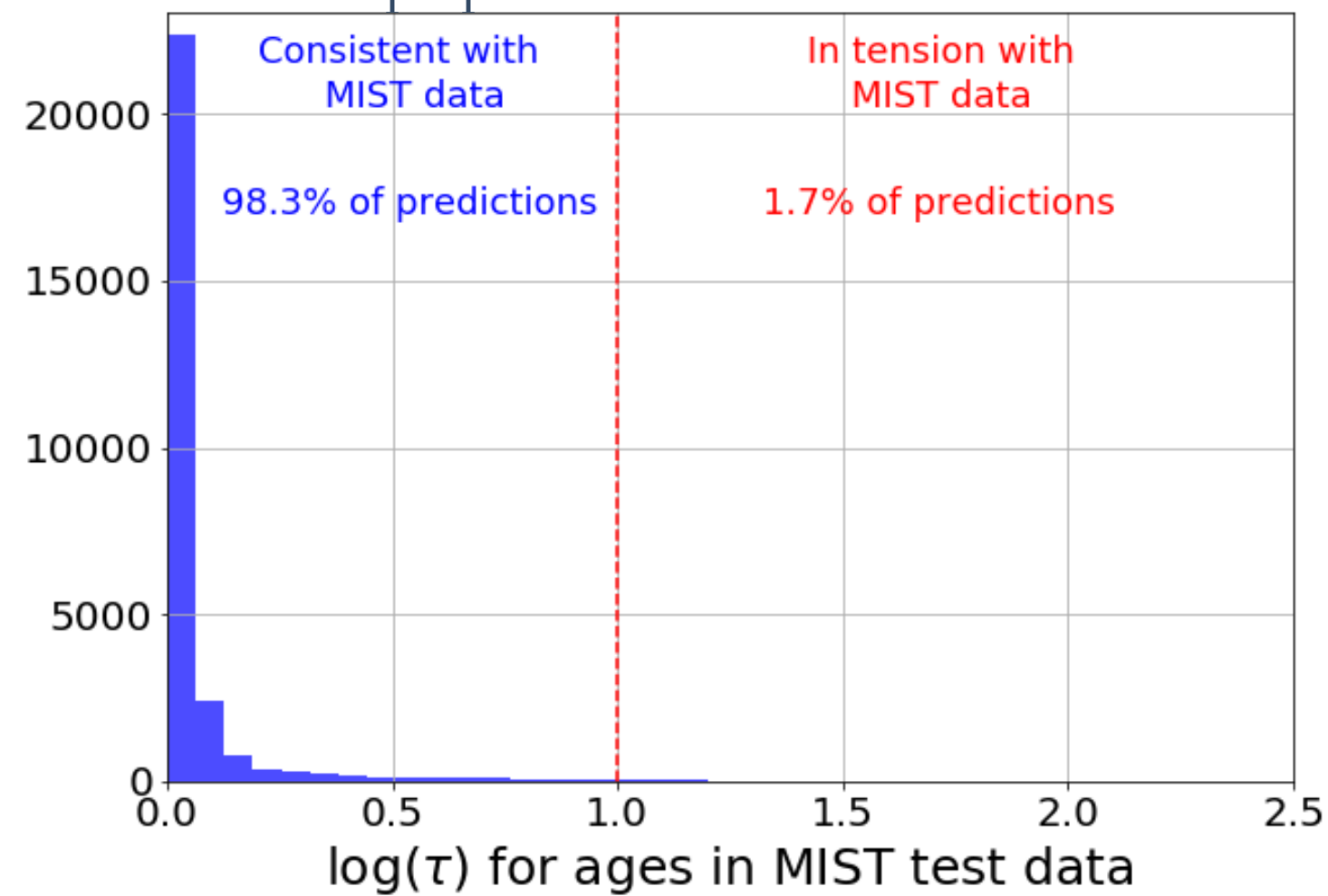
P(m, age)

Garraffo et al. 2021

Quantifying performance on test *MIST* synthetic data and on observed data



Garraffo et al. in prep.



Garraffo et al. 2021



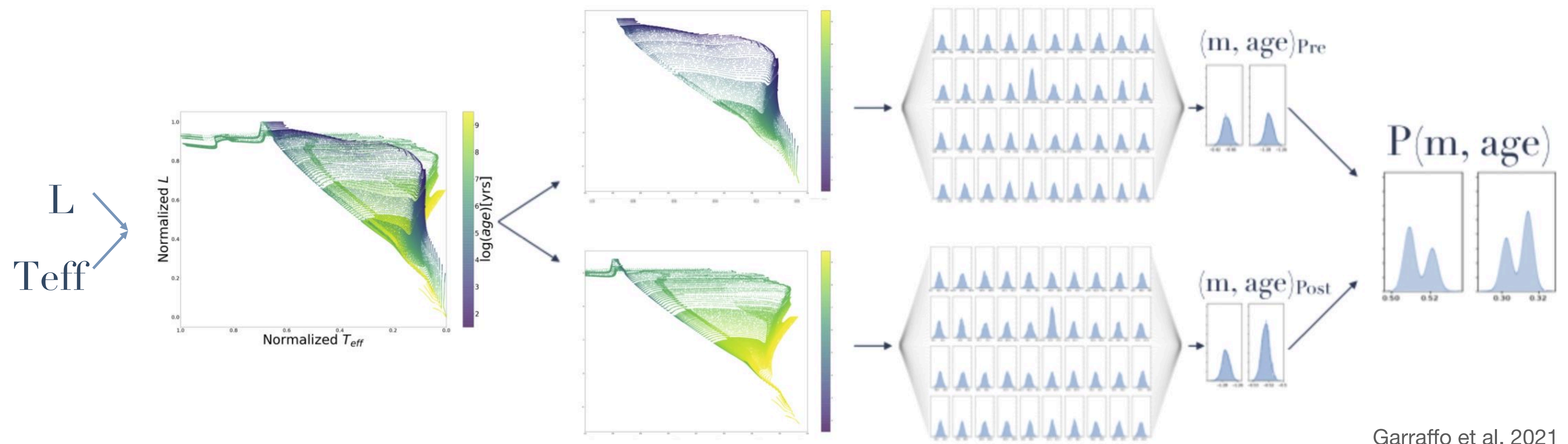
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Anya Phillips

Automatic Stellar Characterization for Gaia



Garraffo et al. 2021



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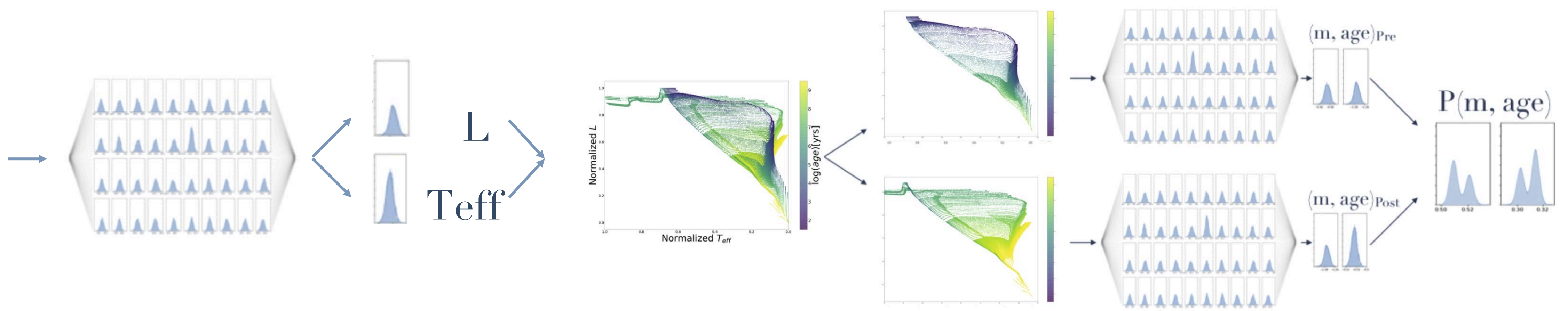


Anya Phillips

Automatic Stellar Characterization for Gaia

One Step Approach: directly from photometry

Gaia Photometry



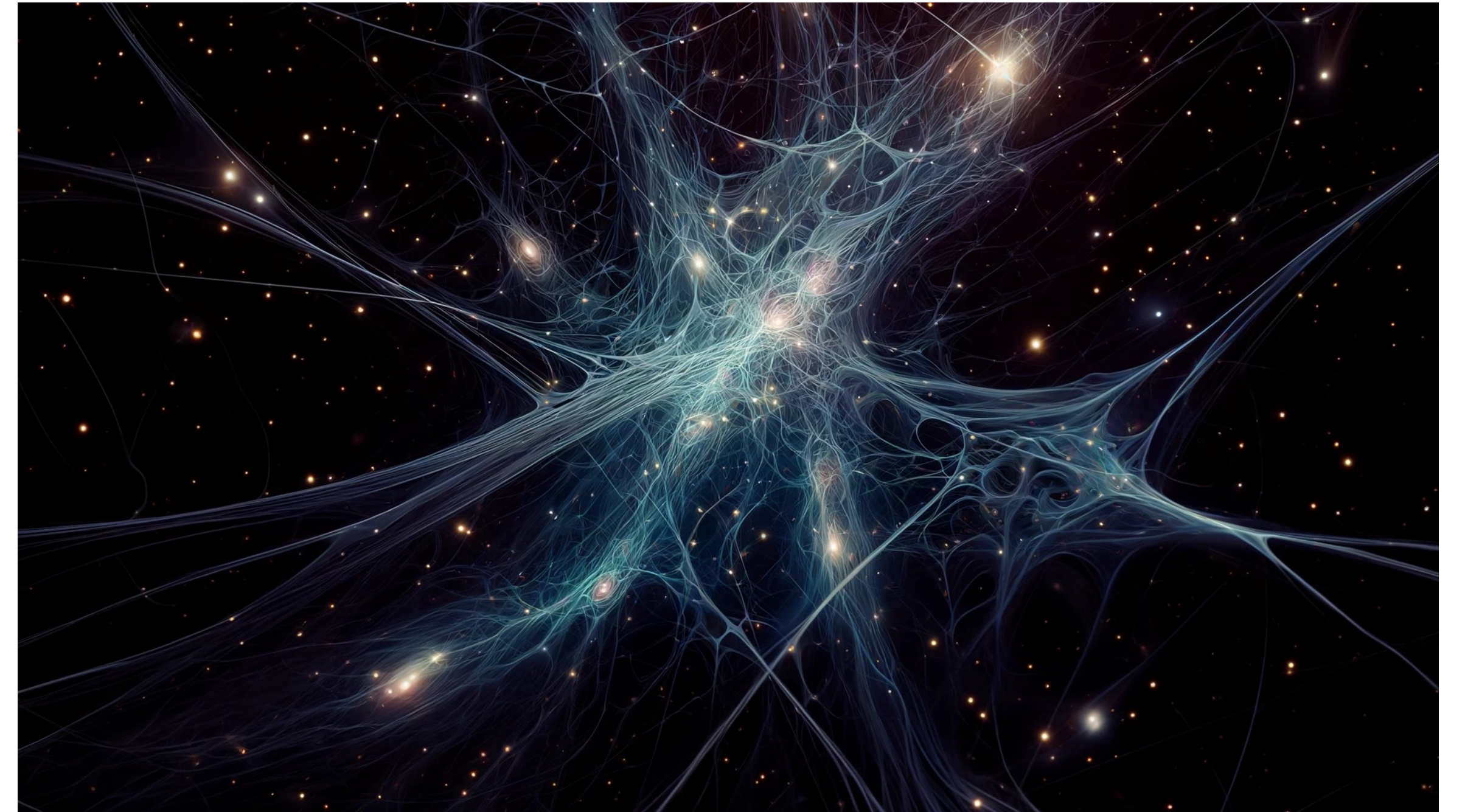
Phillips et al. in prep

Diffusion Models for Astrophysics

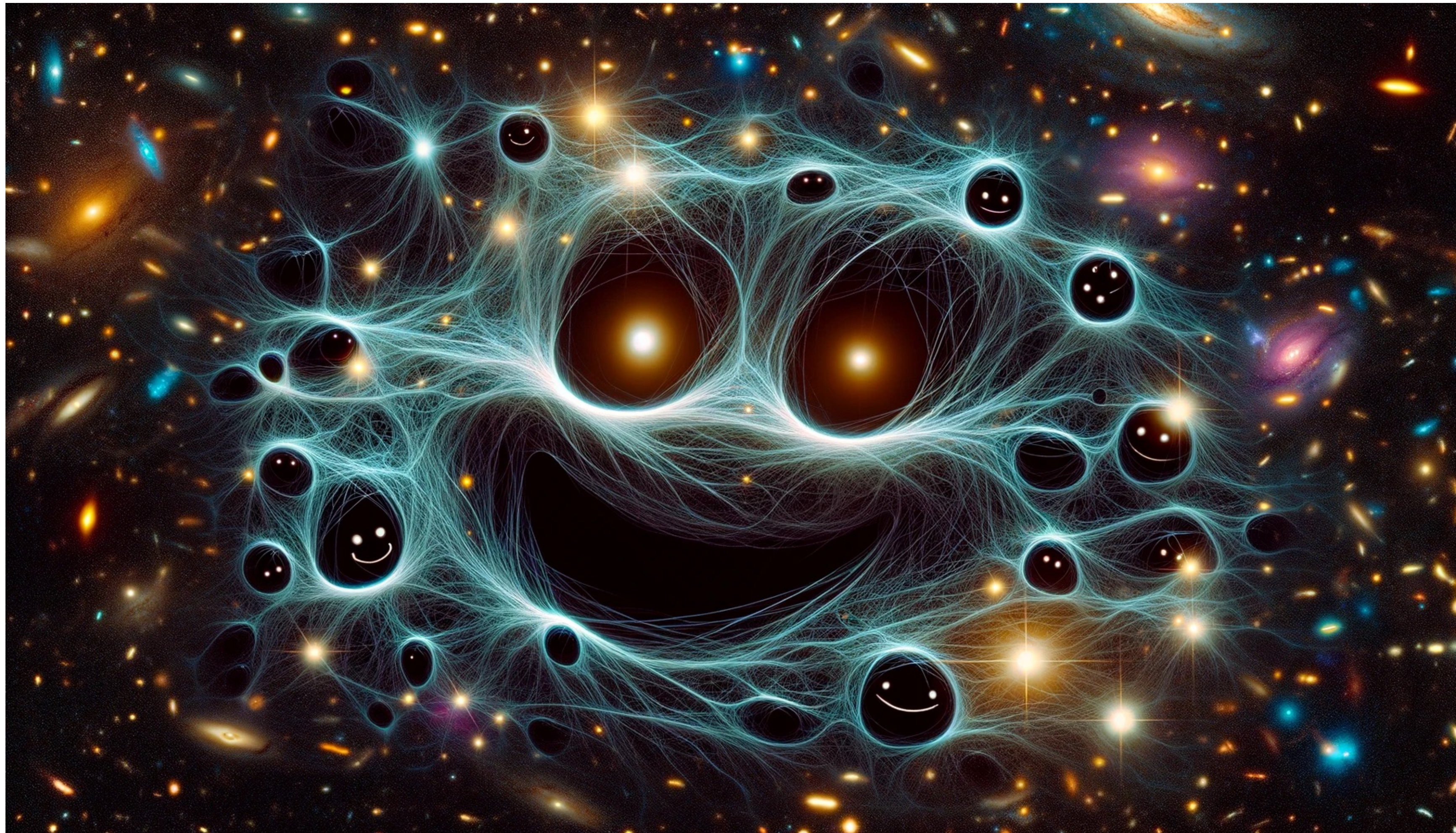
DALL-E prompt:
A dark matter field

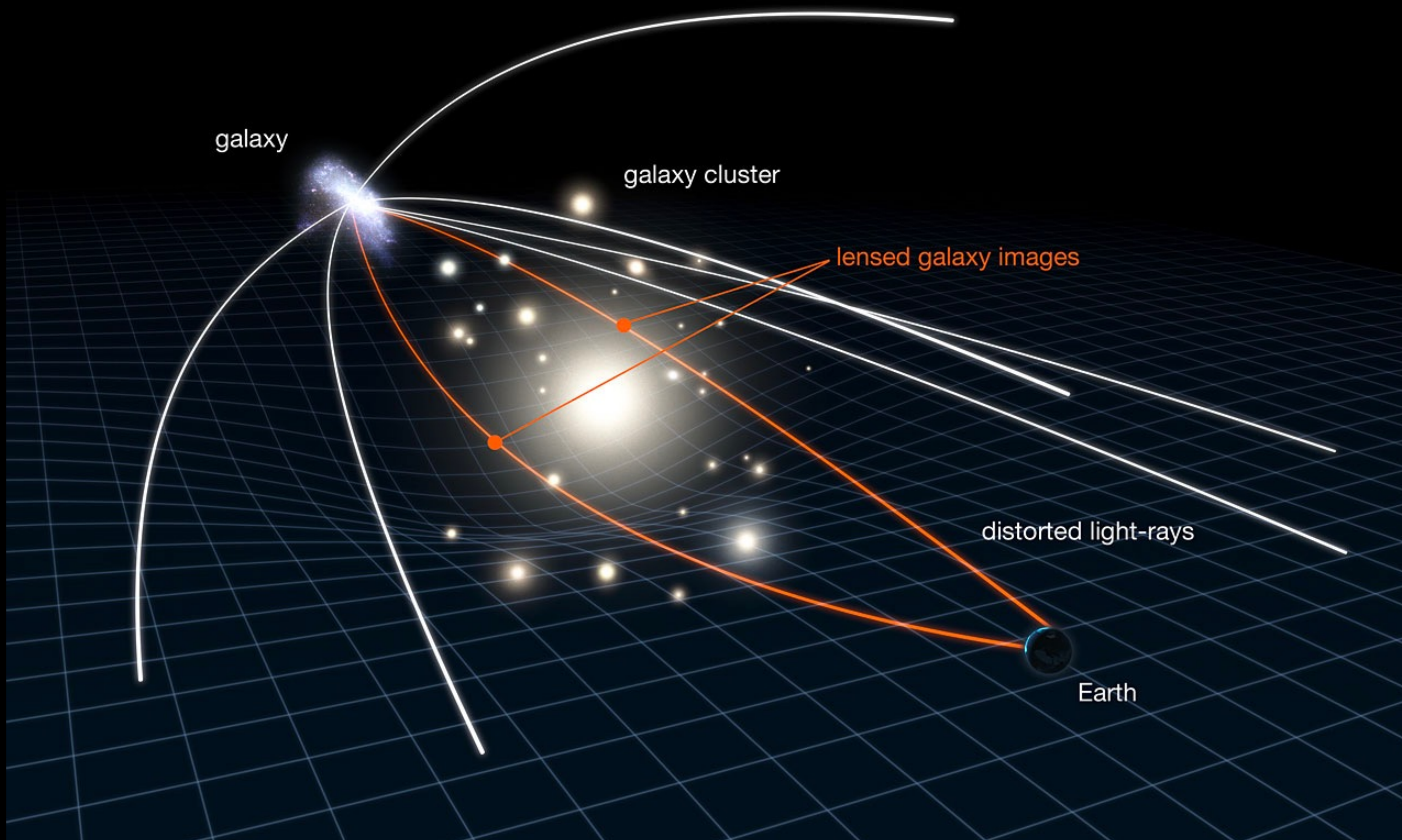


DALL-E prompt:
Dark matter field from a cosmological simulation,
showing filaments of dark matter in intergalactic medium



Diffusion Models for Astrophysics





galaxy

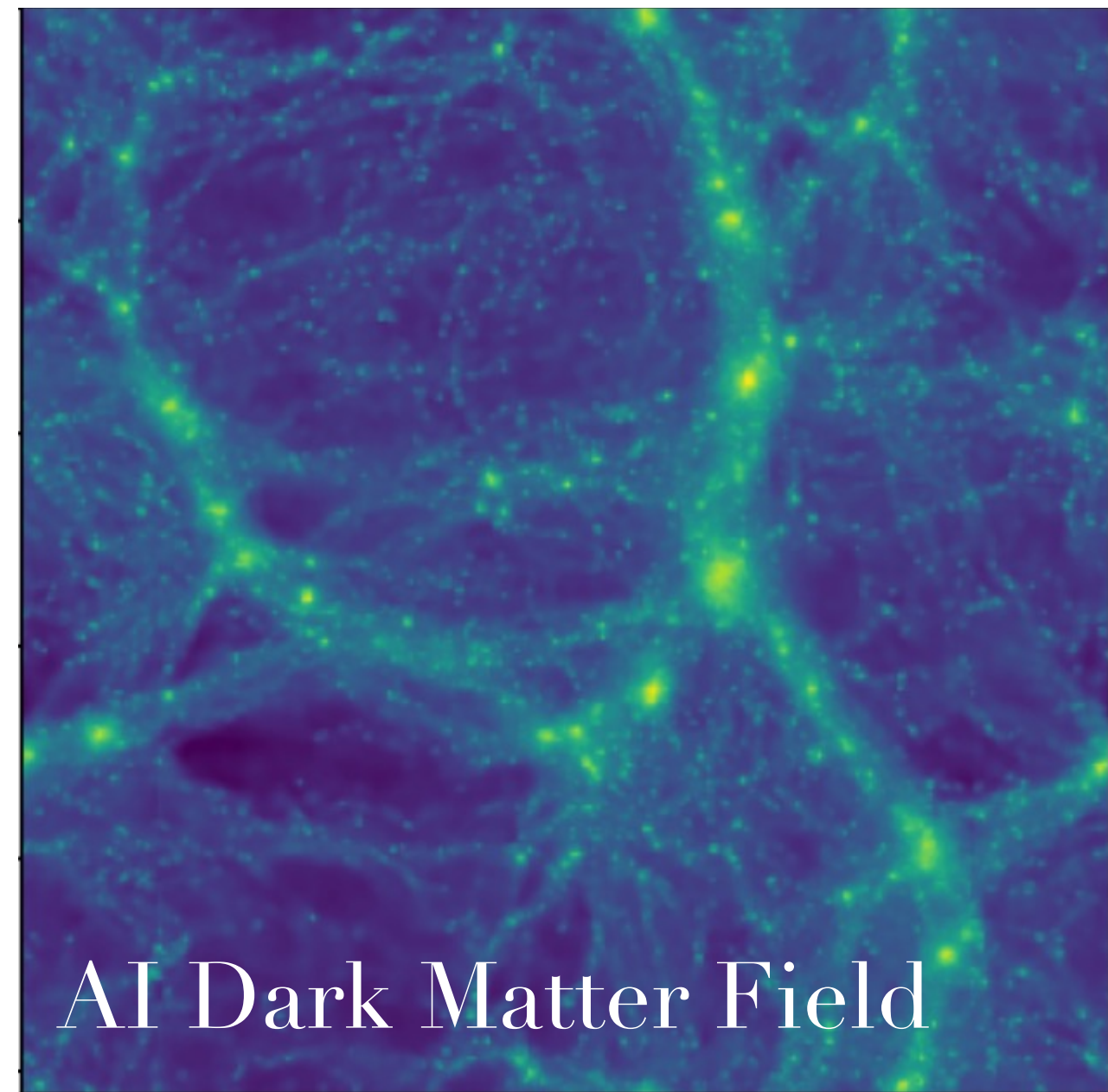
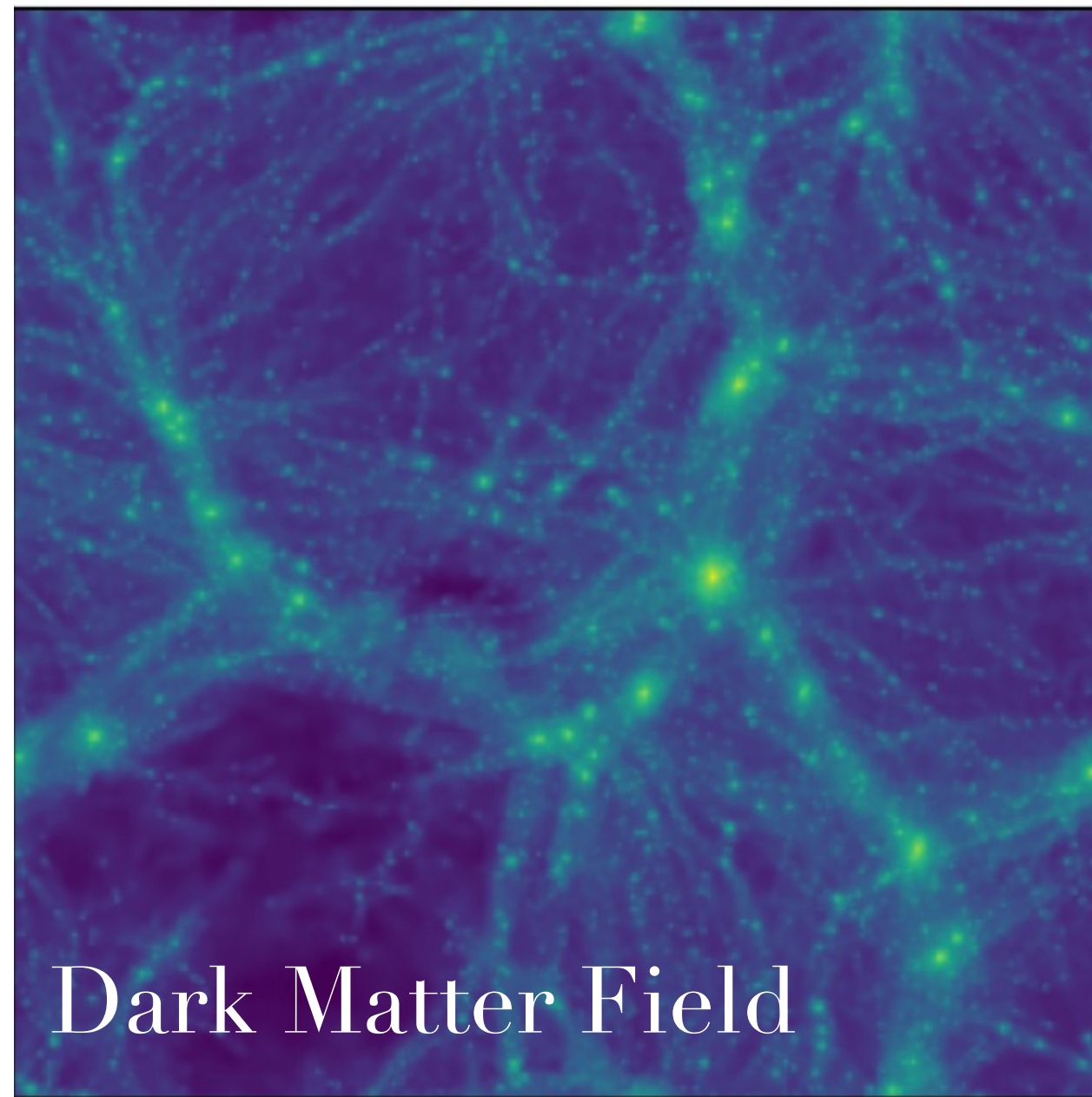
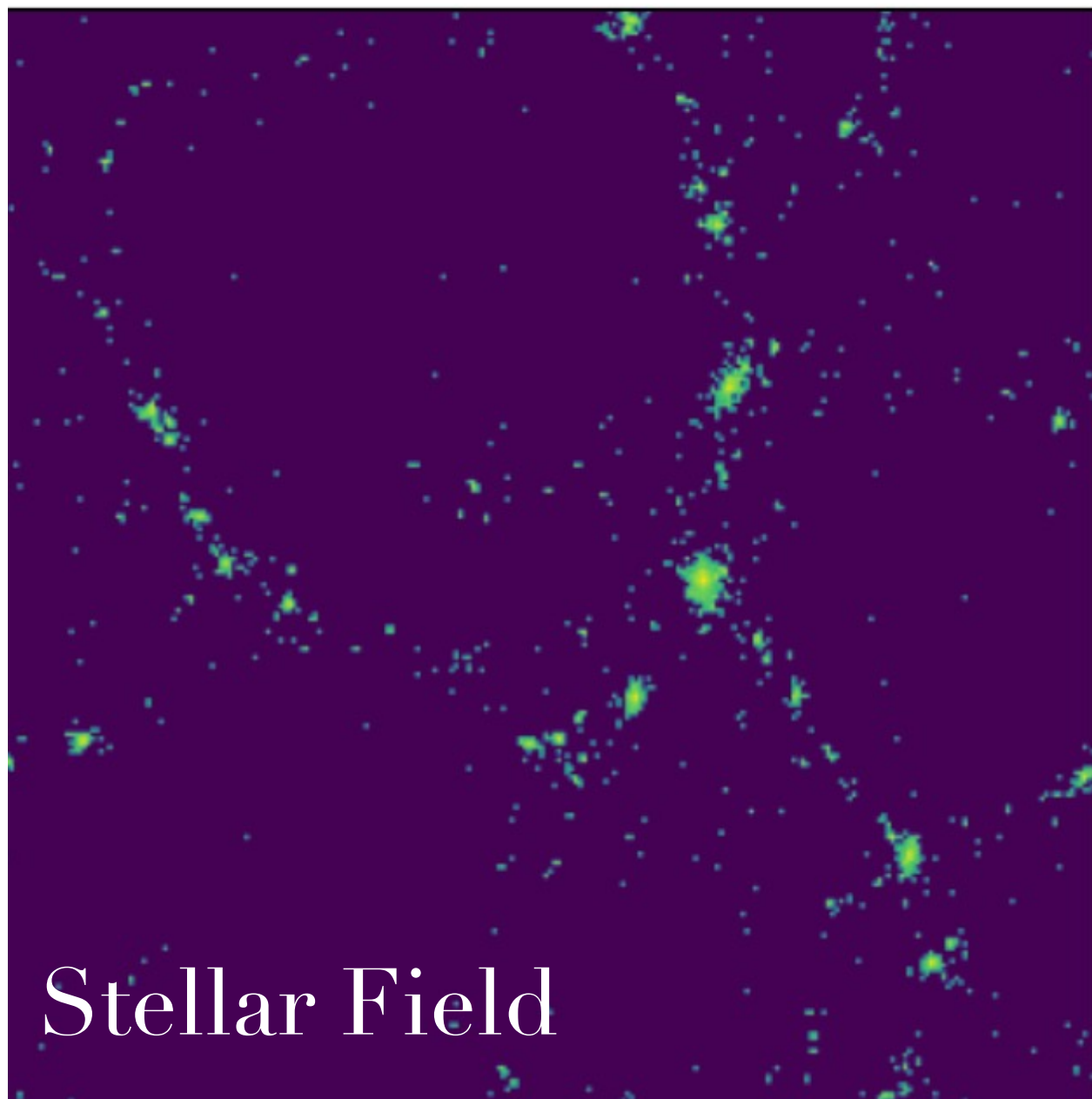
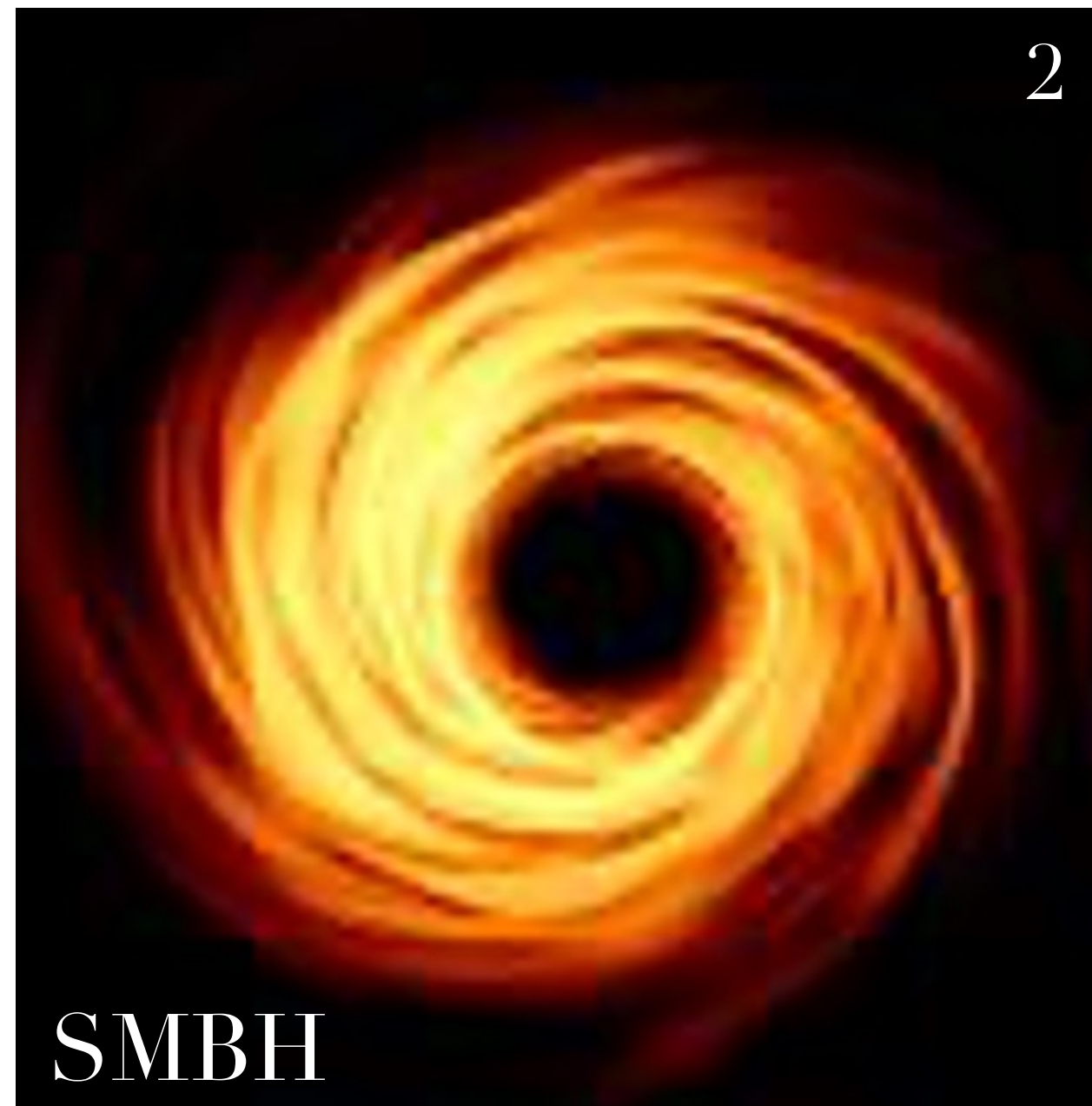
galaxy cluster

lensed galaxy images

distorted light-rays

Earth





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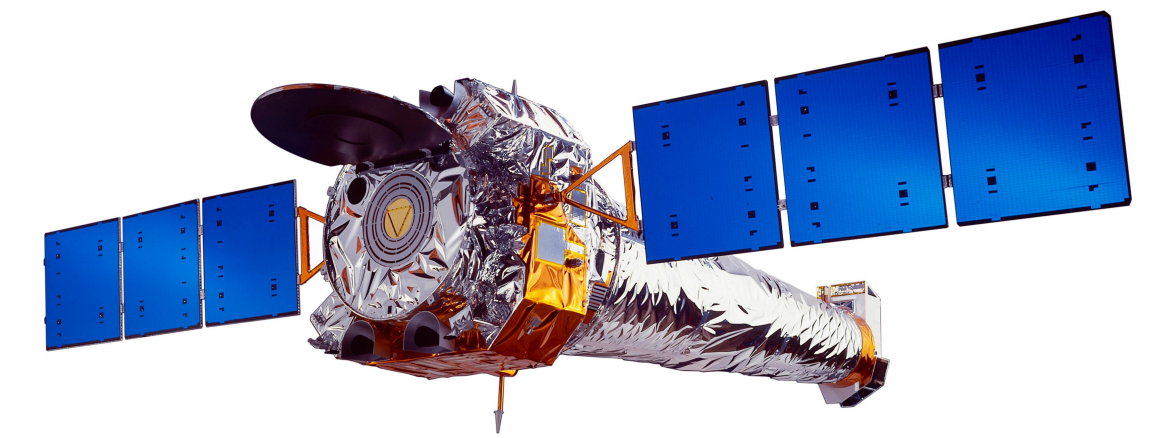
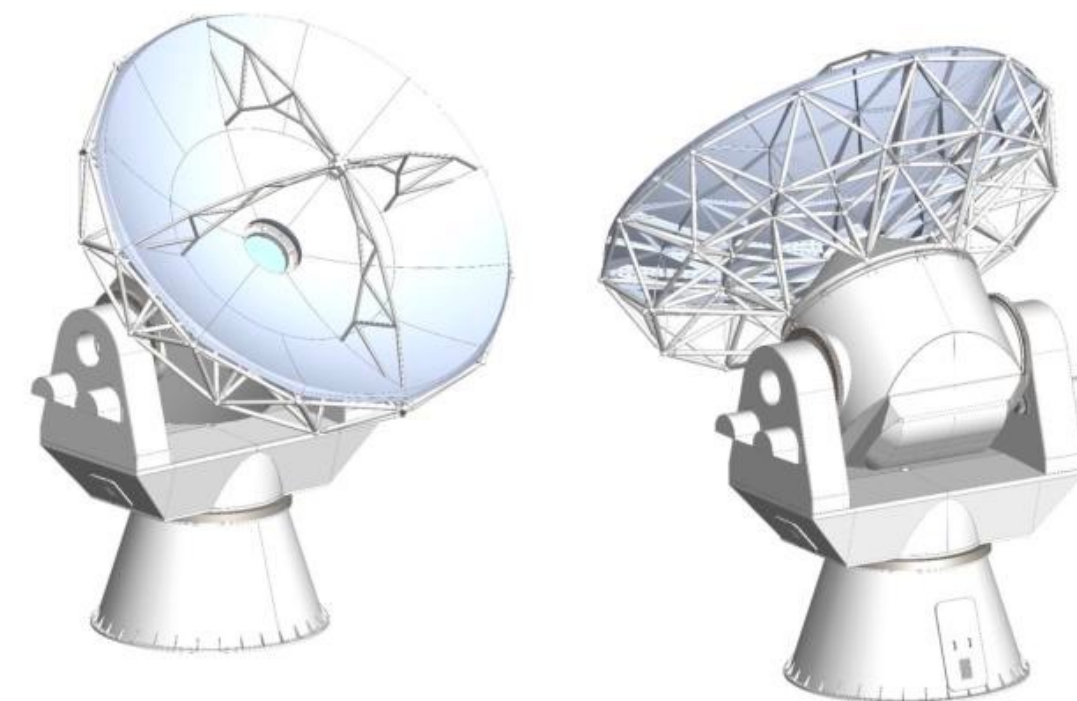
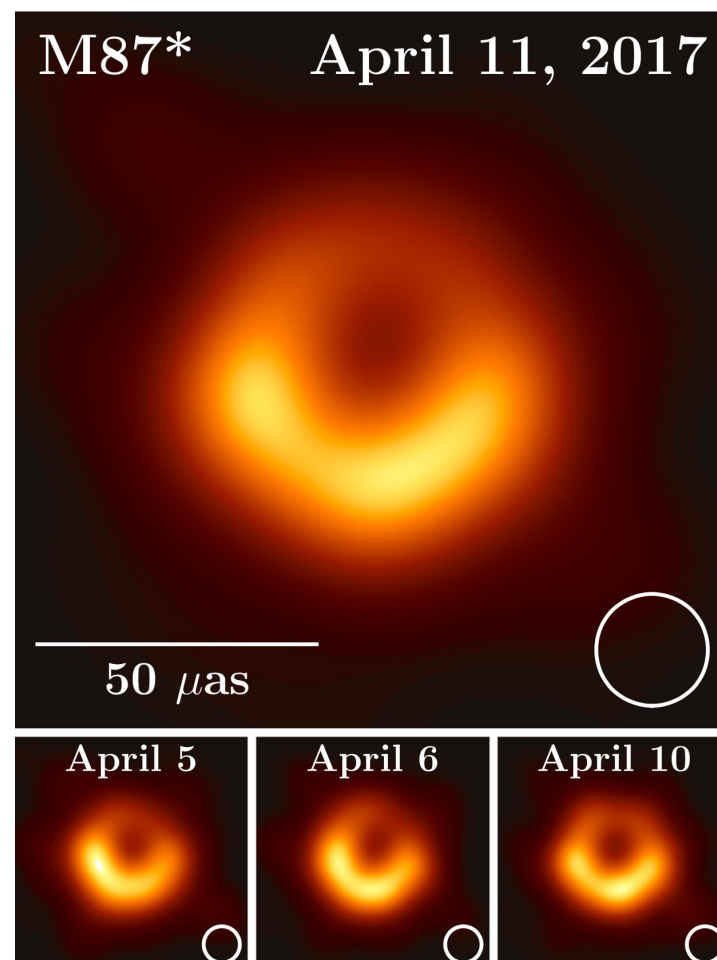
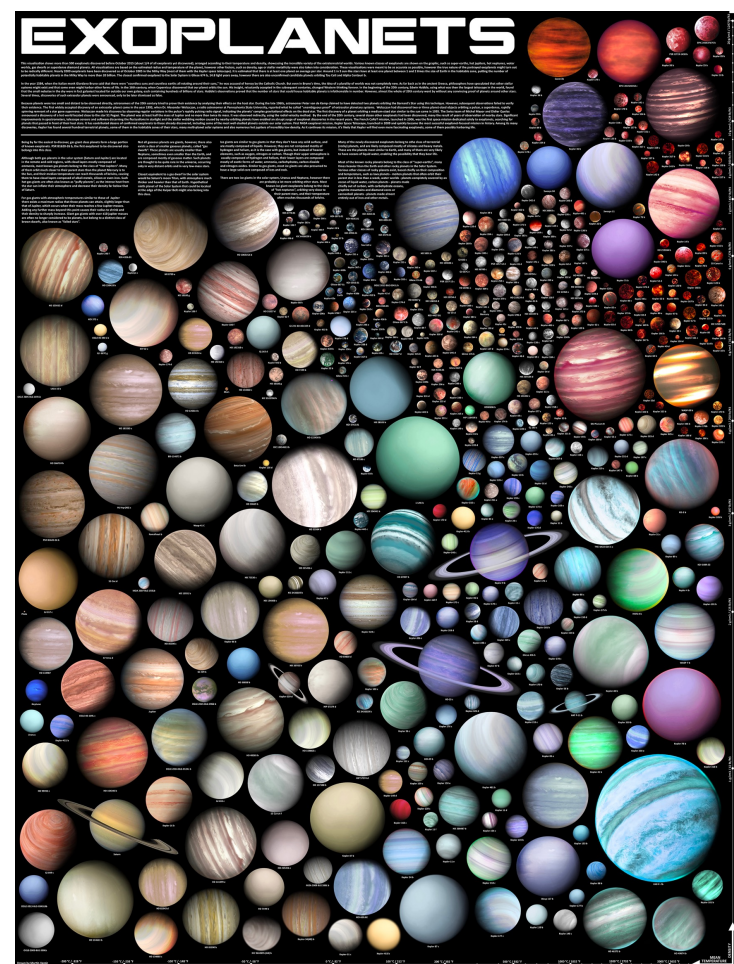
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The CfA

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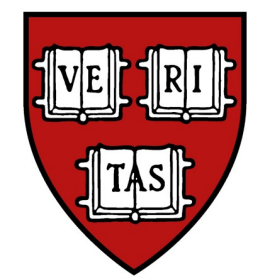
A lot of Astronomy

Data from Ground-based Space & Telescopes

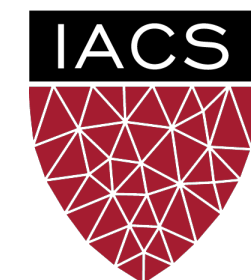
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The Boston Area



Scientific Image Analysis
Group - SIAG



Harvard John A. Paulson School of Engineering and Applied Sciences
IACS Institute for Applied
Computational Science



HDSI | Harvard Data
Science Initiative



MIT EECS

Electrical Engineering | Computer Science | Artificial Intelligence + Decision-making



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Harvard University
Faculty of Arts & Sciences

AI+Physics @MIT

A home for the intersection of artificial intelligence and physics at MIT

International CHASC Astro-Statistics Collaboration



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Northeastern University

Khoury College of Computer Sciences

Data Science



Google DeepMind



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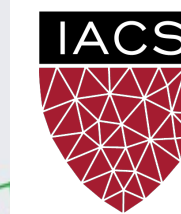
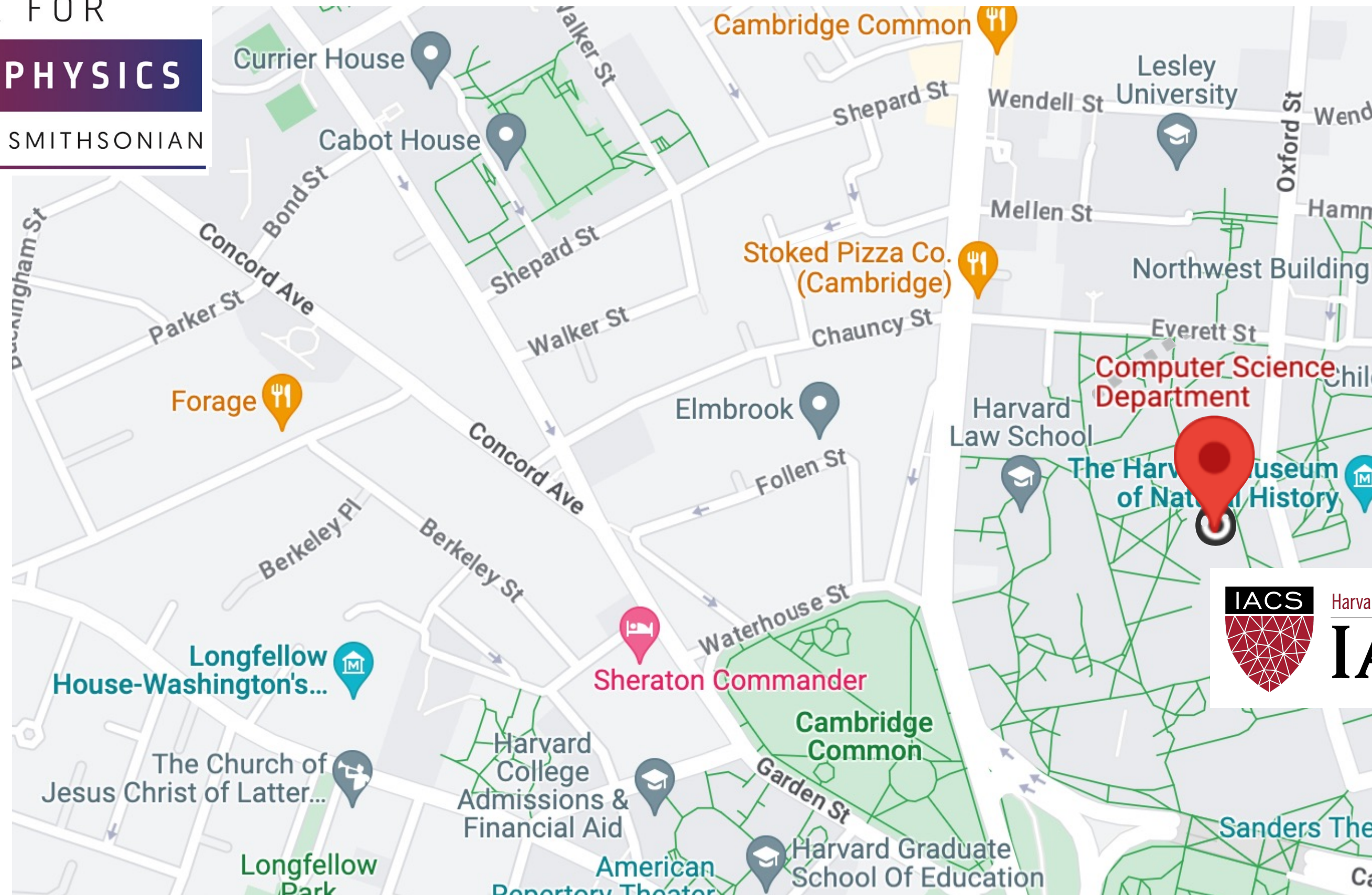
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Harvard John A. Paulson School of Engineering and Applied Sciences

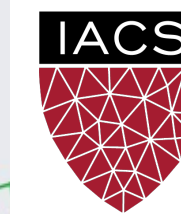
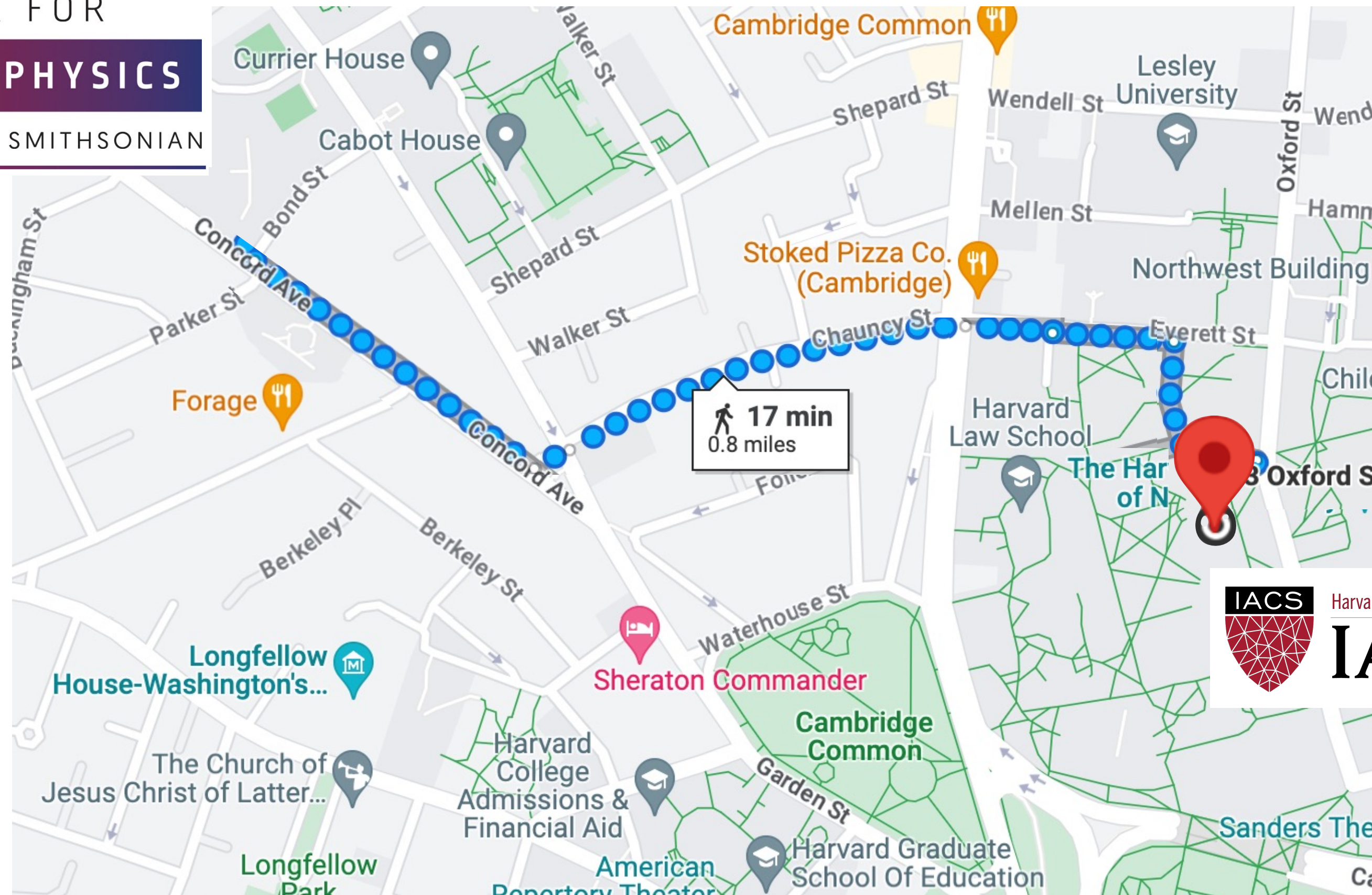
IACS Institute for Applied Computational Science

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Harvard John A. Paulson School of Engineering and Applied Sciences

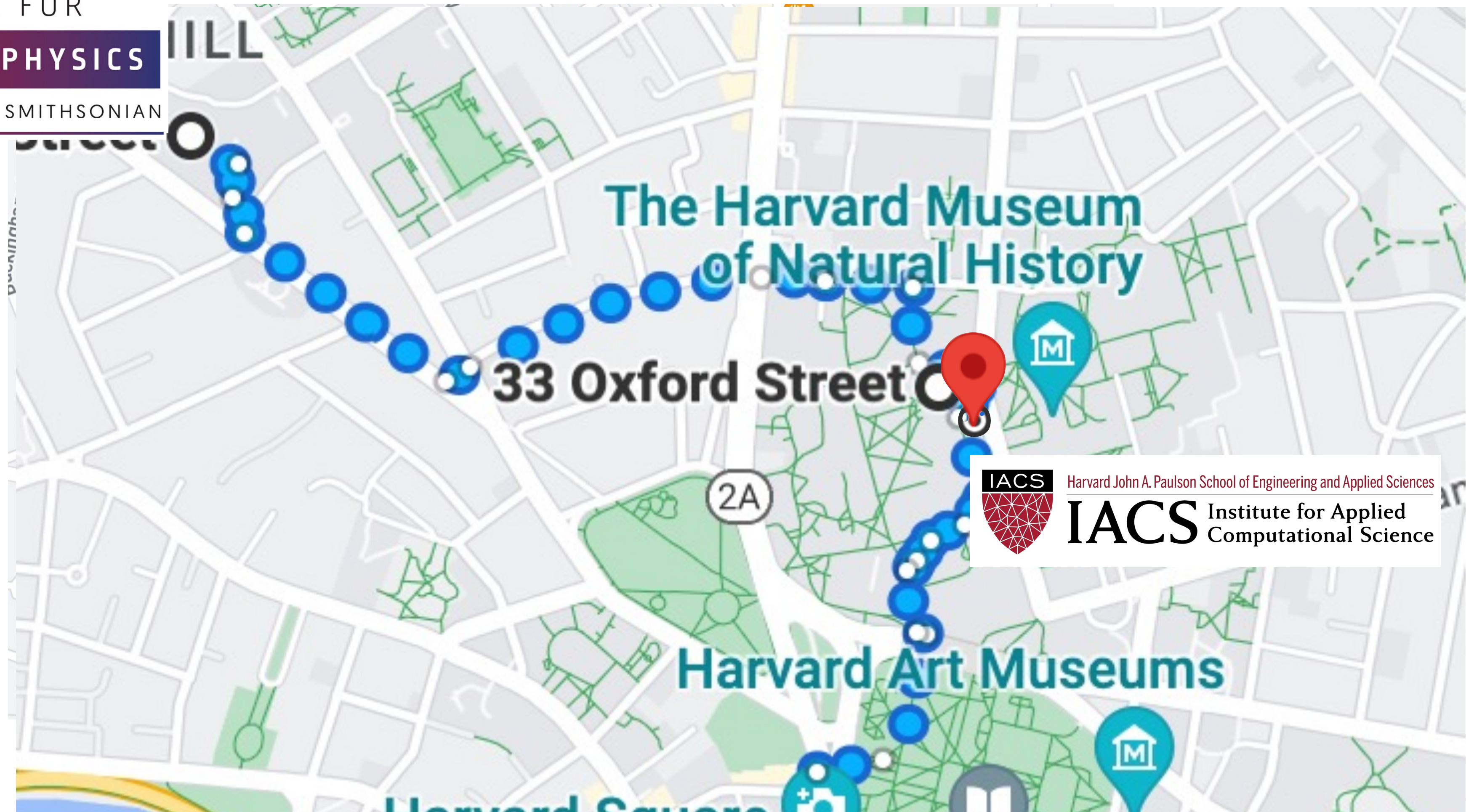
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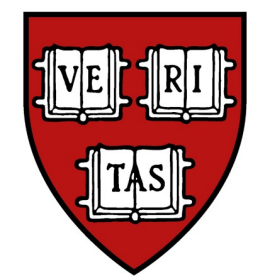


IACS Harvard John A. Paulson School of Engineering and Applied Sciences
IACS Institute for Applied Computational Science

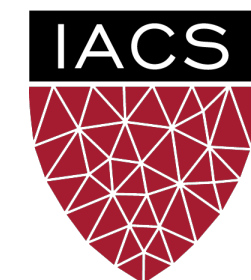
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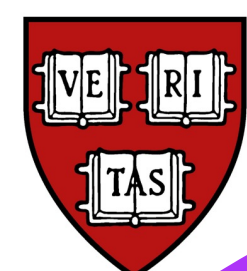
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Why AstroAI?

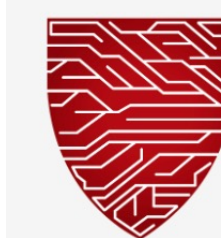
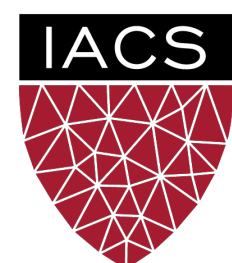
Harvard John A. Paulson School of Engineering and Applied Sciences

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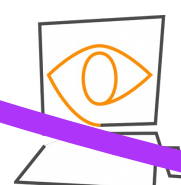
Khoury College of Computer Sciences

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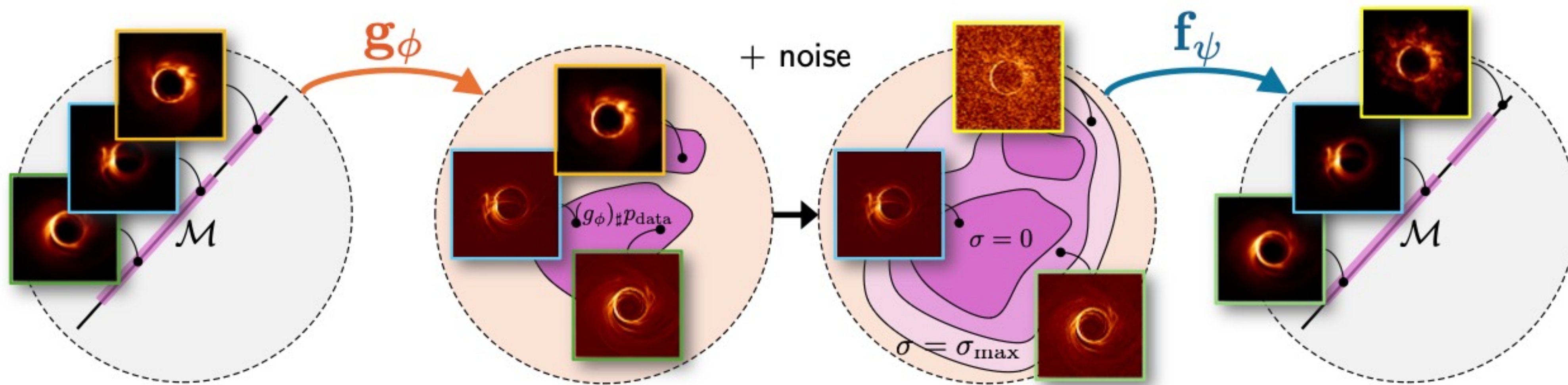
HARVARD & SMITHSONIAN

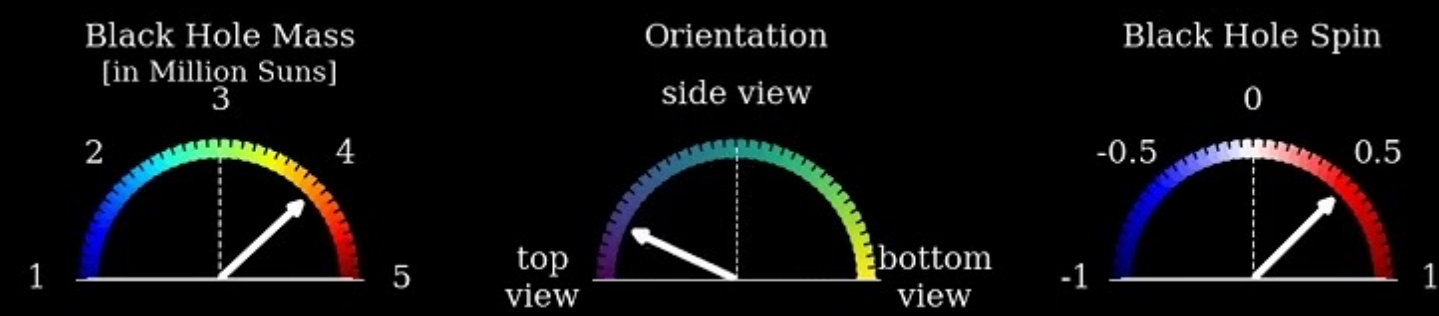


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Constrained Diffusion Models

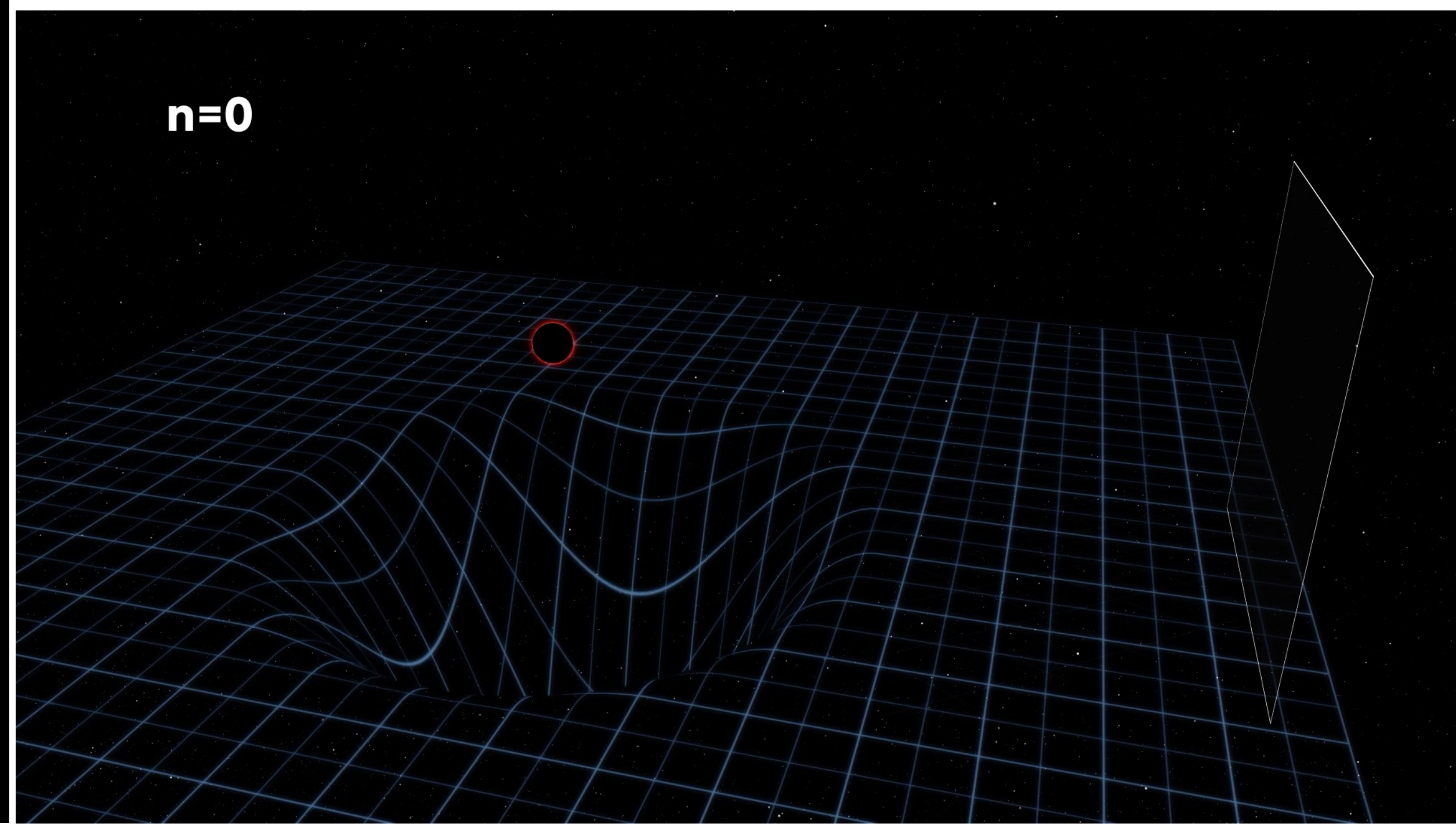
Mirror Diffusion Models for Constrained Generation





C. M. Fromm (Würzburg), Y. Mizuno (Shanghai), Z. Younsi (London), O. Foth (Amsterdam)
 H. Olivares (Nijmegen), A. Nathanail (Athens), A. Cruz-Orso, L. Weih and L. Rezzolla (Frankfurt)

GRMHD Simulations and Best-bet Model for Sagittarius A*
 ITP Goethe University, Frankfurt



Imaging a BH - Charles Gammie's group

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AI Experts



Bill Freeman, CS



Melanie Weber, A. Math



Robin Walters, CS



David Alvarez-Melis, CS

AstroAI Leadership



Cecilia Garraffo



Jack Steiner



Rafael Martinez



Kari Haworth



Ashley Villar



Phill Cargile



Doug Finkbeiner



Floor Broekgaarden



Carol Cuesta-Lazaro



Josh Wing



Alex Gagliano



Nayantara Mudur

The Team

Physicists



Adam Foster
AtomDB

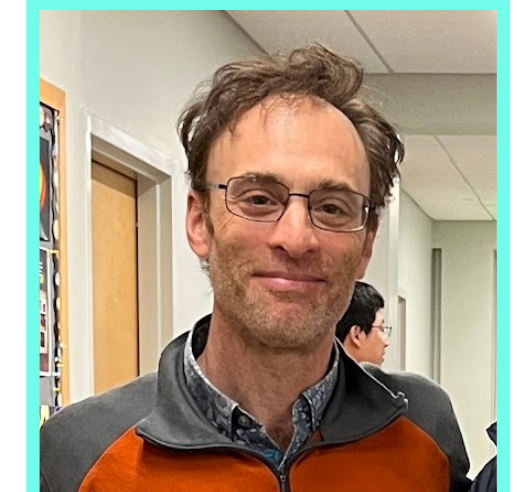


Iouli Gordon
HITRAN

Astronomers



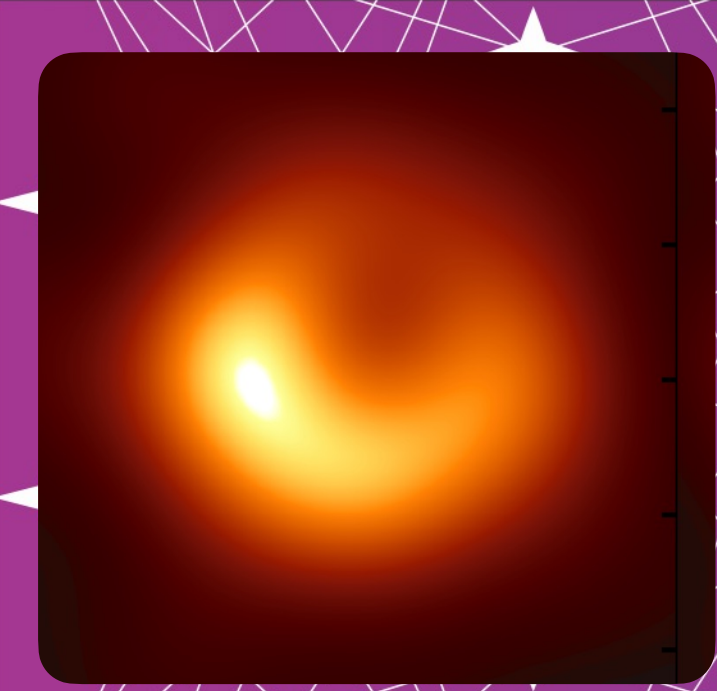
Mercedes Lopez-Morales



Shep Doeleman, EHT



Alberto Acomazzi
NASA / ADS



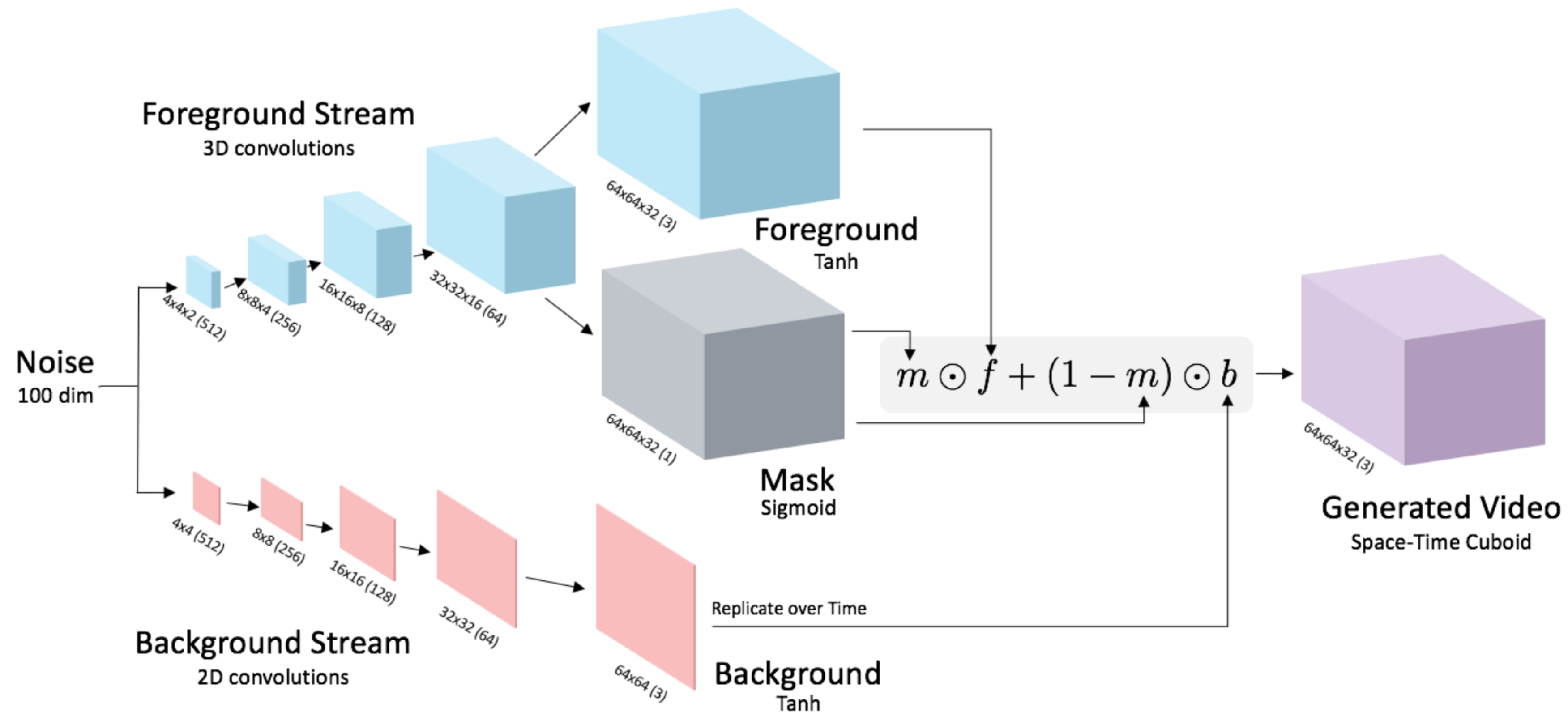
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David Loving

Generative Model for Black Holes' Dynamics



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Stellar
Spectra



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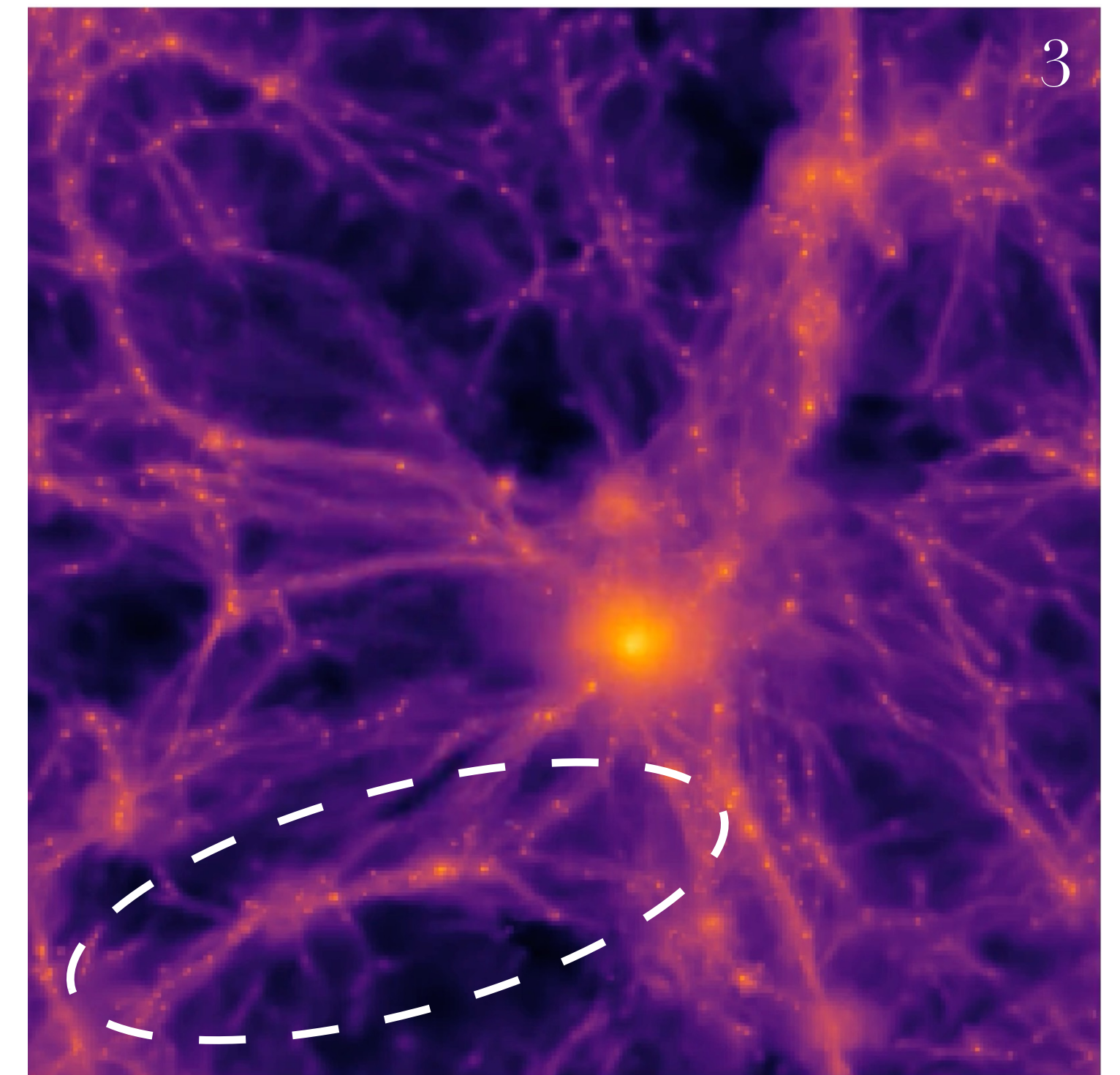
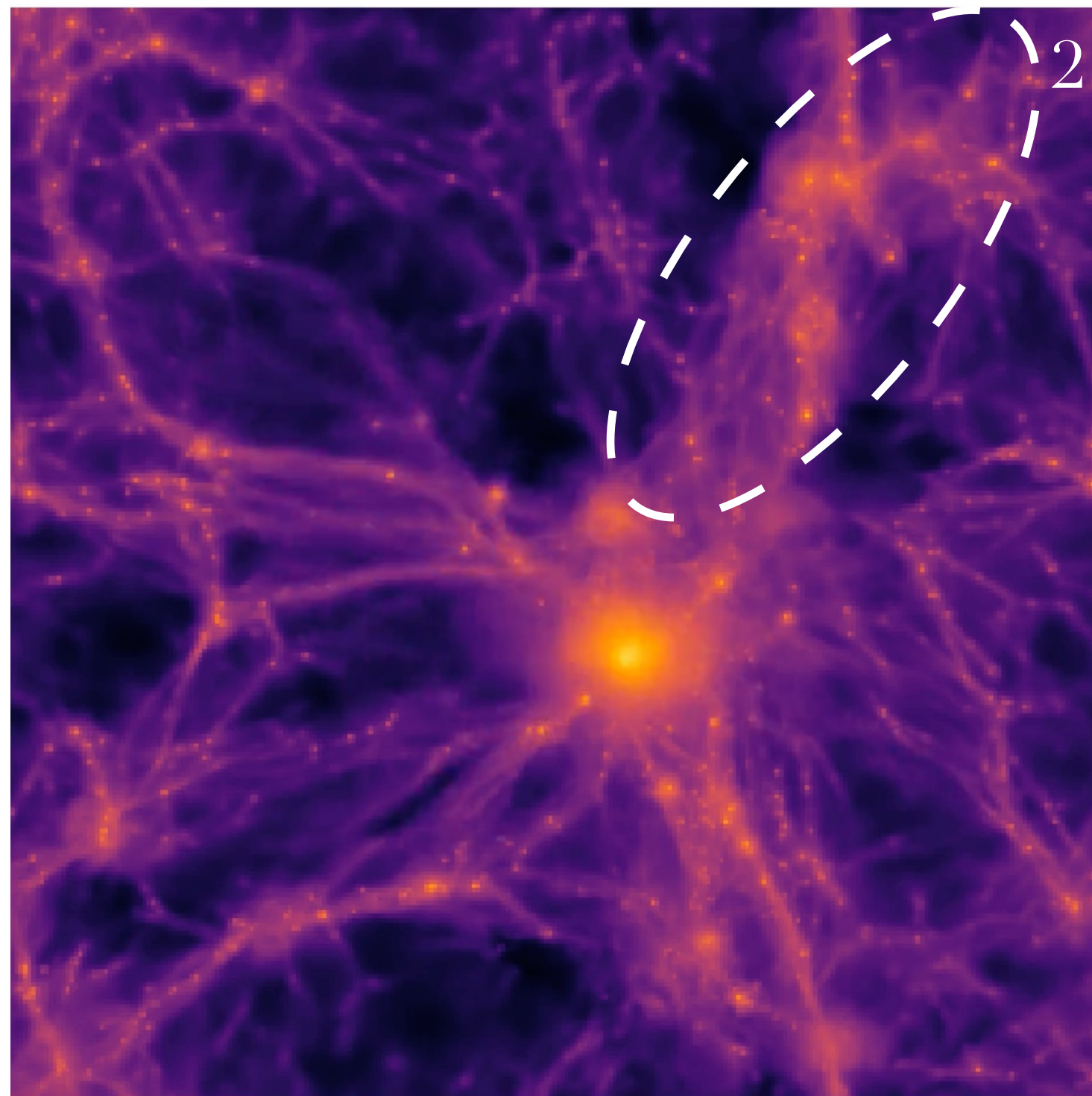
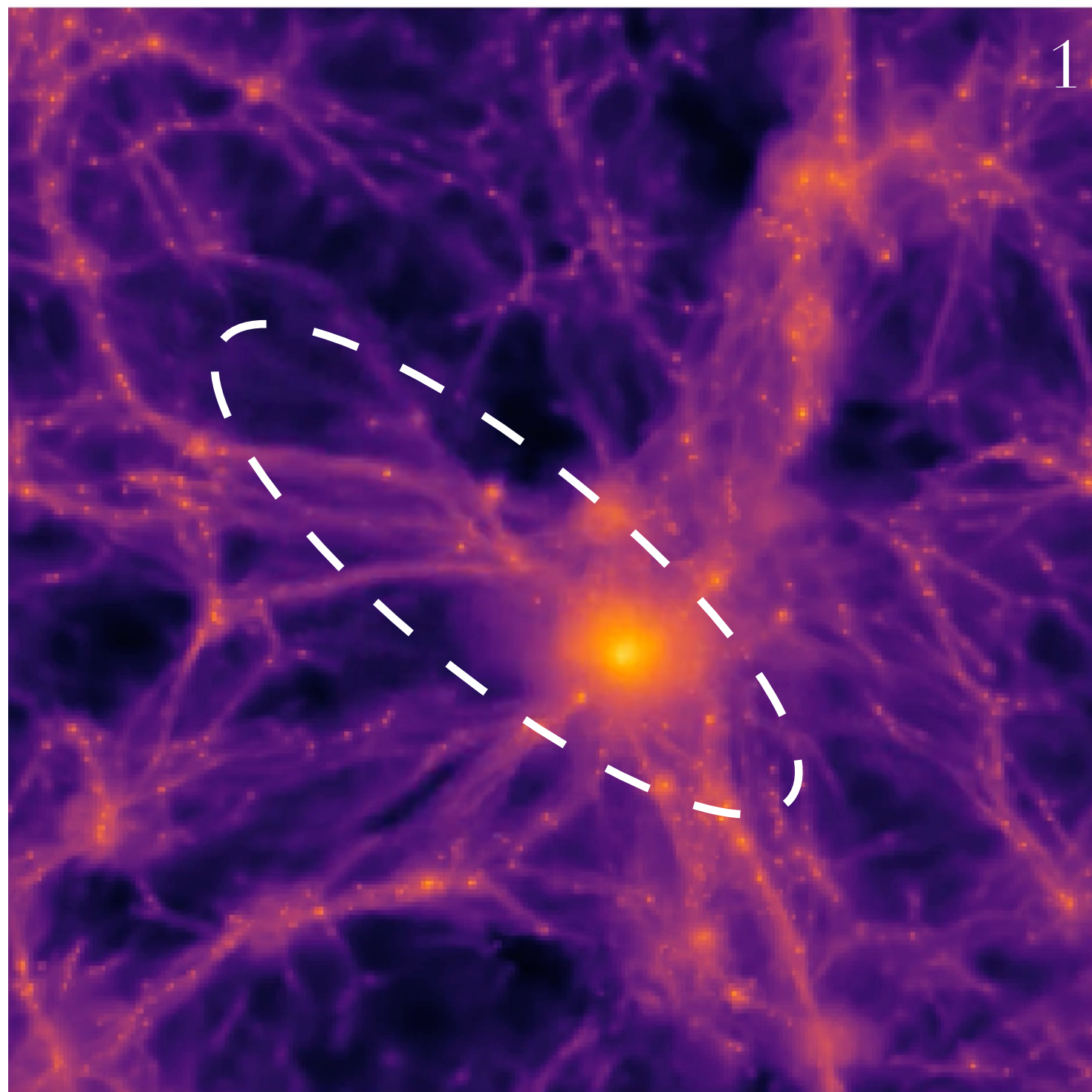
Stellar
Spectra



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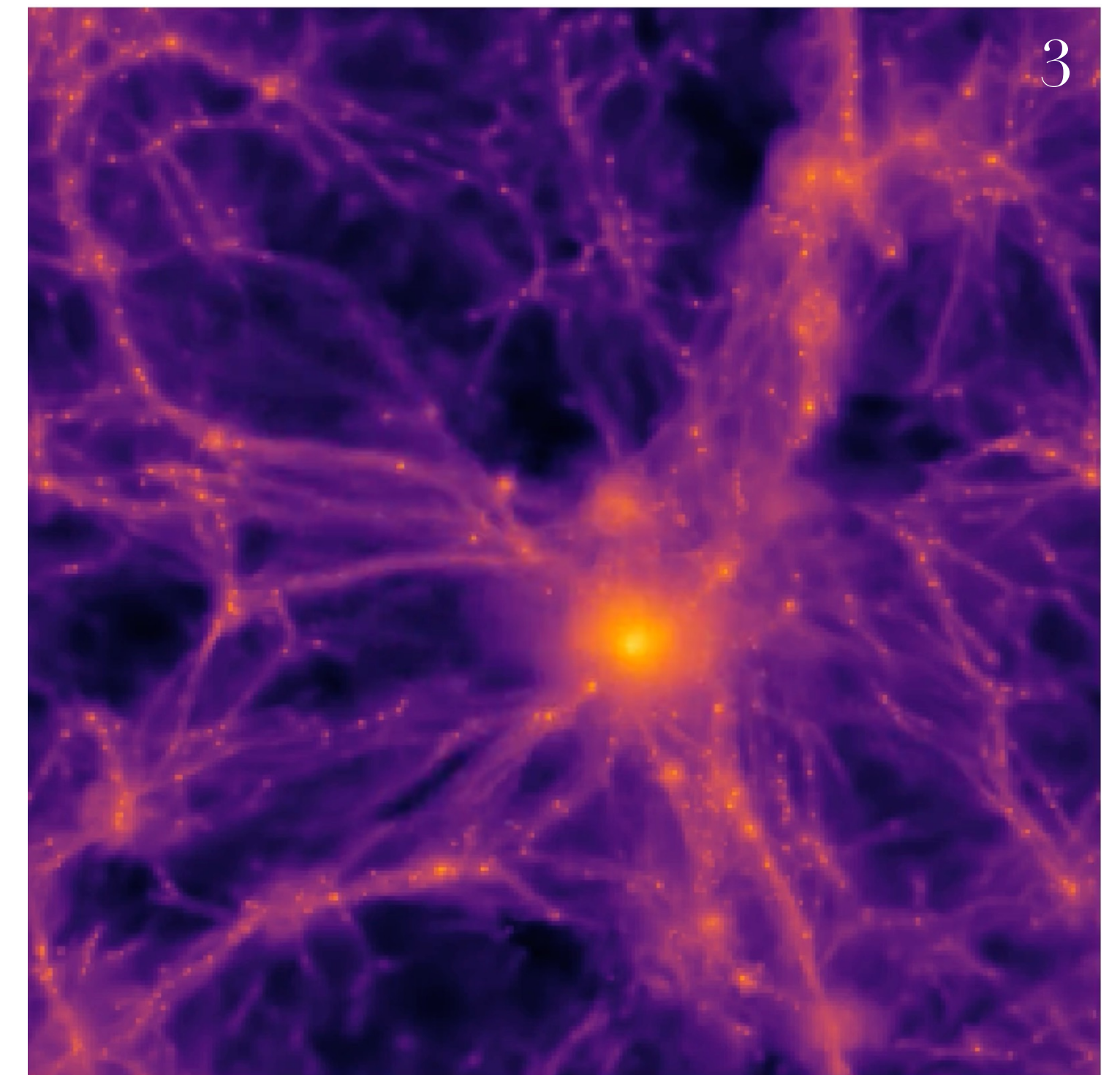
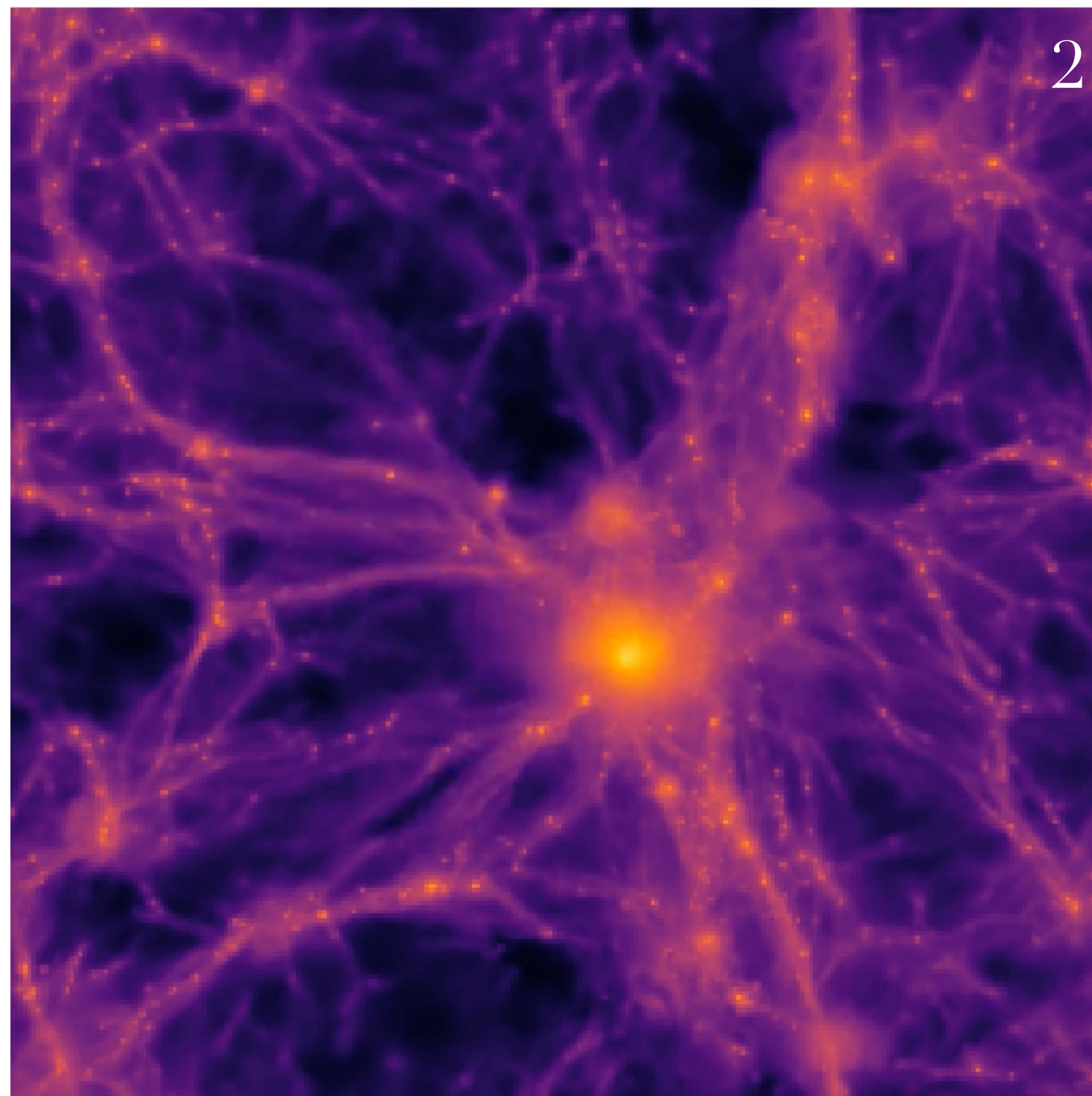
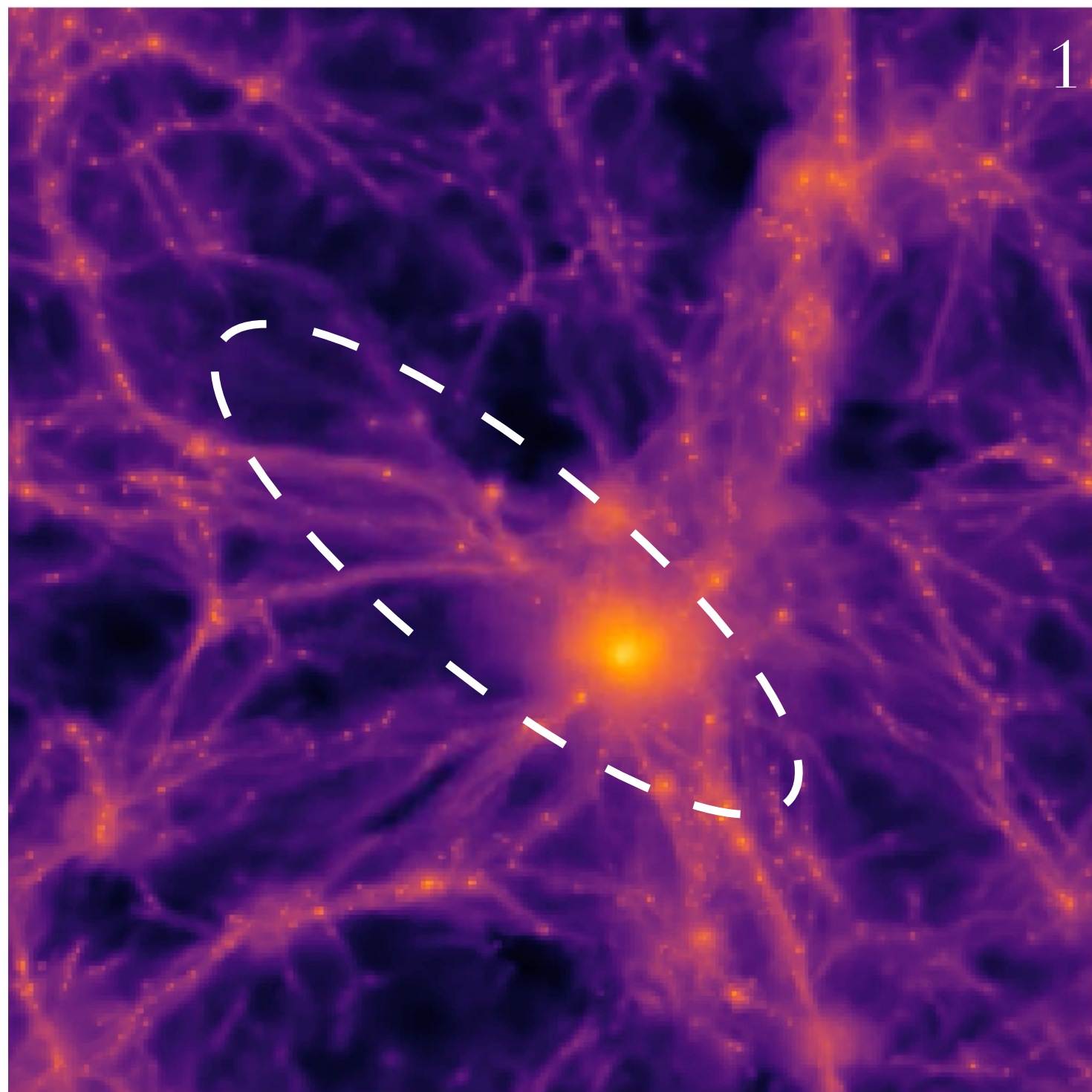
Galaxy Filament AI-Infill




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Galaxy Filament AI-Infill





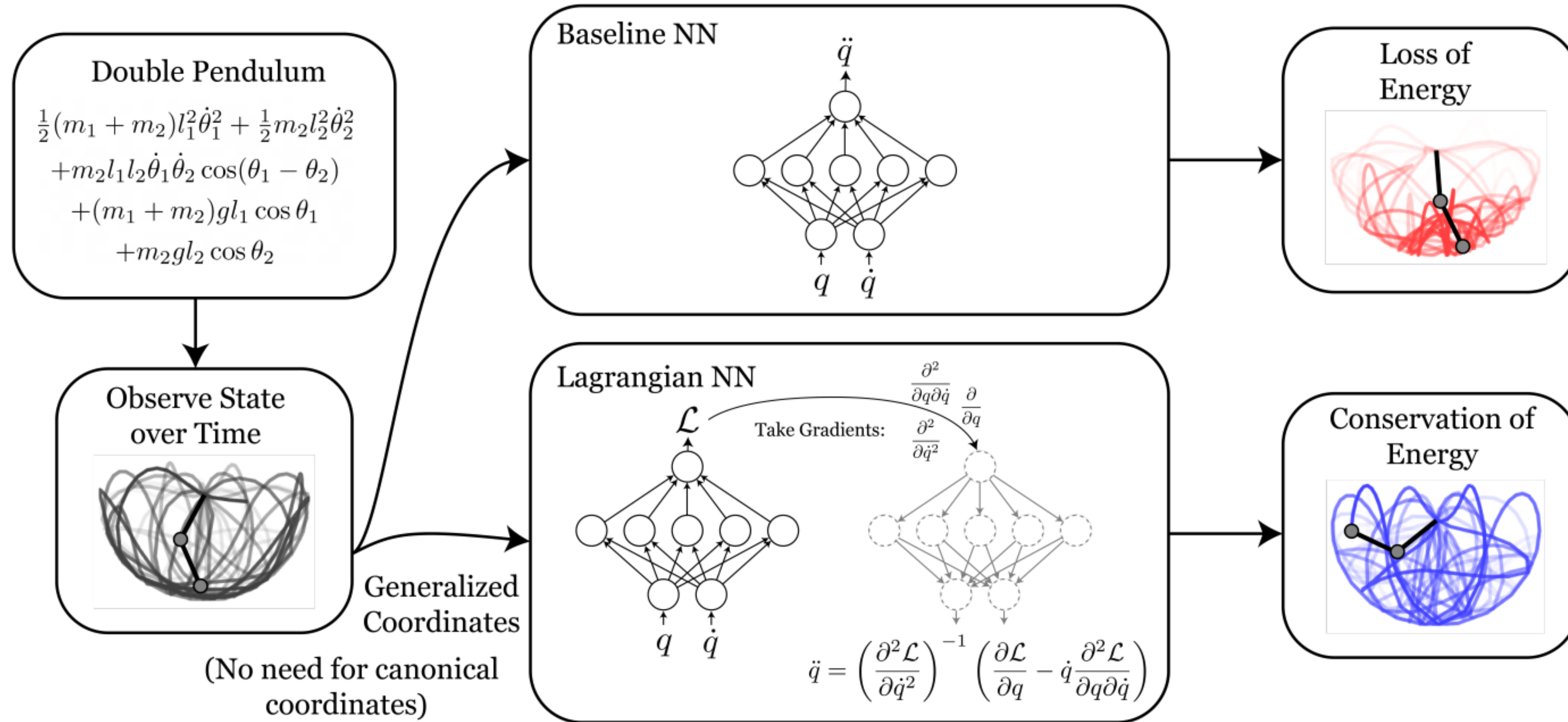
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The Scientific Questions

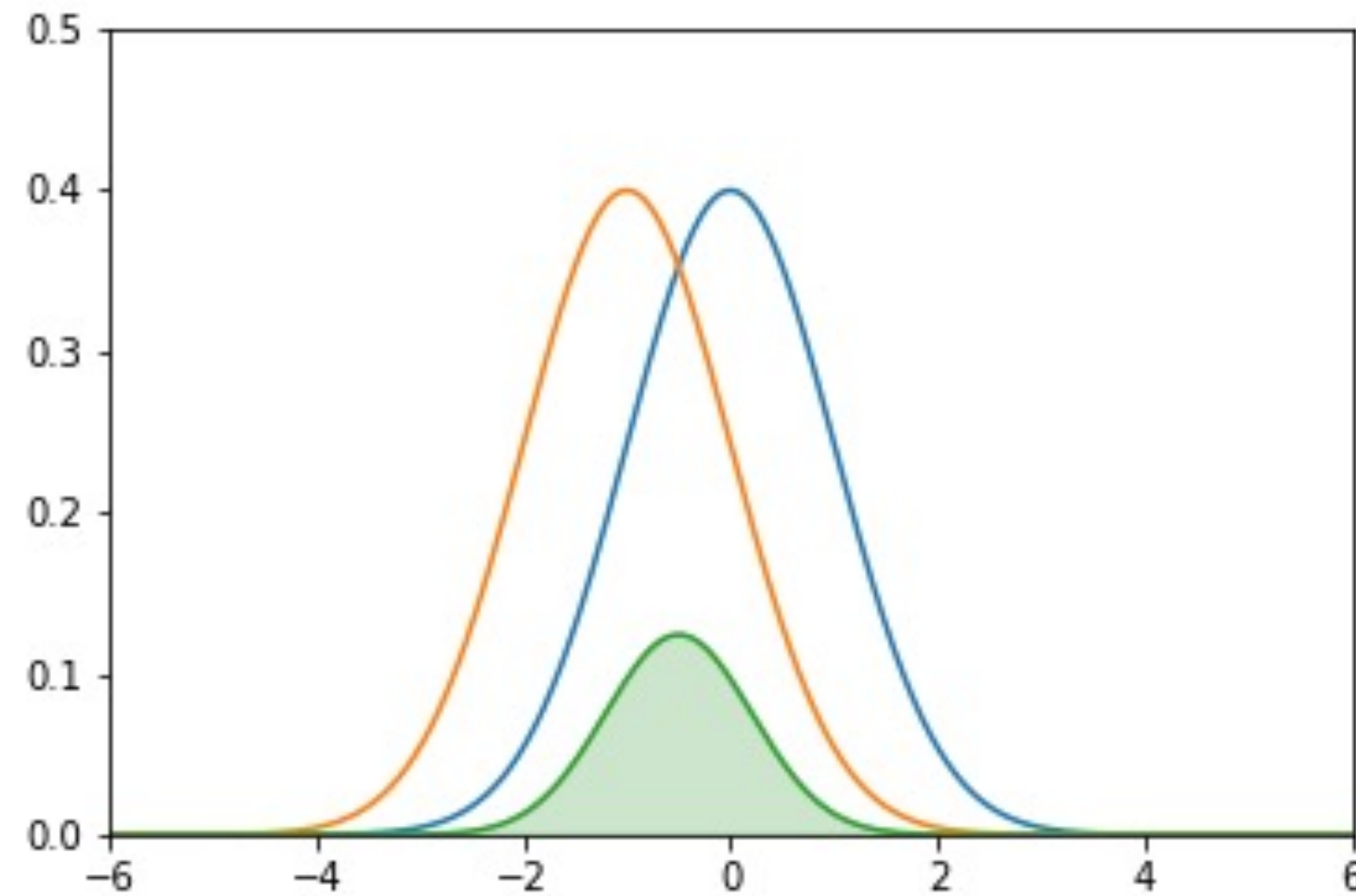
- *Are we alone in the Universe?*
- *How do Black Holes form and evolve?*
- *What are the unique events in the dynamic sky?*
- *What is our Universe made of and how did it start?*
- *Can we extract new understanding from our collective knowledge?*
- *What are the fundamental laws of physics?*

Lagrangian Neural Networks



StelNet: A Hierarchical Bayesian Neural Network

Comparing distributions



$$\int \bar{P}_A \bar{P}_B dx = \bar{\varepsilon} |_{\max A = \max B}$$

$$\int \bar{P}_A \bar{P}_B dx = \varepsilon < \bar{\varepsilon}$$

$$\tau = \frac{\bar{\varepsilon} |_{\max A = \max B}}{\varepsilon} \quad \text{Tension}$$

A large tension means that the null hypothesis ($\max A = \max B$) is unlikely

Jeffrey's scale:

$\log \tau < 1$
not significant

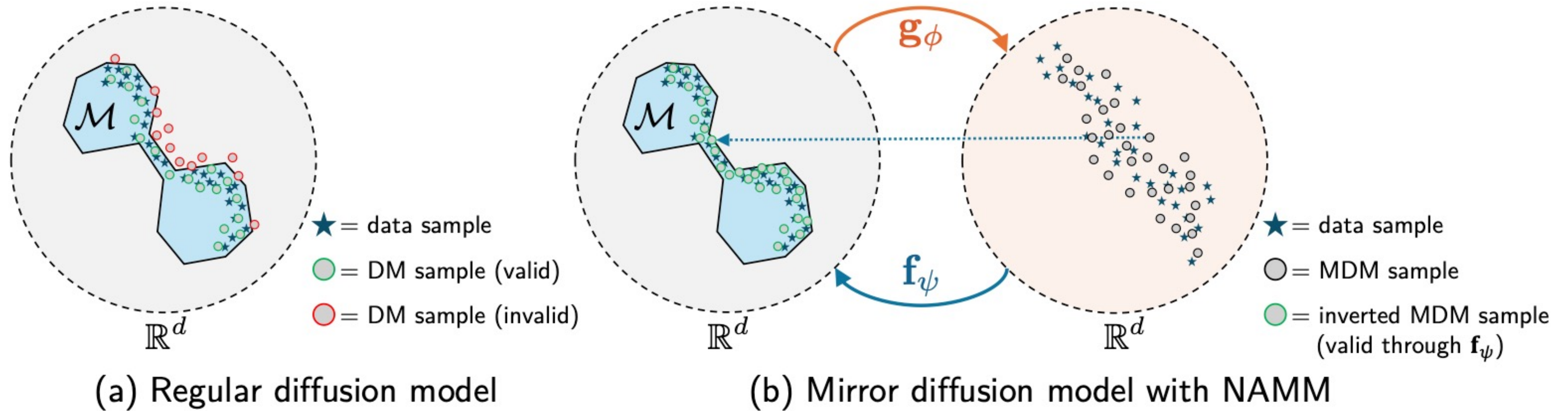
$1 < \log \tau < 2.5$
substantial

$\log \tau > 5$
highly significant

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Soft Constraints



Physical GenAI

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Symmetric Diffusion for Models with Conservation Laws

$$T : \phi \mapsto \phi + \Delta\phi$$

$$\& \quad \mathcal{L} \xrightarrow{T} \mathcal{L}$$

$$\implies \quad \partial_\mu j^\mu = 0 \quad , \quad j^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \Delta\phi$$

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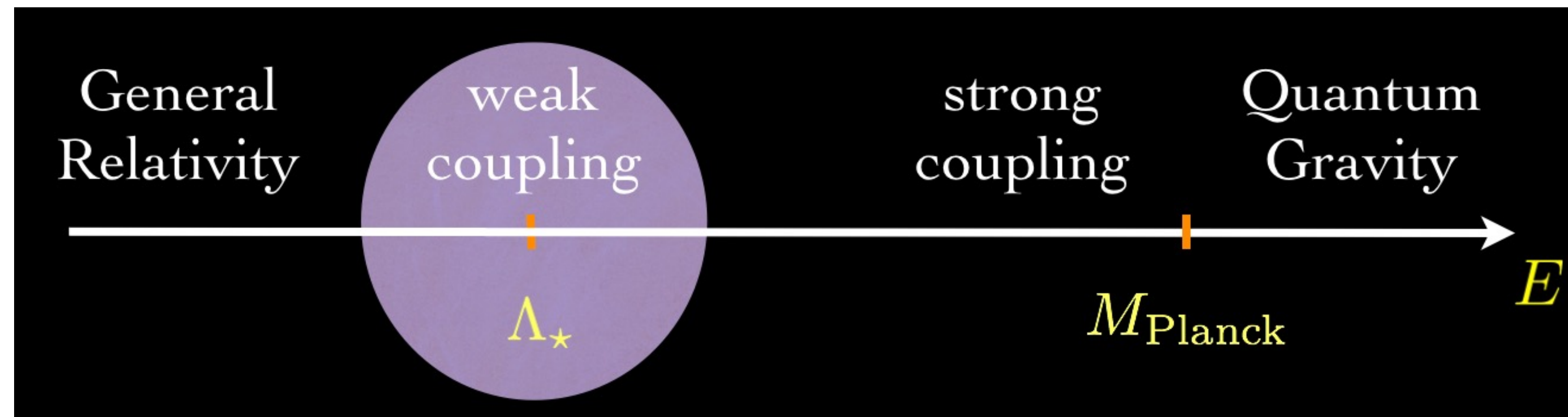
Towards a Quantum Theory of Gravity



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Classical vs Quantum Gravity



It is generally understood that **GR is a low energy effective theory** of a more general theory of Gravity. Low energy means **low space-time curvature** (large distance): there must be a scale at which higher-derivative terms arise

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Higher Order Gravity

$$\mathcal{L} = \int d^4x \sqrt{-g} (R - 2\Lambda)$$

Einstein-Hilbert Action
General Relativity

Einstein Gauss Bonnet
Lovelock Gravity

$$\mathcal{L} = \int d^4x \sqrt{-g} (R - 2\Lambda + \alpha \left(\frac{1}{3} R^2 - 2R_{\alpha\beta} R^{\alpha\beta} + R_{\alpha\beta\mu\nu} R^{\alpha\beta\mu\nu} \right))$$

A **single combination** at every order leads to second order Euler-Lagrange equations [[Lovelock, 1971](#)].
It is **non-trivial** iff $D \geq 2k + 1$ (for a k -th order term in the Riemann curvature).

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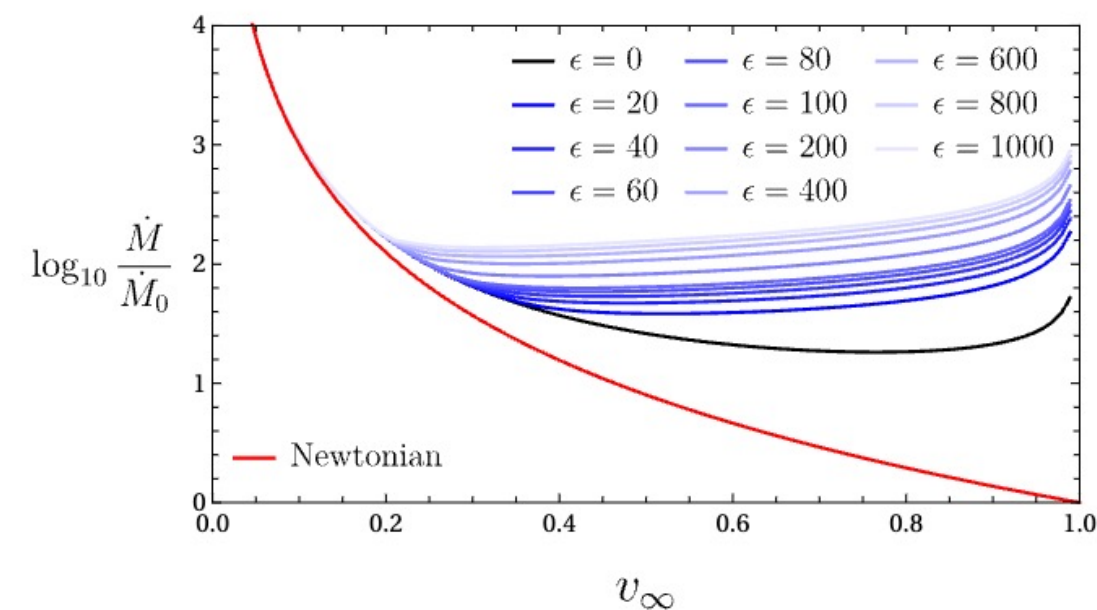
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Natural Extensions of GR

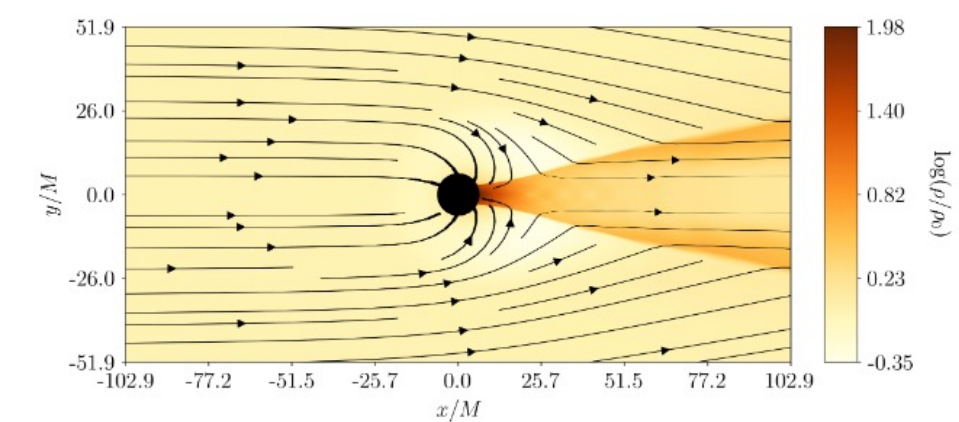
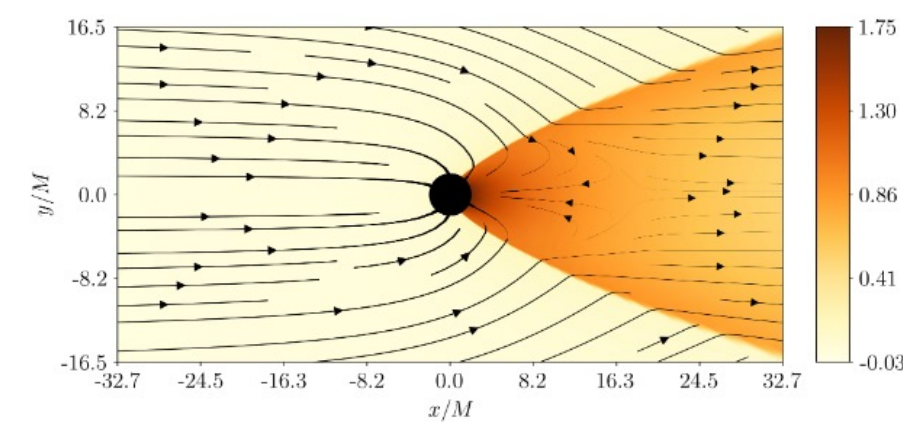
Cubic Gravity

$$\mathcal{L} = \int d^4x \sqrt{-g} (R - 2\Lambda + \sum_{n=2} \lambda_n \ell_\star^{2n-2} \mathcal{R}_{(n)})$$

Interestingly enough, higher curvature terms **magnify the black holes accretion rate** [Edelstein, Rivadulla Sánchez, Rodríguez Moris, Tejada, 2024])



where $\epsilon = \lambda_3 L_\star^4 / M^4$, both for wind and spherical accretion. They also tend to **increase the contrast in density** and **decrease the aperture angle of the shock cone**

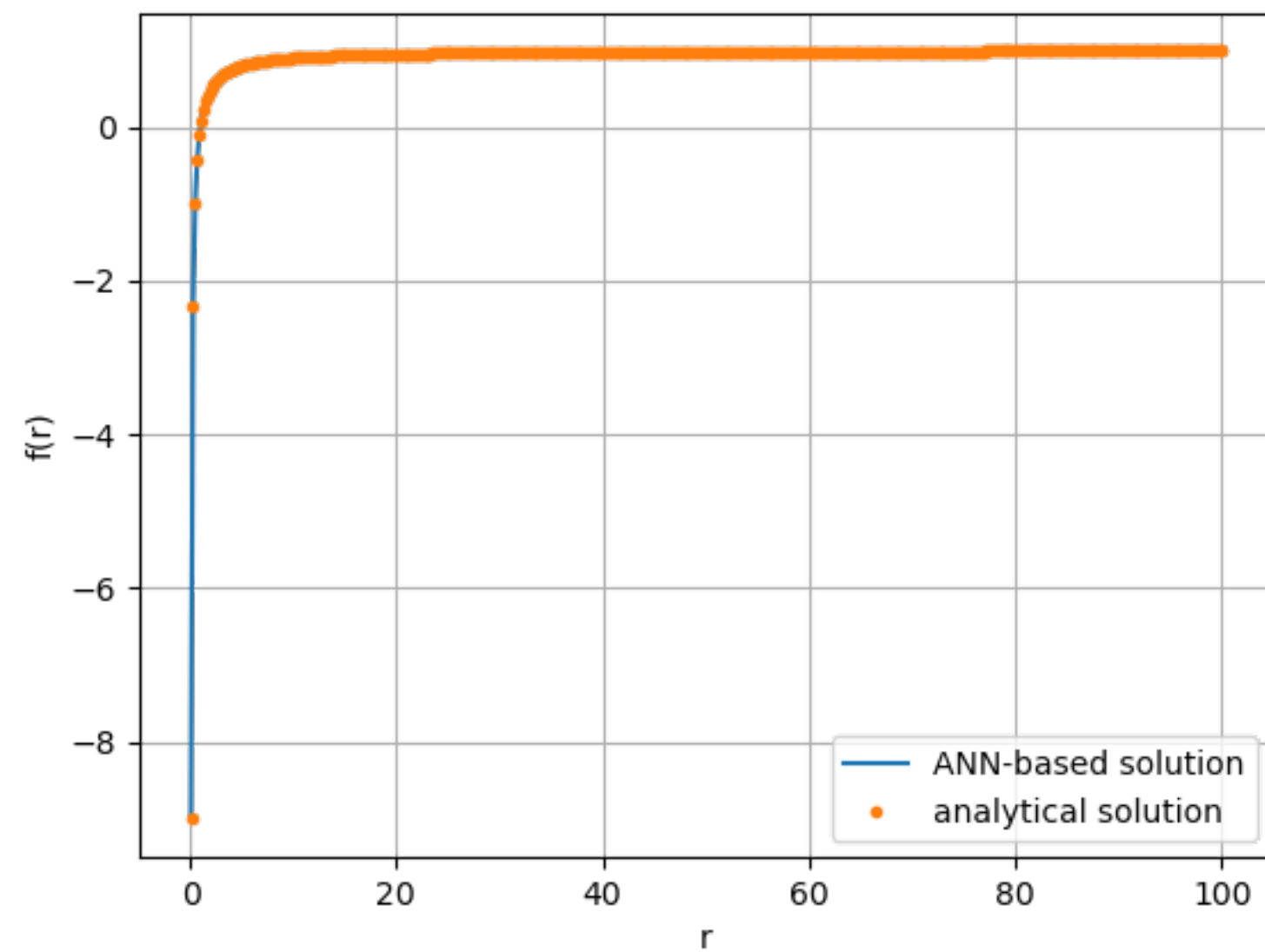


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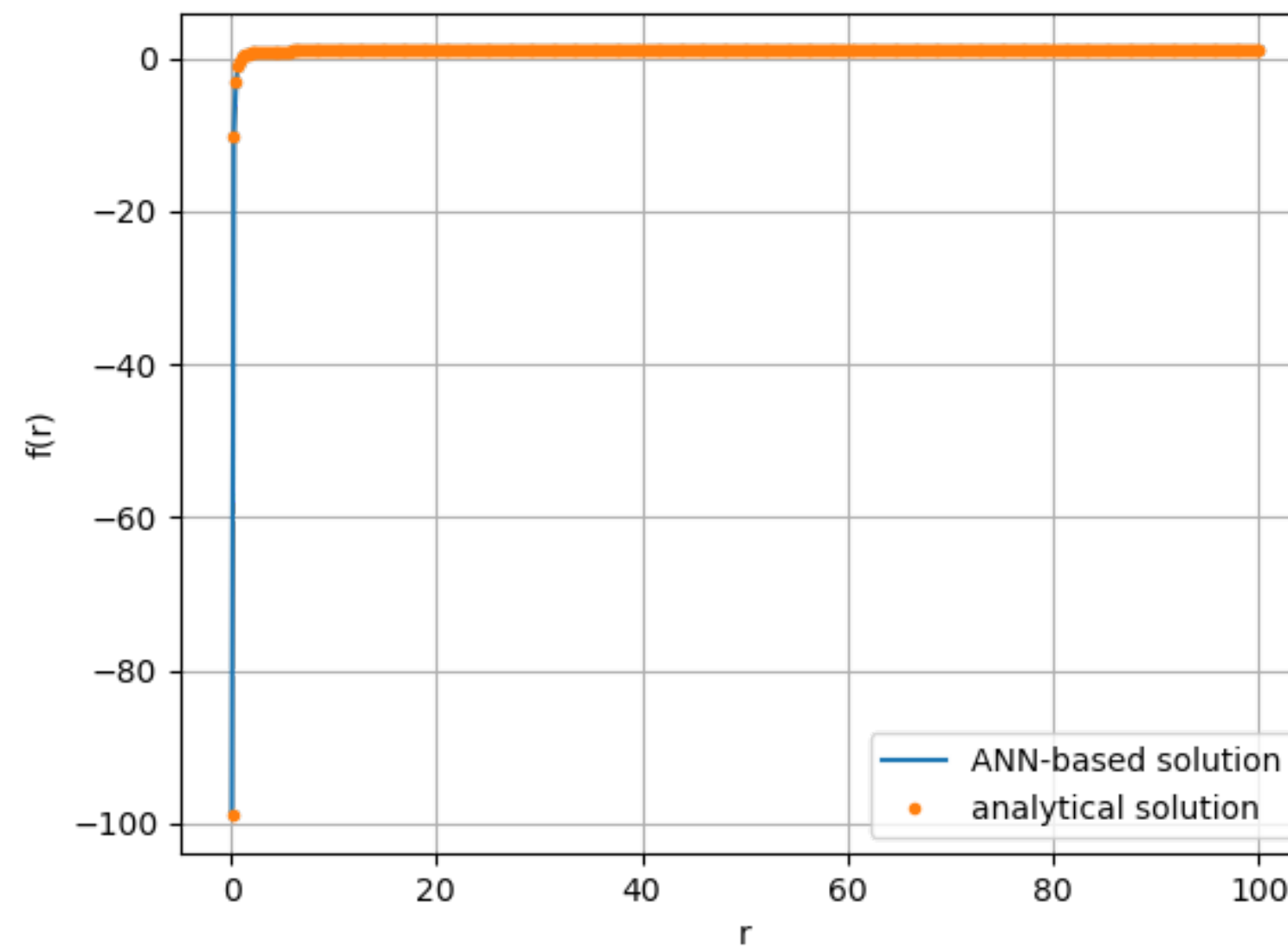
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Finding Solutions in Seconds

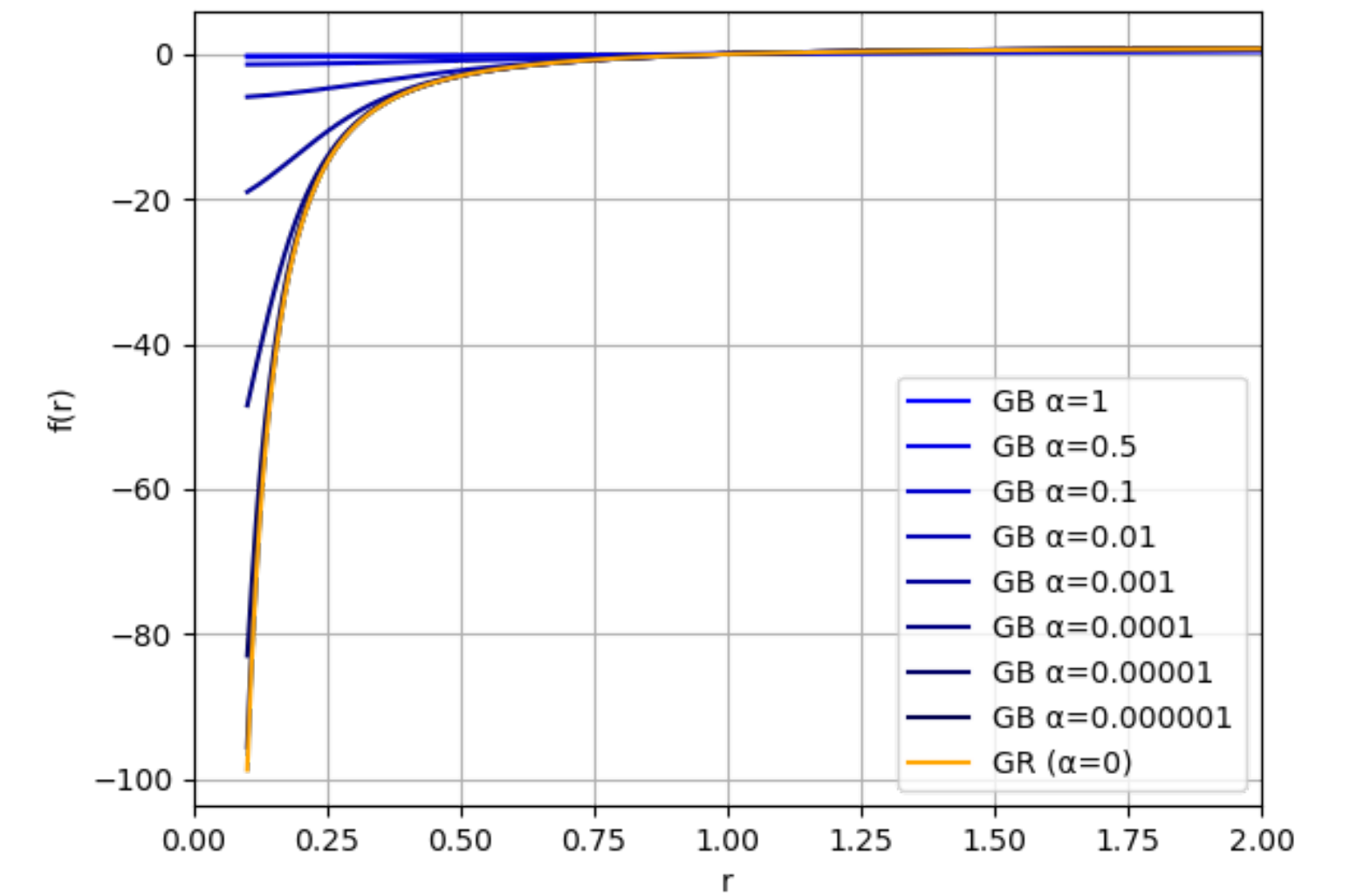
Schwarzschild BH



Schwarzschild BH in 5D



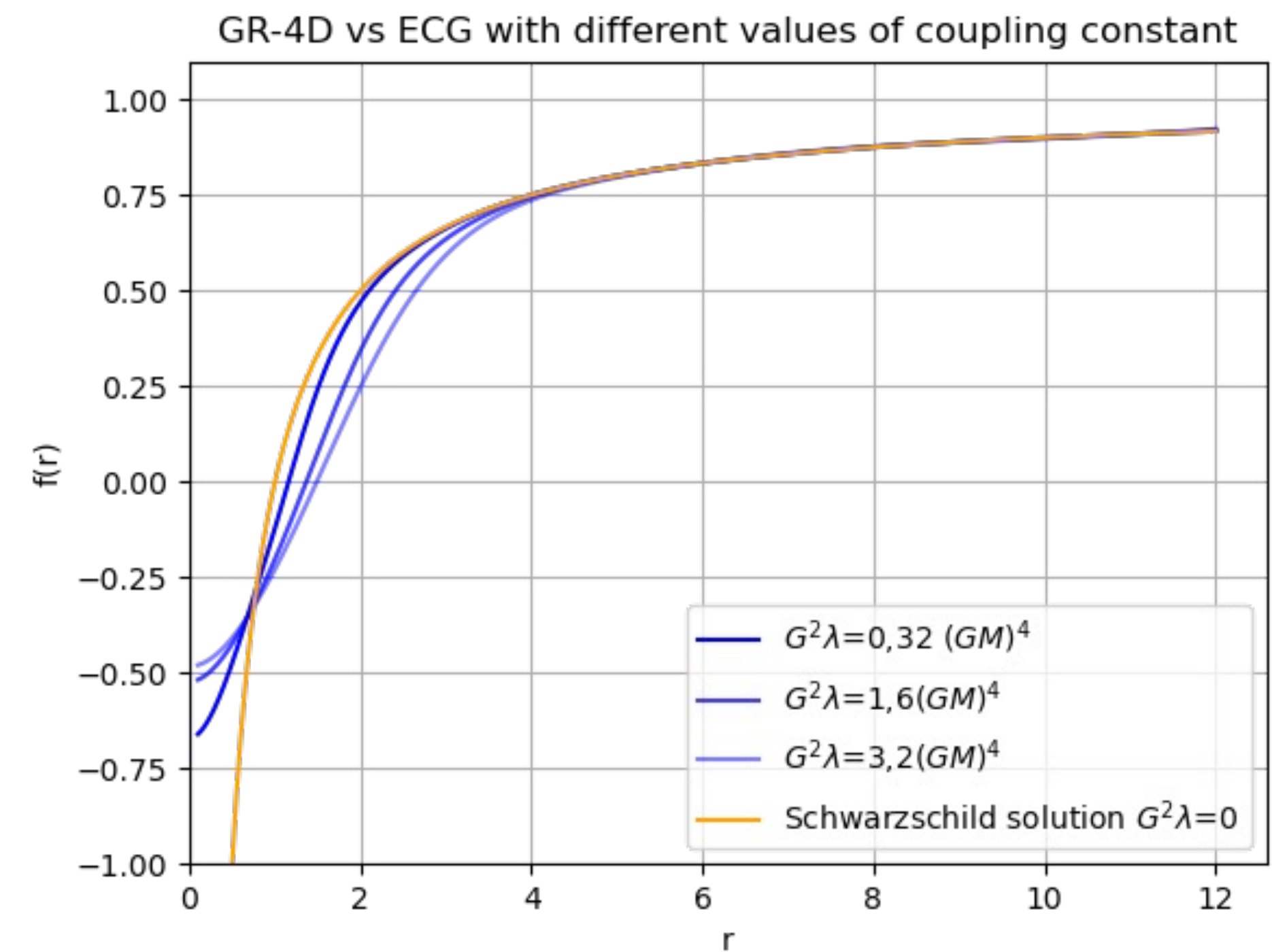
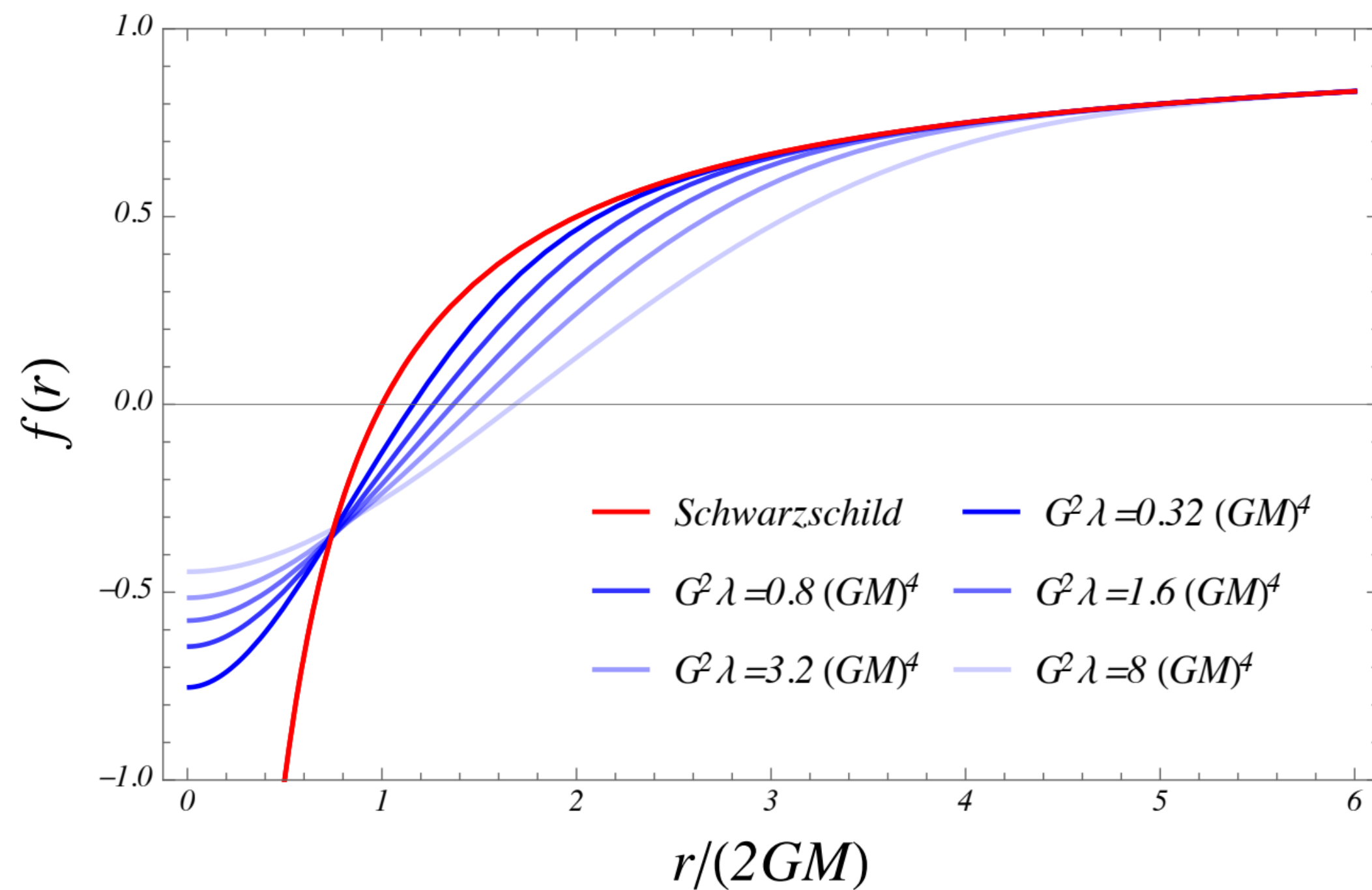
GR-5D vs Gauss Bonnet with different values of coupling constant



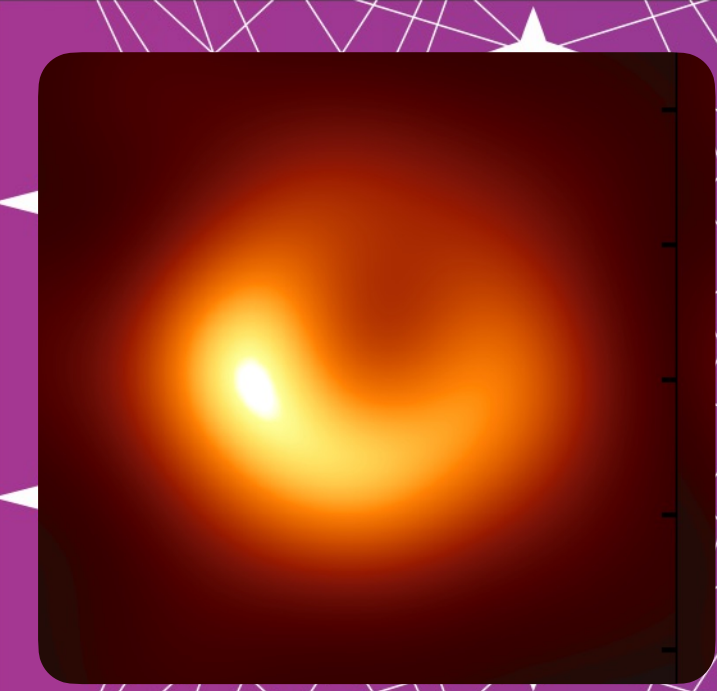
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Finding Solutions in Seconds

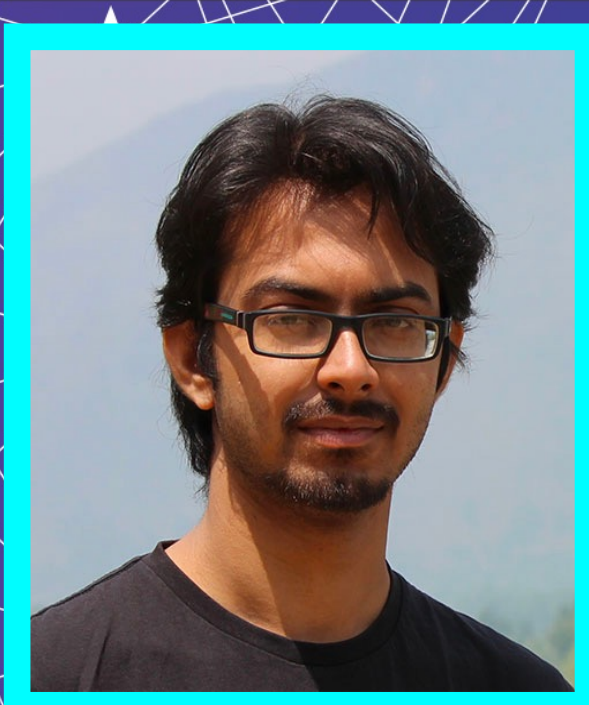


Breaking the Multiscale Barrier



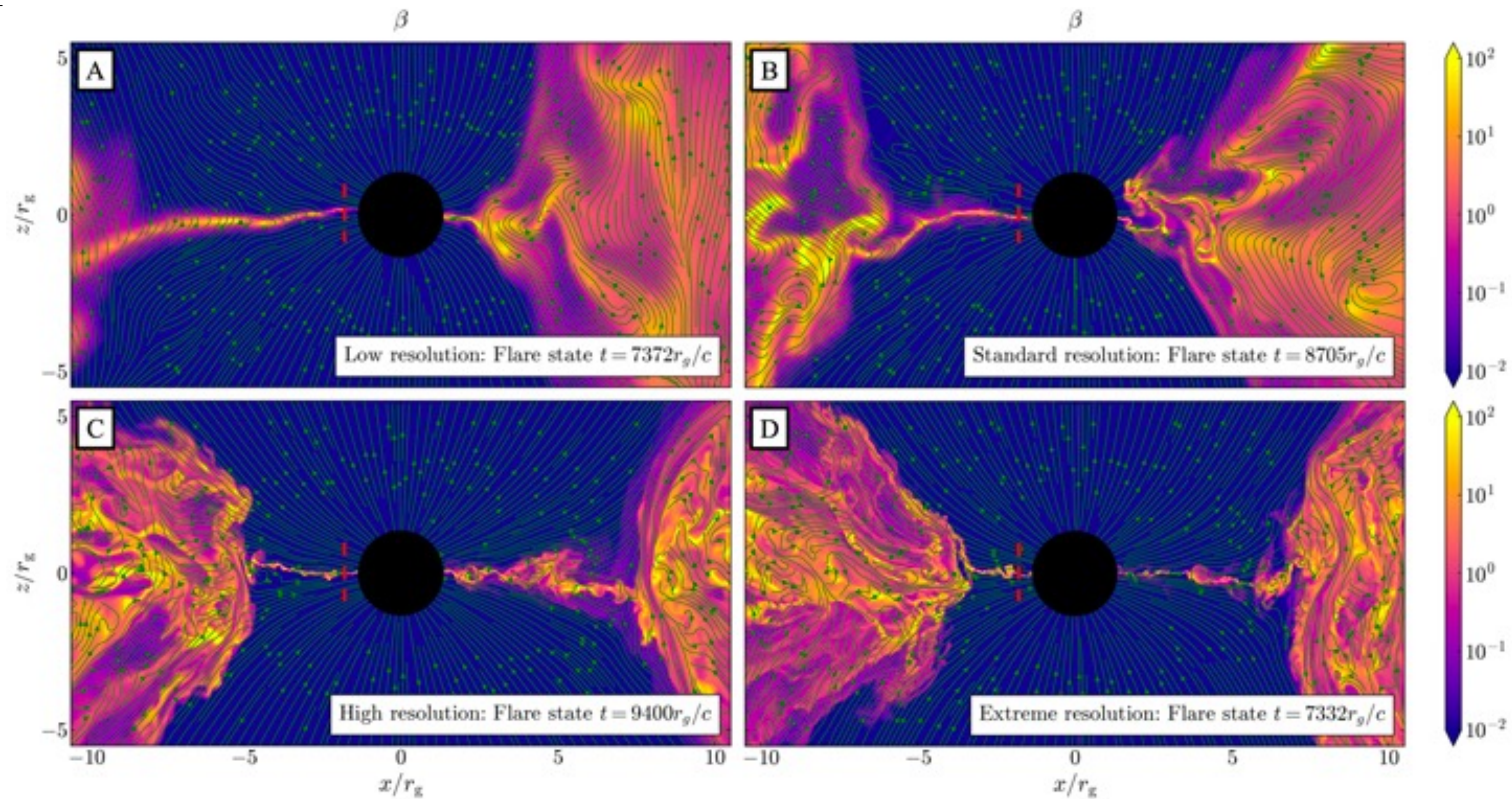
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Koushik
Chatterjee

Super resolution Model for GRMHD simulations for EHT



The Scientific Questions

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AI for Astronomy

Probabilistic

Physical

Interpretable

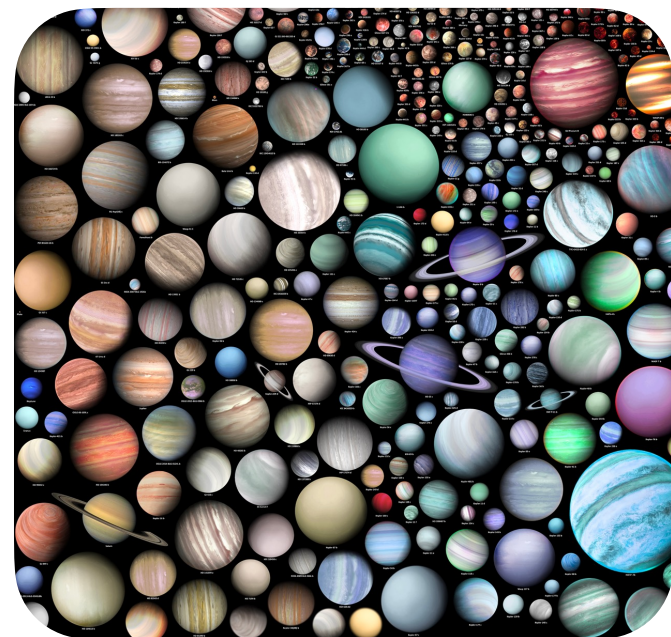
Robust

Multimodal

Multi-Scale

Generative

Open
Source



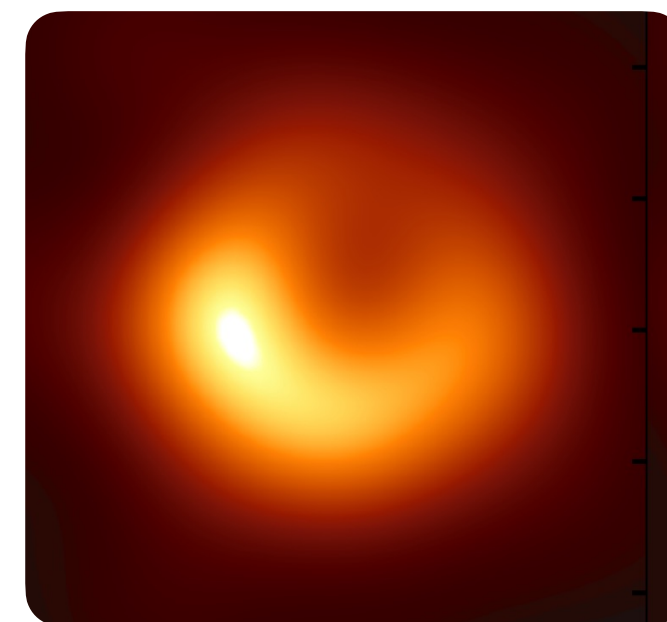
Biomarkers



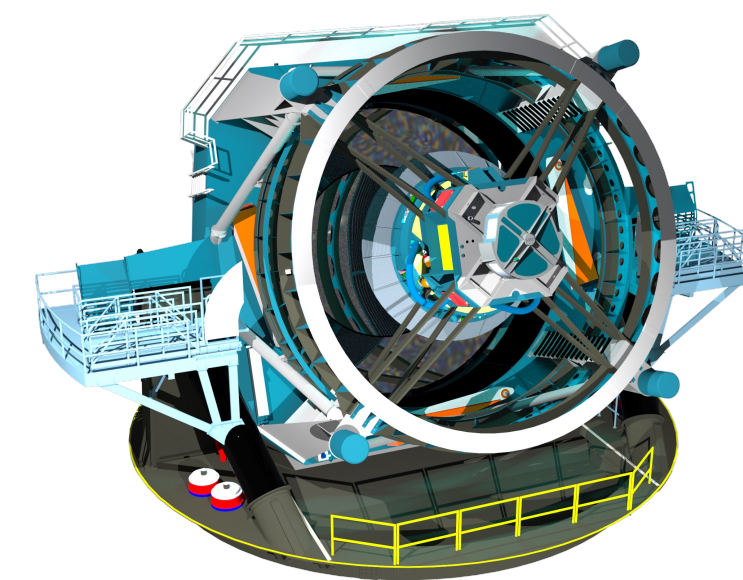
Stars



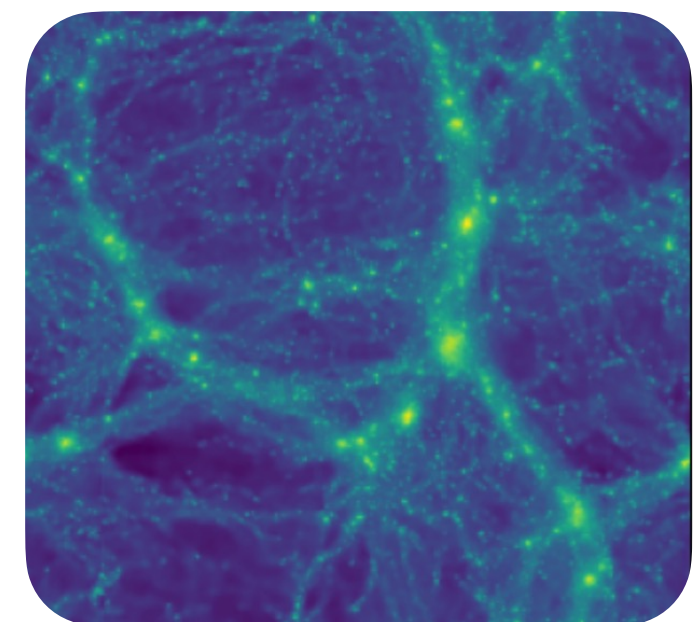
**LLMs for
Astronomy**



Black Holes



Dynamic Sky

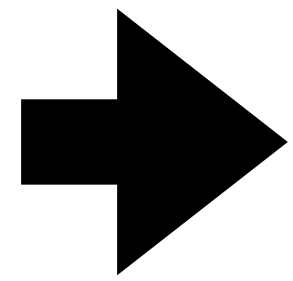
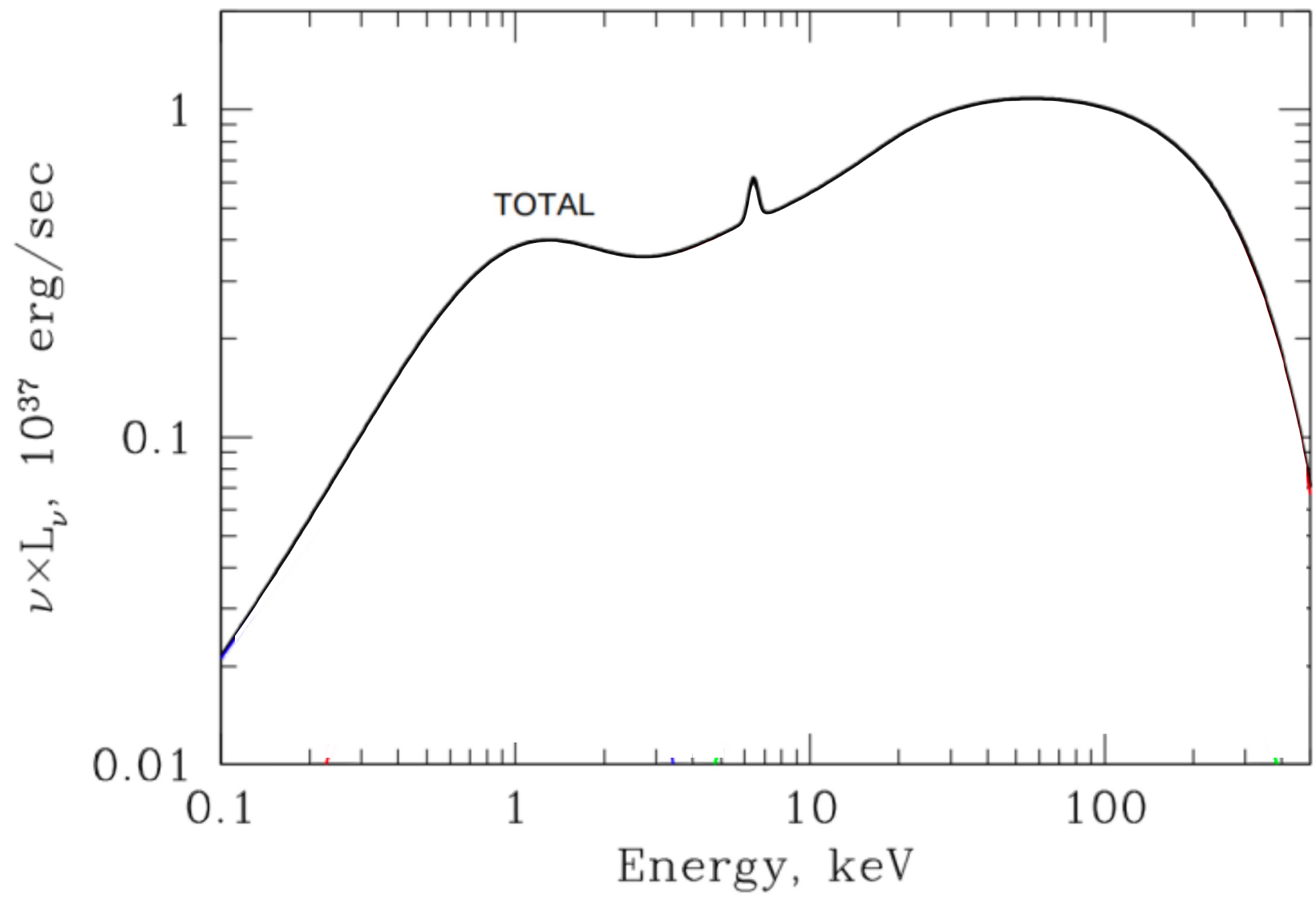


Cosmology

The Projects

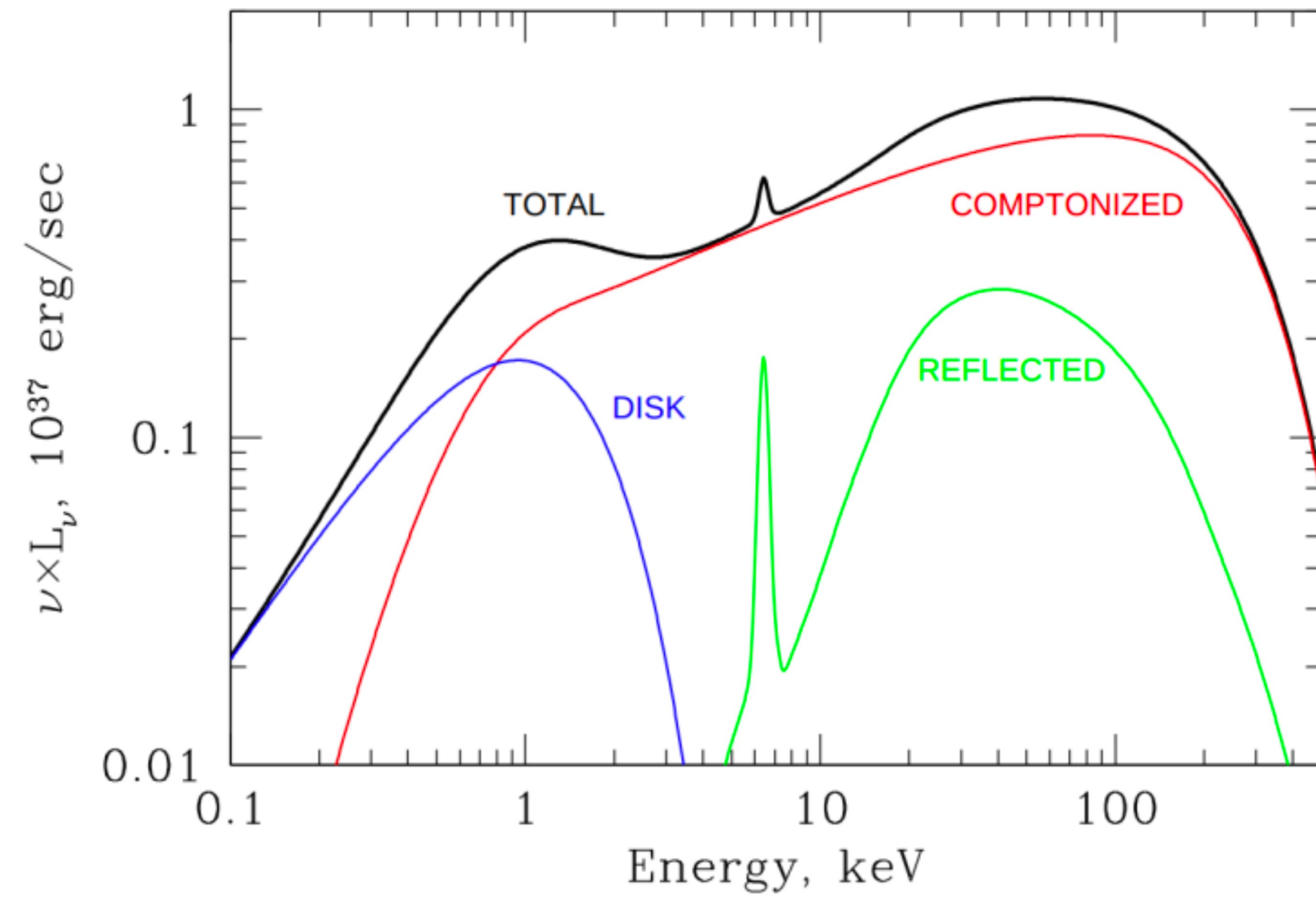


Jack Steiner



Expert

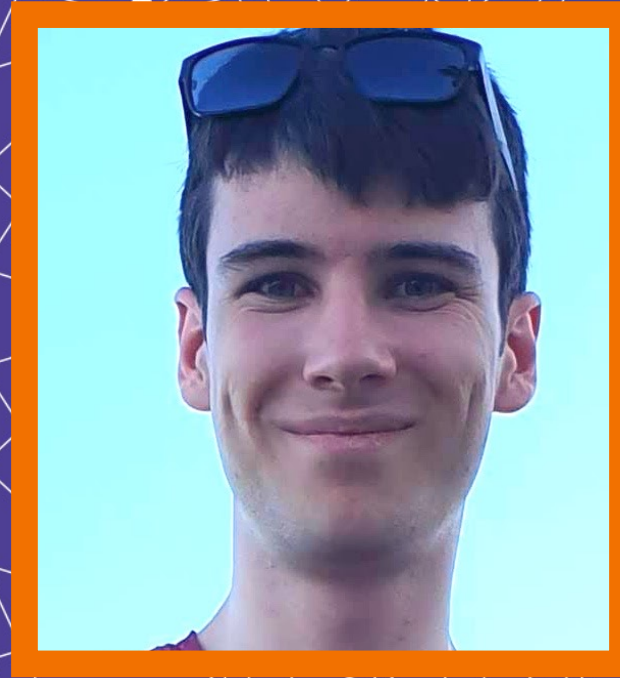
10,000 times!



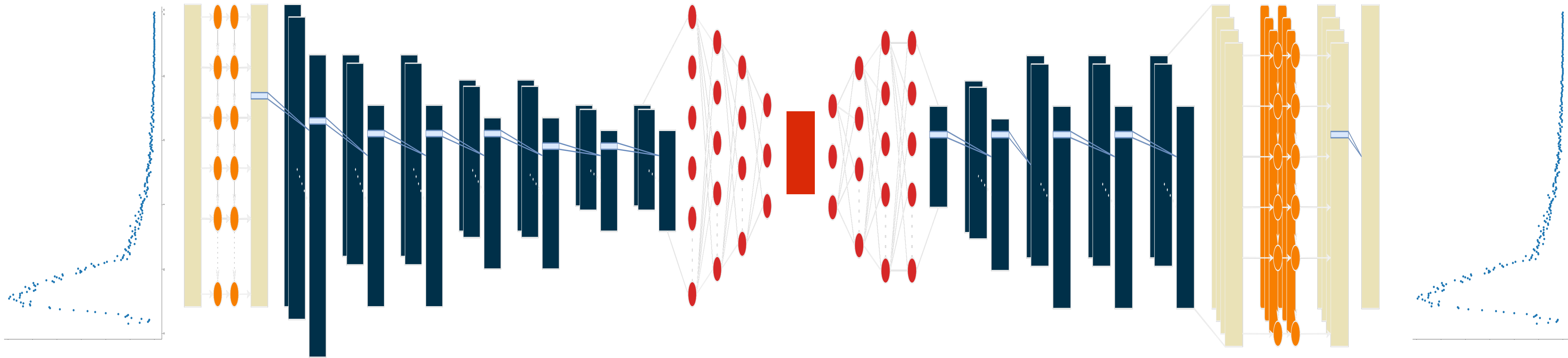
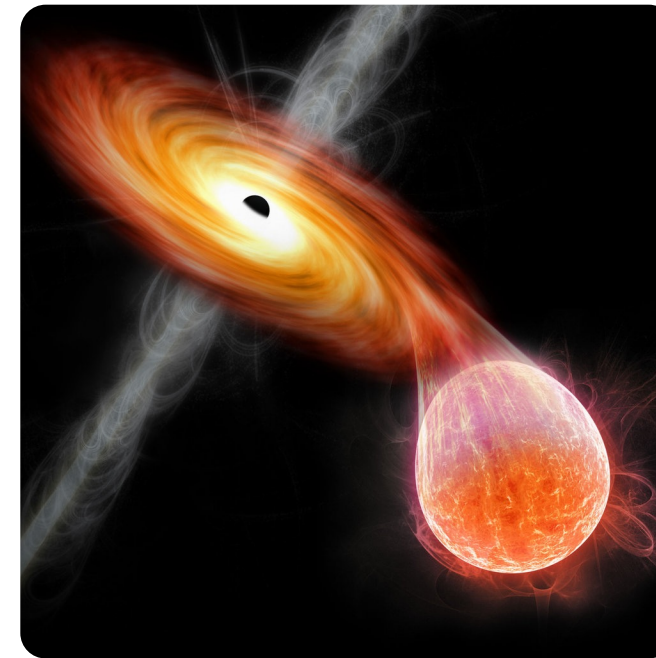
**Physical Parameters:
T, M, Spin**

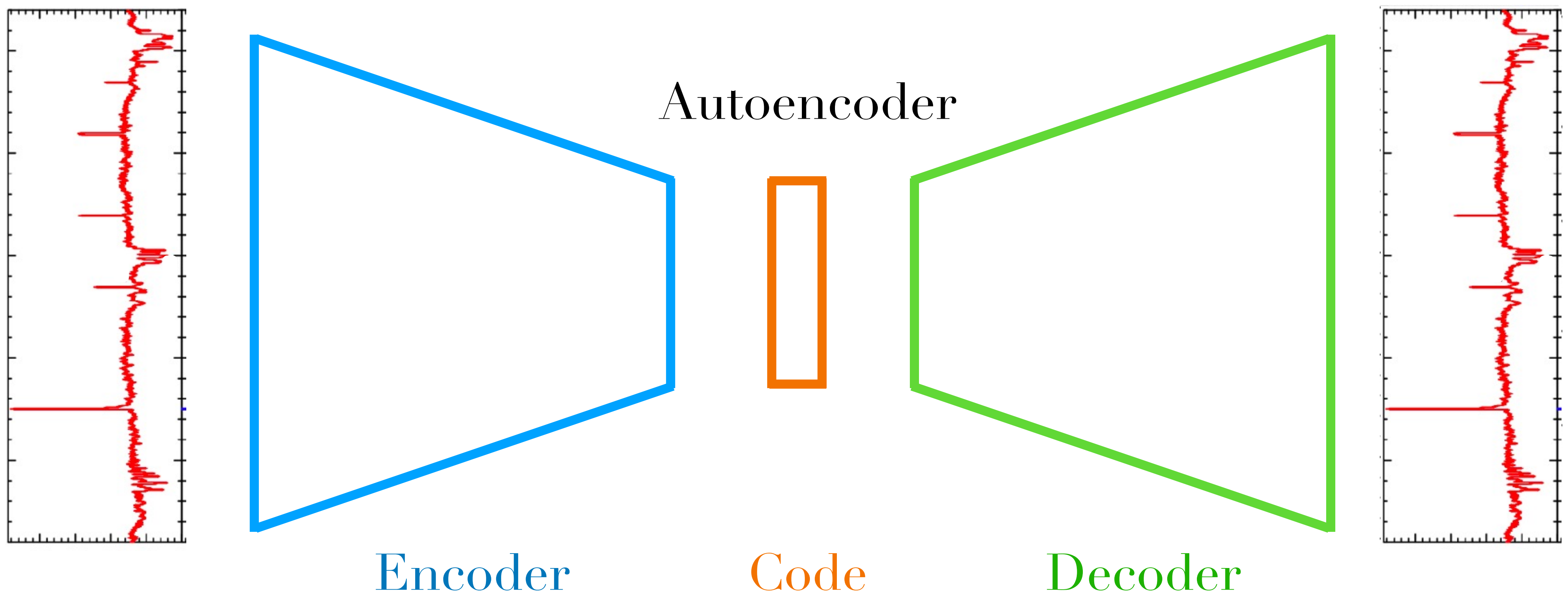
ASTROAI

Enabling Next Generation Astrophysics



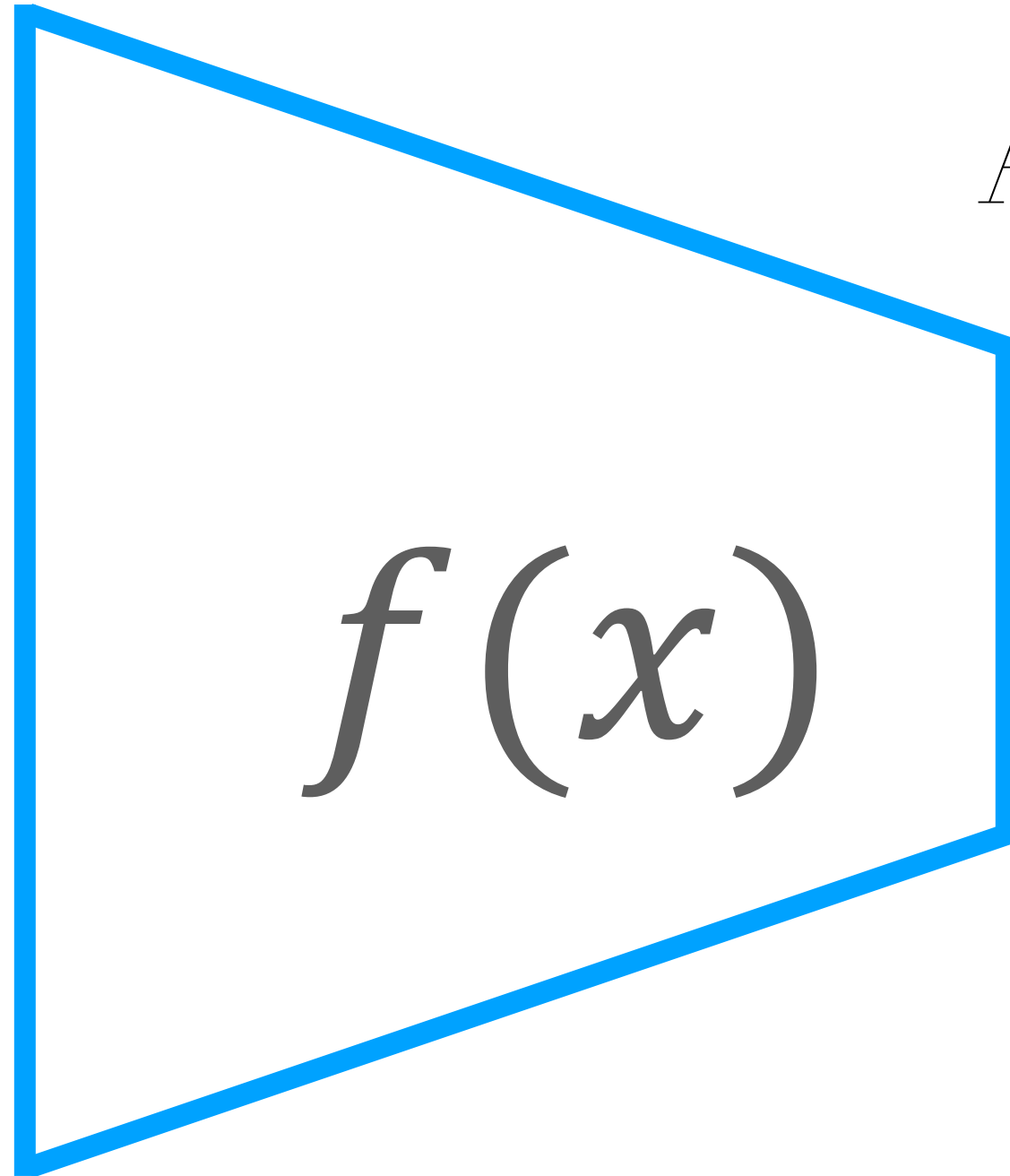
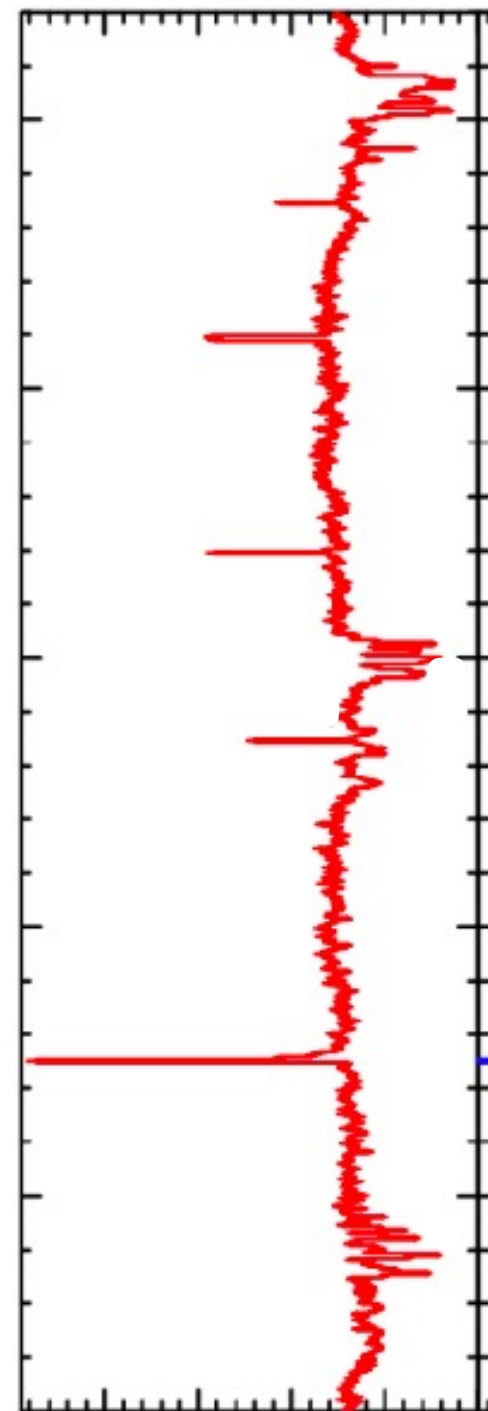
Ethan Tregidga



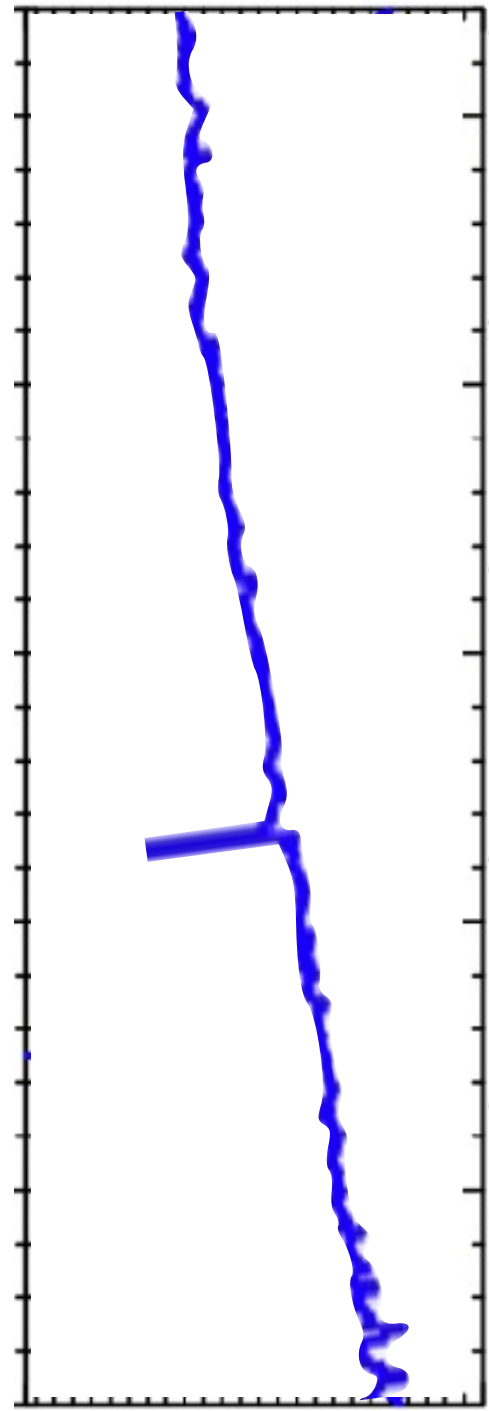
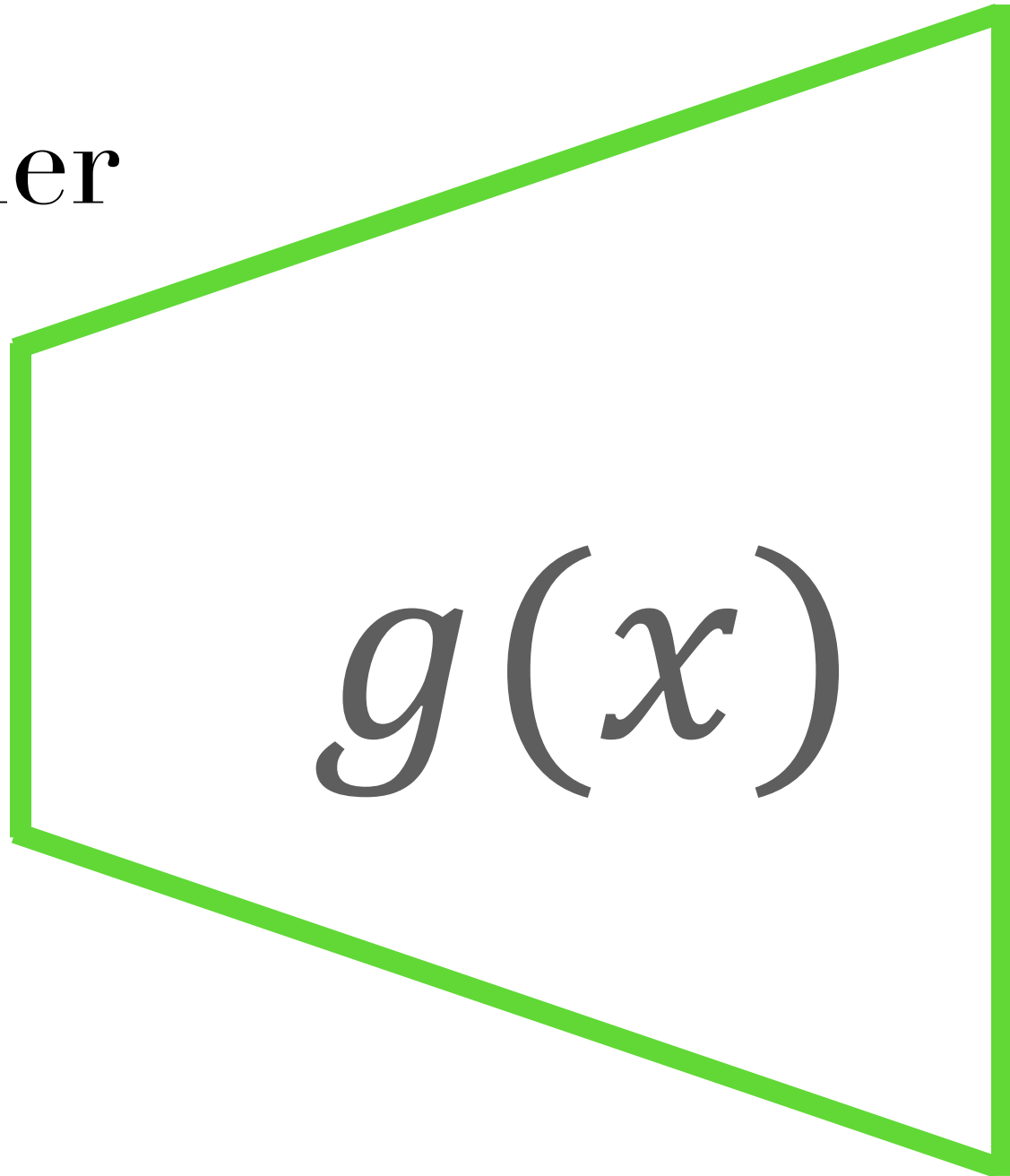
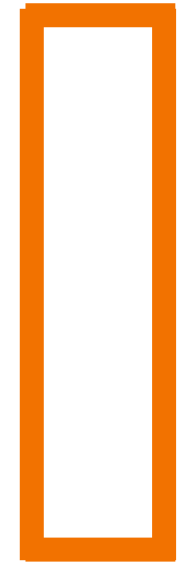


Primer Centro de IA en
Astrofísica

ASTROAI



Autoencoder



Encoder

Code

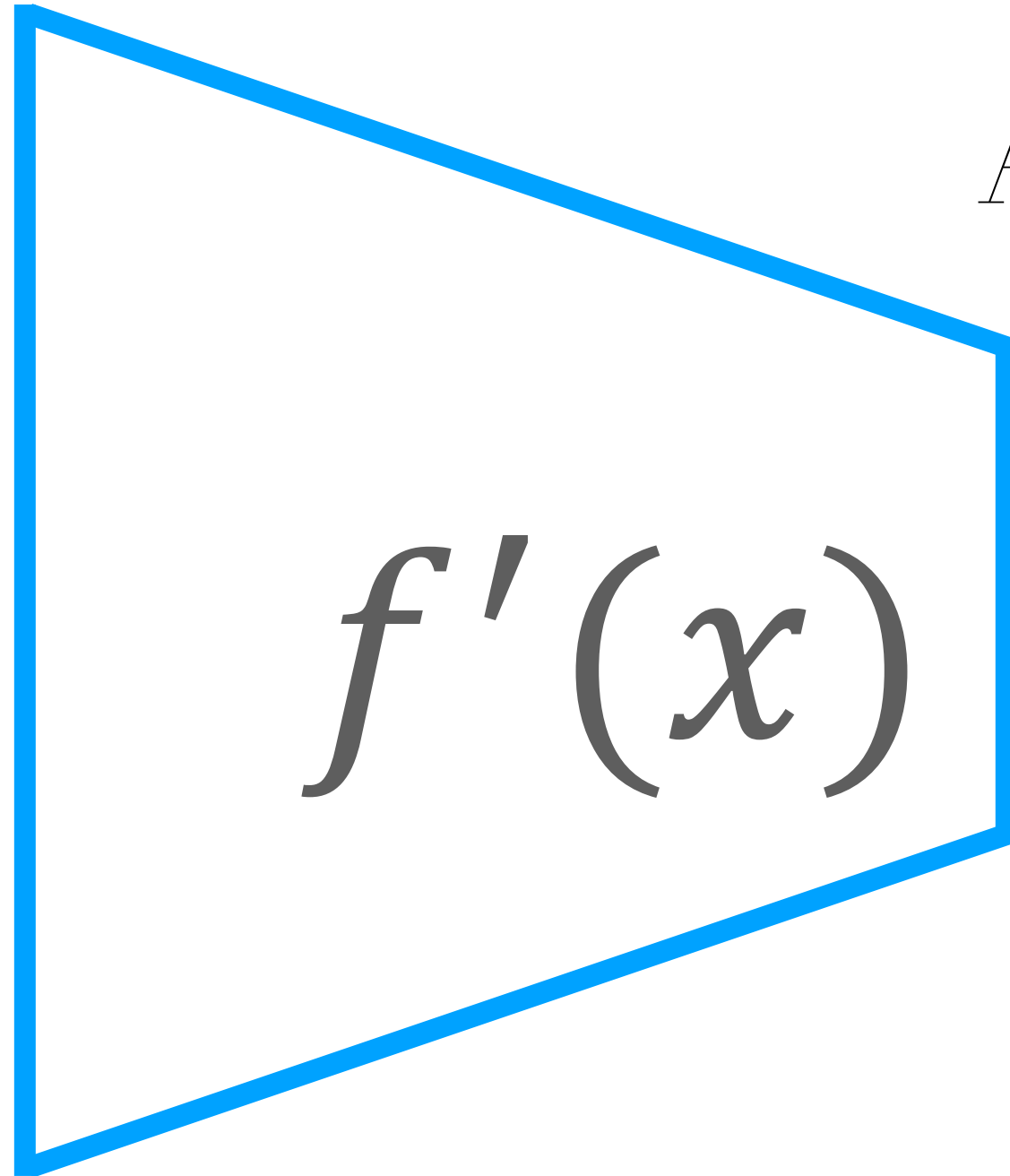
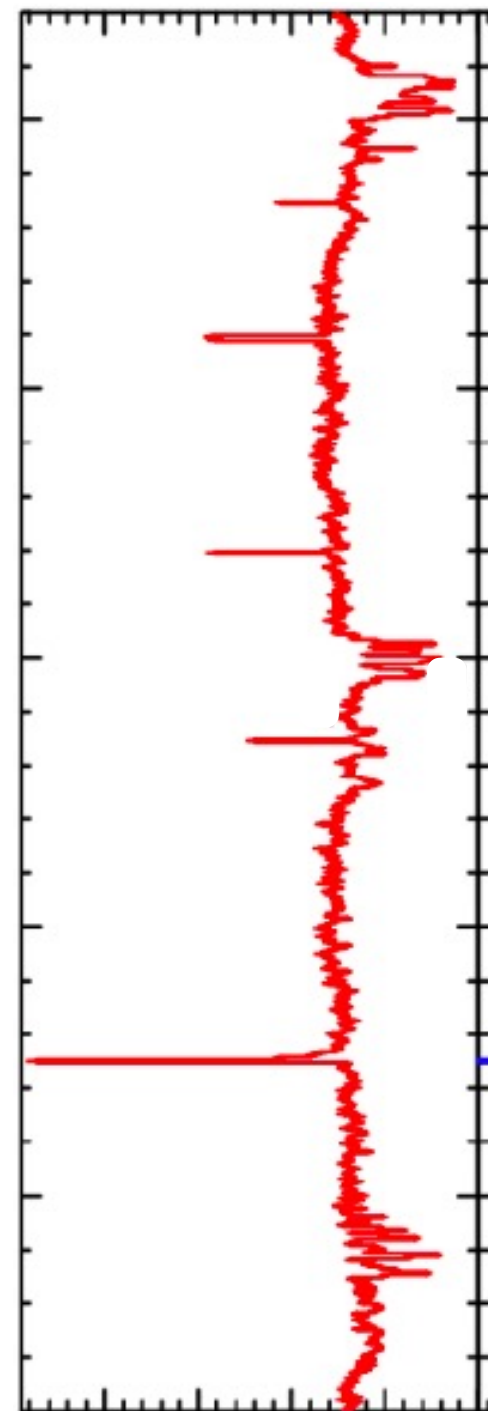
Decoder



Forward Pass

Primer Centro de IA en
Astrofísica

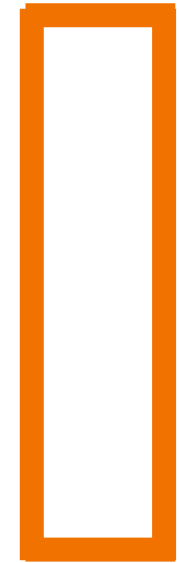
ASTROAI



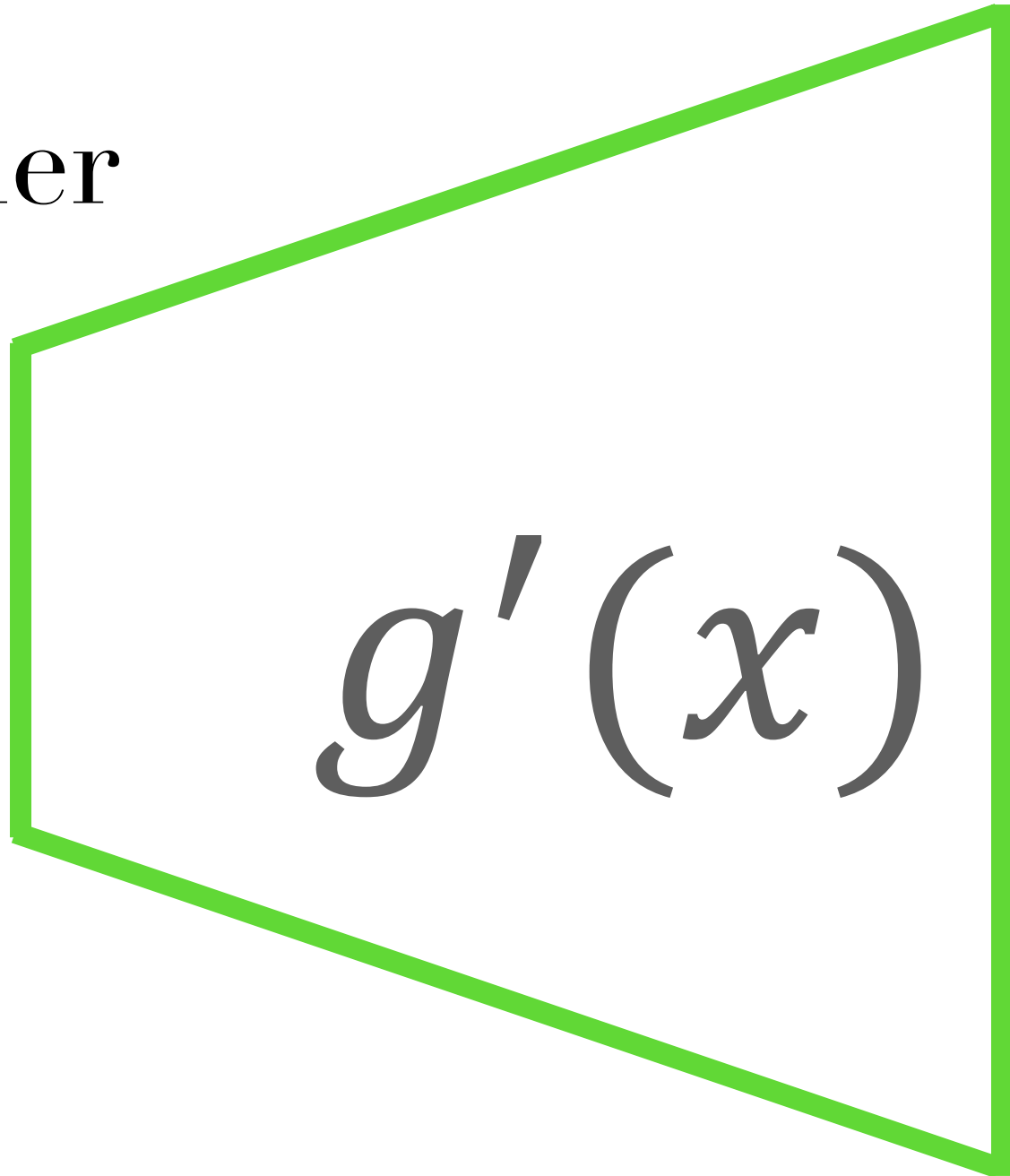
$$f'(x)$$

Encoder

Autoencoder

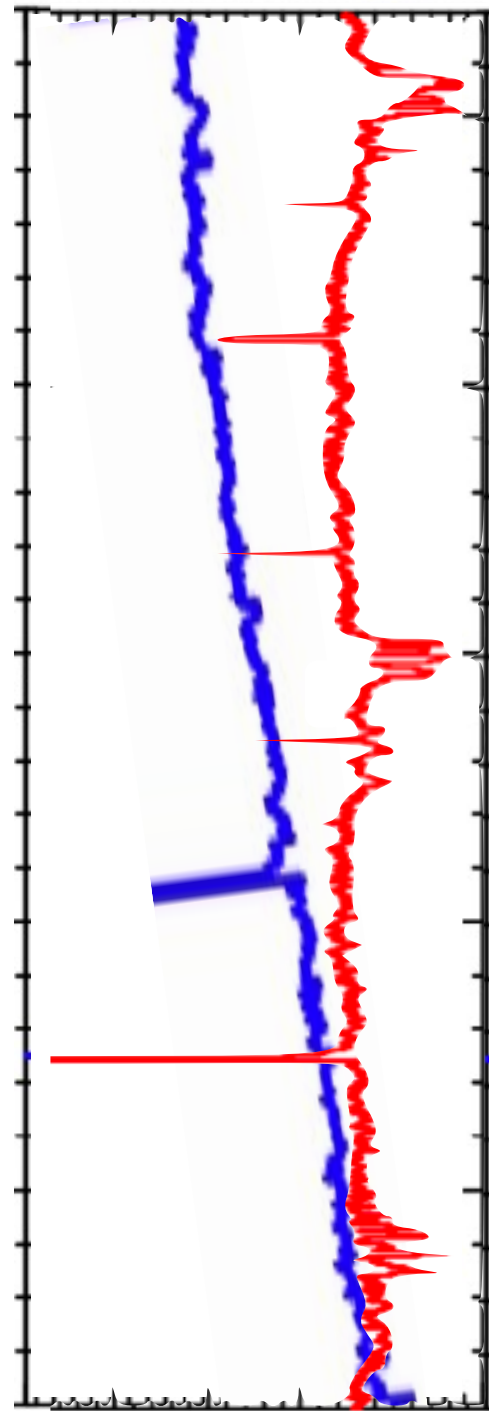


Code



$$g'(x)$$

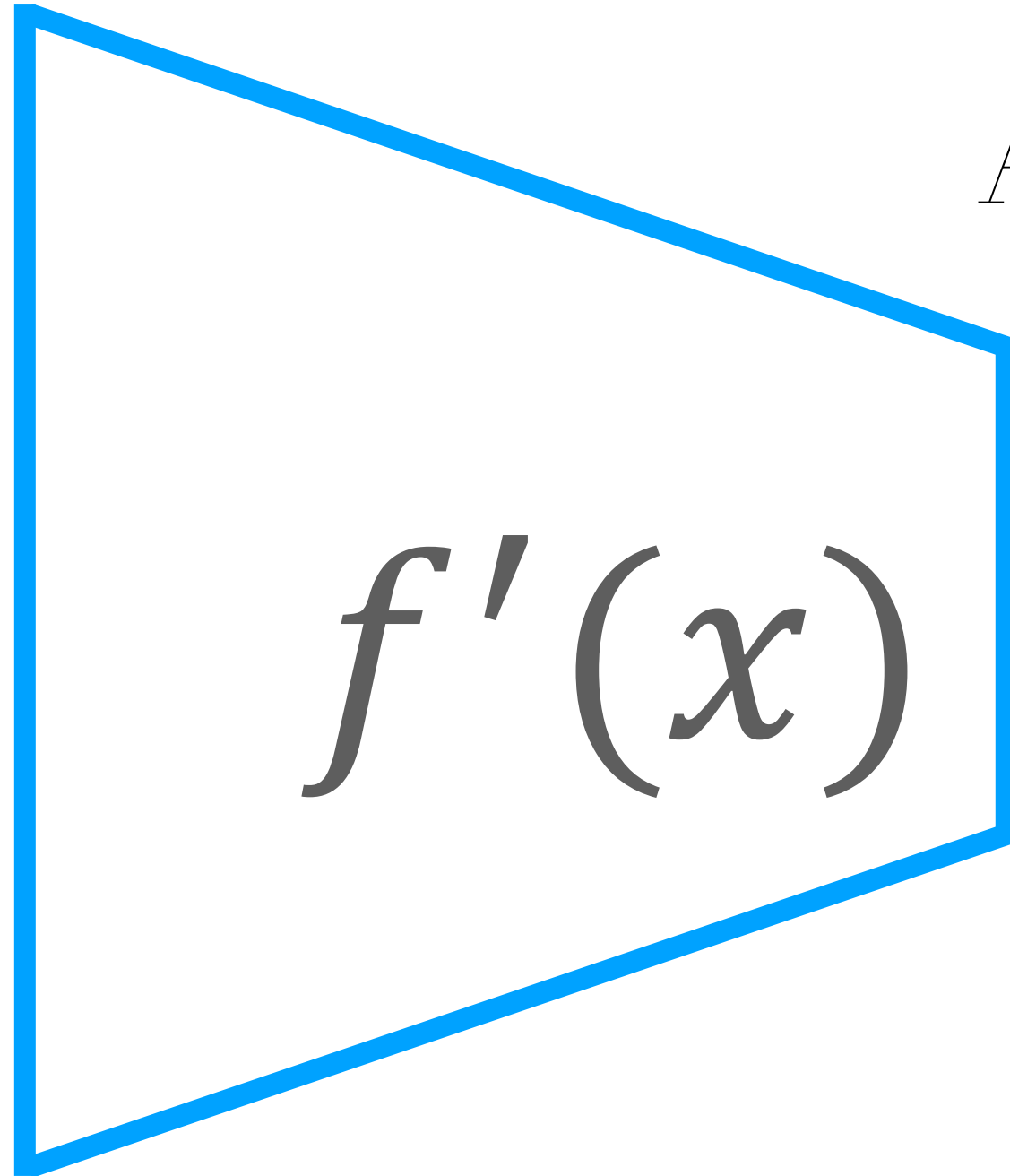
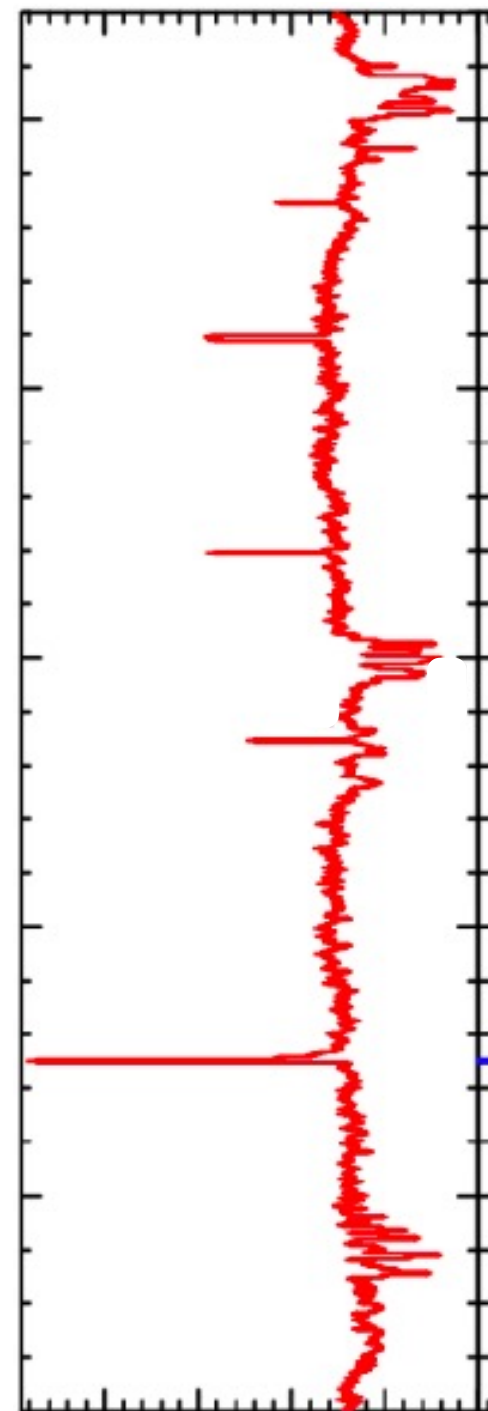
Decoder



Back Propagation

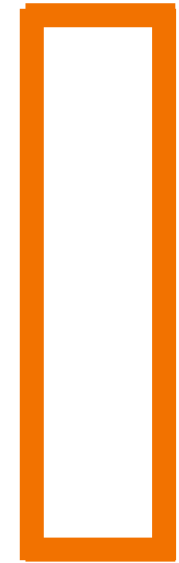
Primer Centro de IA en
Astrofísica

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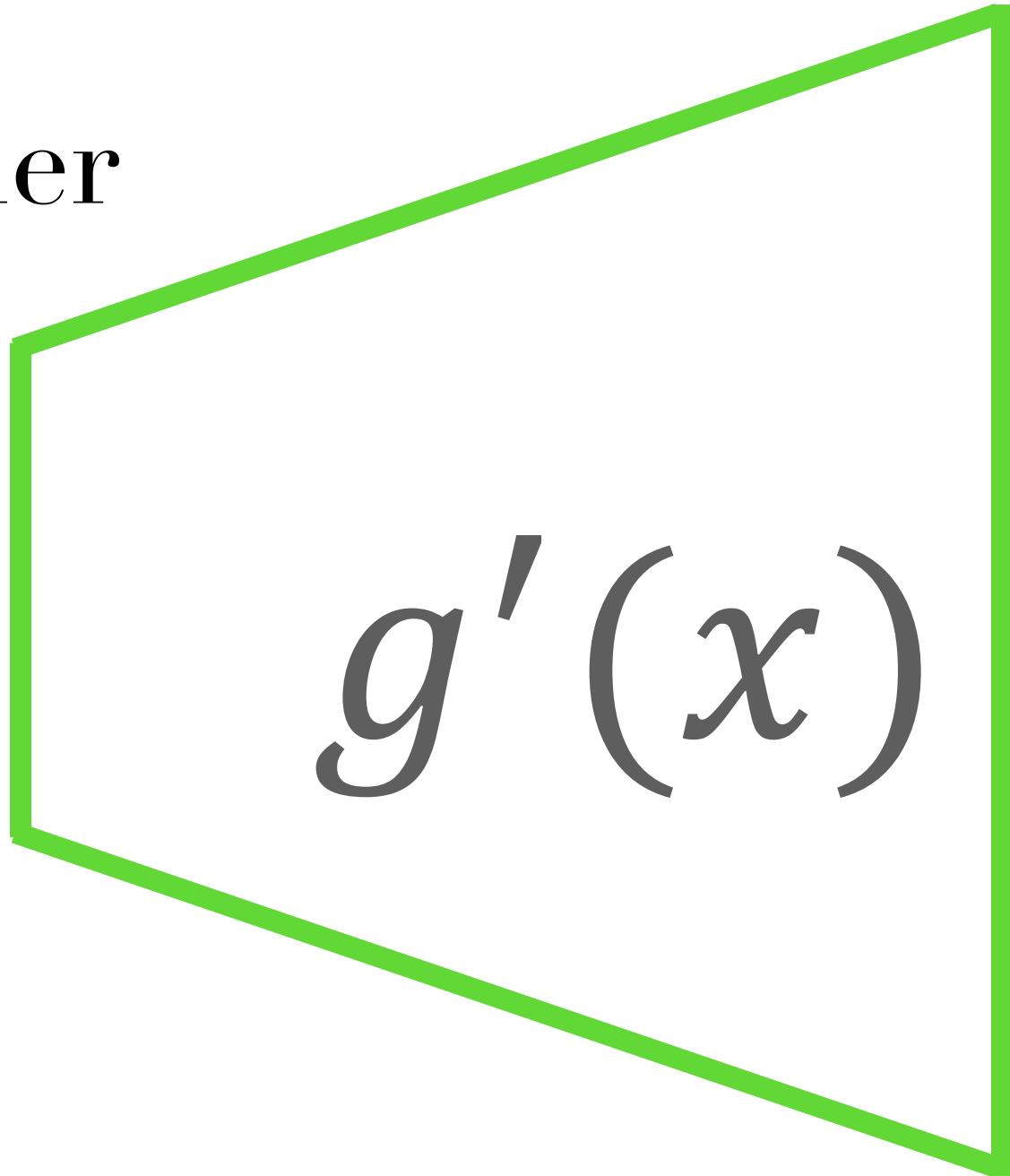


Encoder

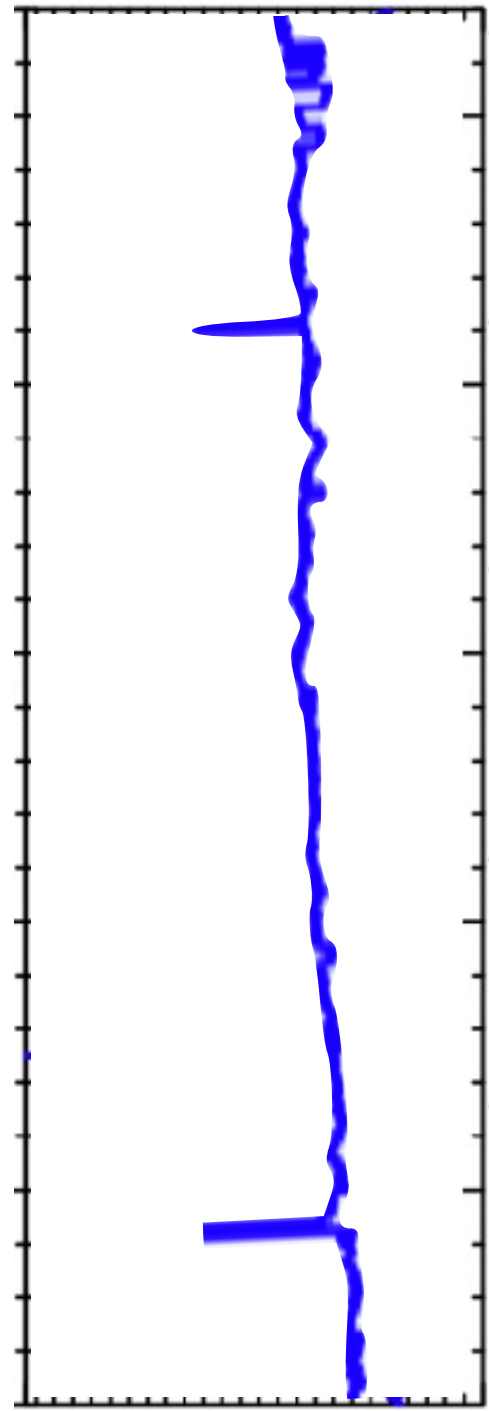
Autoencoder



Code



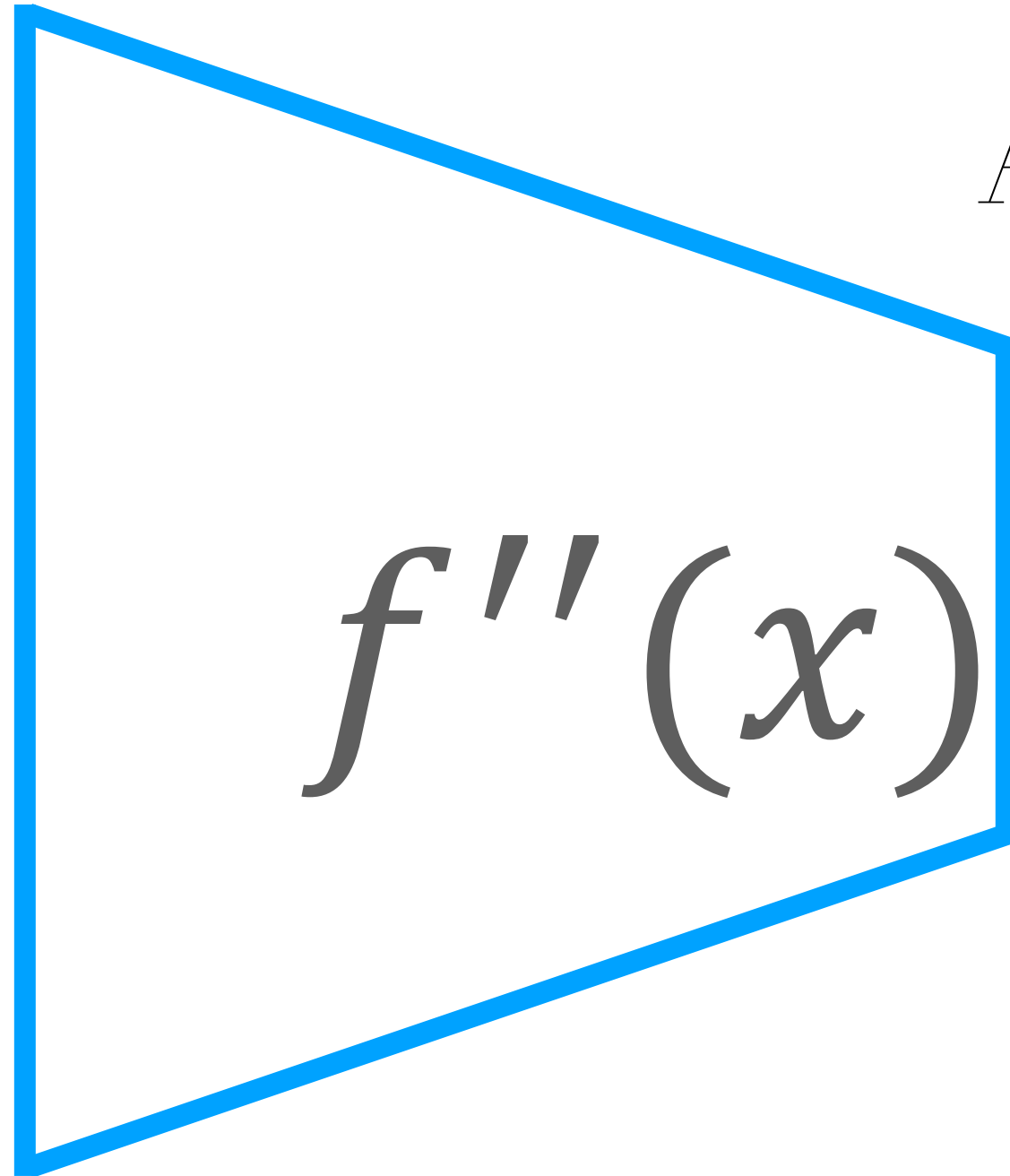
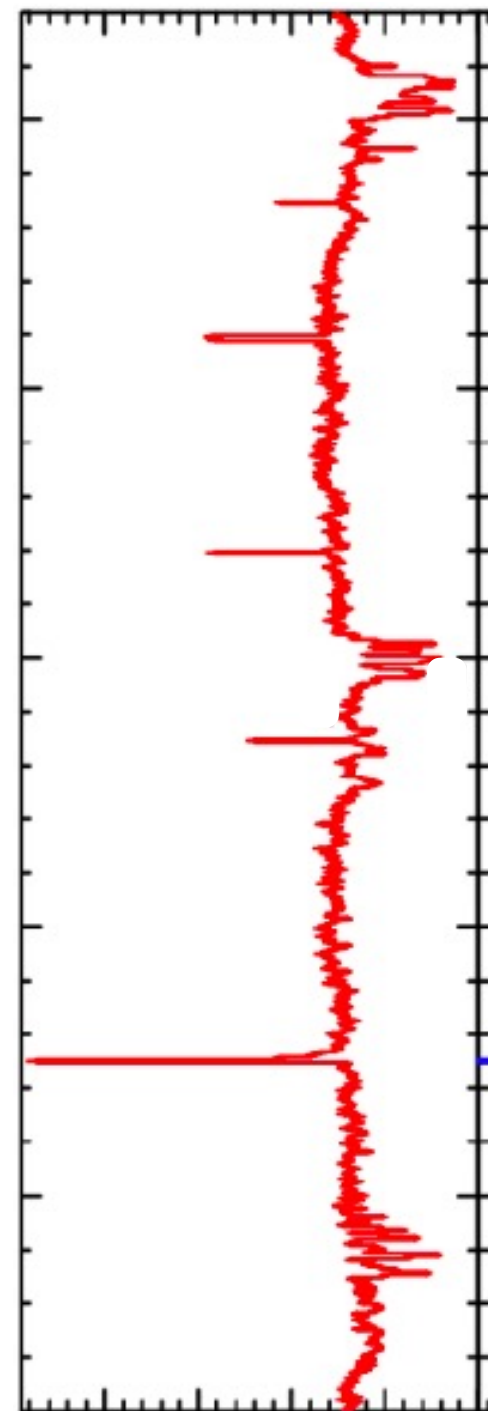
Decoder



Forward Pass

Primer Centro de IA en
Astrofísica

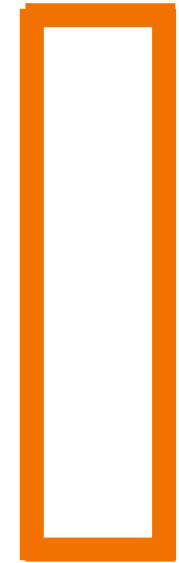
ASTROAI



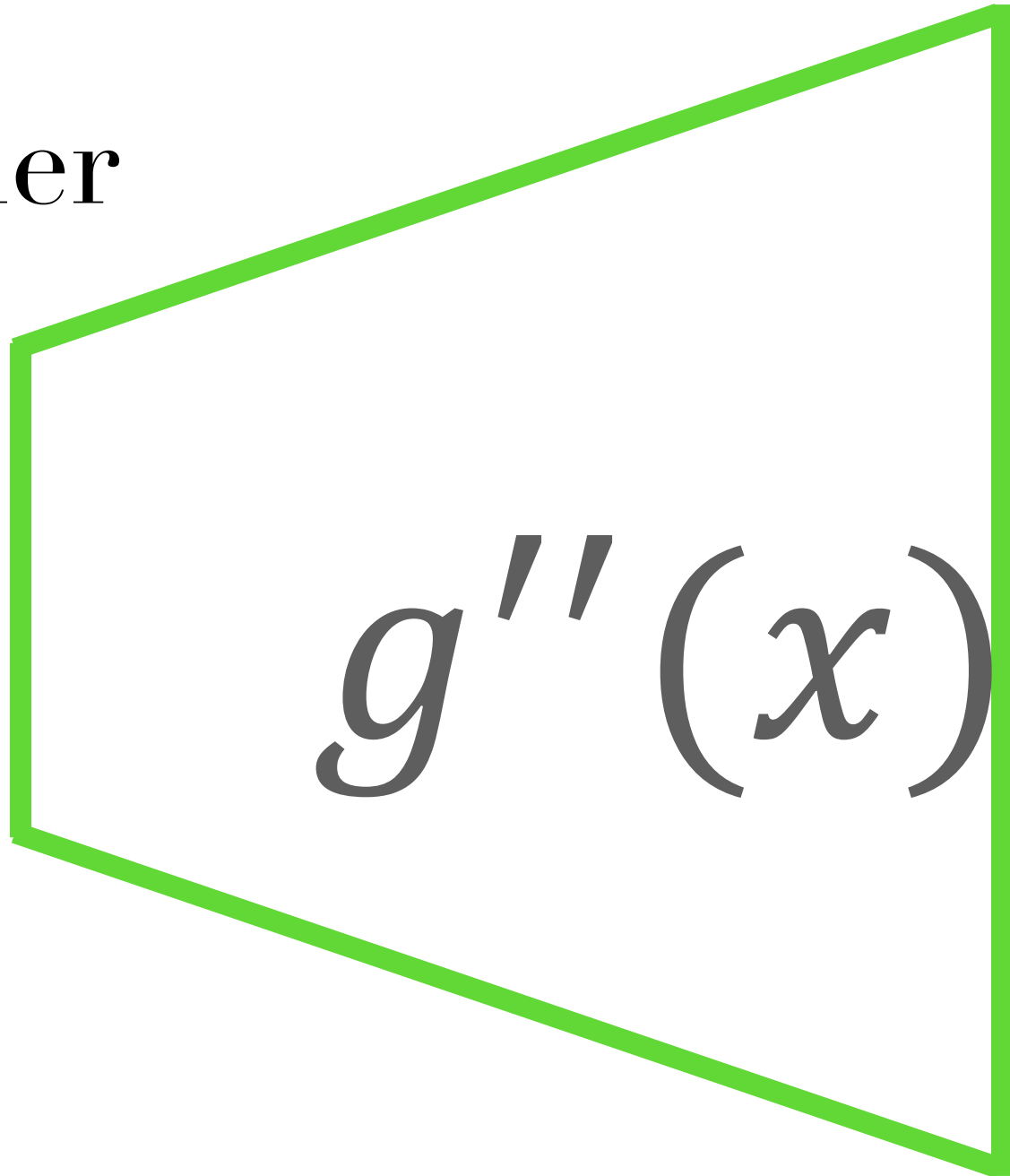
$$f''(x)$$

Encoder

Autoencoder

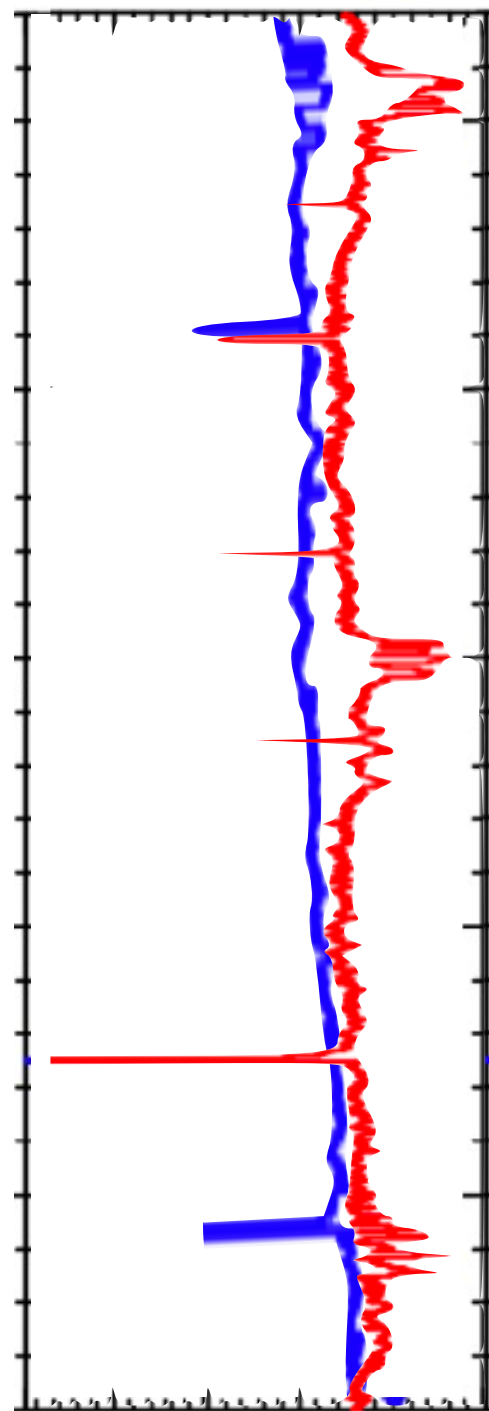


Code

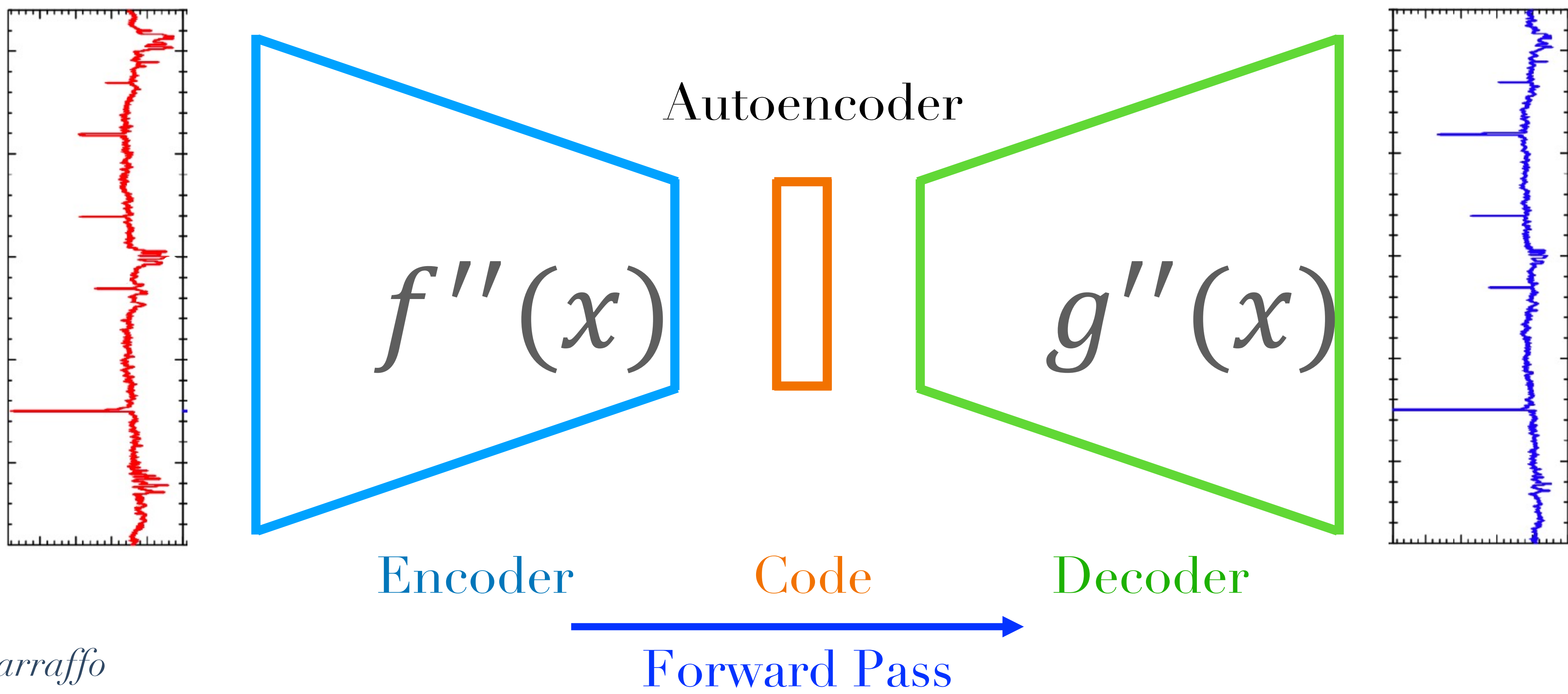


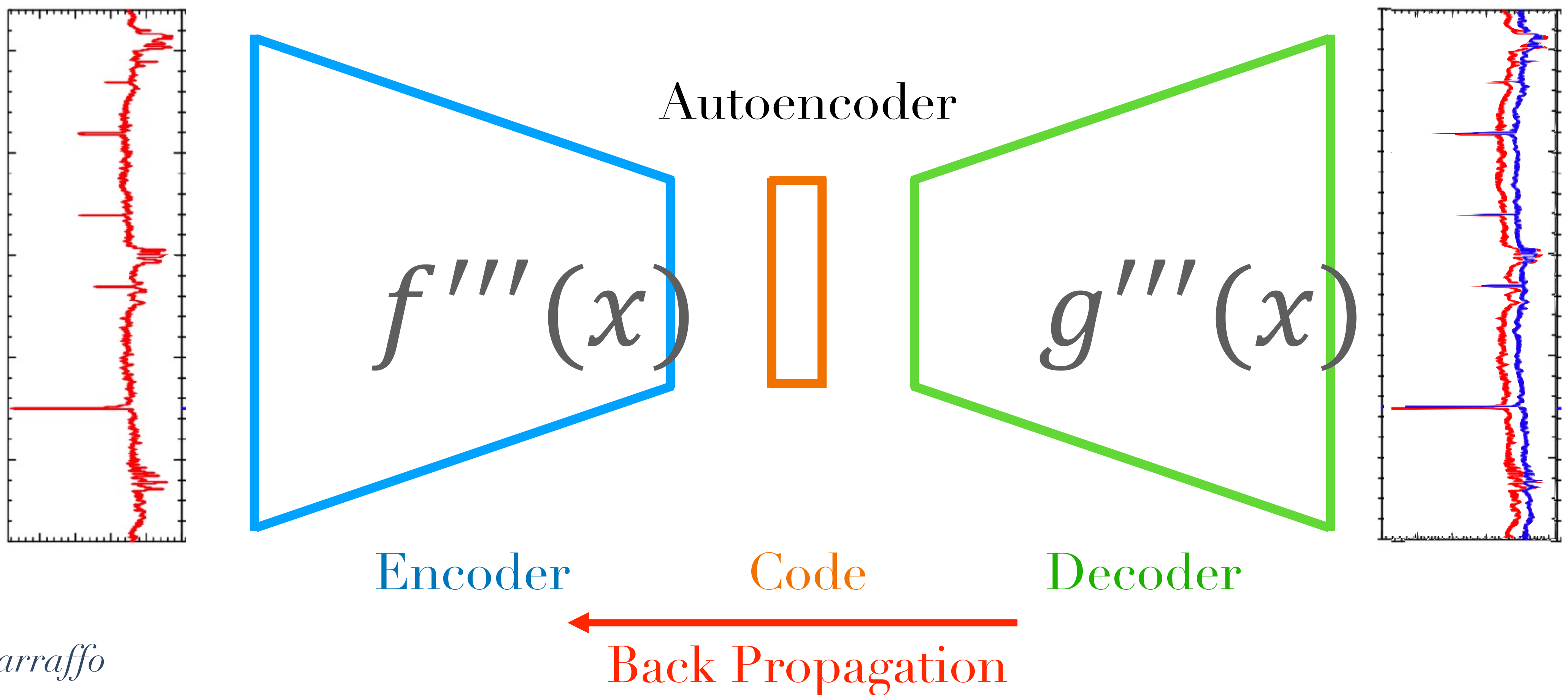
$$g''(x)$$

Decoder



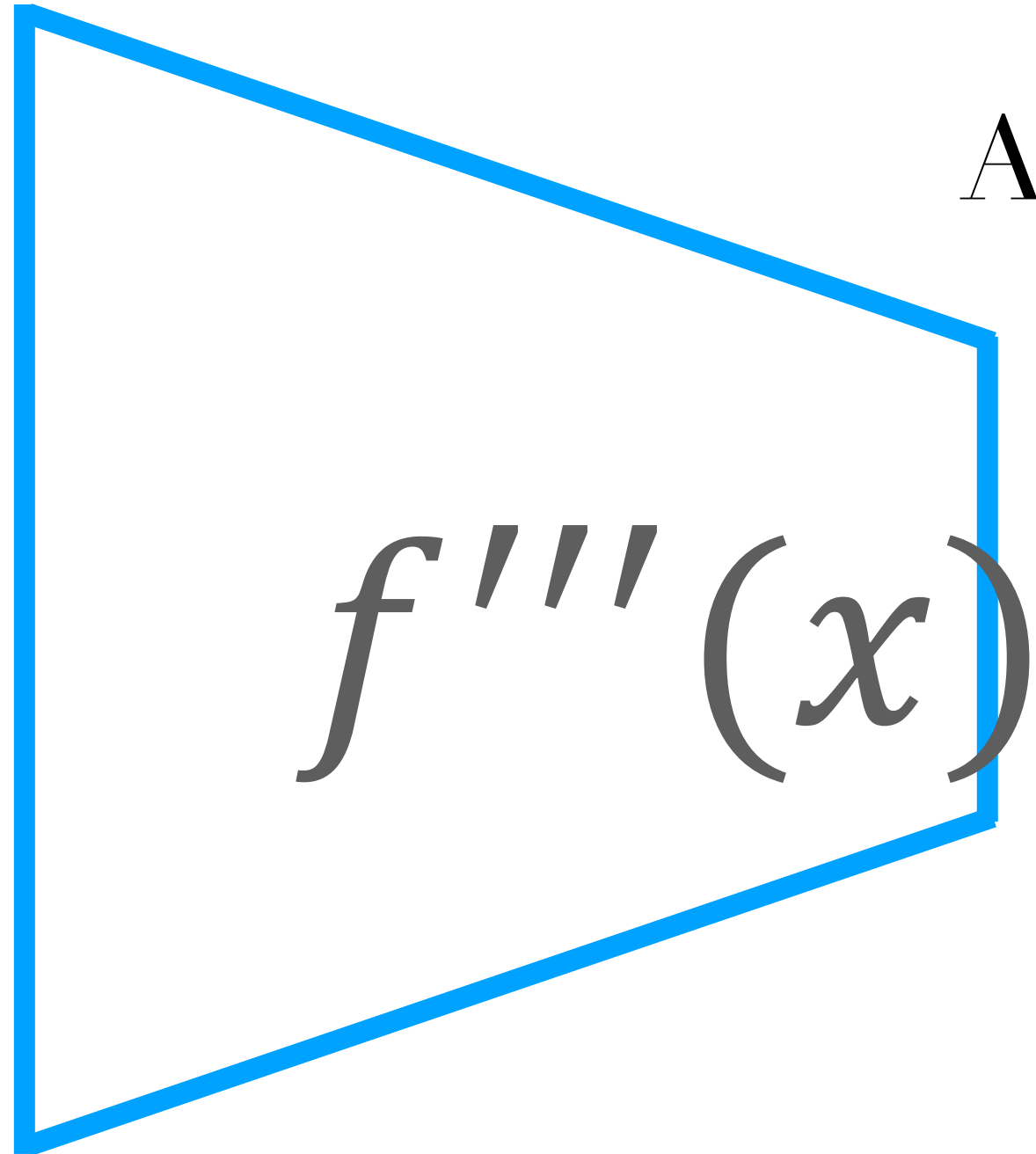
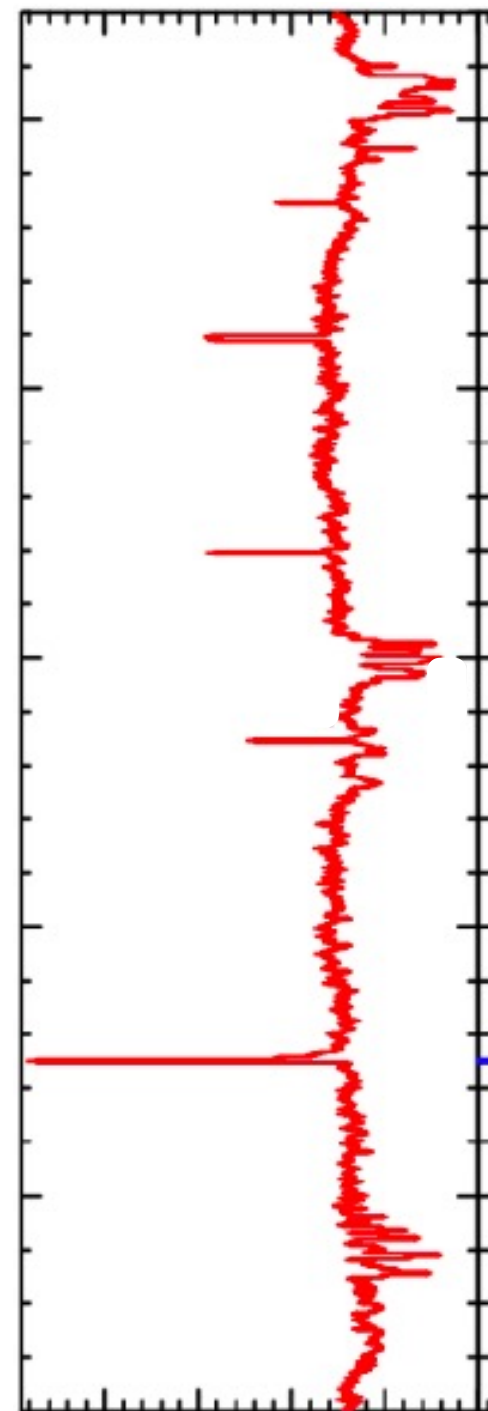
Back Propagation





Primer Centro de IA en
Astrofísica

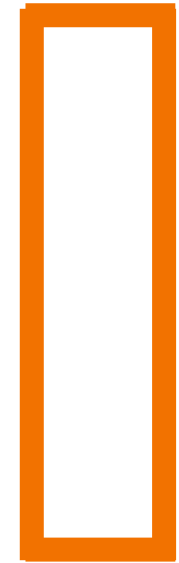
ASTROAI



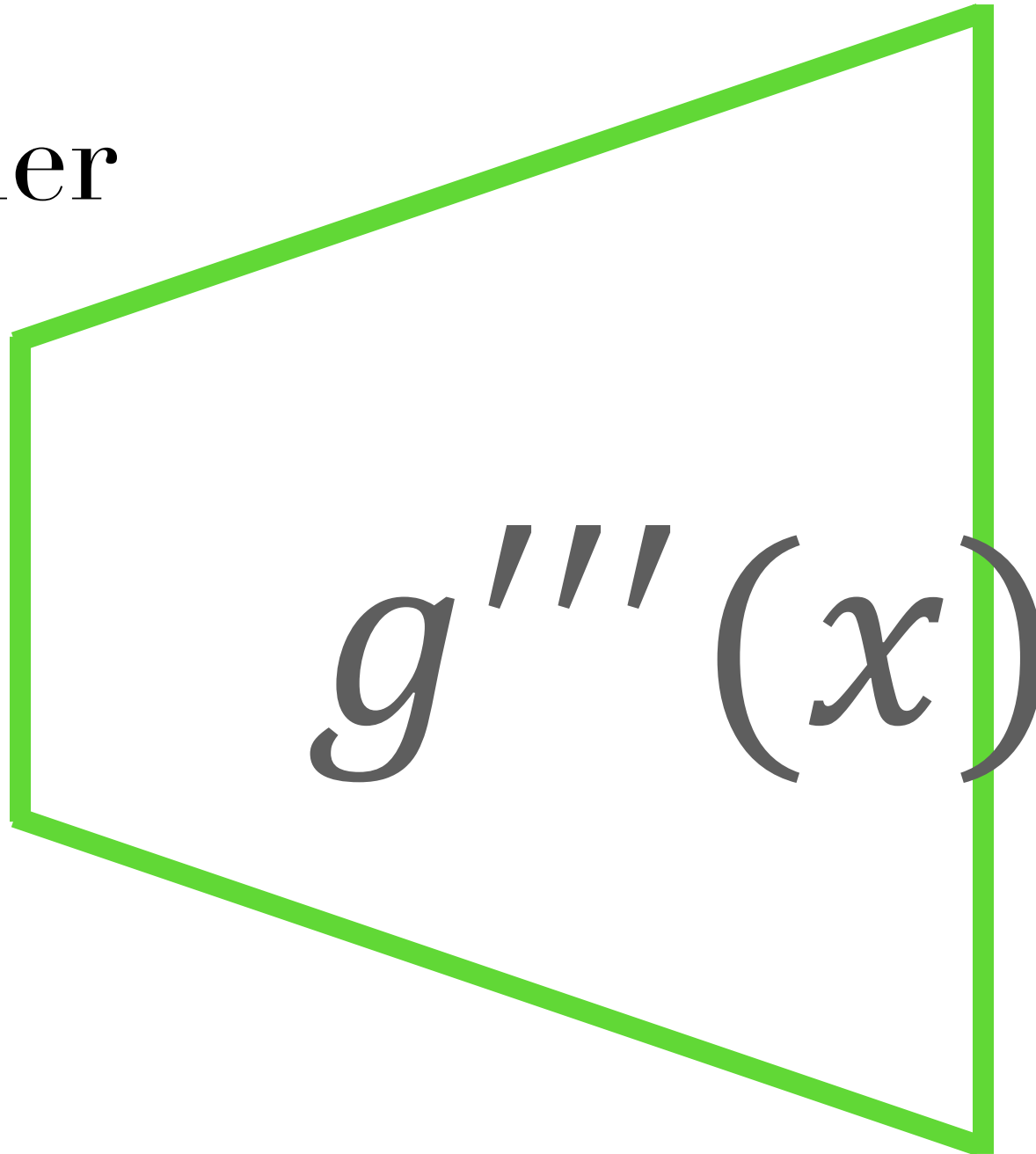
$$f'''(x)$$

Encoder

Autoencoder

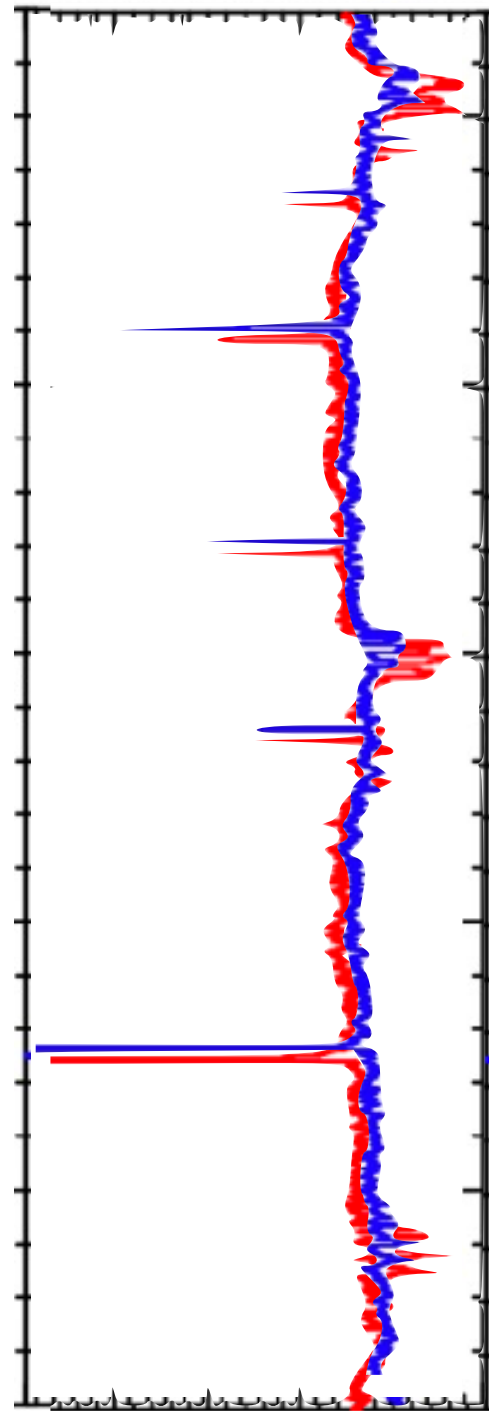


Code



$$g'''(x)$$

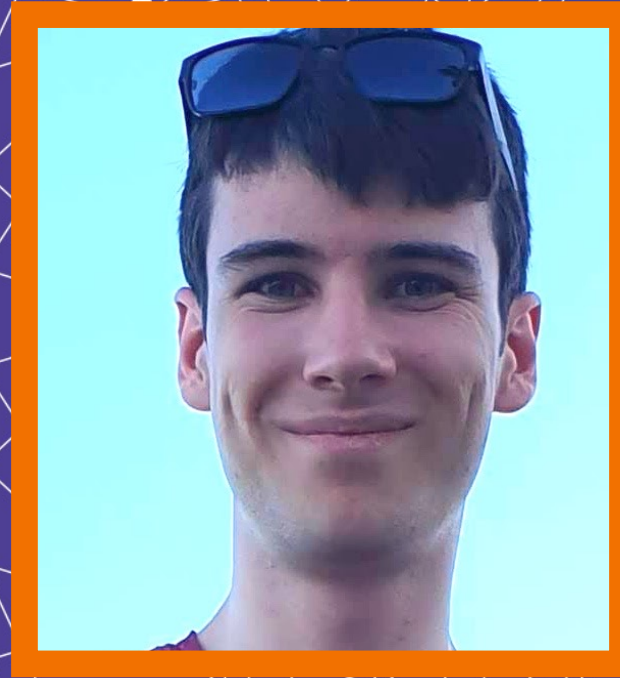
Decoder



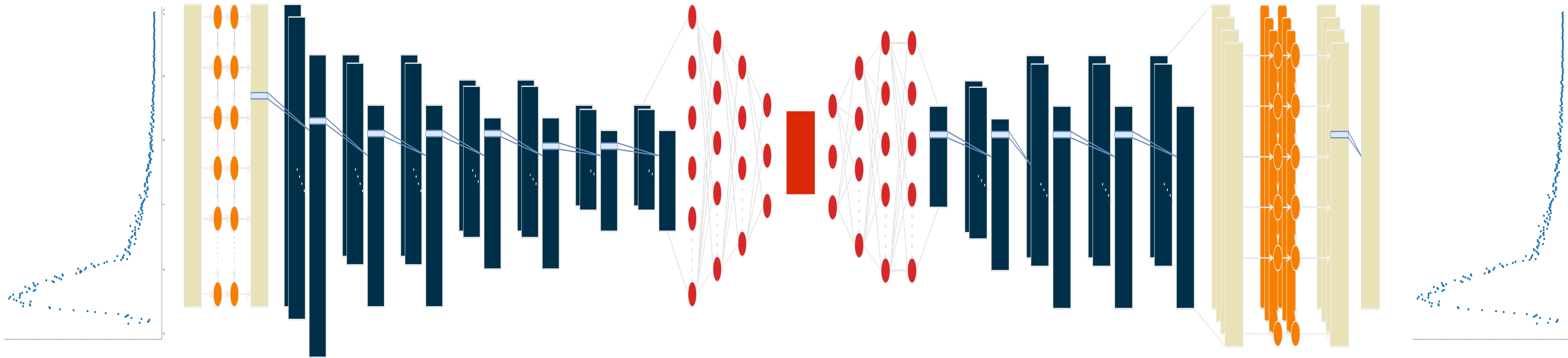
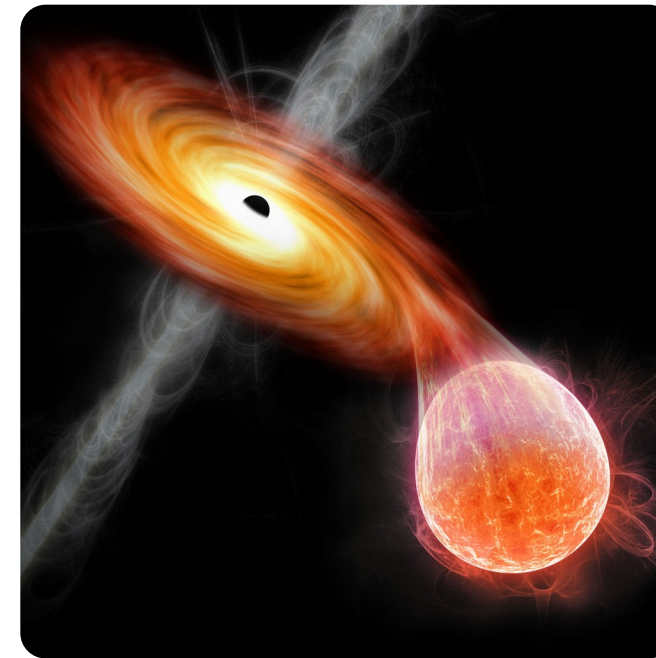
Forward Pass

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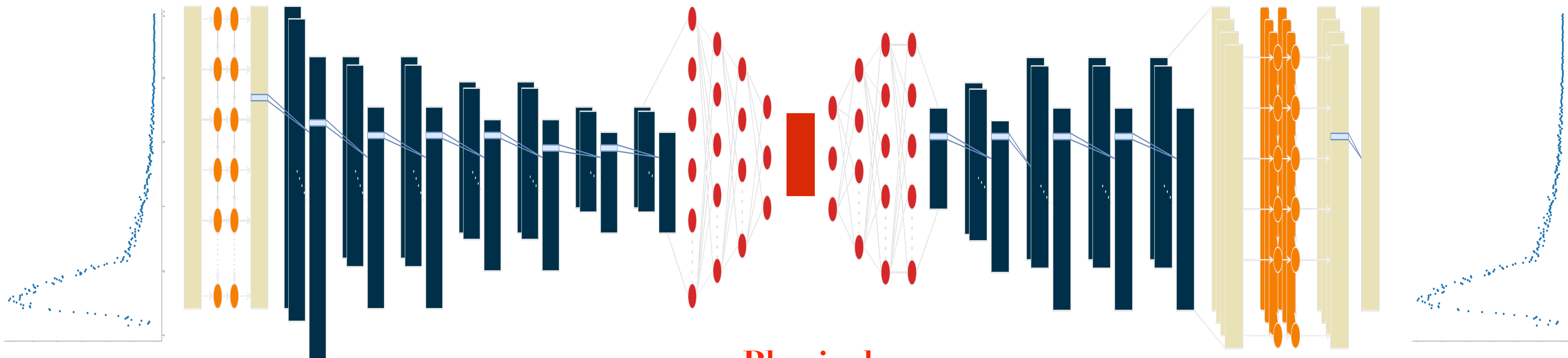
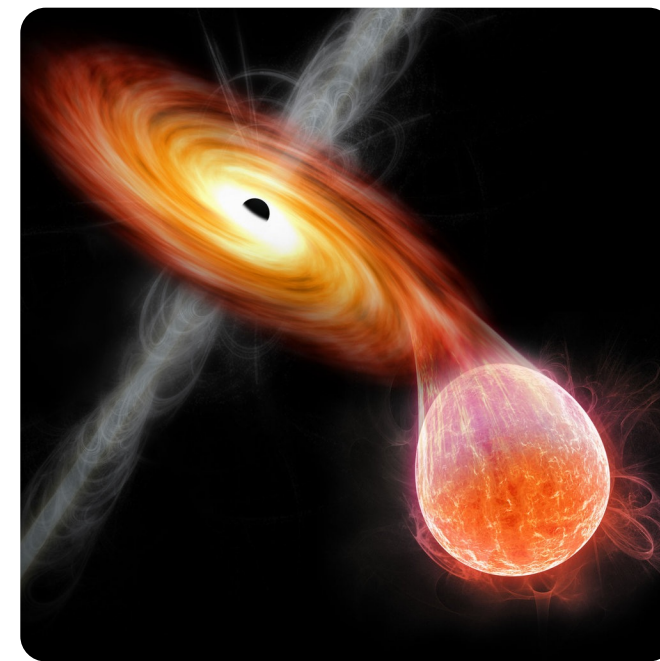


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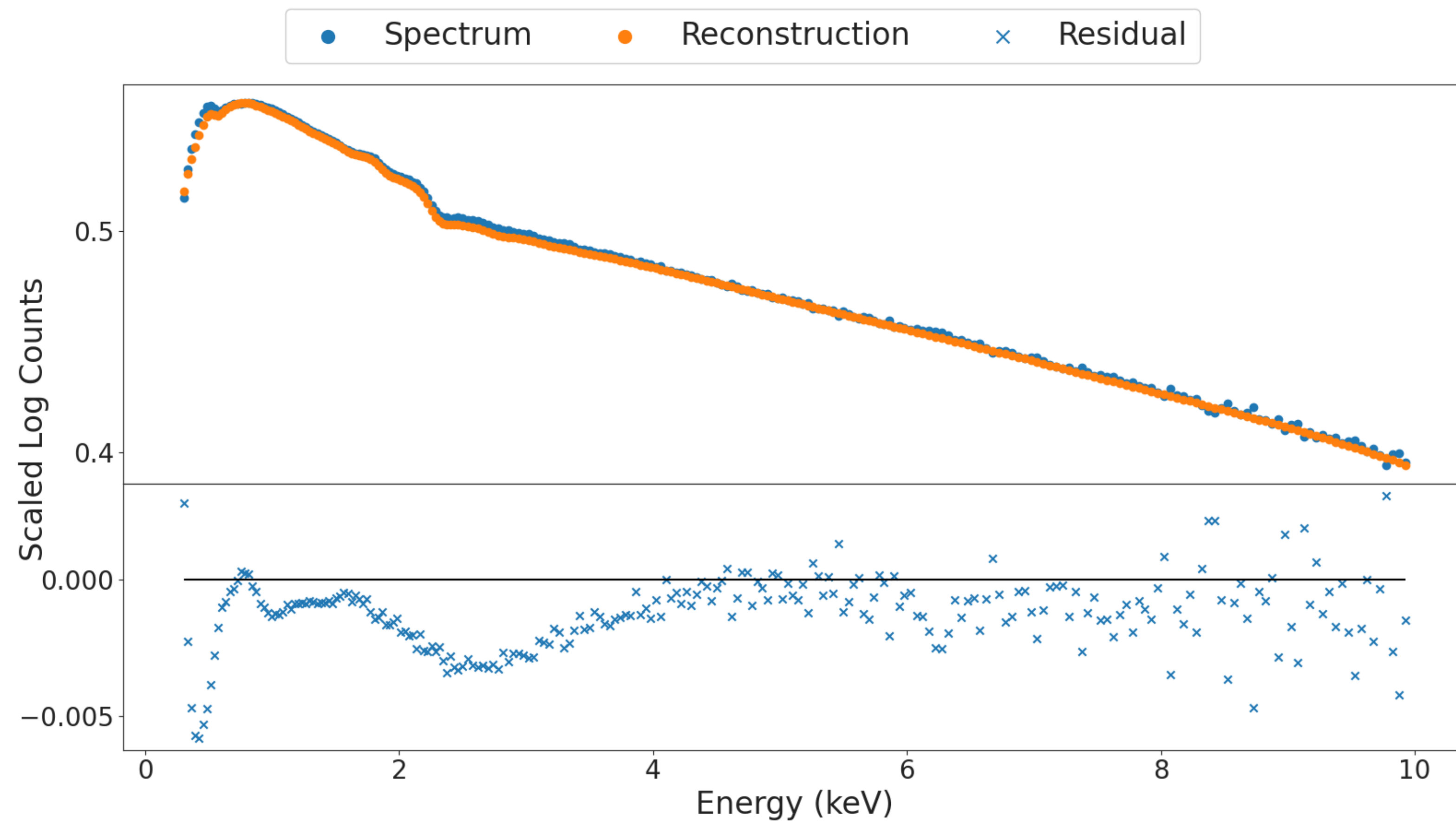
**Physical
Parameters**

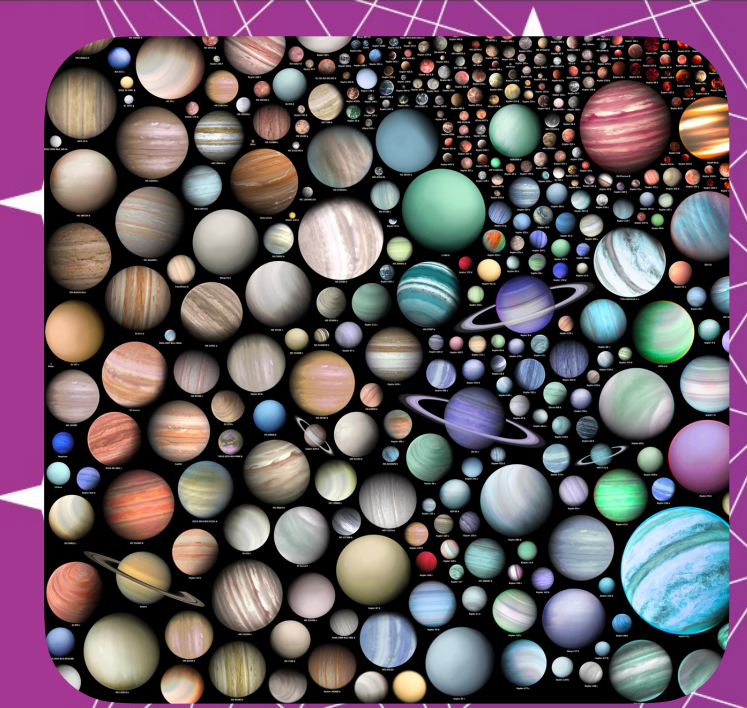
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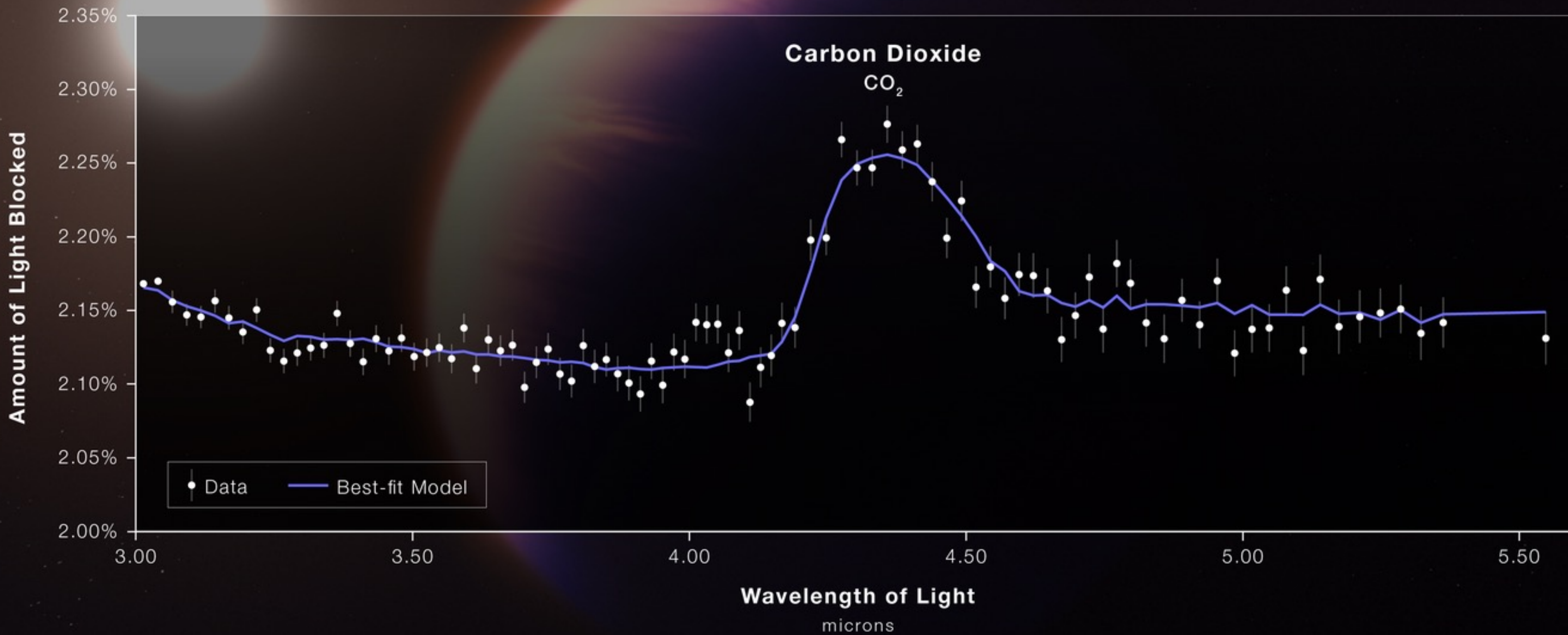


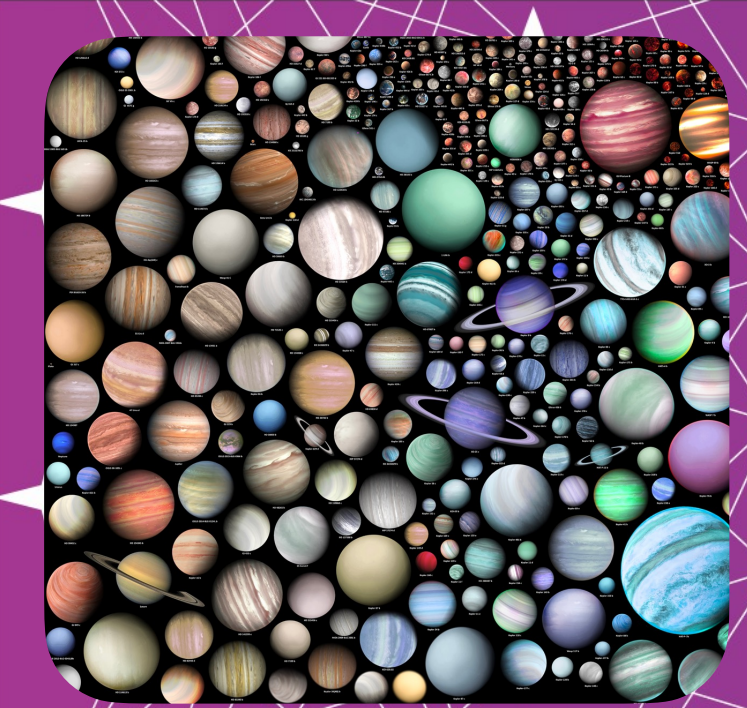
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Mayeul Aubin





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Mayeul Aubin



Ethan Tregigda



Carol Cuesta-Lazaro



Iouli Gordon



Mercedes López-Morales



Javier Viana

Students

Astronomers

AI Experts

Spectroscopists

AstroAI



Robert Hargreaves



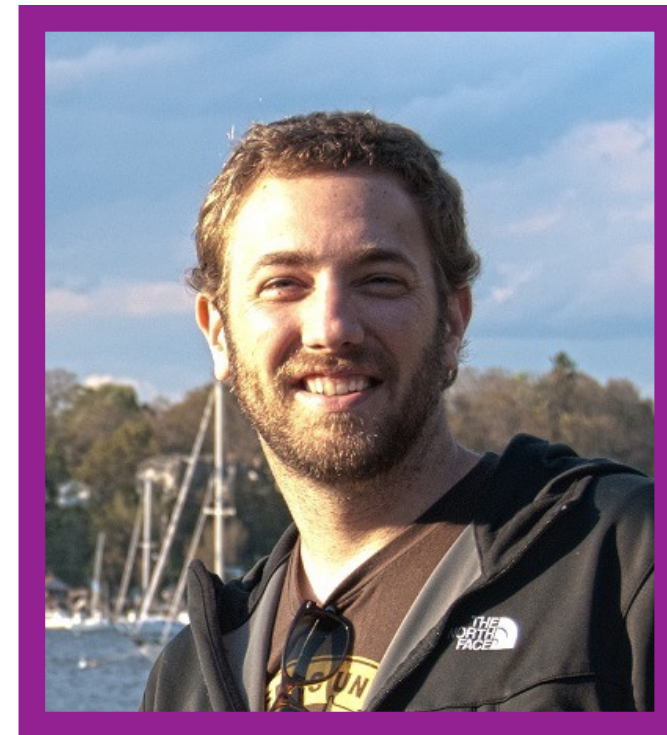
Cecilia Garraffo



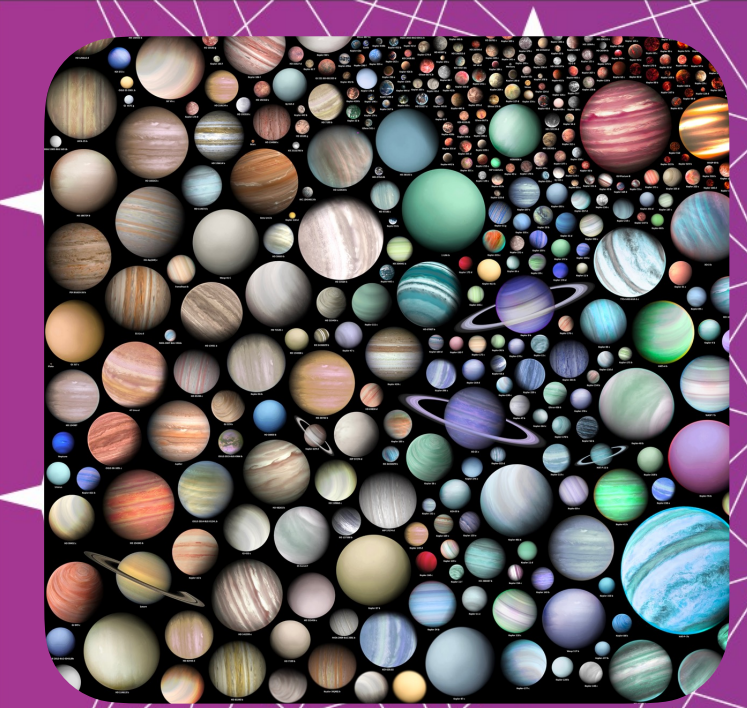
Vladimir Makhnev



Jeremy Drake



Phillip Cargile



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Mayeul Aubin



Ethan Tregigda



Carol Cuesta-Lazaro



Iouli Gordon



Mercedes López-Morales



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AI Experts



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Cecilia Garraffo



Vladimir Makhnev



Jeremy Drake

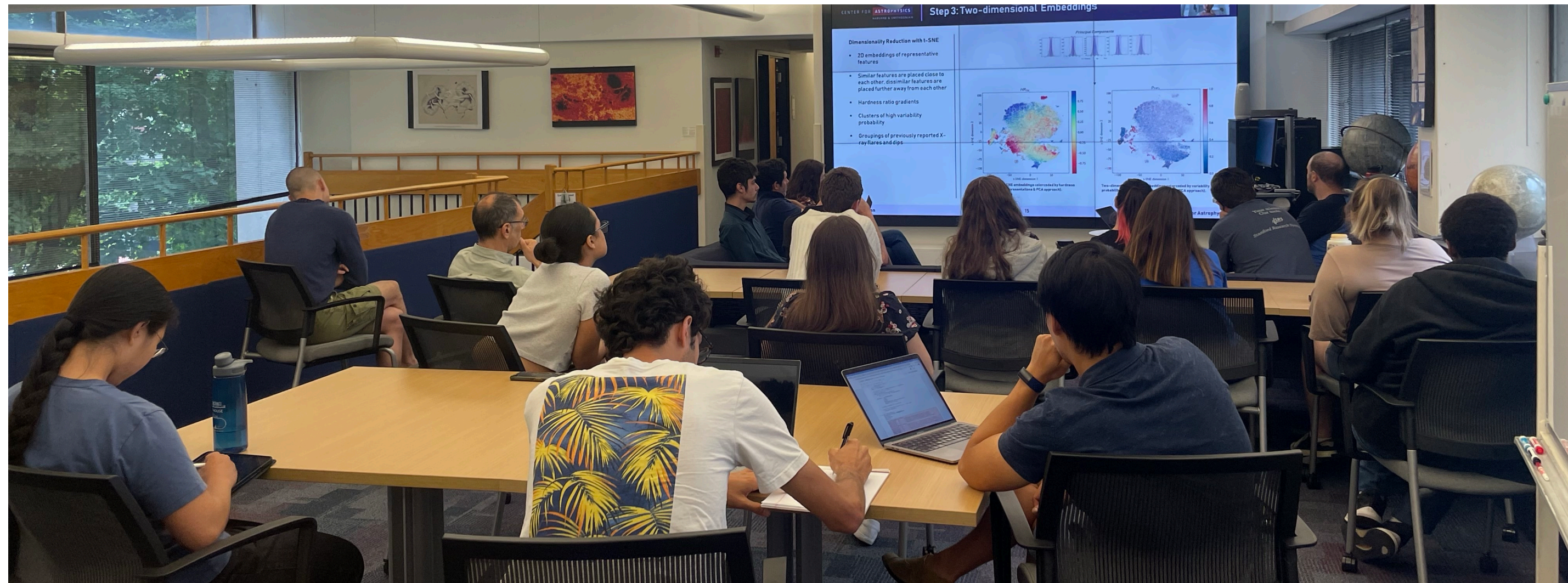


Phillip Cargile

Spectroscopists

AstroAI

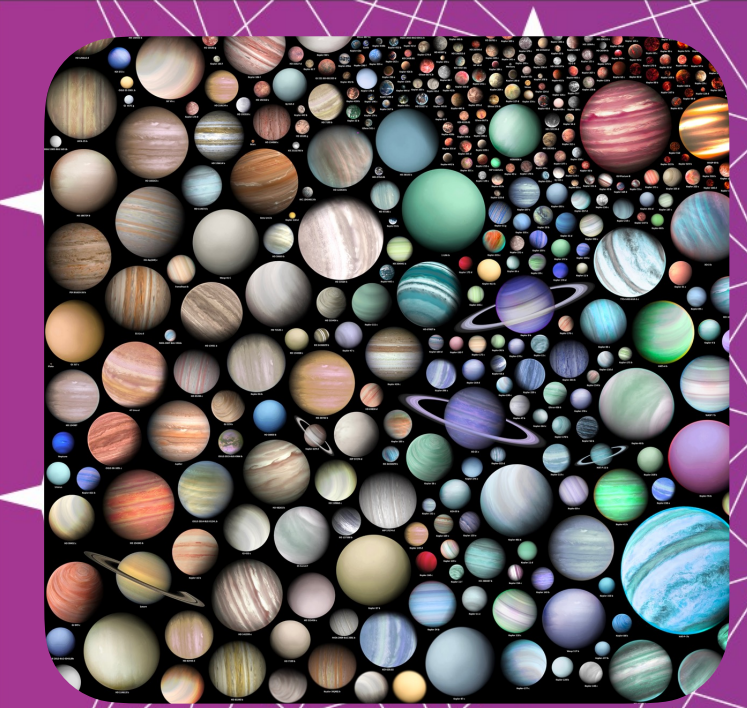
Building Community:



Hybrid AstroAI meetings every Monday. Join us!

www.astroai.cfa.harvard.edu





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Bill Freeman, CS



Robin Walters, CS



Brandon Feng, CS



David, CS



Yuanyuan, CS

Students

Astronomers

AI Experts

Spectroscopists

AstroAI



Sara Seager



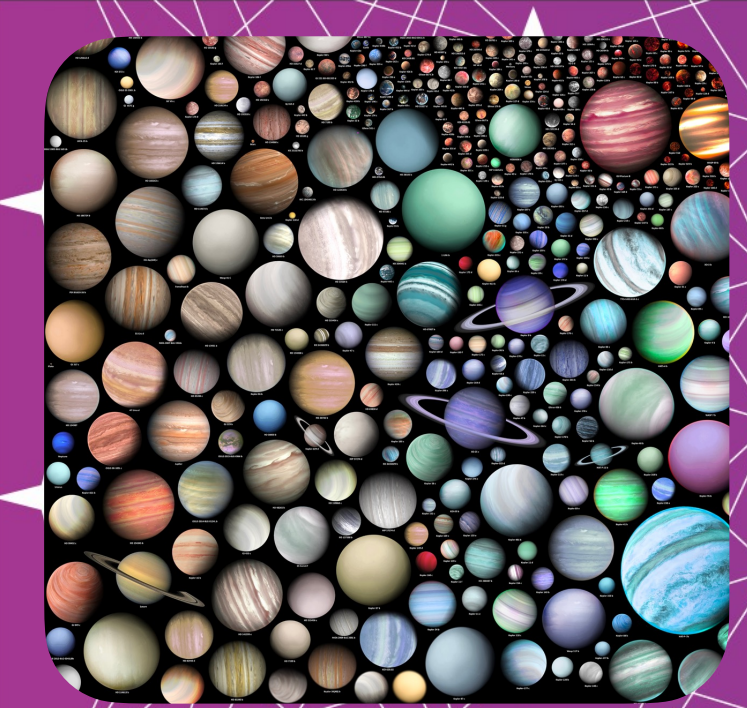
Cecilia Garraffo



Iouli Gordon



Eddie, CS

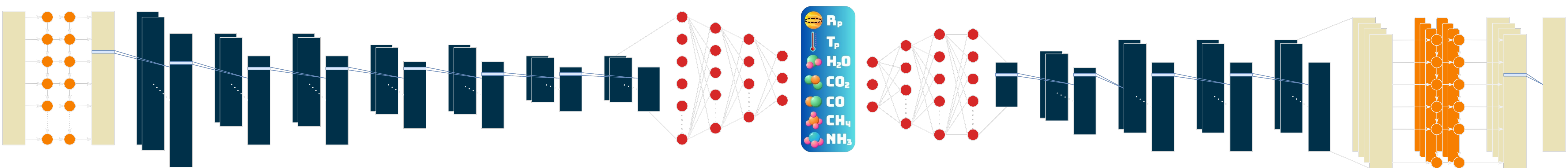


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● Spectrum

● Reconstruction

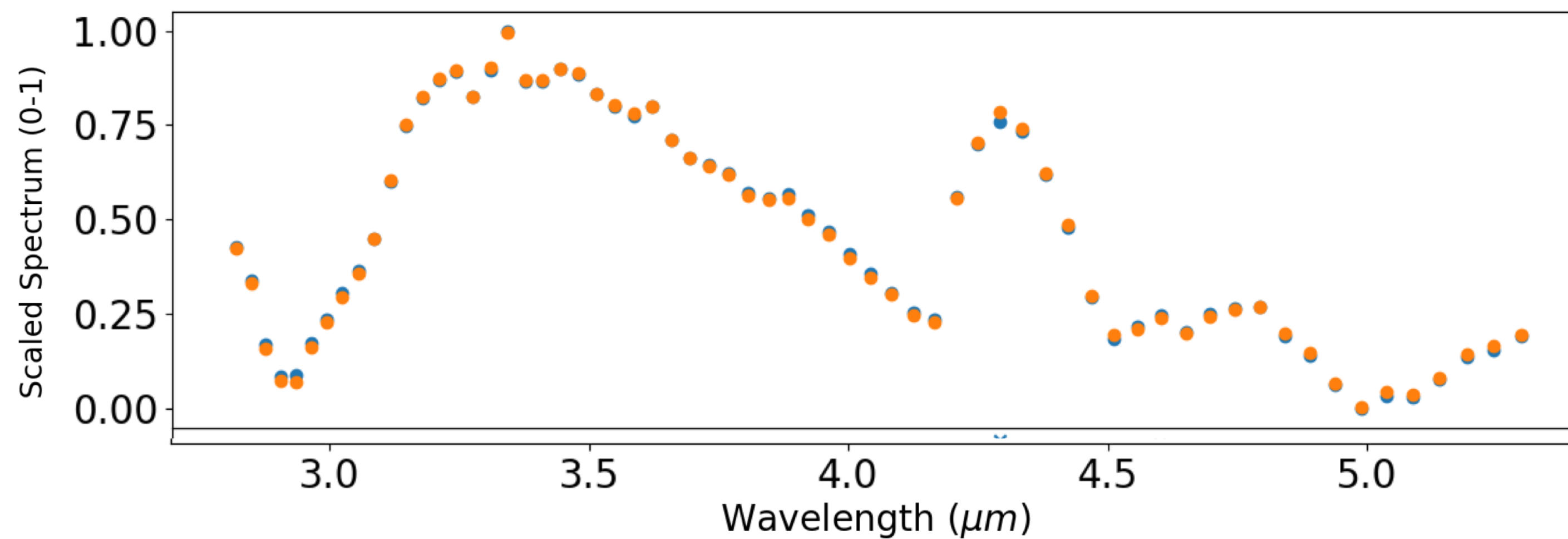
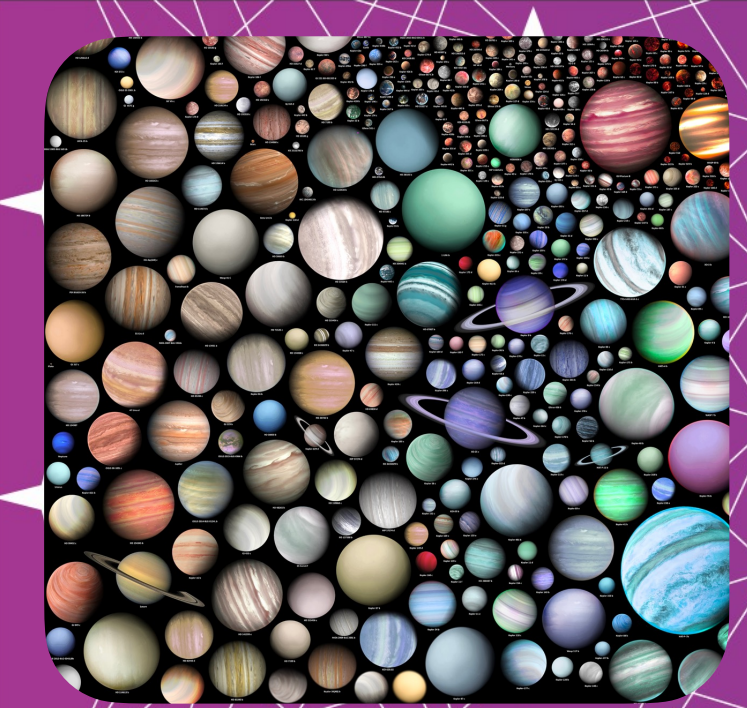


Figure 2: Reconstruction of a spectrum by the decoder



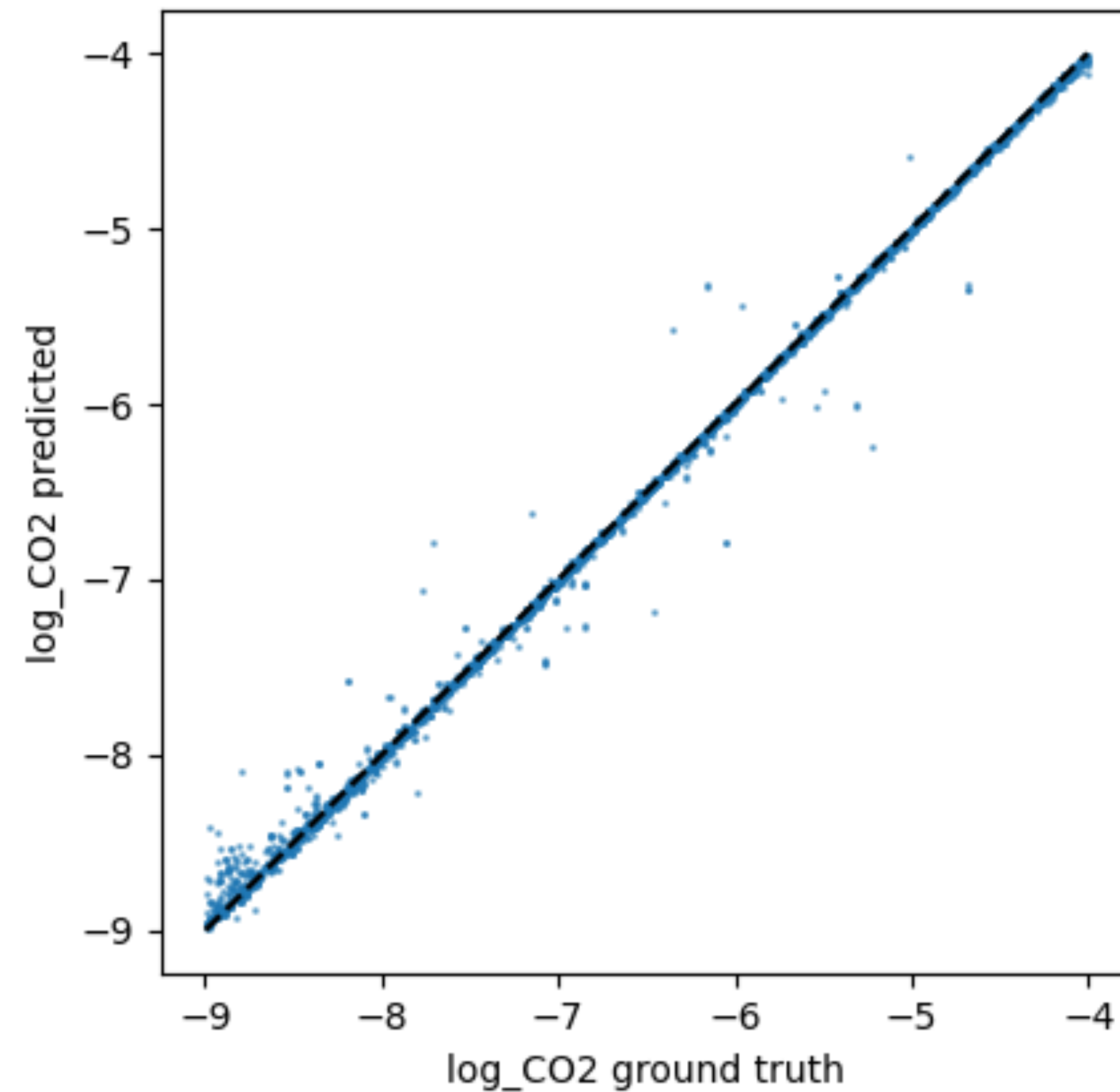
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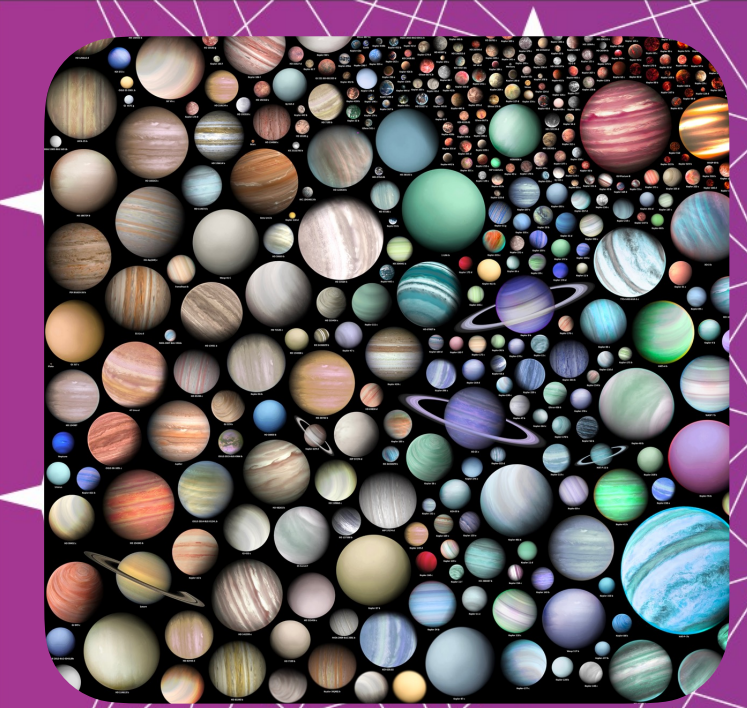


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The encoder can reliably predict the target parameters

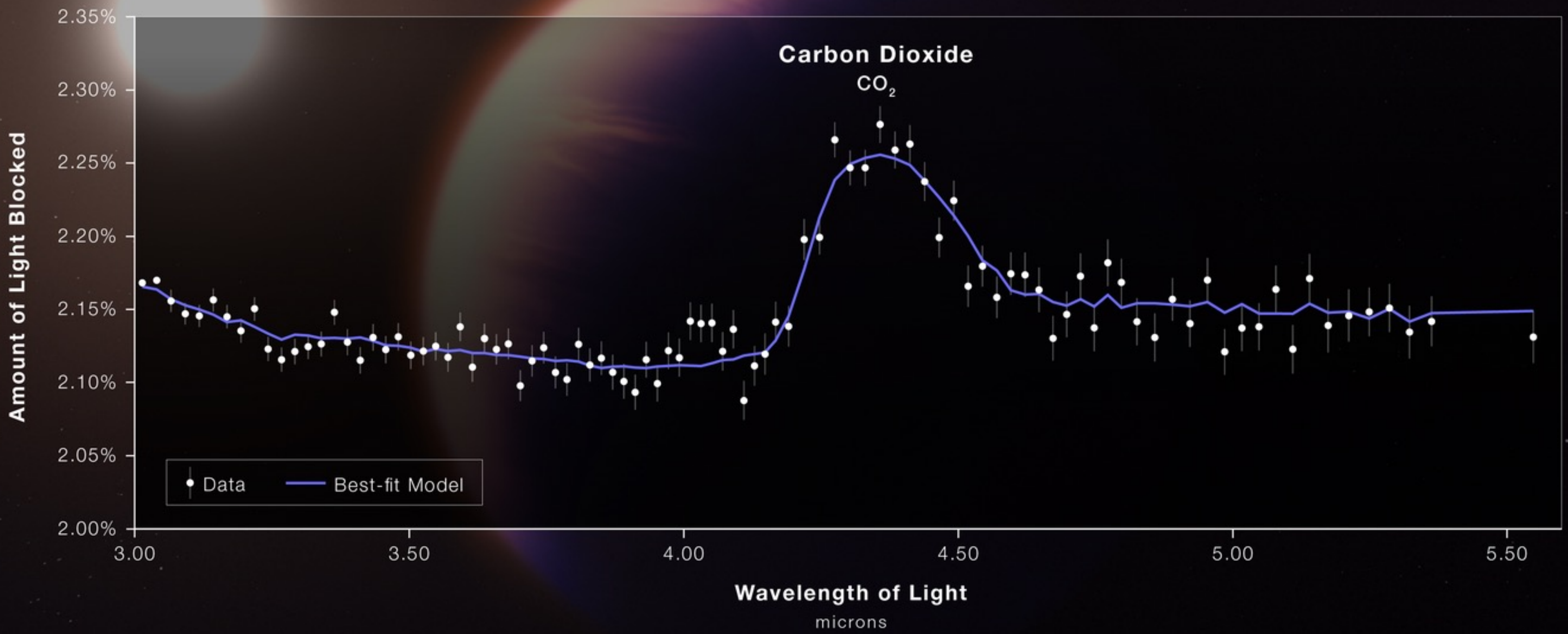


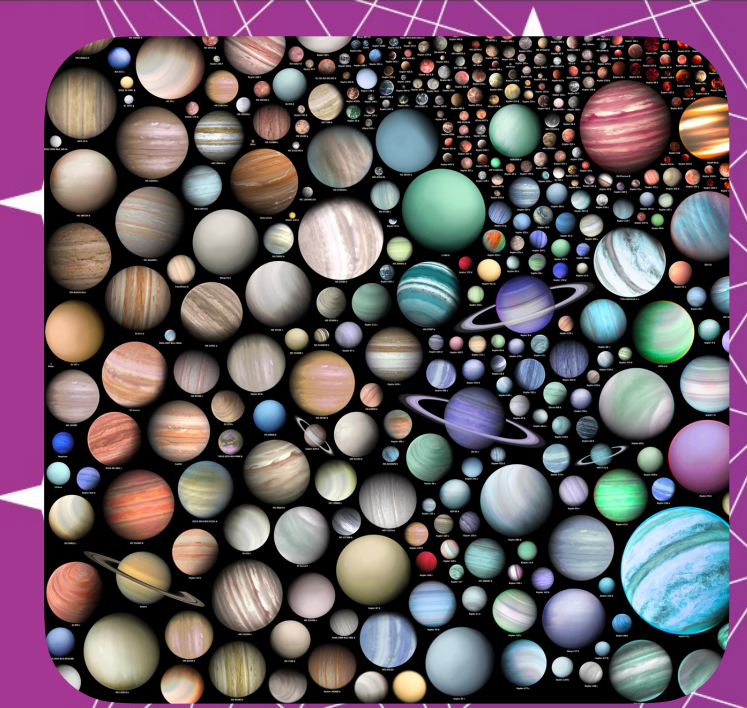
Prediction of the mass fraction of CO2 in the atmosphere by the encoder



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The 2023 Ariel Data Challenge: Scientists invite AI experts to help study exoplanets

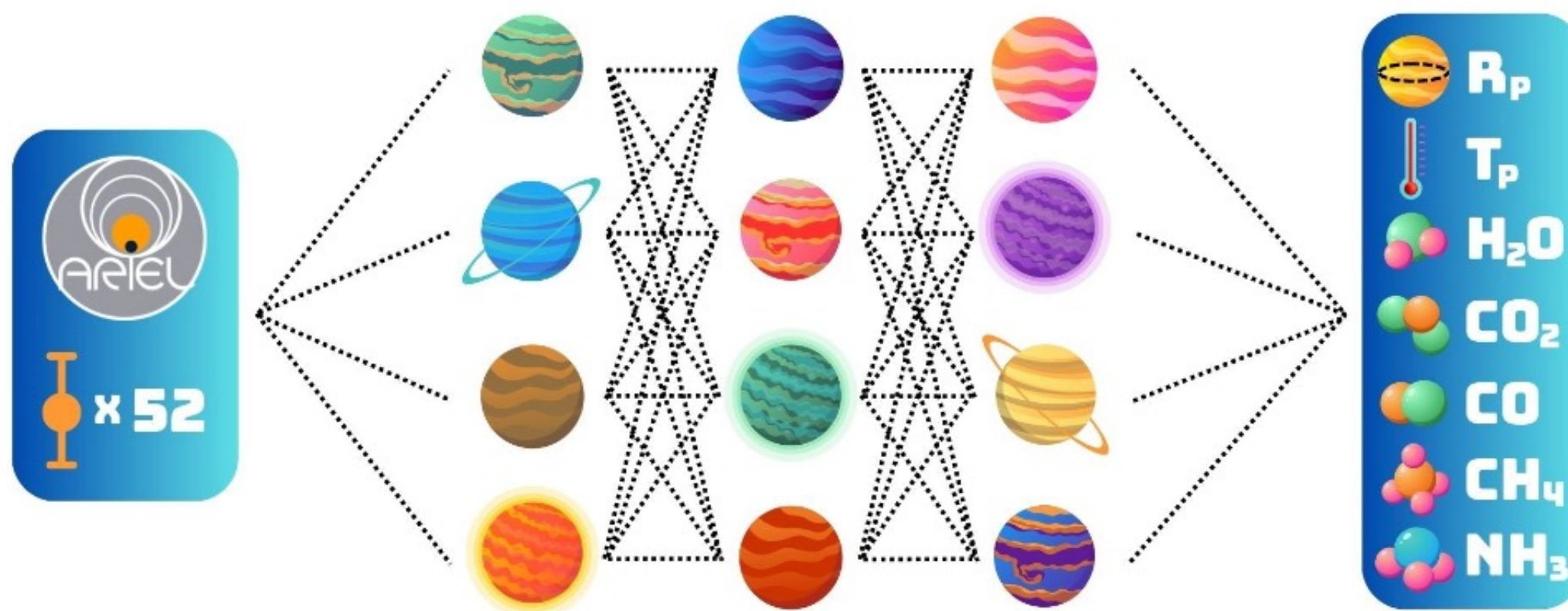
"Astronomers are struggling to keep up with the complexity and volume of incoming exoplanetary data. The challenge is an excellent platform to facilitate cross-disciplinary solutions with AI experts."



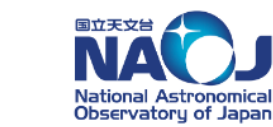
Quite a lot harder than last year

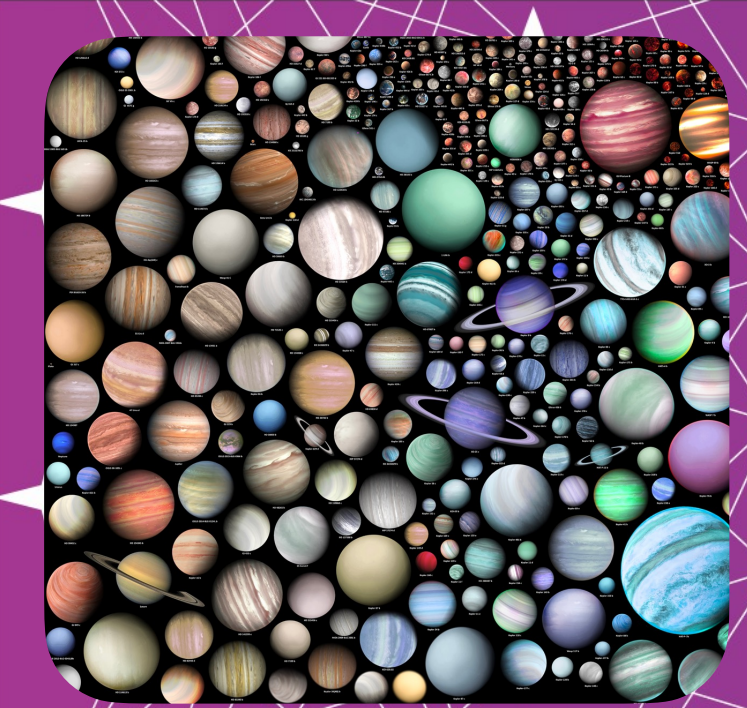


Mayeul Aubin



Science and Technology Facilities Council





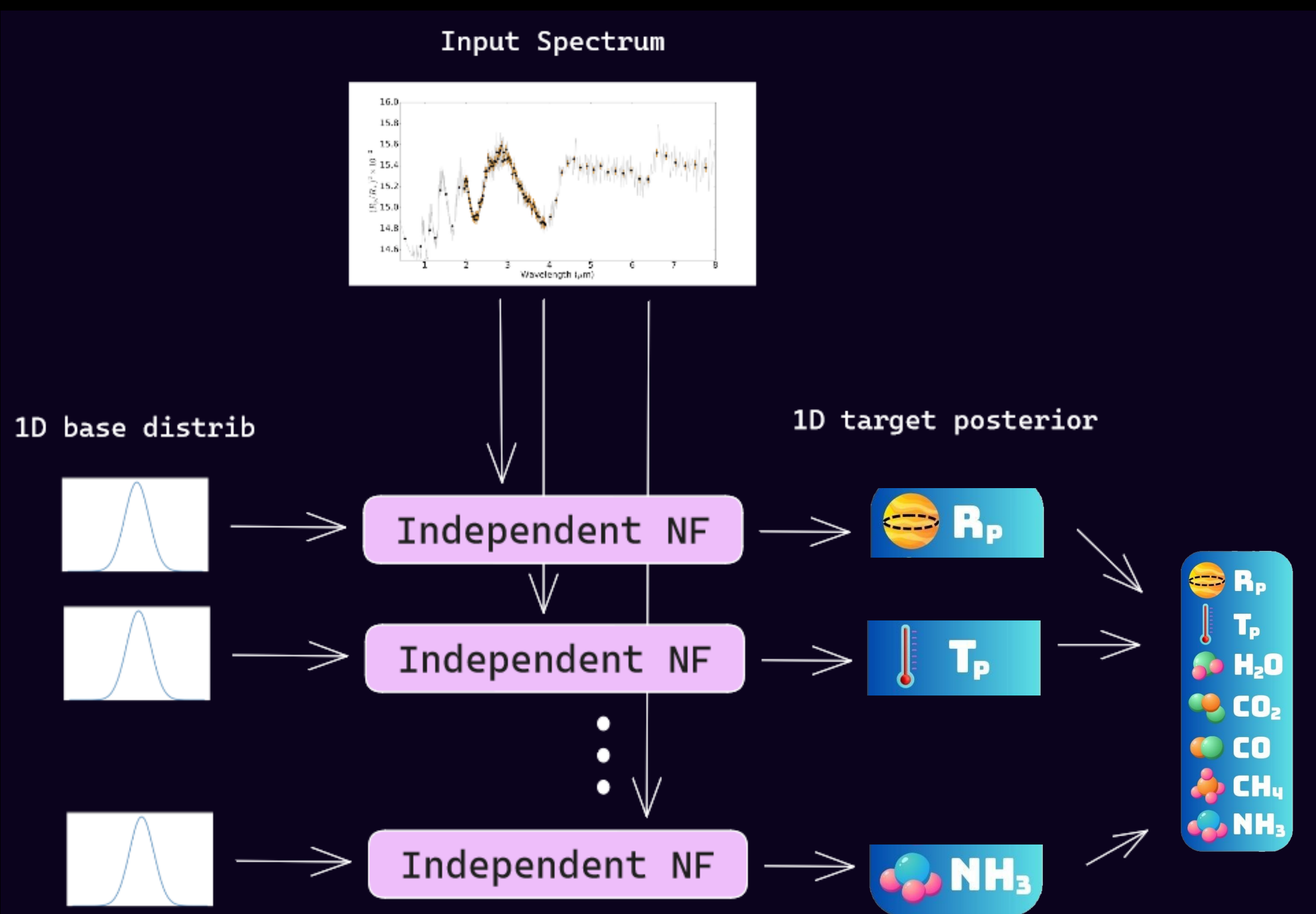
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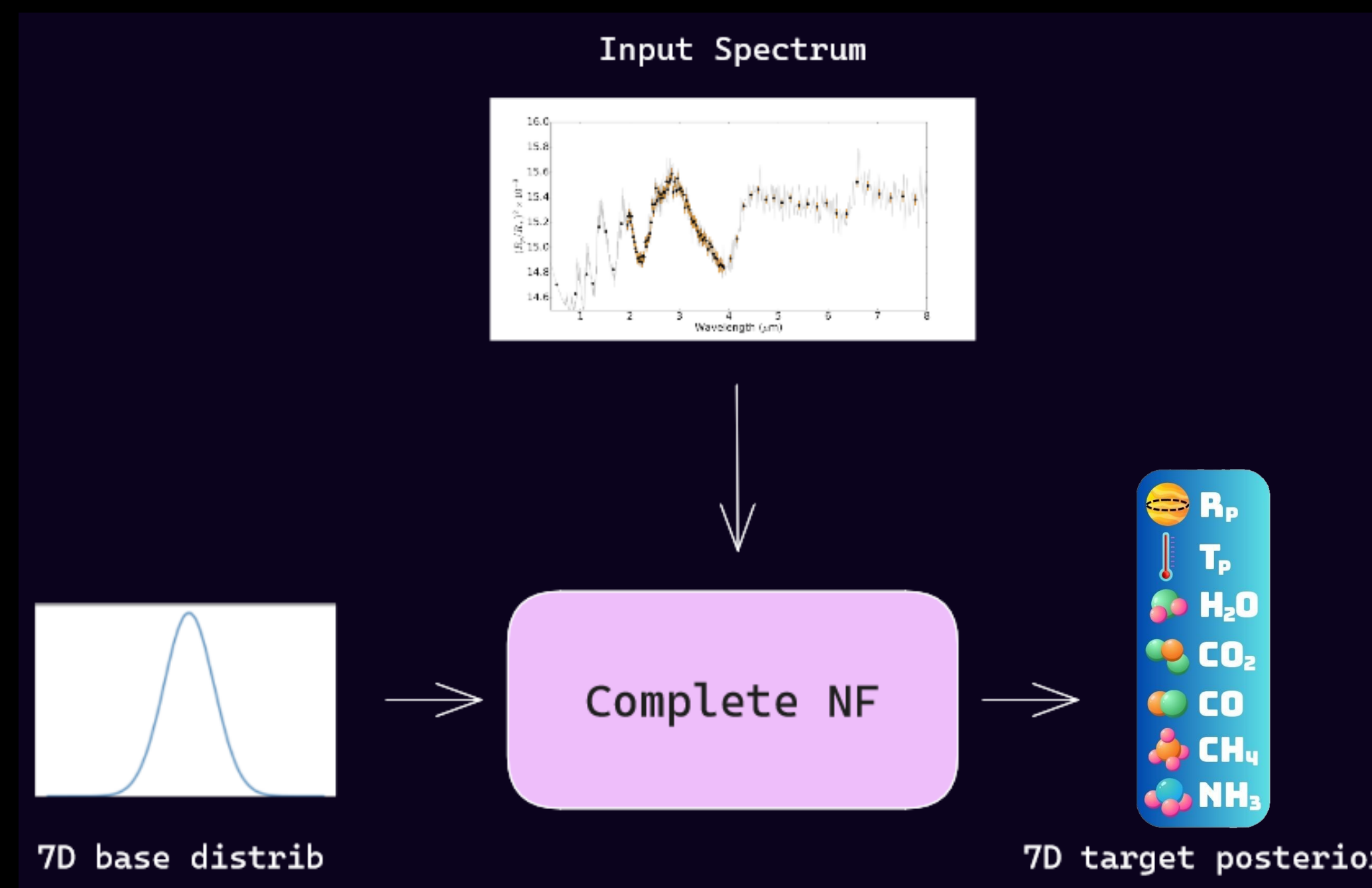


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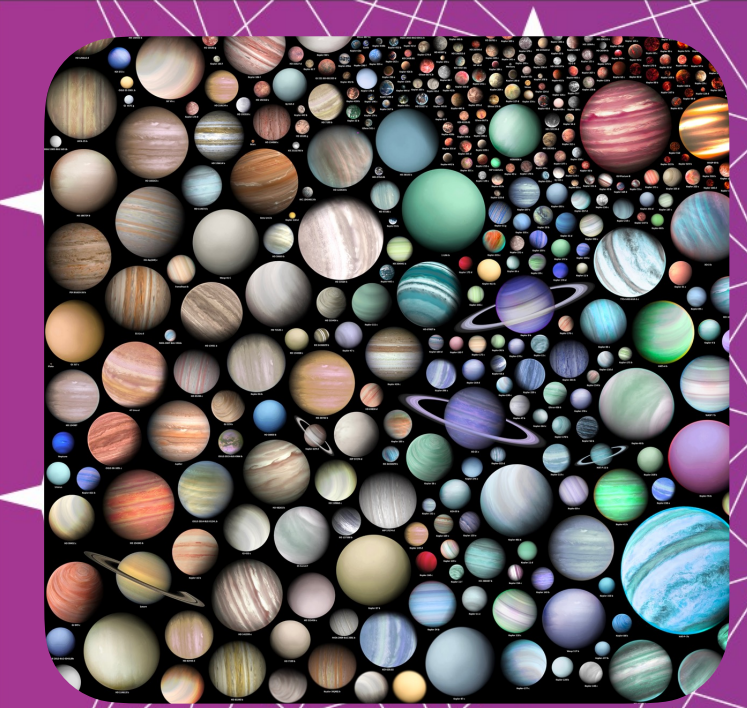
We used 7 independent normalising flows



A set of independent Normalising Flows

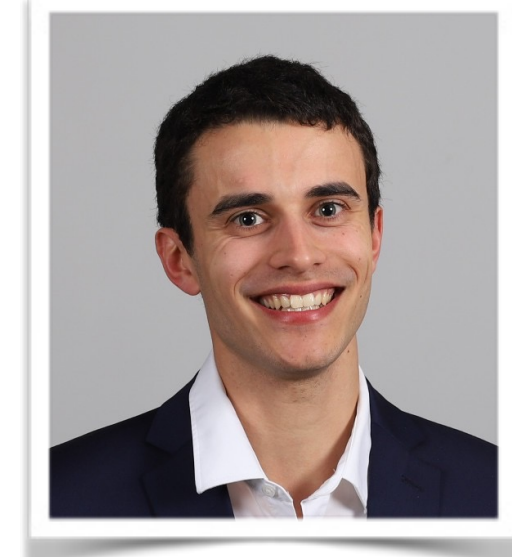


One complete Normalising Flow



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Mayeul Aubin

Leader Board

In-competition

Rank	Name	Score
1	Mayeul_Aubin	679
2	gators	666
3	Les3Stagios	650
4	asweet	618
5	caokyhan	615
6	hieucao	610
7	dungpt	602
8	aescalantelopez	596
9	MALTO	595
10	brian_jonestown_massacre	586
11	inosen_infinity	582
12	diogo4u	560

Simulation-based Inference for Exoplanet Atmospheric Retrieval: Insights from winning the Ariel Data Challenge 2023 using Normalizing Flows

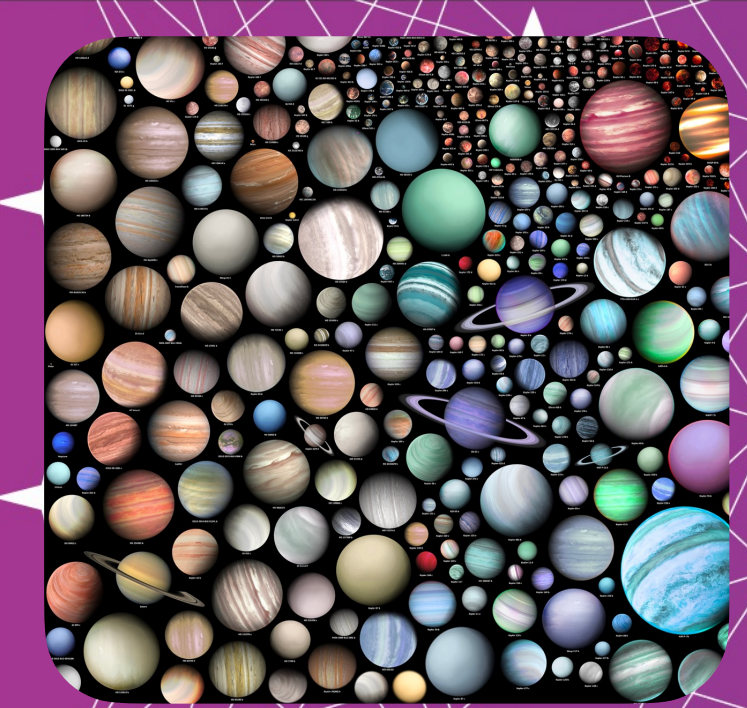
Mayeul Aubin^{1,2*}, Carolina Cuesta-Lazaro^{3,4}, Ethan Tregidga^{1,5}, Javier Viaña⁶, Cecilia Garraffo^{1,7}, Iouli E. Gordon⁸, Mercedes López-Morales⁸, Robert J. Hargreaves⁸, Vladimir Yu. Makhnev⁸, Jeremy J. Drake⁷, Douglas P. Finkbeiner³, and Phillip Cargile⁹

Exoplanet Atmospheric Parameter Retrieval: The AstroAI winning model for the 2023 Ariel Data Challenge using Normalizing Flows

MAYEUL AUBIN,^{1,2} CAROLINA CUESTA-LAZARO,^{3,4} ETHAN TREGIDGA,^{1,5} JAVIER VIAÑA,⁶ CECILIA GARRAFFO,^{1,7} IOULI E. GORDON,⁸ MERCEDES LÓPEZ-MORALES,⁸ ROBERT J. HARGREAVES,⁸ VLADIMIR YU. MAKHNEV,⁸ JEREMY DRAKE,⁷ DOUGLAS P. FINKBEINER,⁹ AND PHILLIP CARGILE³

ASTROAI
1st of 293 teams!

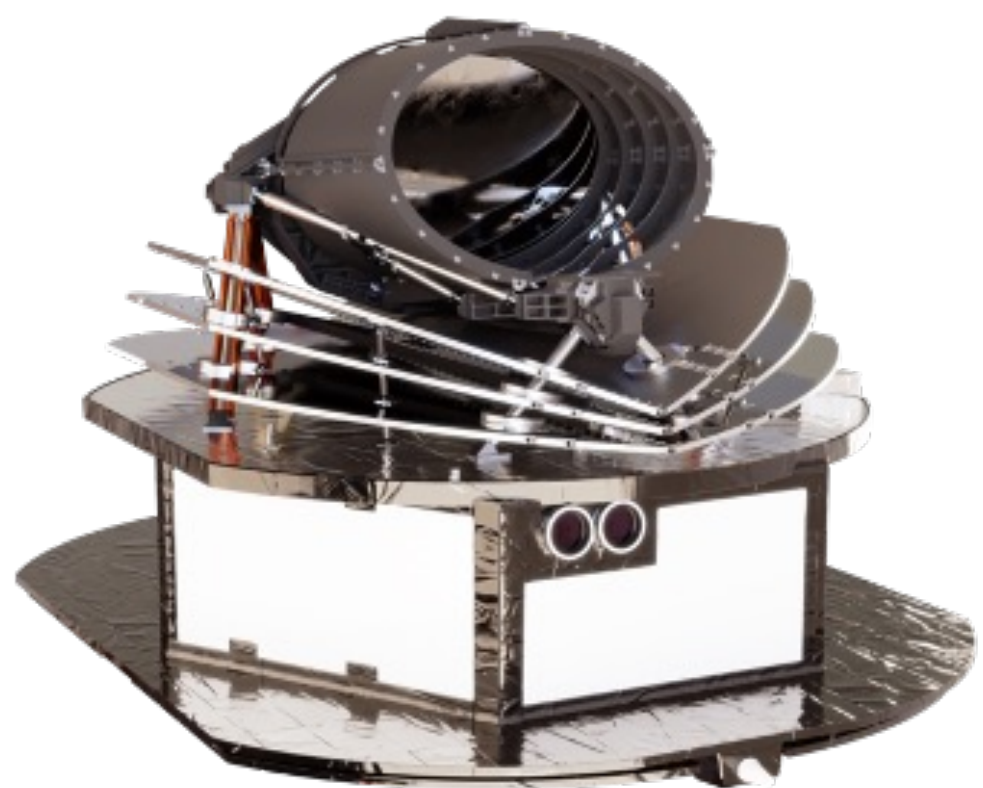




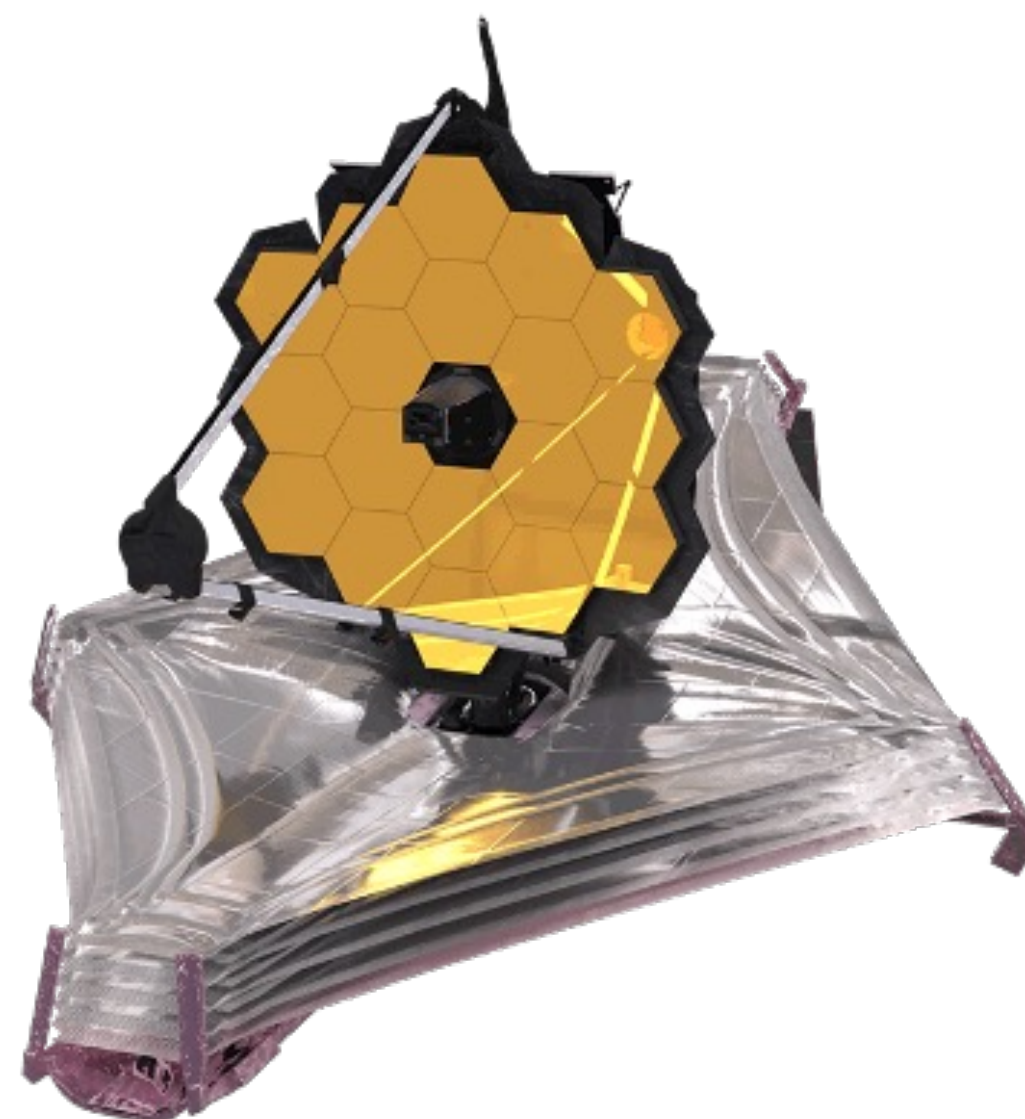
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Next Small Steps: Generalize for other missions.



Ariel Space Mission



JWST

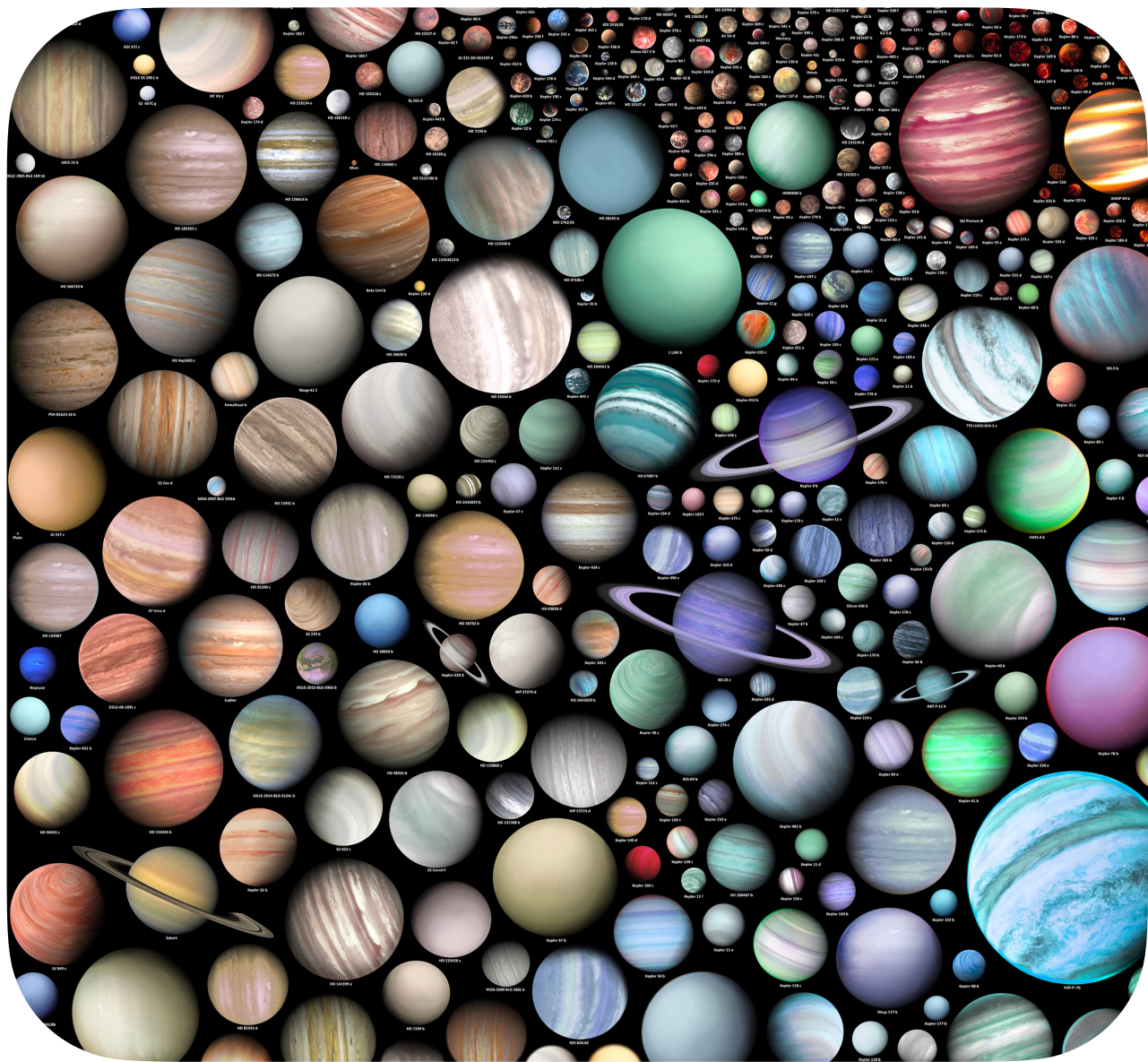


Nancy Grace Roman
Space Telescope

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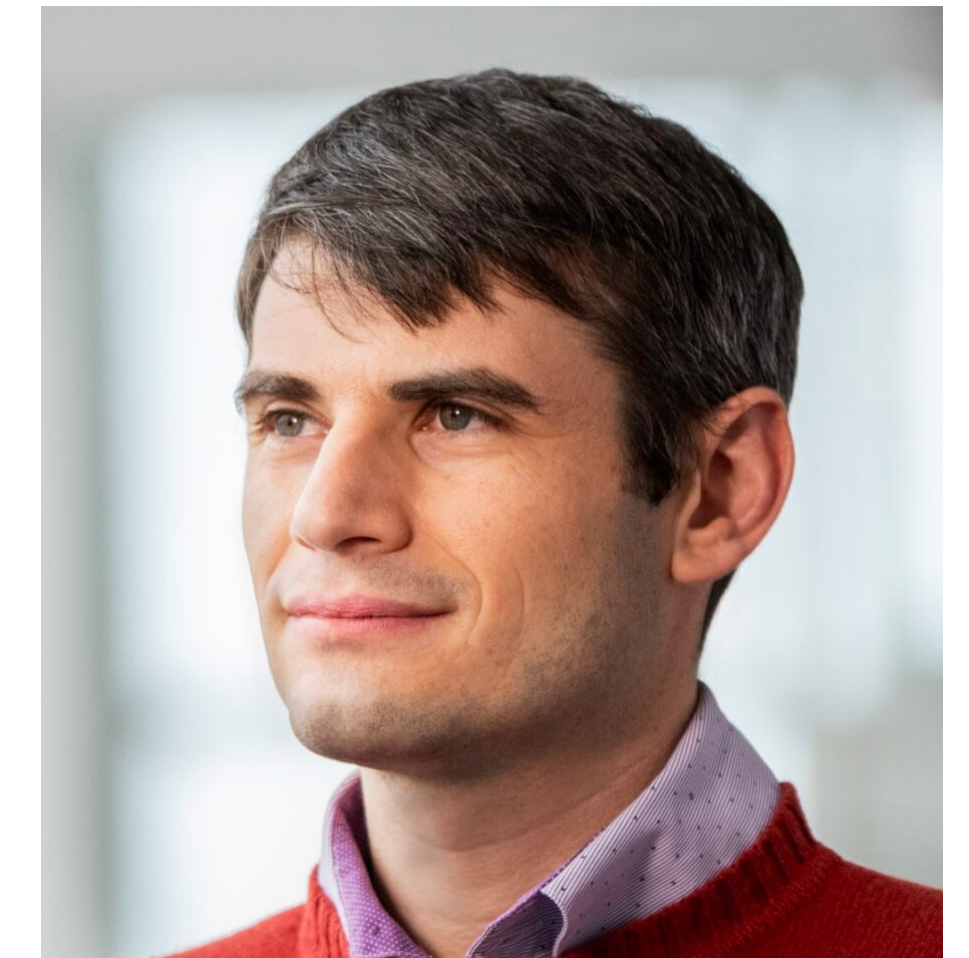
Exoplanet Atmospheres & Biosignatures Team



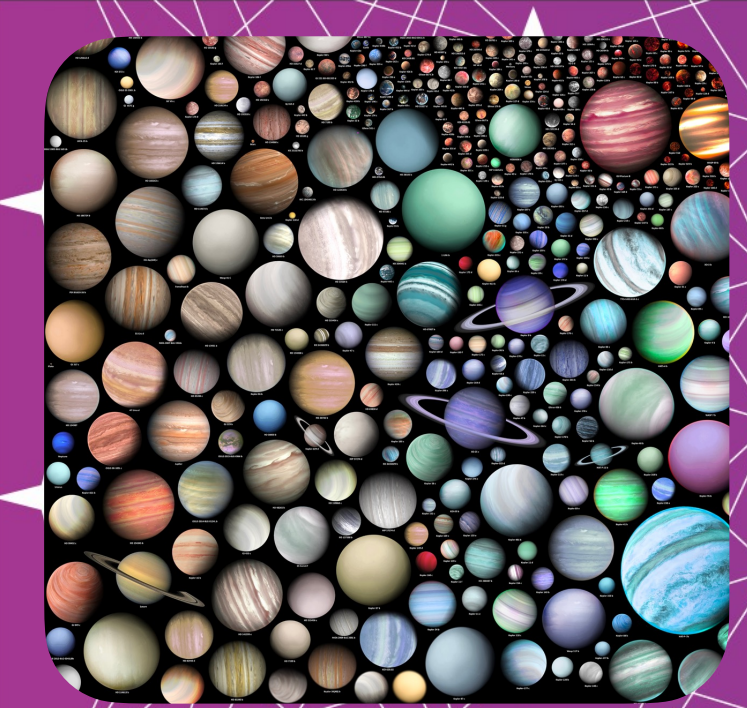
Mercedes López-Morales



Bill Freeman



Robin Walters

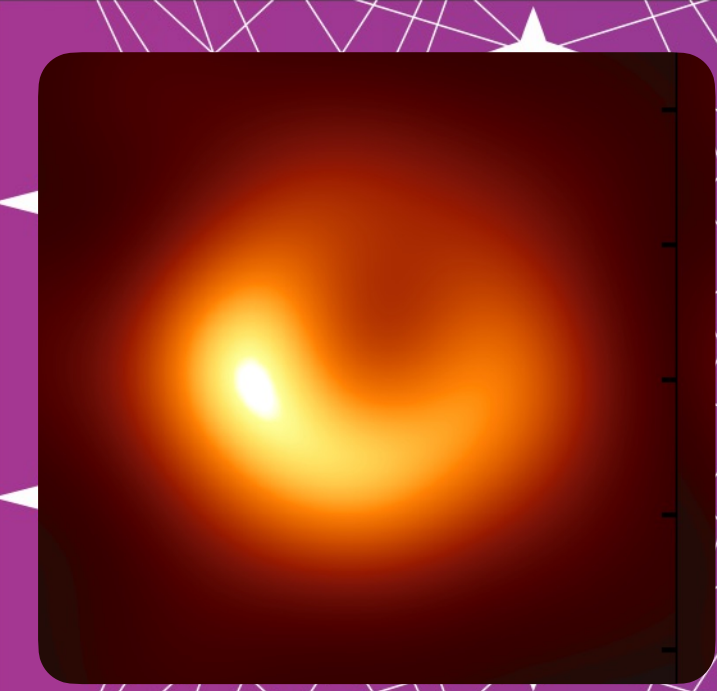


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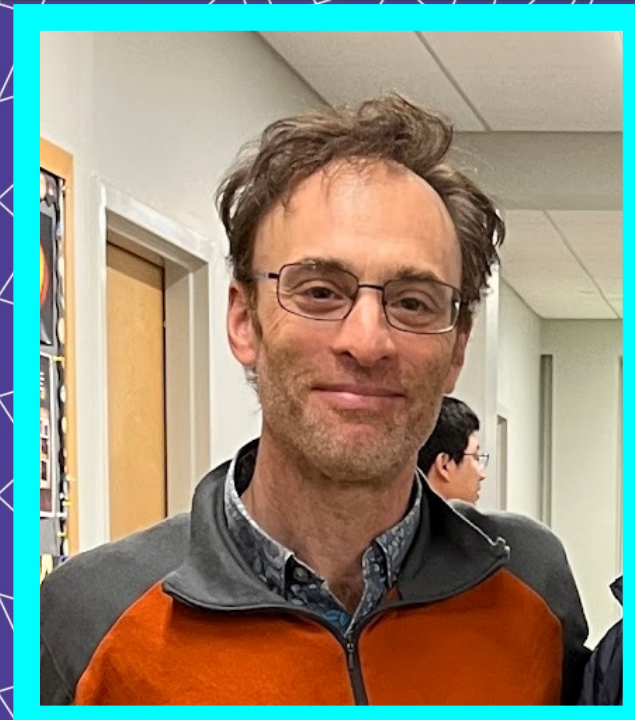


Breakthrough: Find Life Elsewhere in the Universe!



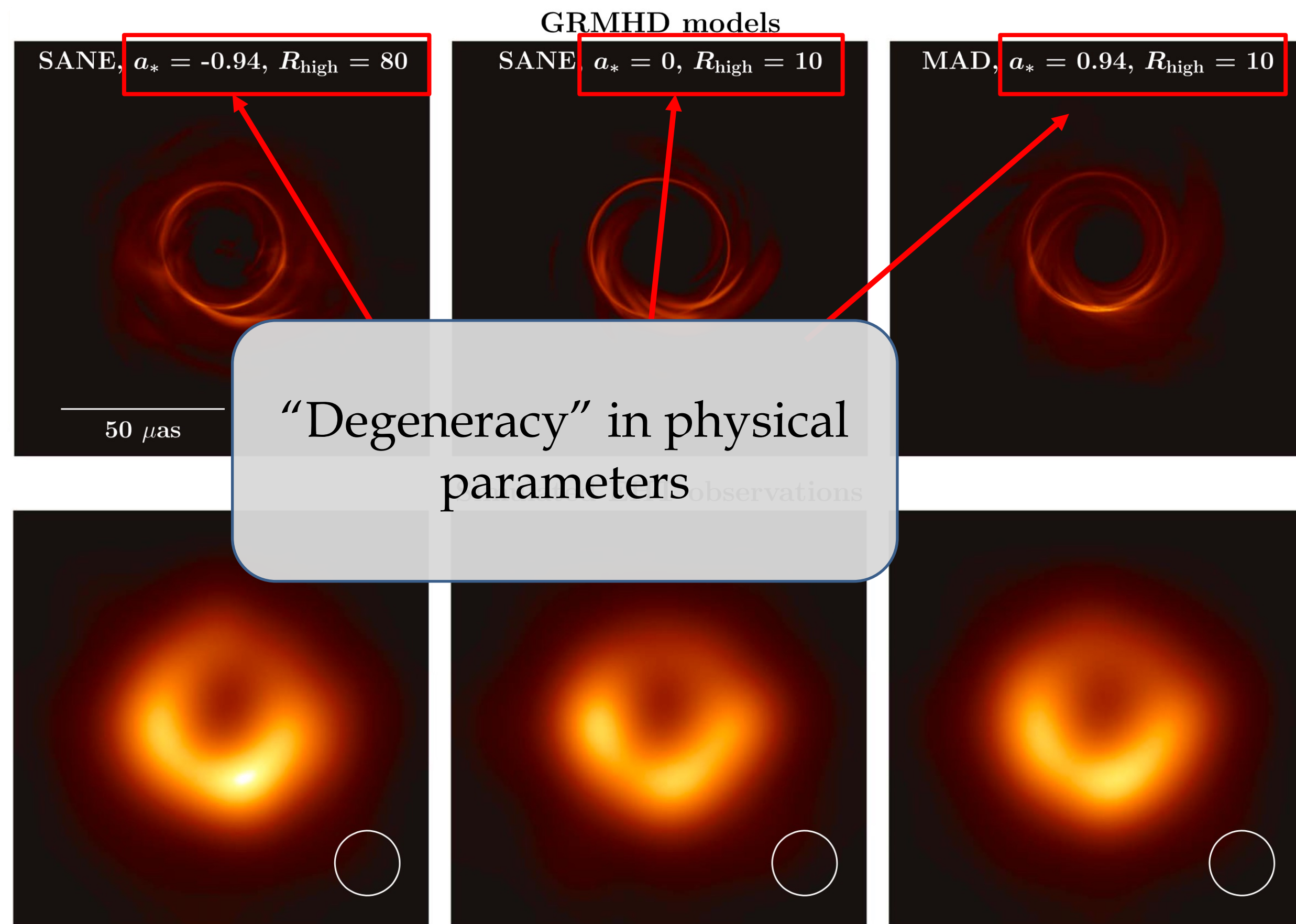
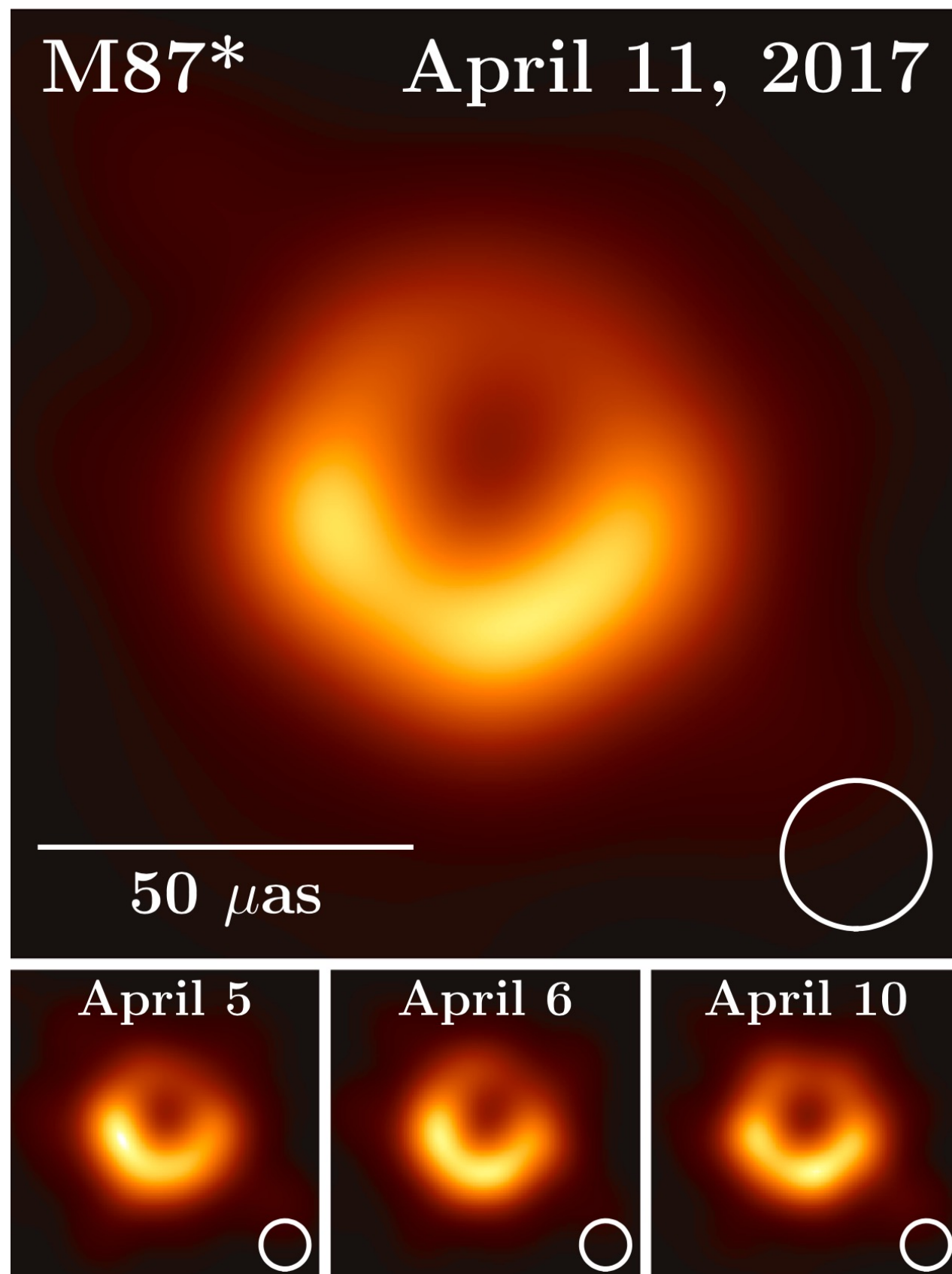
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Shep Doeleman

Supermassive BHs: EHT



ASTROAI

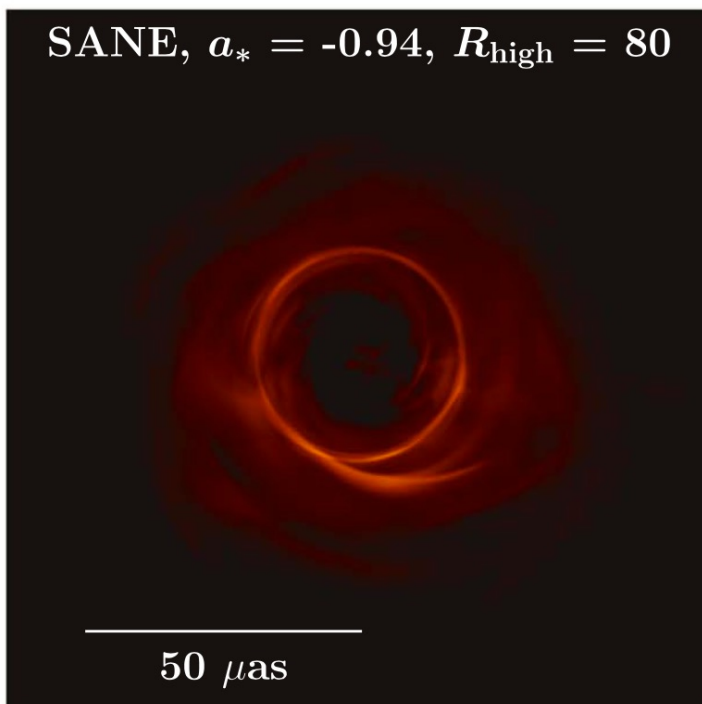
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We have data from two sources:

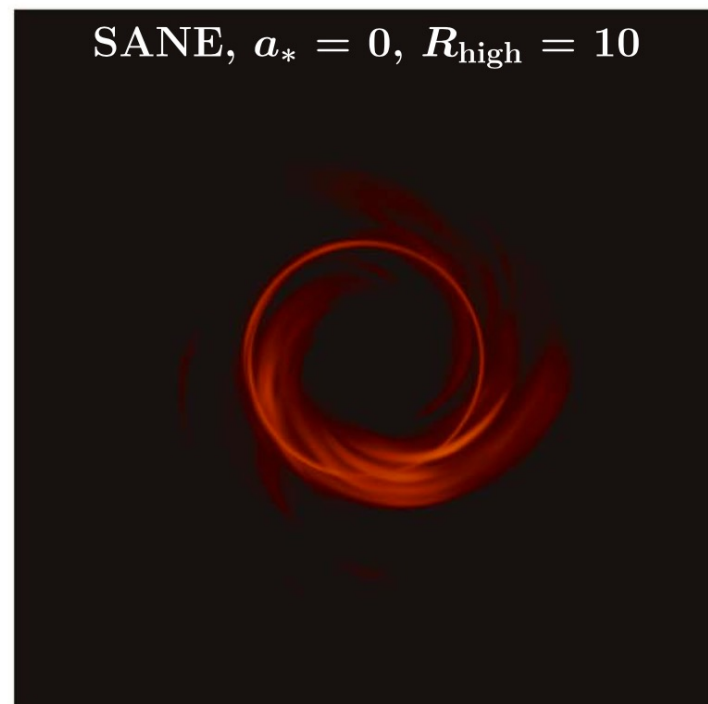
- GRMHD simulated images

GRMHD models

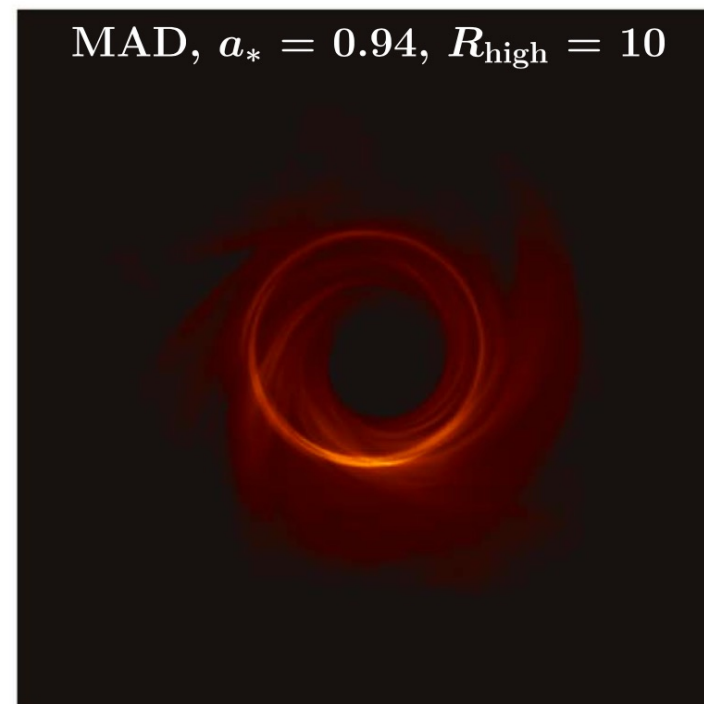
SANE, $a_* = -0.94$, $R_{\text{high}} = 80$



SANE, $a_* = 0$, $R_{\text{high}} = 10$

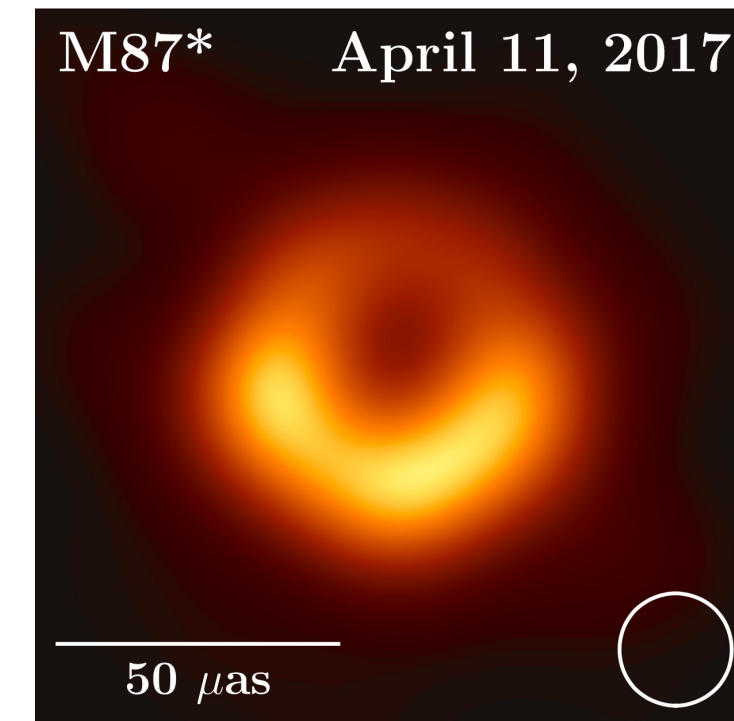


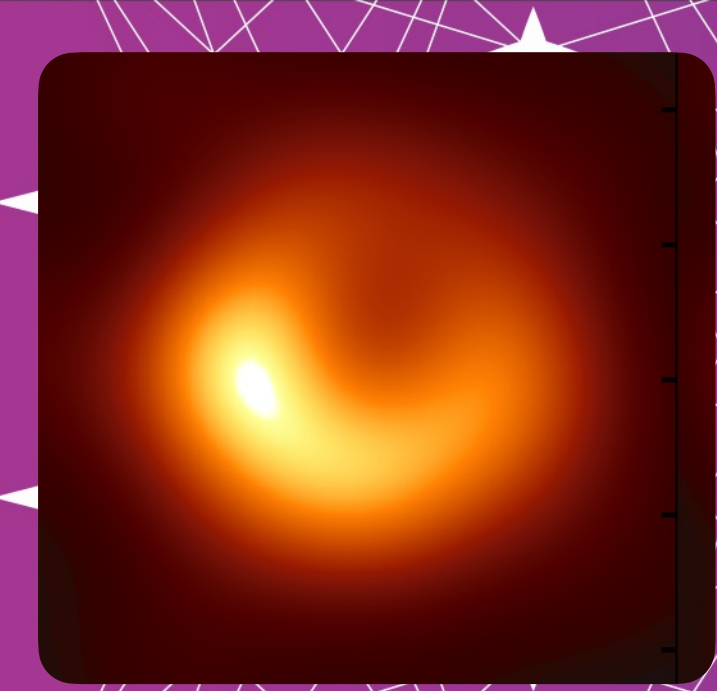
MAD, $a_* = 0.94$, $R_{\text{high}} = 10$



- Real EHT observations

M87* April 11, 2017



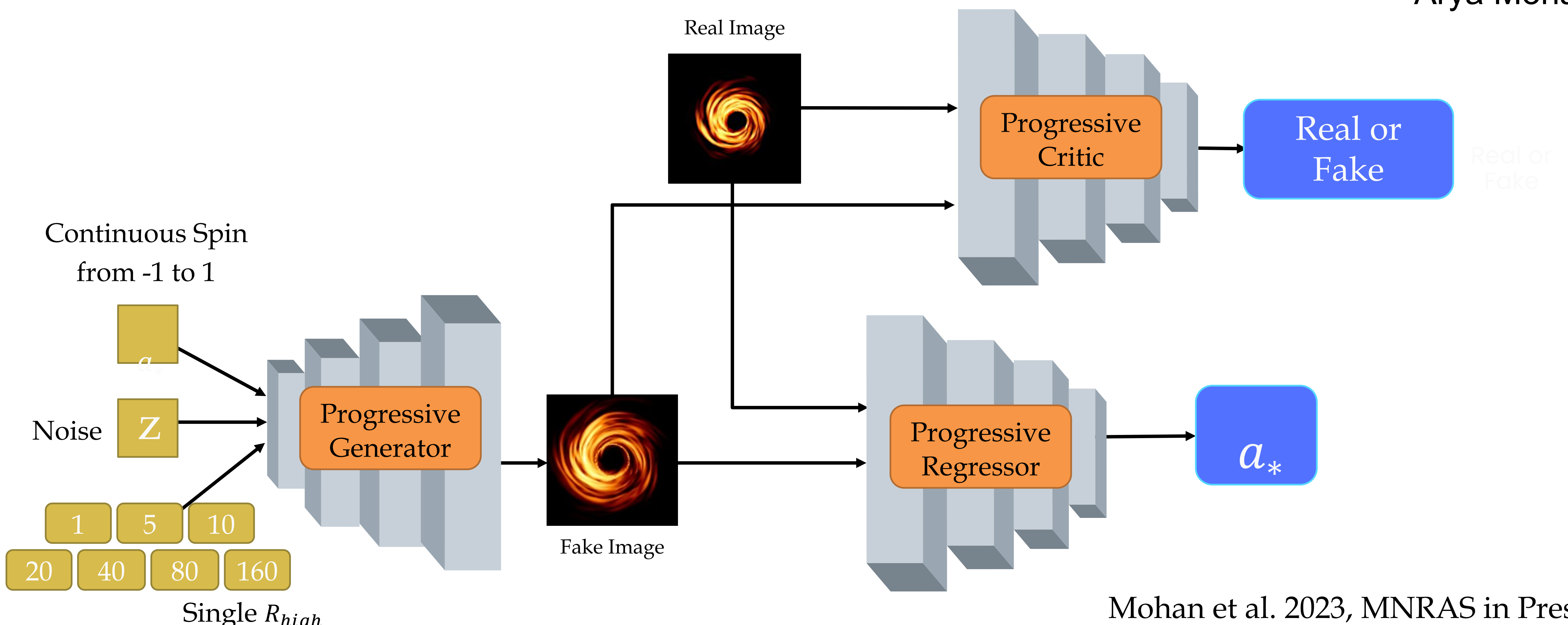


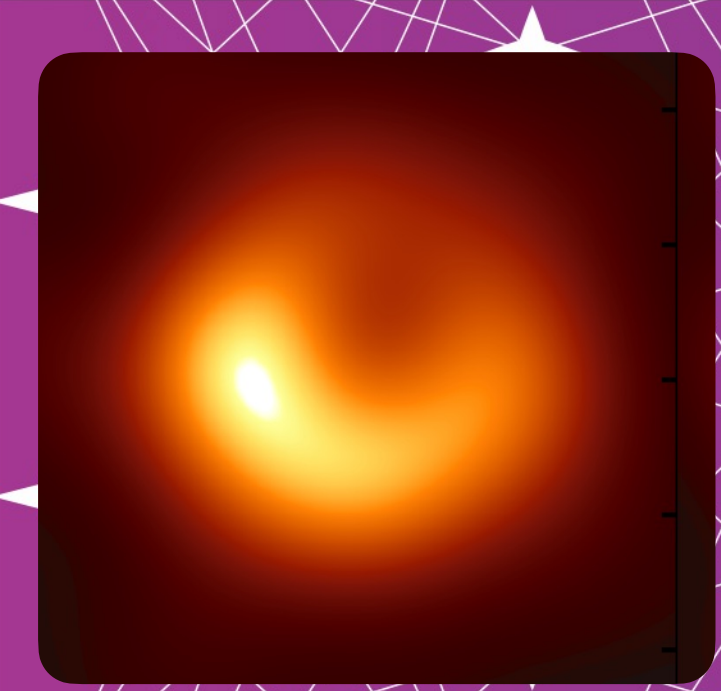
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Arya Mohan

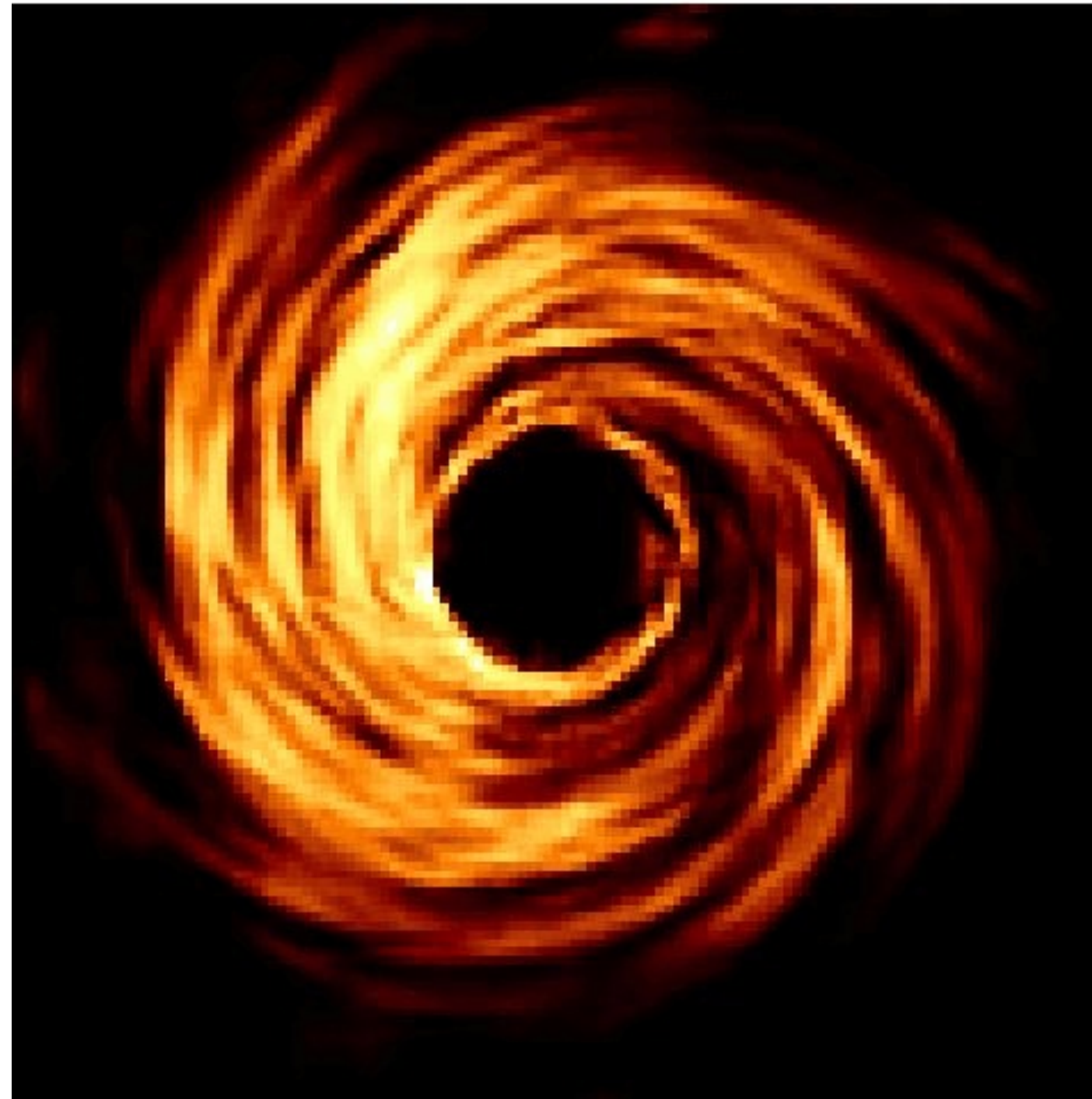


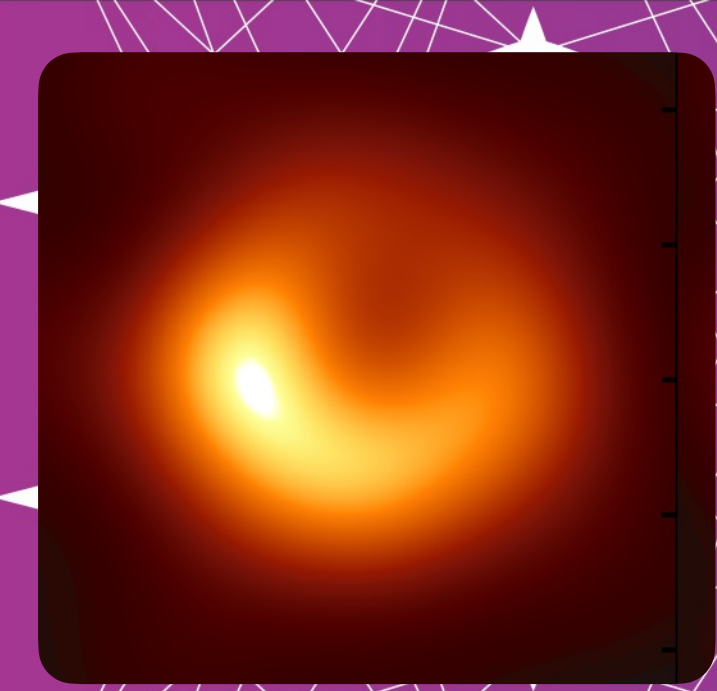


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$a = -0.4$





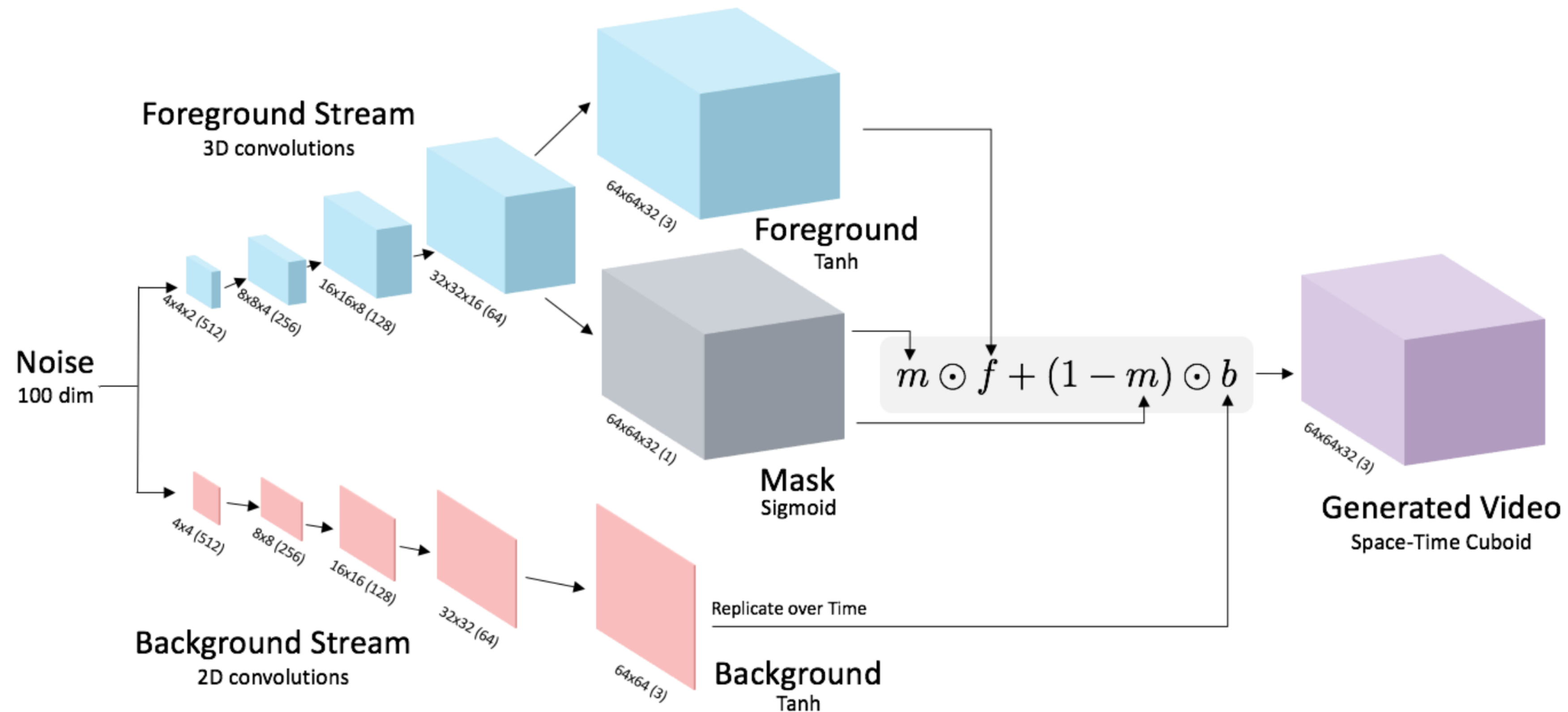
ASTROAI

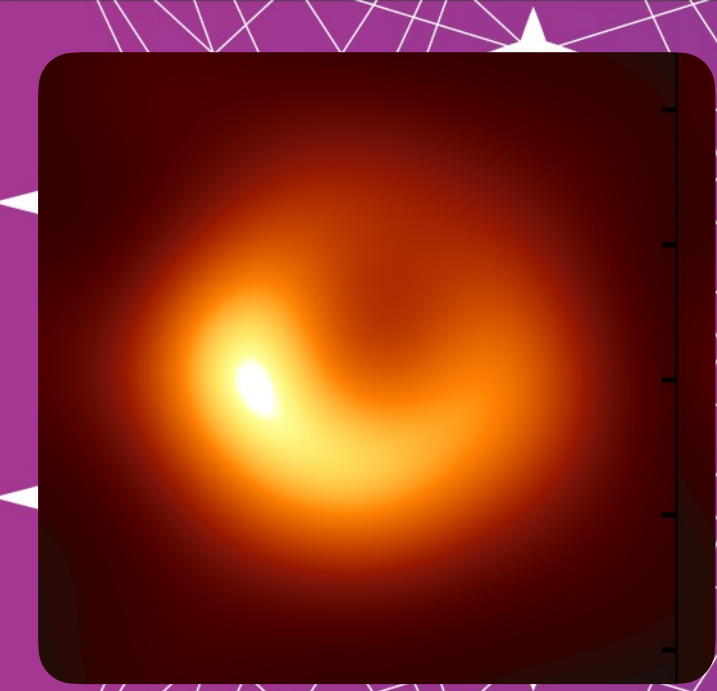
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David Loving

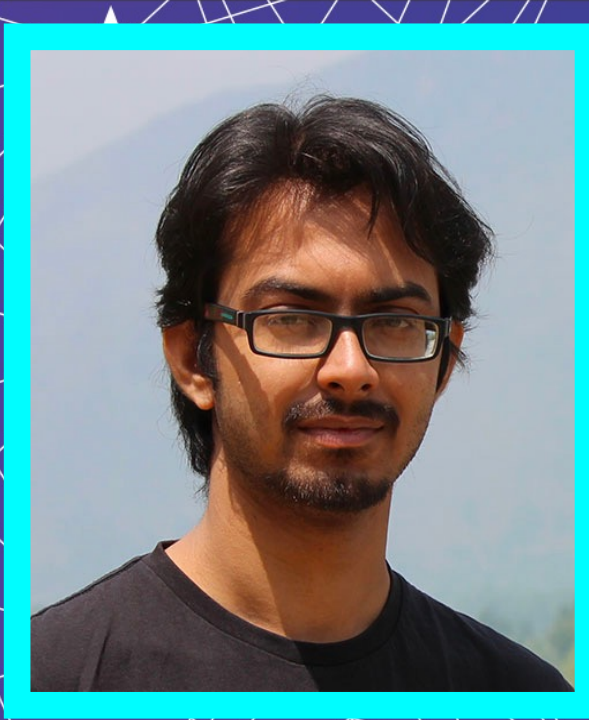
Generative Model for Black Holes' Dynamics





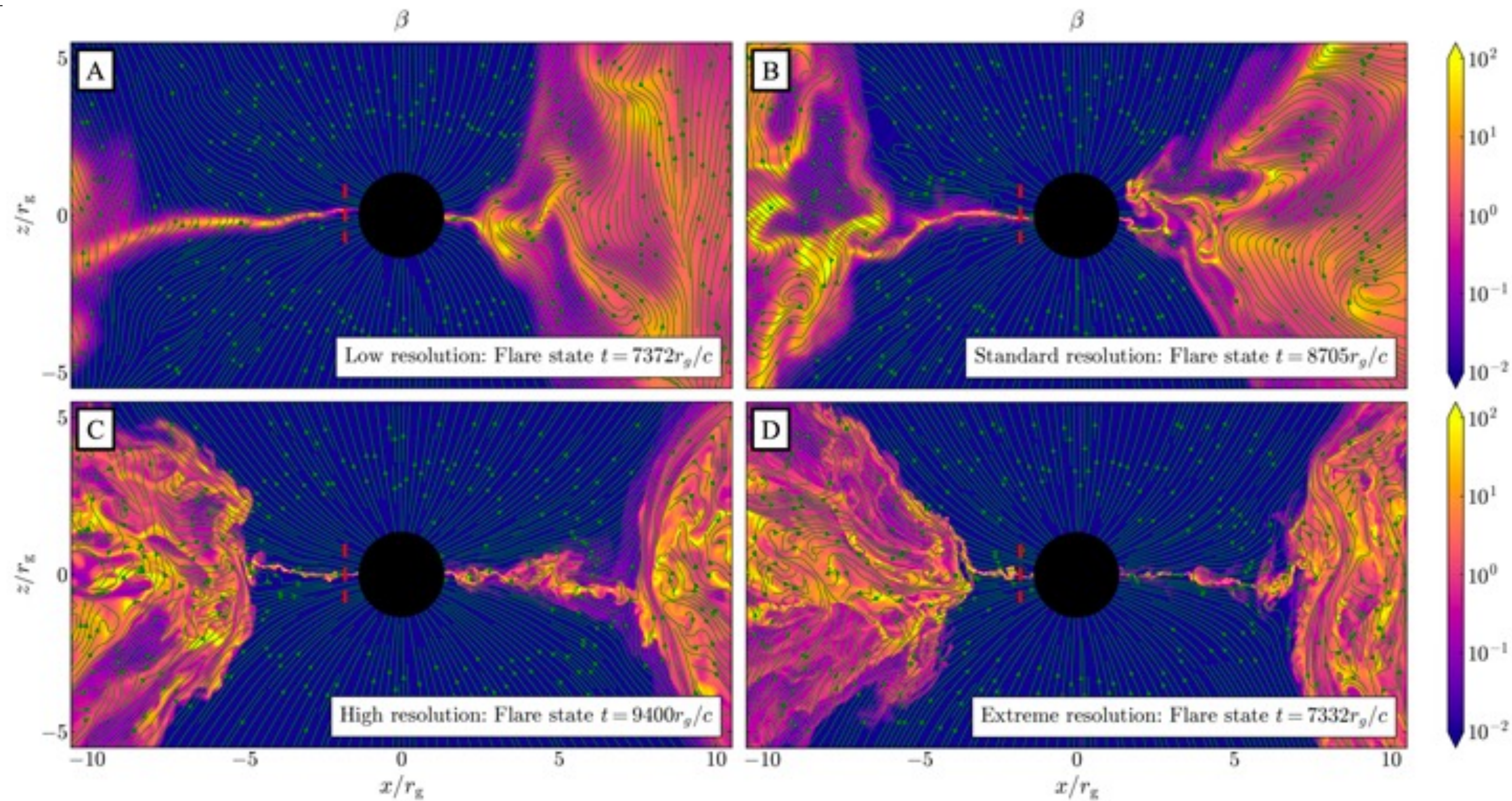
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Koushik
Chatterjee

Super resolution Model for GRMHD simulations for EHT



The Impact

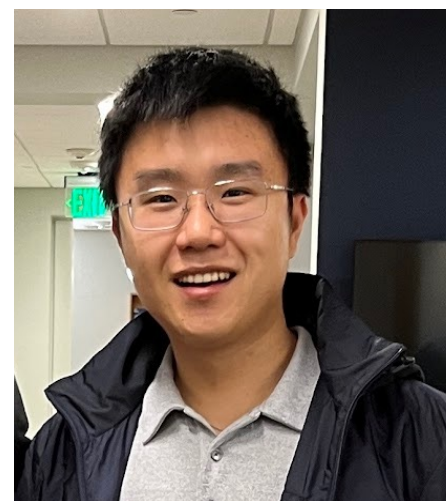
The Students



Thaddaeus
Kiker



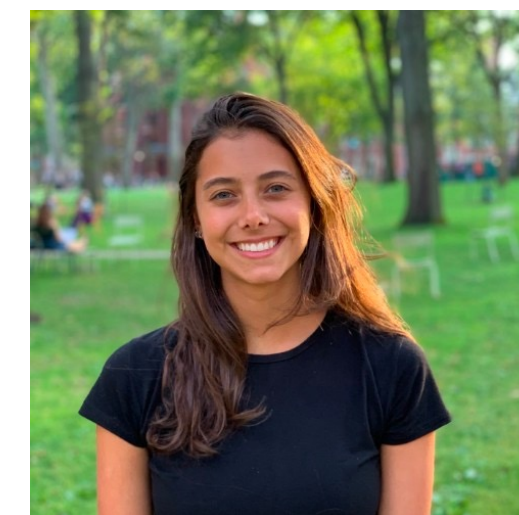
Aryan Mohan



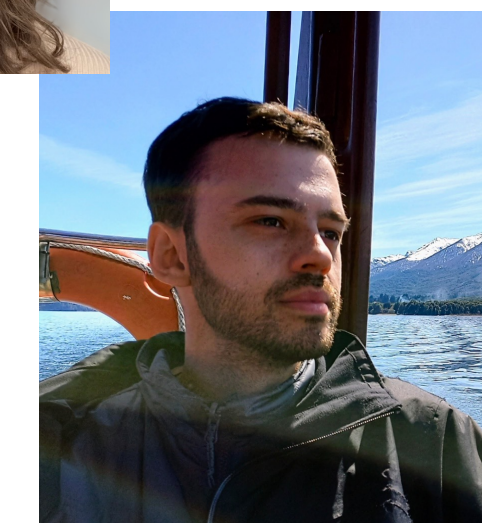
Tao Tsui



Leticia Schettino



Farah Fauth



Benjamin
David Loving
Ricketts



Mayantara
Mudur

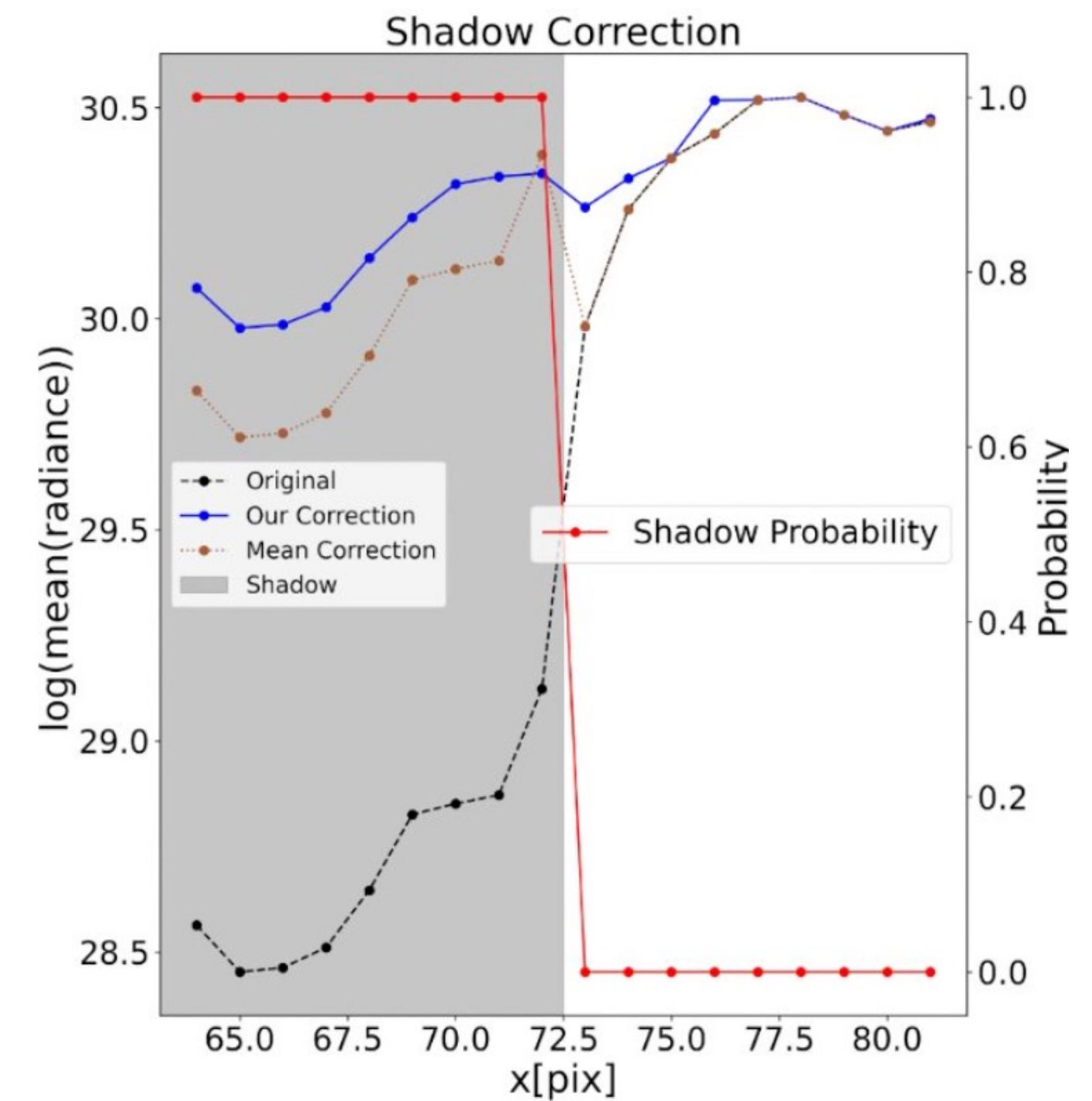
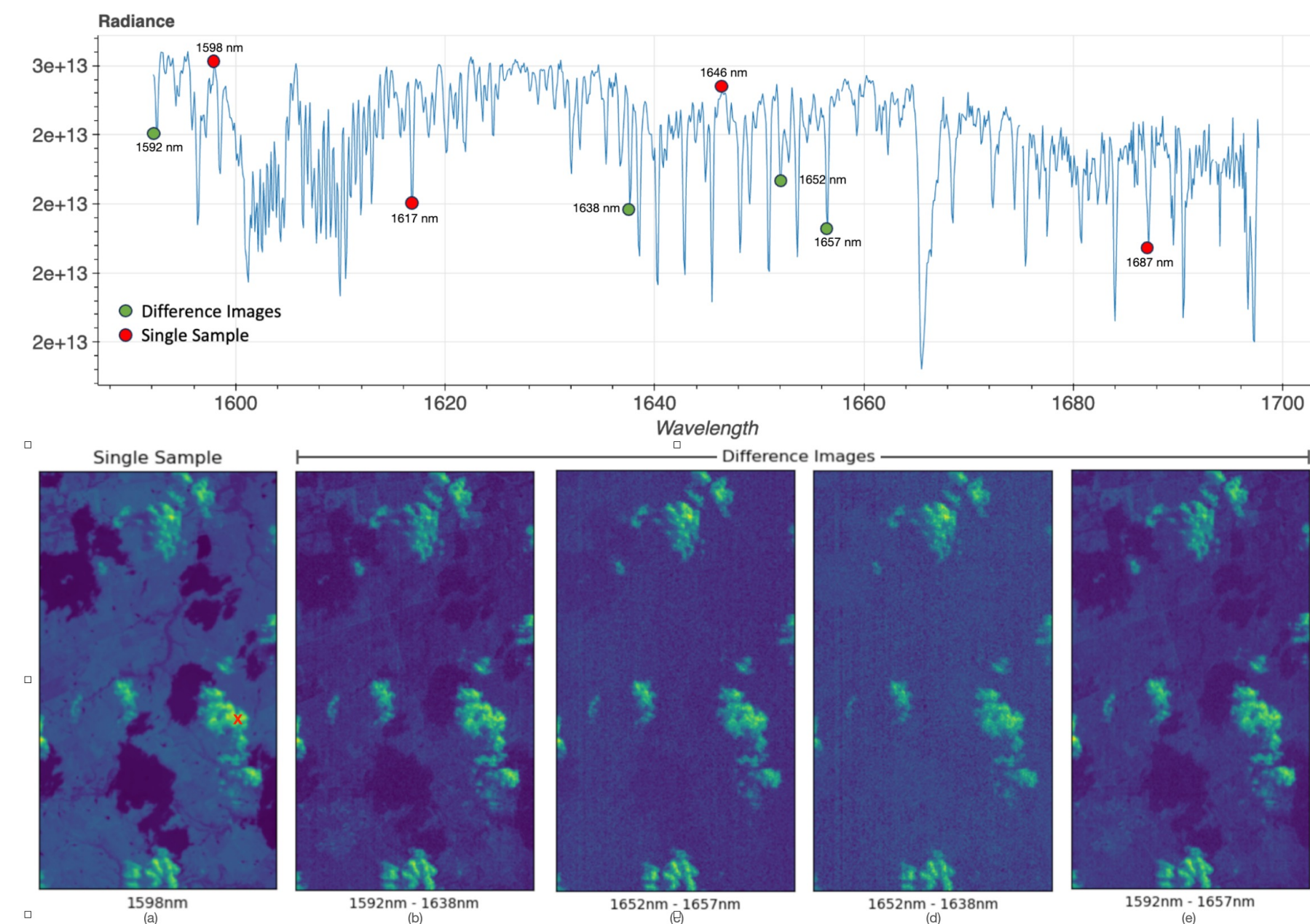
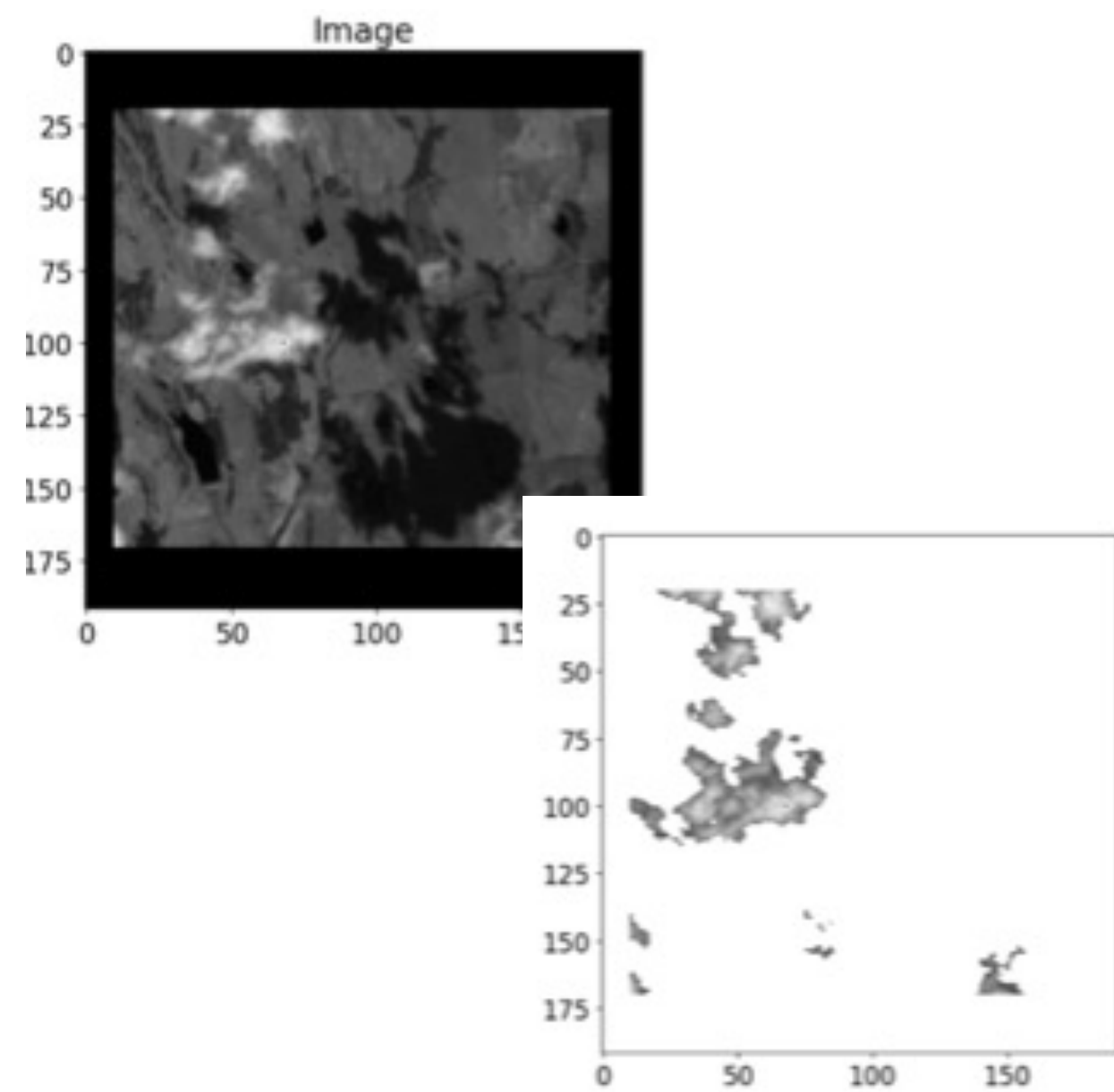


Lily Pan





MethaneSAT: Enhanced Cloud Filtering / Correction



1. MethaneSAT Cloud Filtering Pipeline uses only the image information that let to significant data loss

2. We built an AI model that uses spectral information we enhanced the performance of cloud detection and filtering to 97%

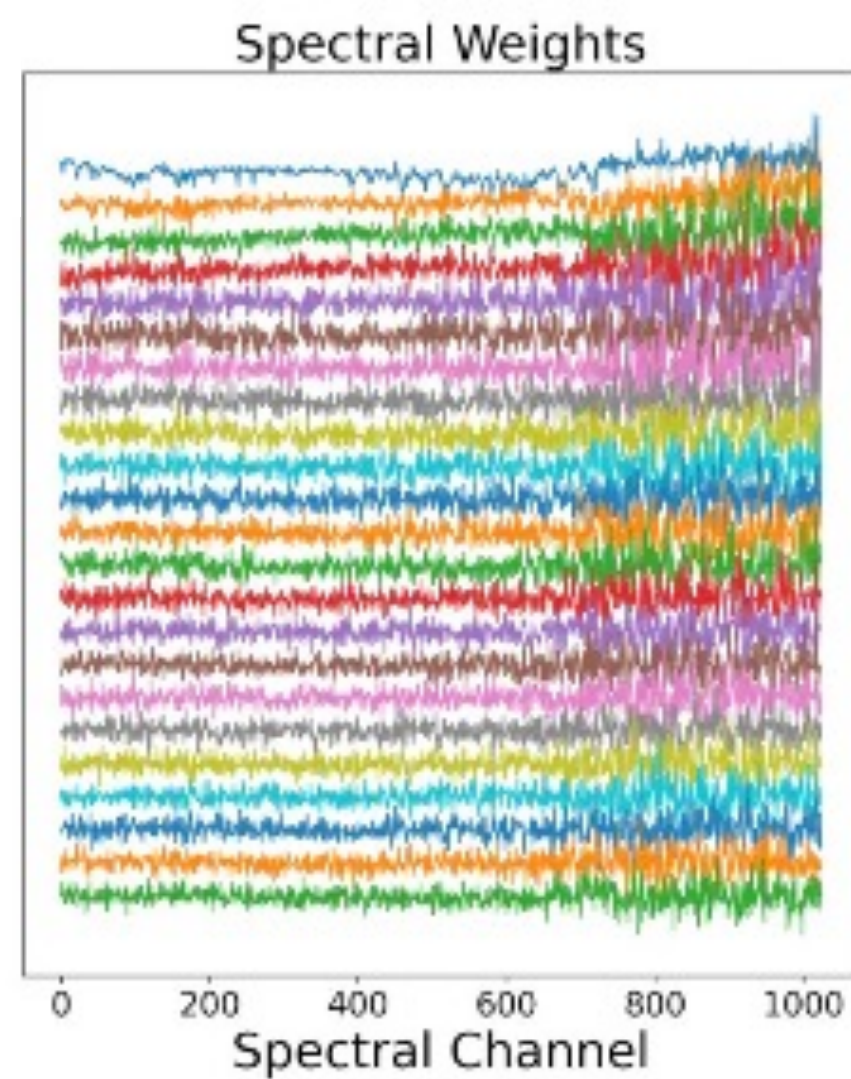
3. We trained an AI model to remove the effect of shadows from the spectra itself, making all the data useable!



MethaneSAT: Enhanced Plume Detection

In Partnership with Google, we are building an AI model to enhance plume detection by using the full spectral information from MethaneSAT data together with Geospatial Data from Google Earth.

MethaneSAT

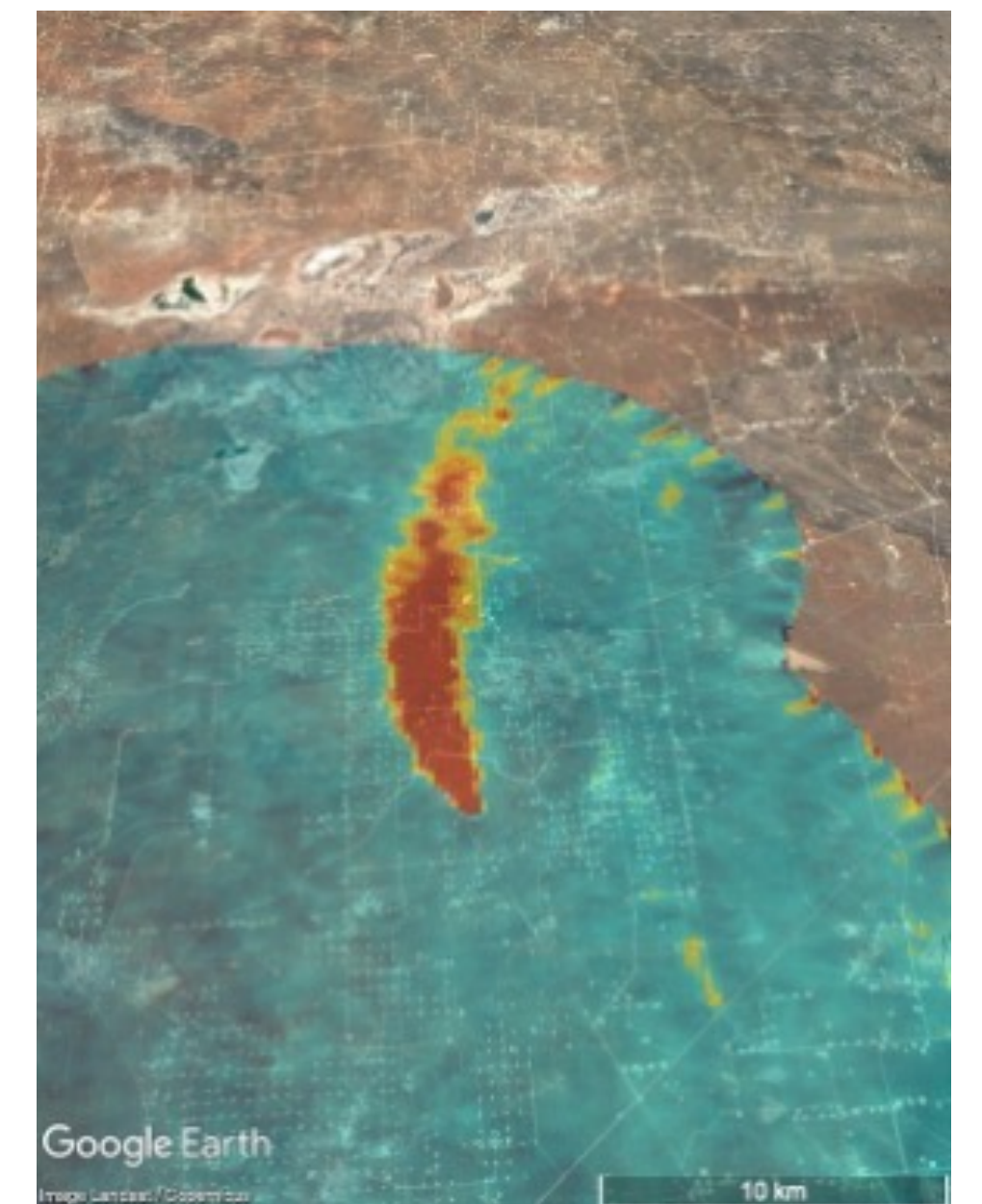


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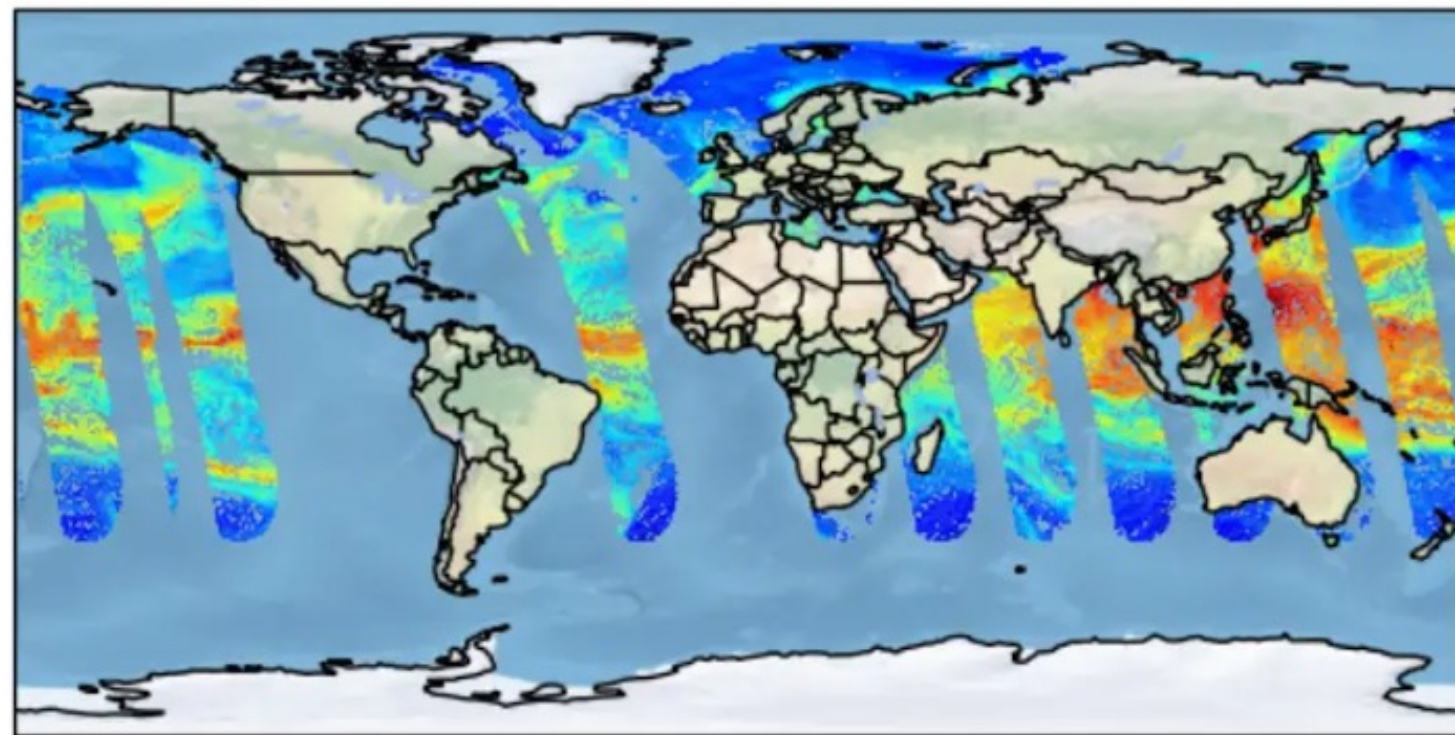
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Reliable Plume Detection

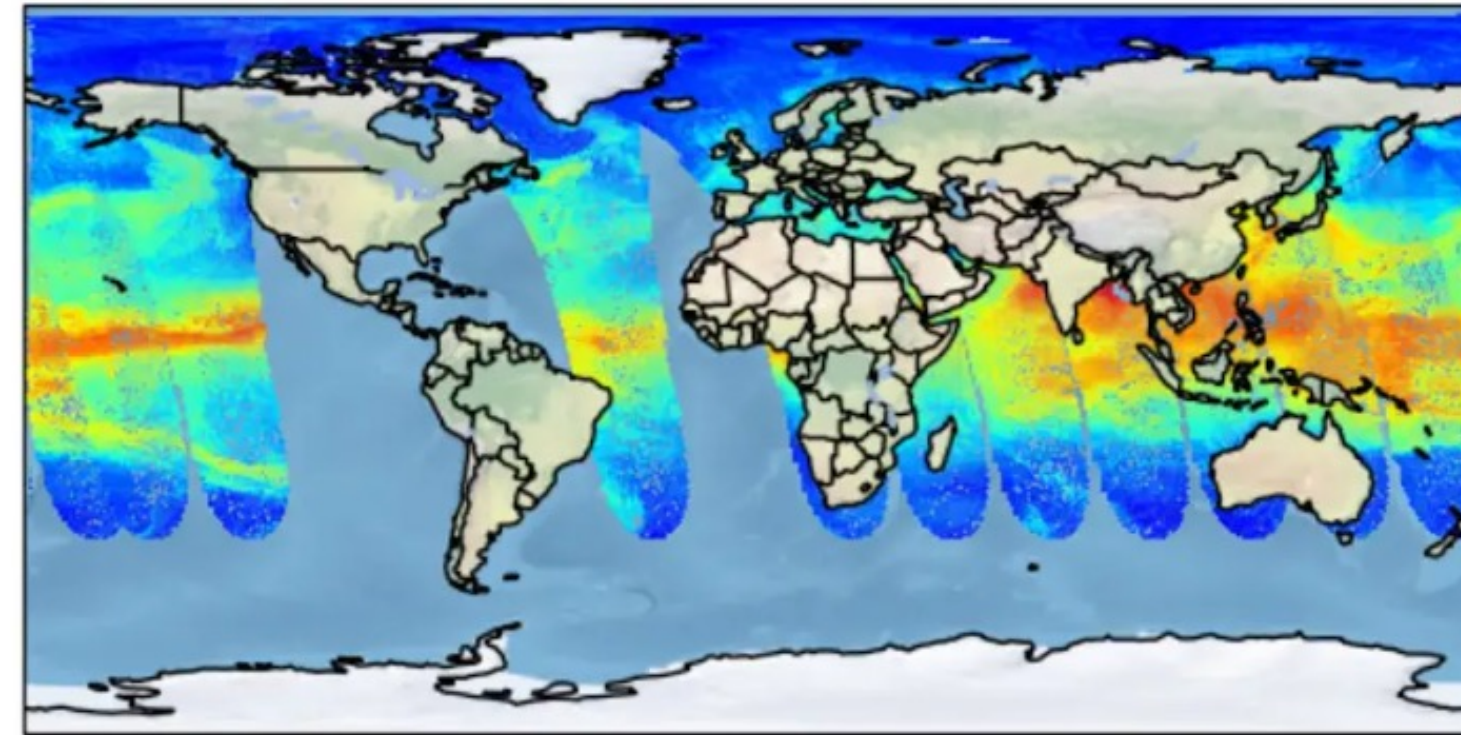




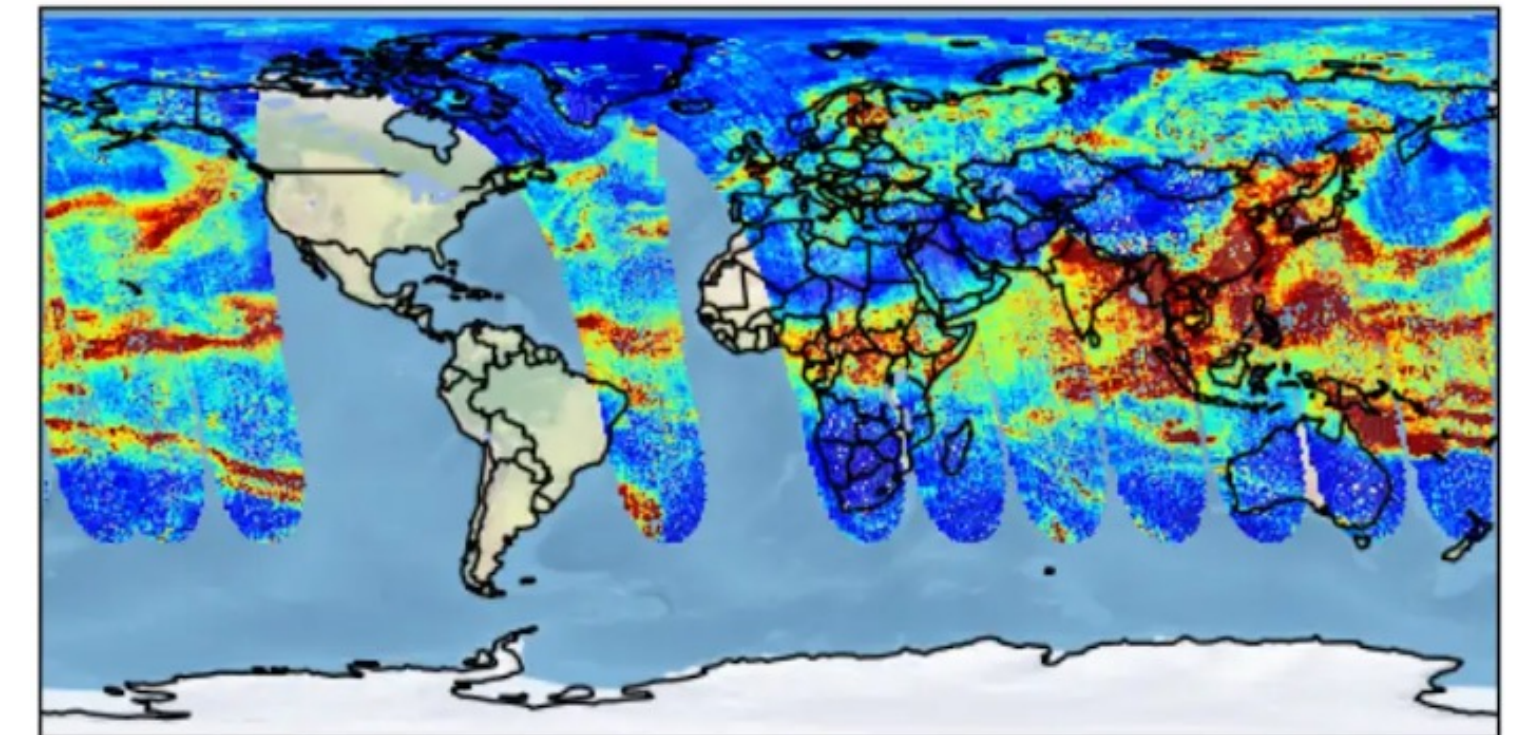
TEMPO: Computer Vision for Water Vapor Imaging



Classic Model strongly dependent on prior assumptions



Light Gradient Boosting (LGB) , prior independent and improved image coverage and quality

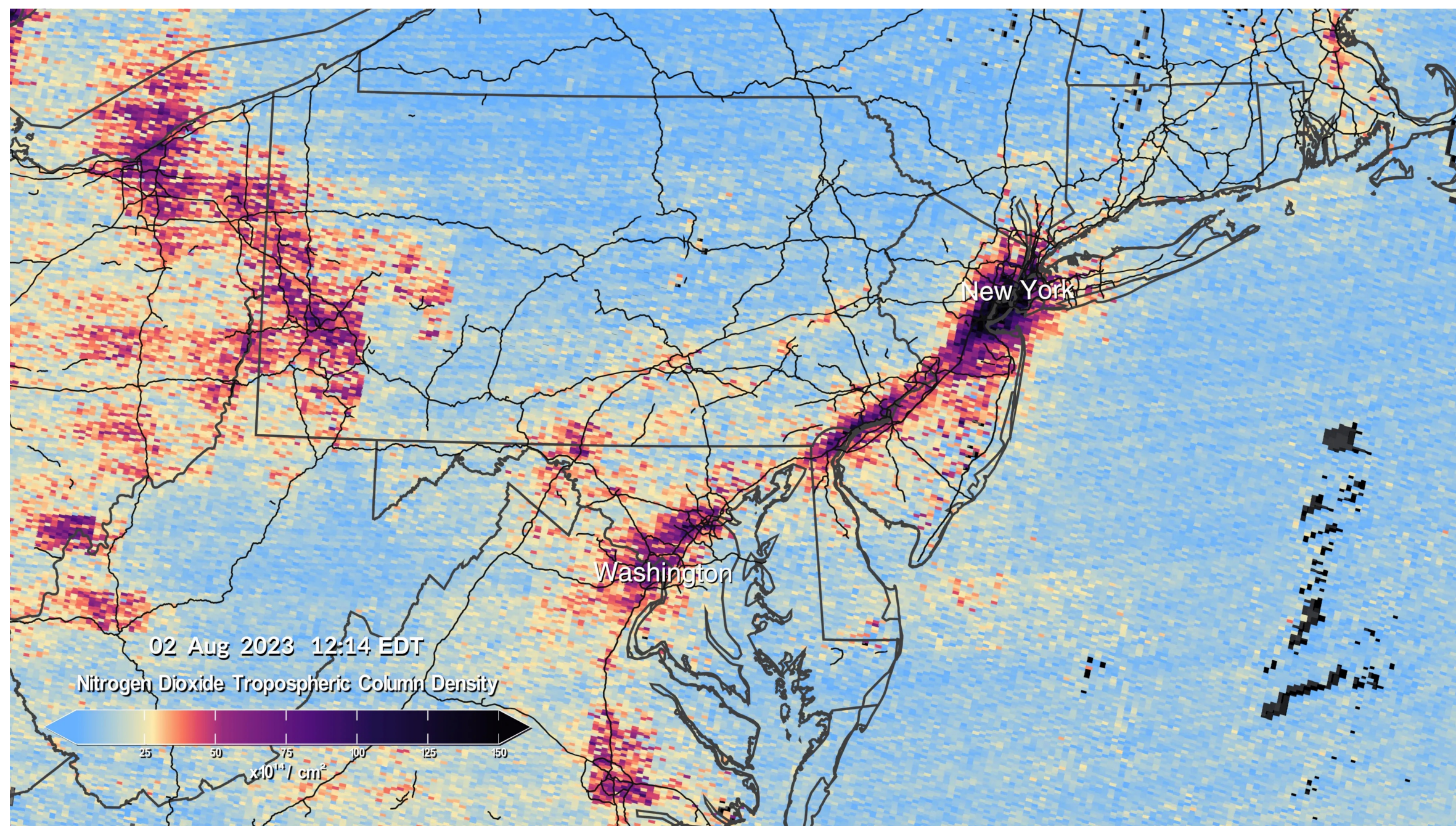


MEaSuRES overestimates in cloudy skies regime and underestimates in clear sky regime.

Goal: Build a well calibrated model to predict pollutants robustly across weather conditions



TEMPO: Resolving the Altitude of Pollutants



Nitrogen dioxide (NO_2) plays a central role in air quality and atmospheric chemistry, and has direct detrimental effects on human health when concentrated near the surface of Earth.

TEMPO is able to successfully retrieve the total column density of pollutants, such as nitrogen dioxide (NO_2), but not its vertical distribution.

We are building a multimodal AI model to integrate TEMPO data with other data (GEOS-CF, EPA Air Quality System, and aircraft profiles like STAQ) to resolve the vertical distribution of pollutants, like NO_2 to assess the air quality where it has human health impact

TEMPO nitrogen dioxide over part of the East Coast on August 2, 2023 at 12:14 EDT. High levels of NO_2 are seen over major urban regions and the I-95 corridor. High levels of NO_2 over Eastern Pennsylvania and Ohio are due to biomass burning.



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The future of *Astronomy* is *AI* driven.
We need to be ready.

Thank you!

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The Lives of Stars Team



Cecilia Garraffo



Phill Cargile

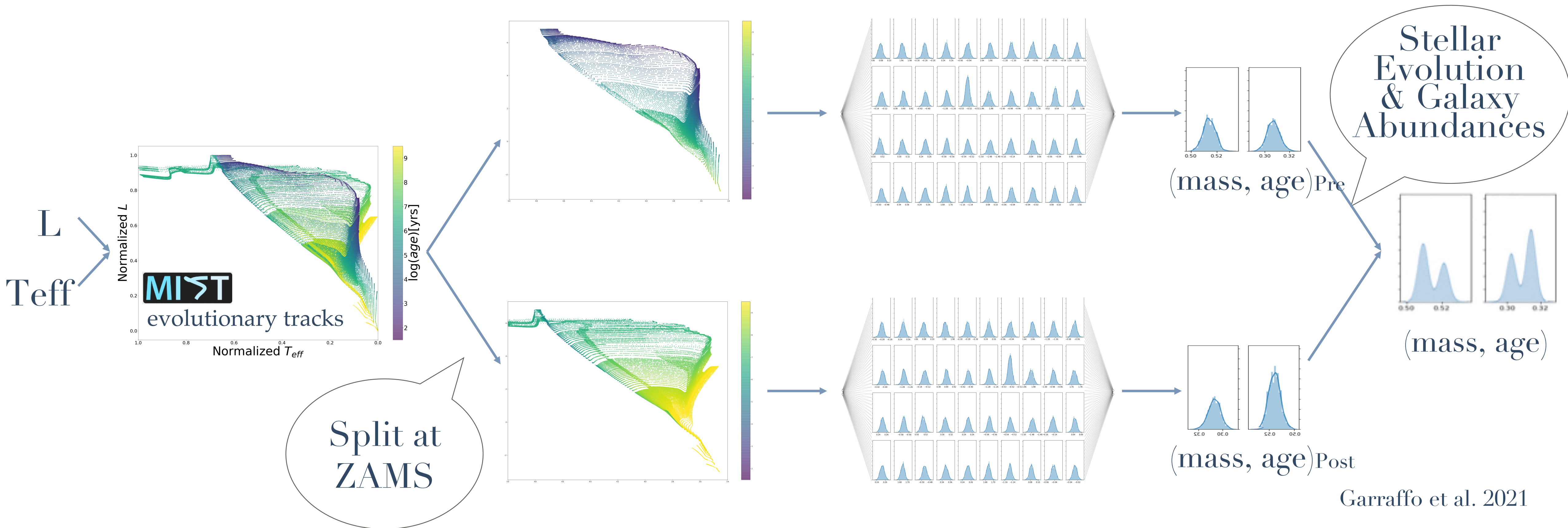


Josh Speagle



ASTROAI

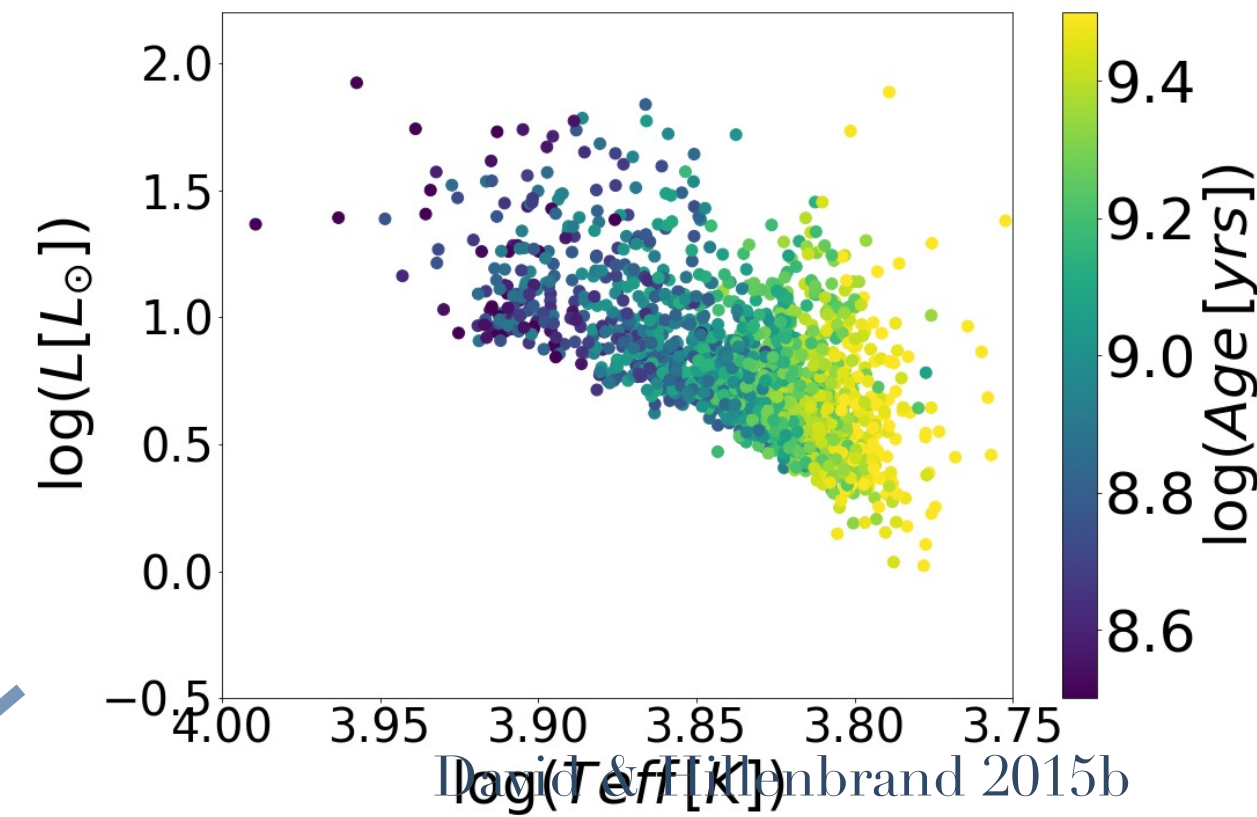
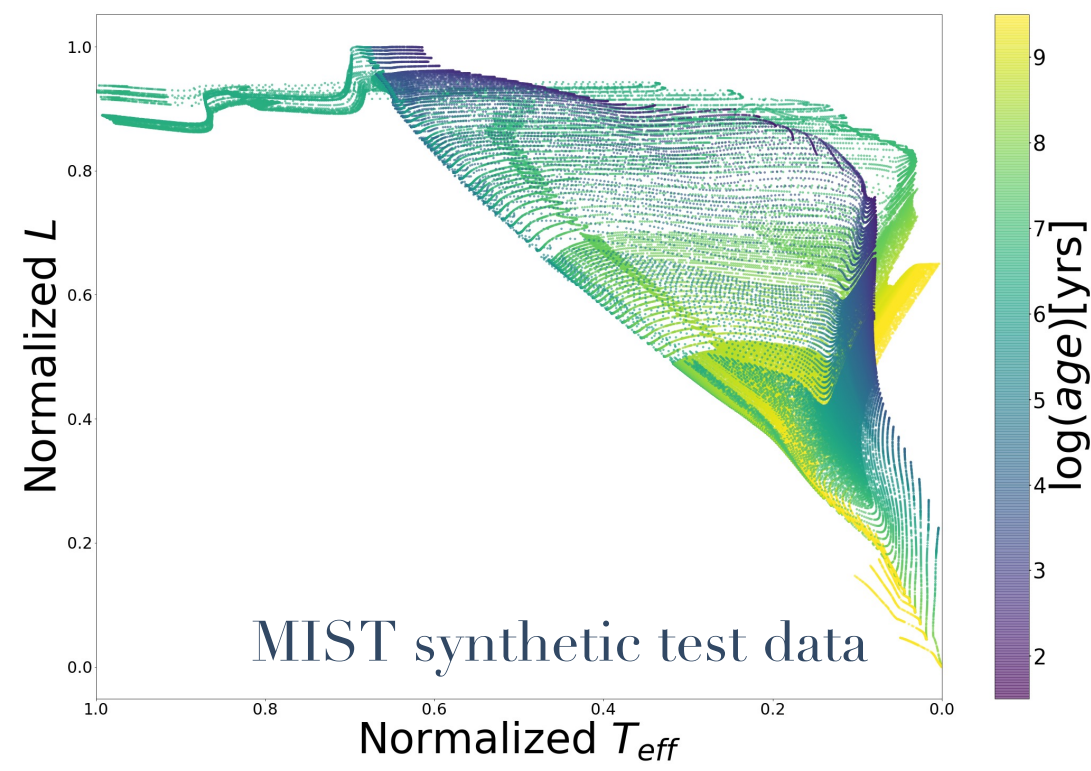
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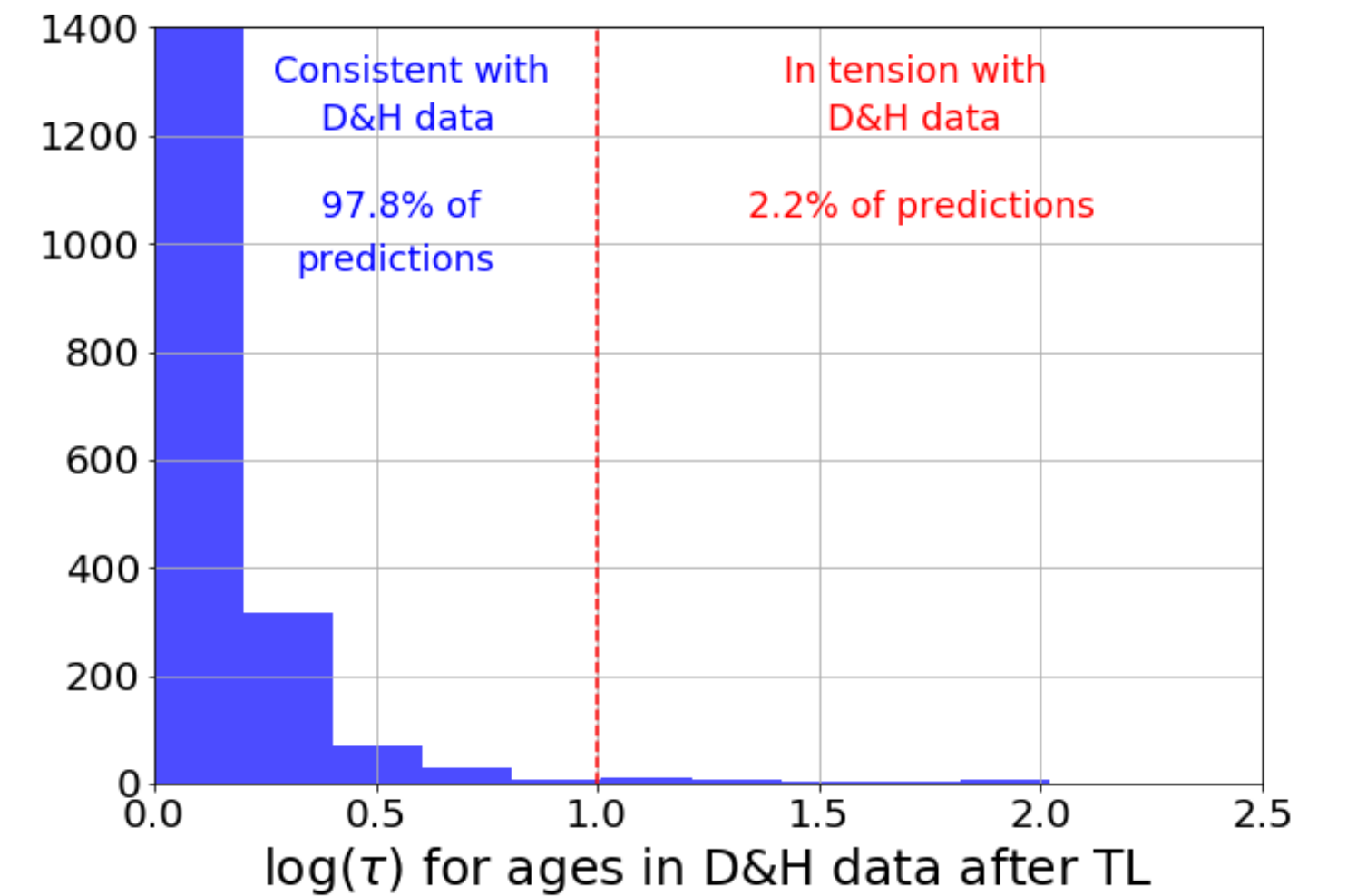
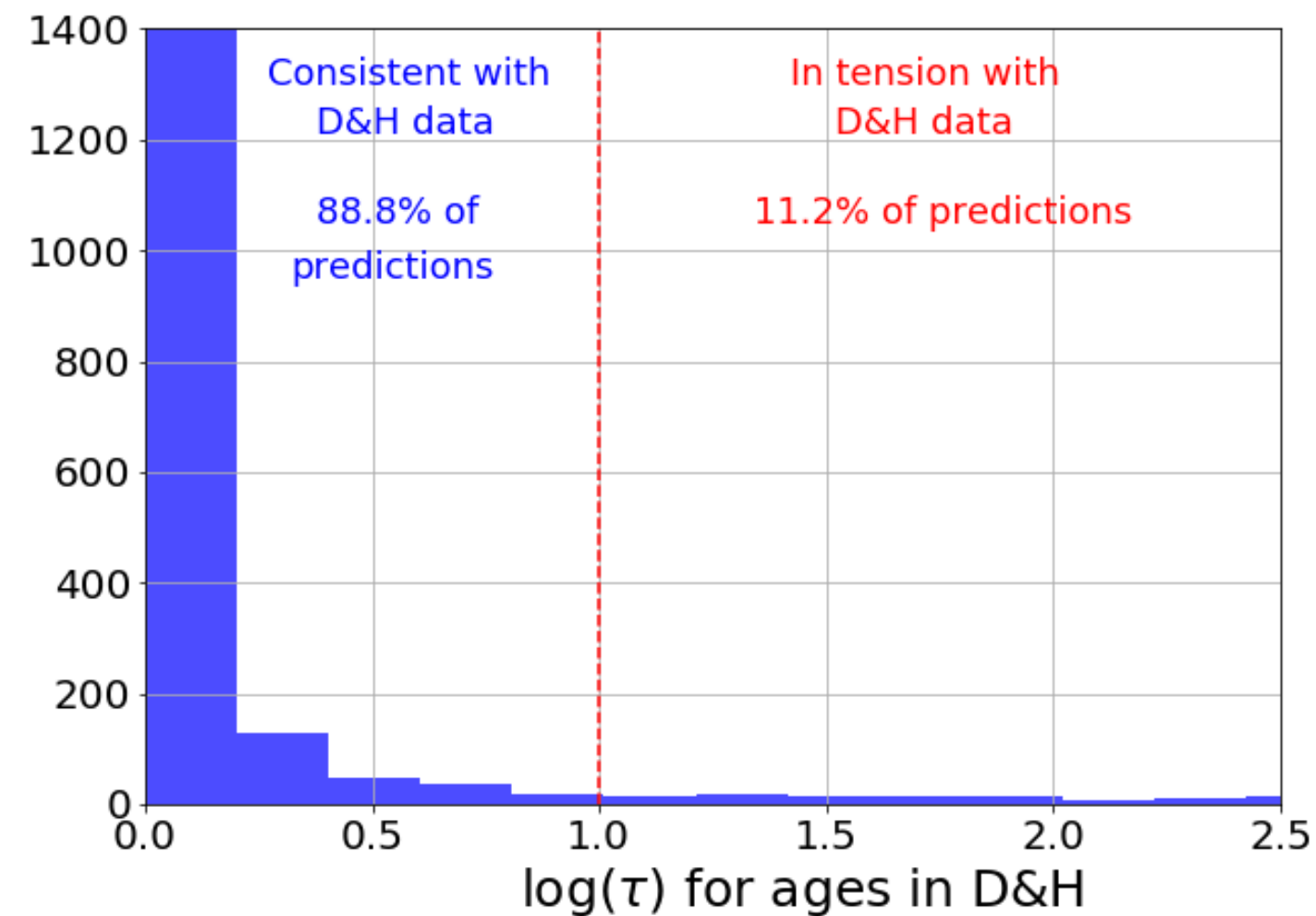
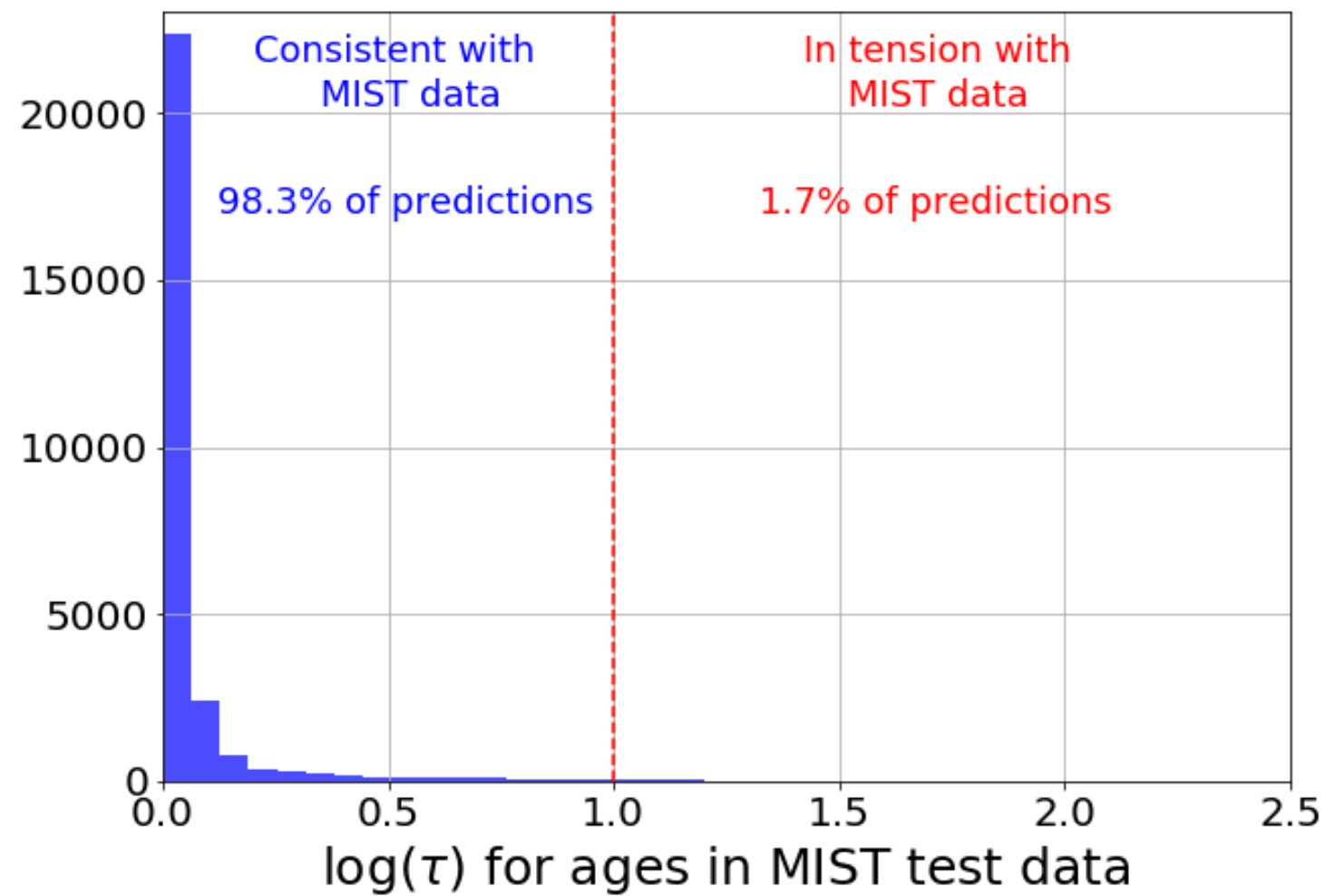
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Using
Transfer
Learning

Garraffo et al. 2021

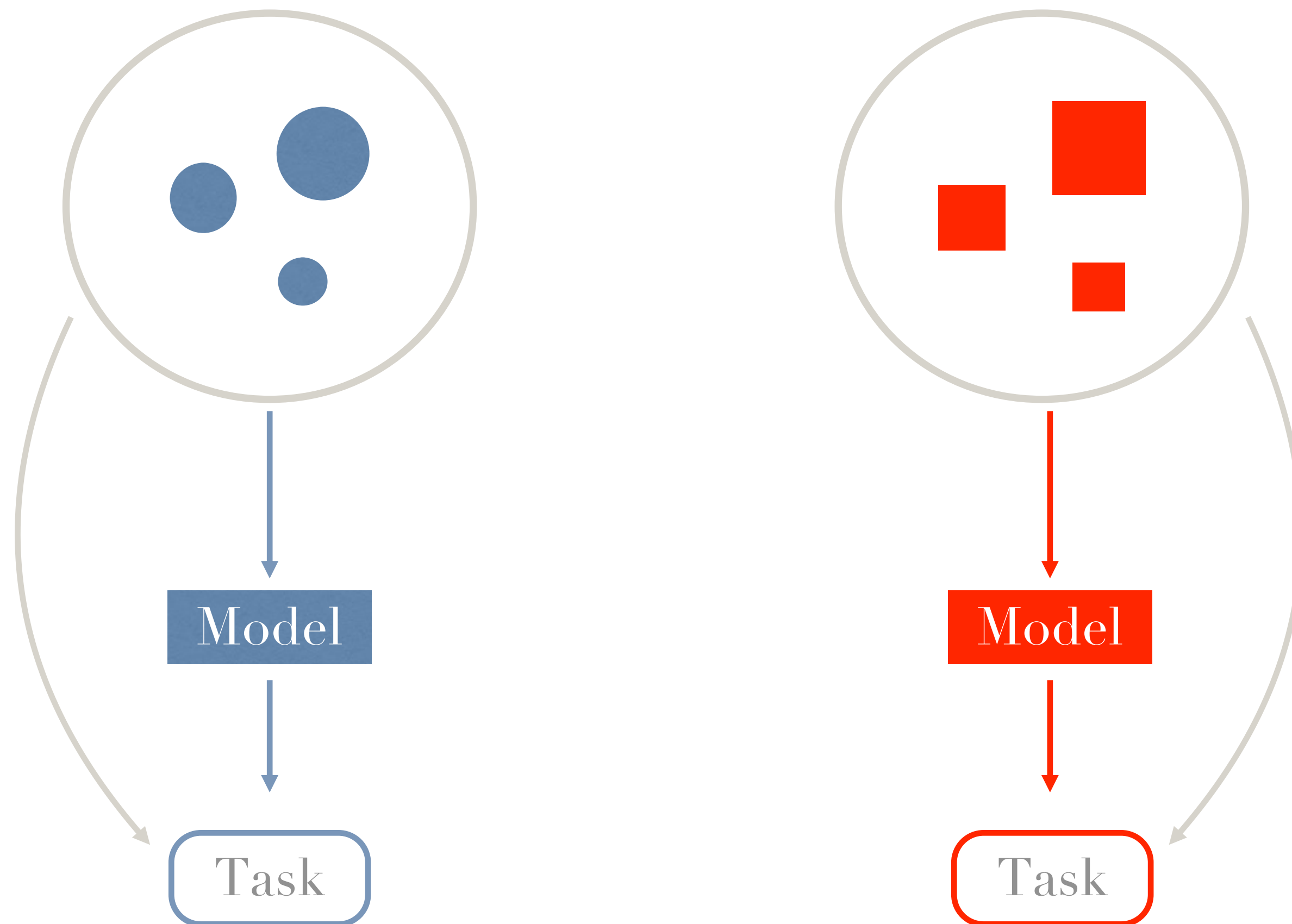




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Traditional Machine Learning





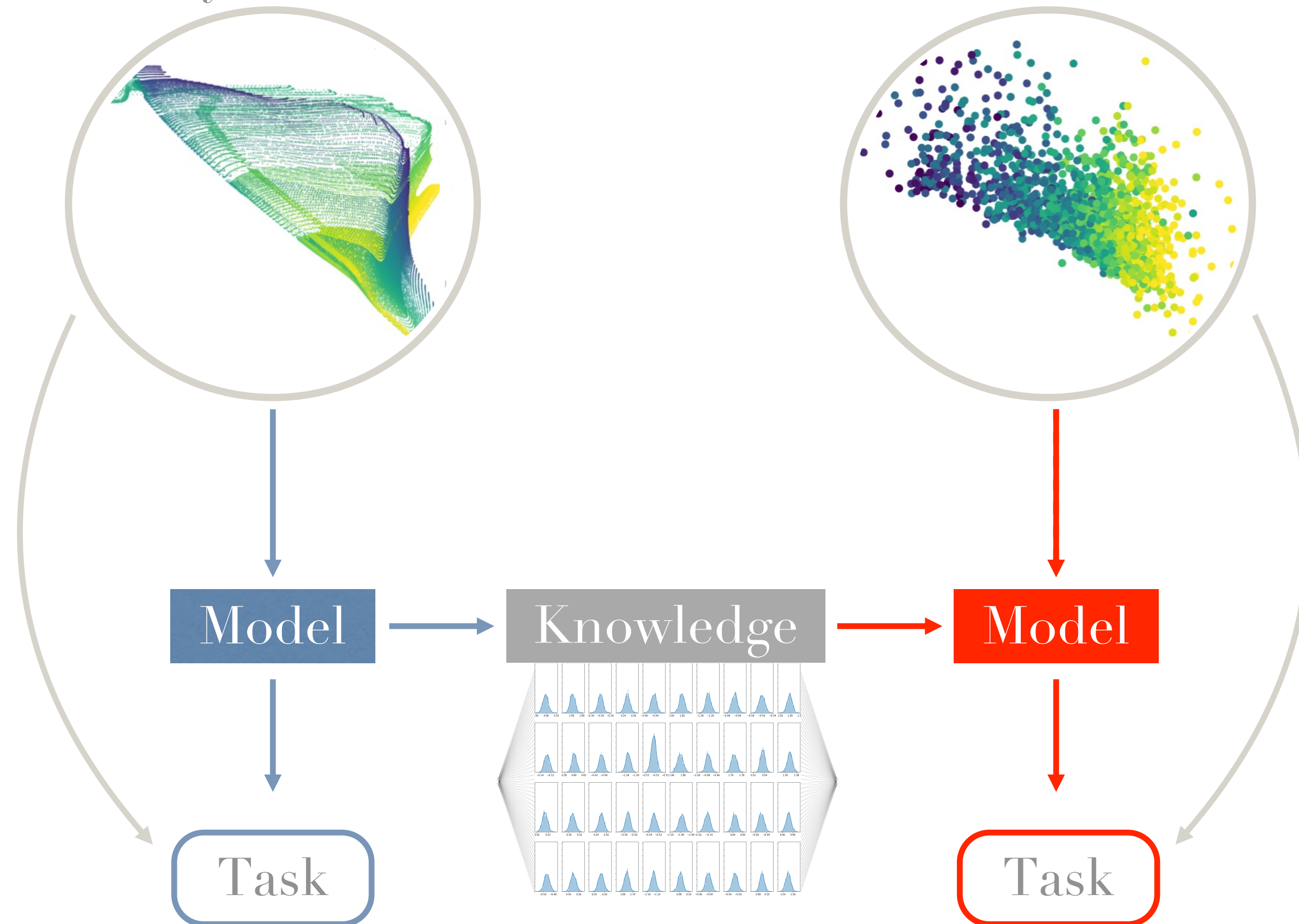
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Transfer Learning

MIST Synthetic data

Observed data





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Pre-ZAMS mass estimation

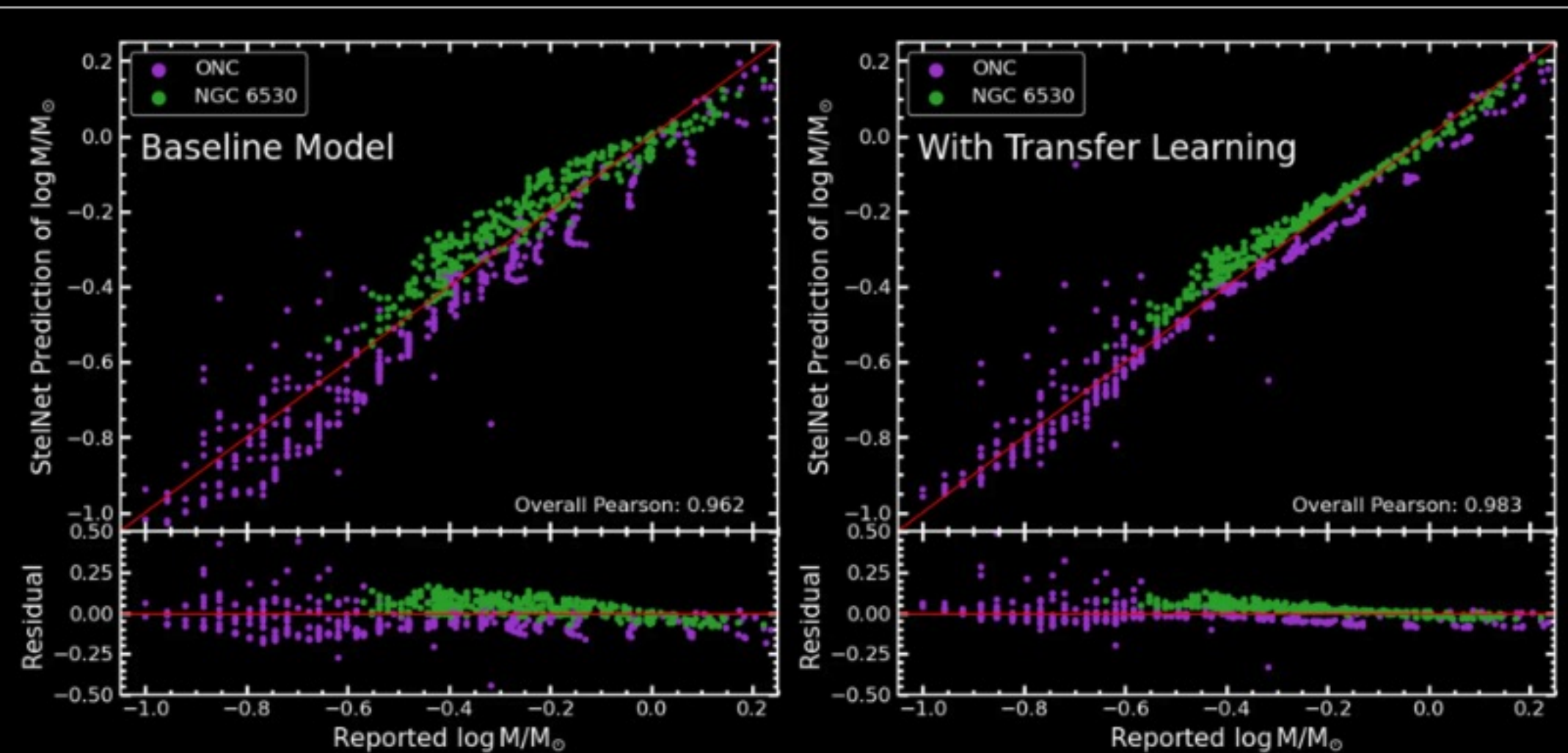
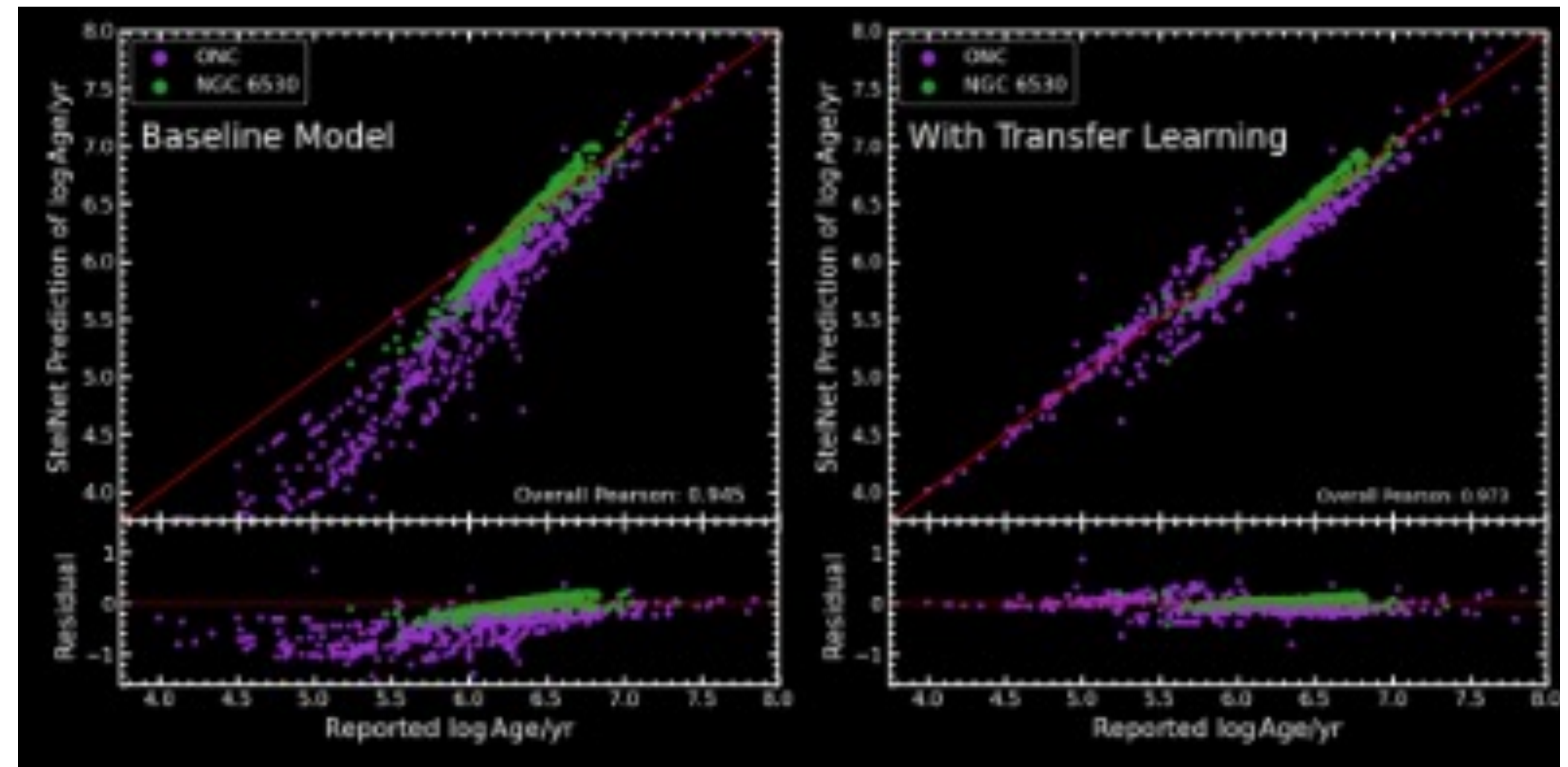


Figure 6. StelNet mass predictions versus reported values for each test catalog of pre-ZAMS stars for the baseline model (left) and the model after transfer learning.



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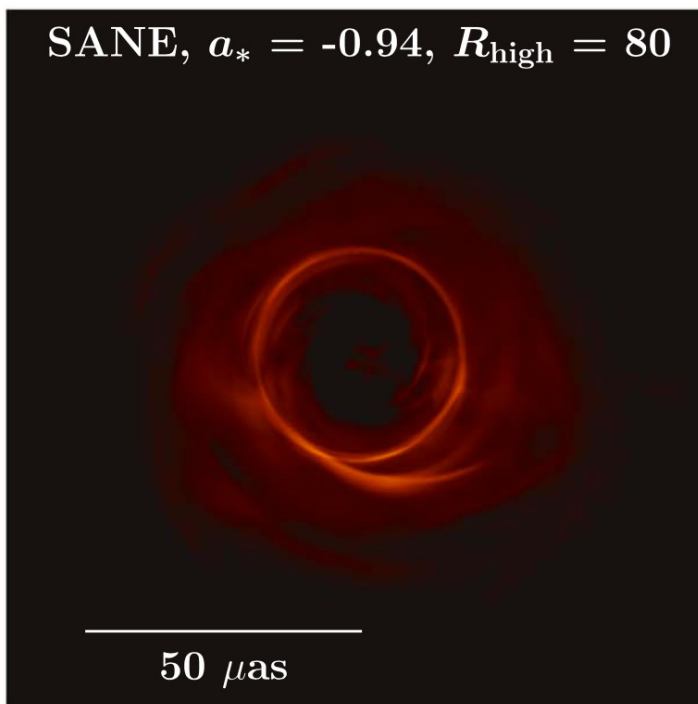
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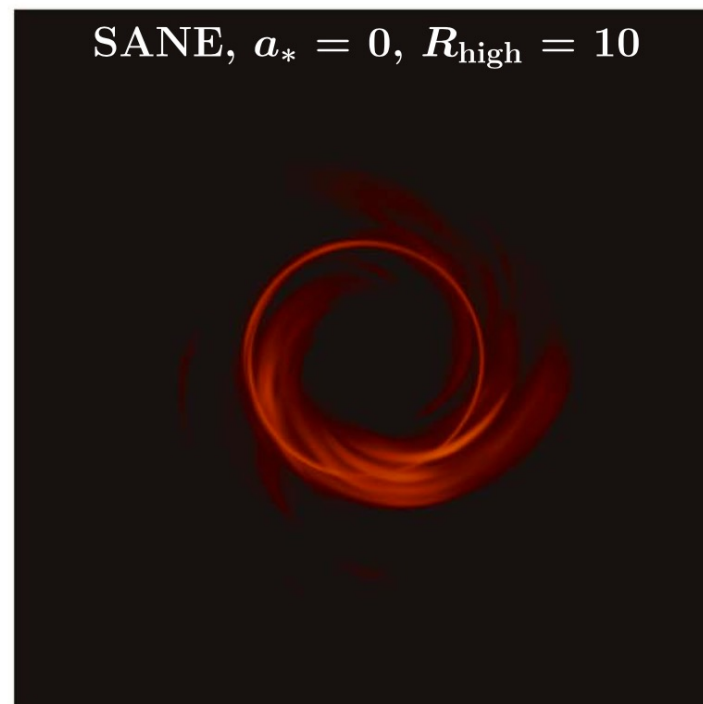
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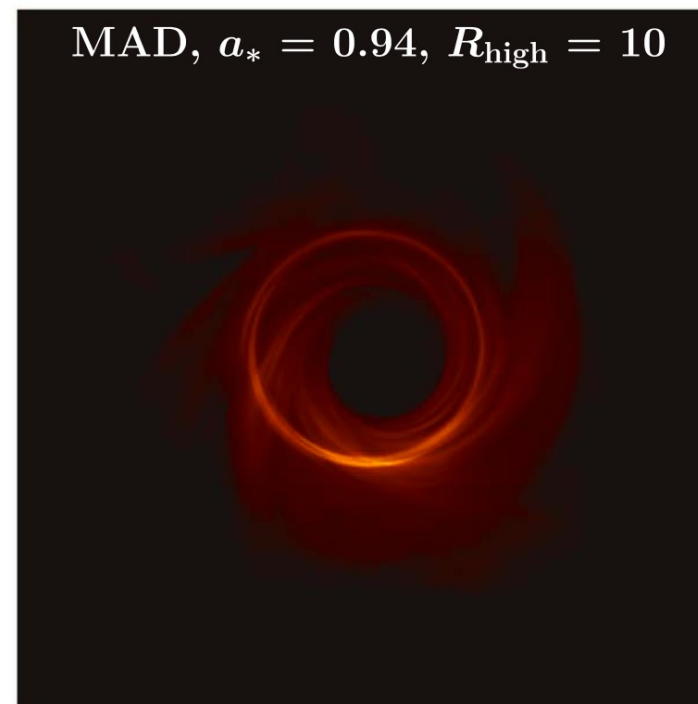
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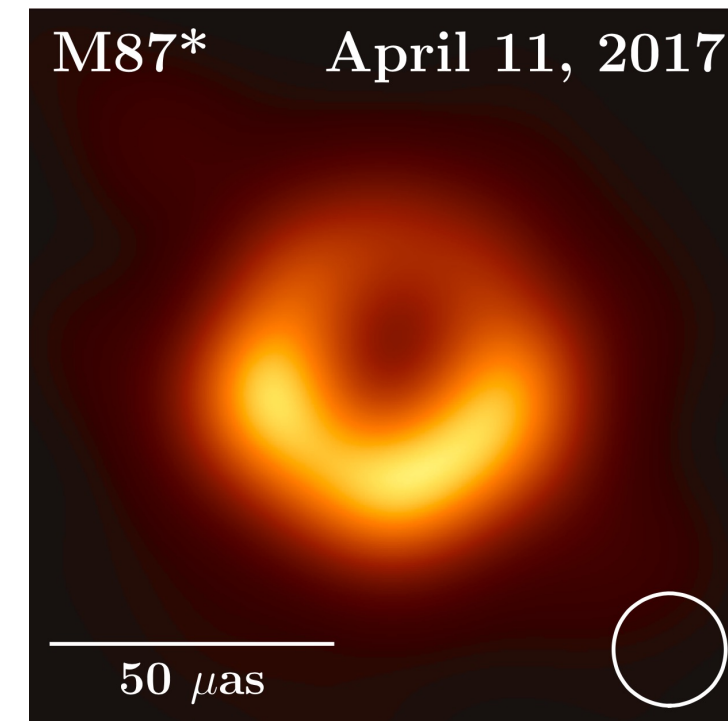


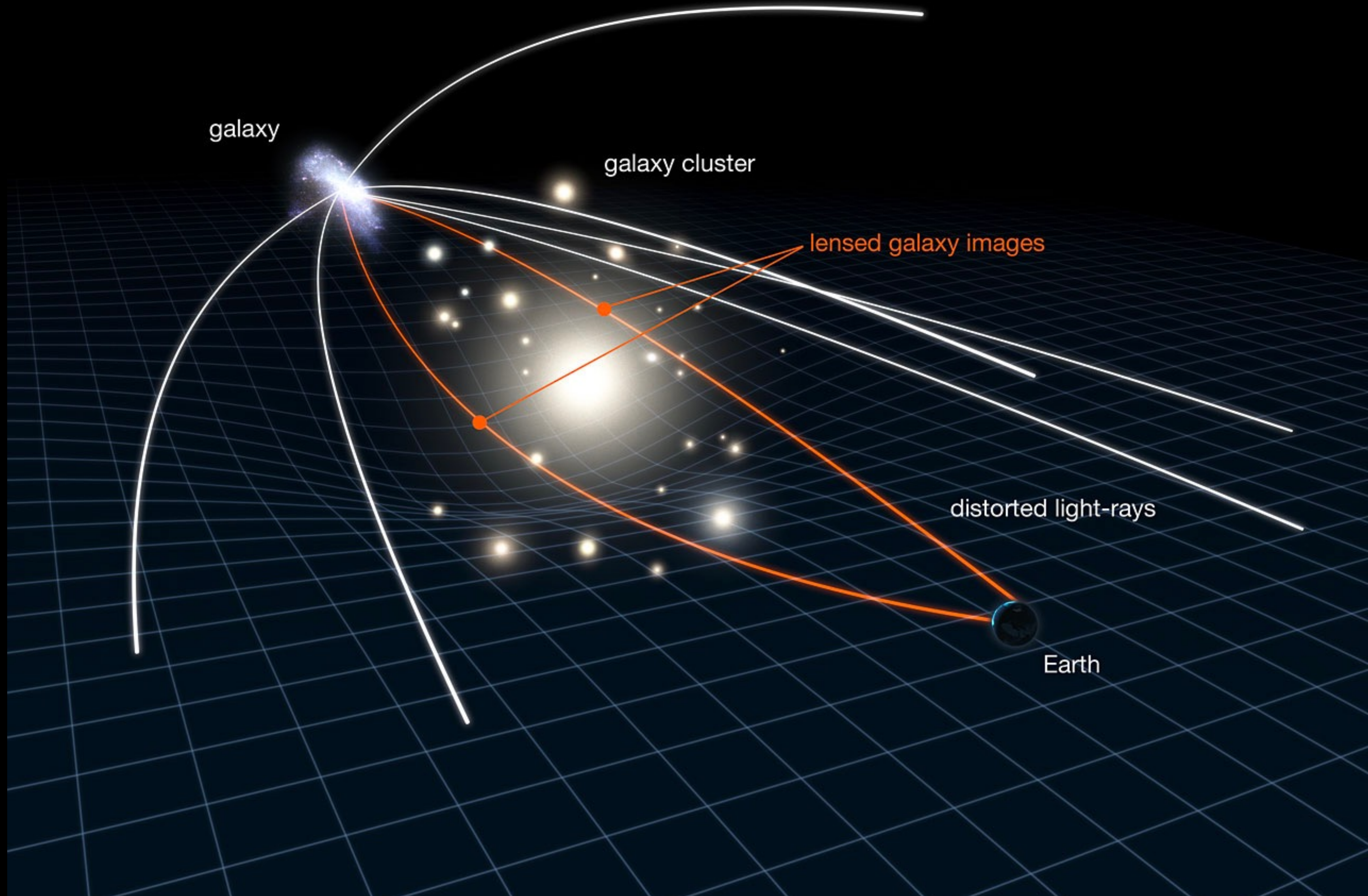
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- Real EHT observations

M87* April 11, 2017







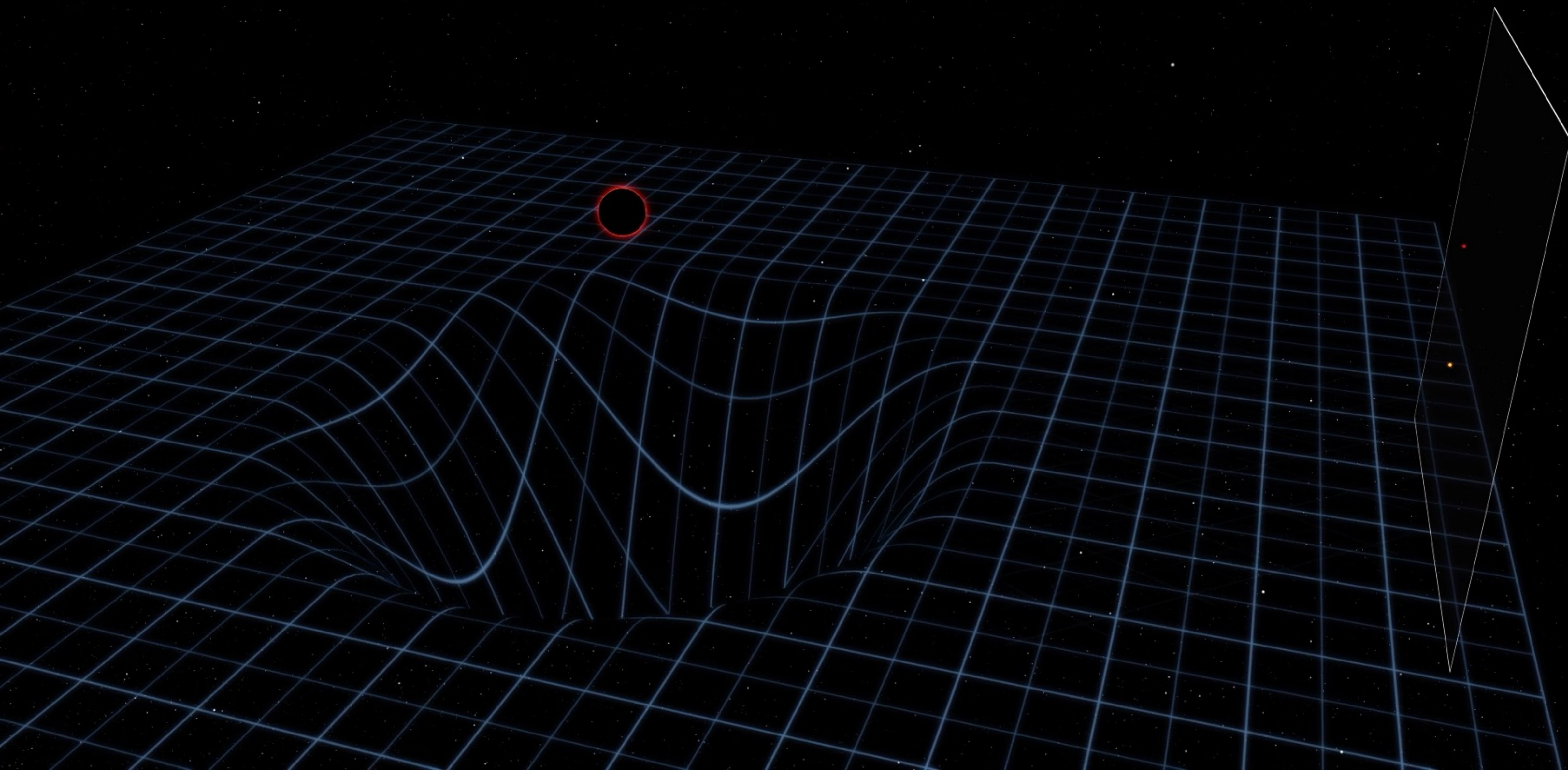
The way we do Astronomy is rapidly changing



New windows into the Universe:

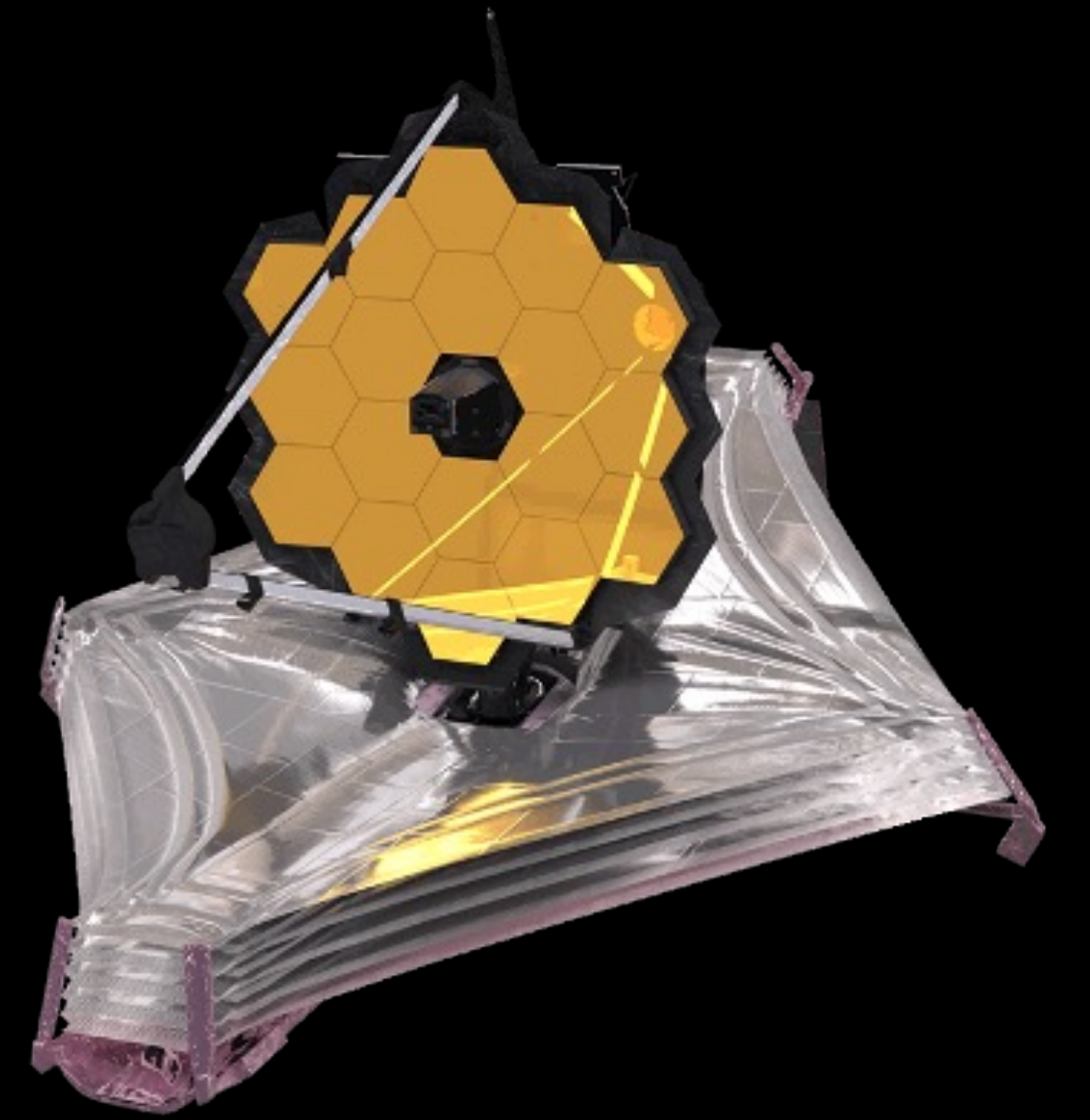


n=0



New windows into the Universe:

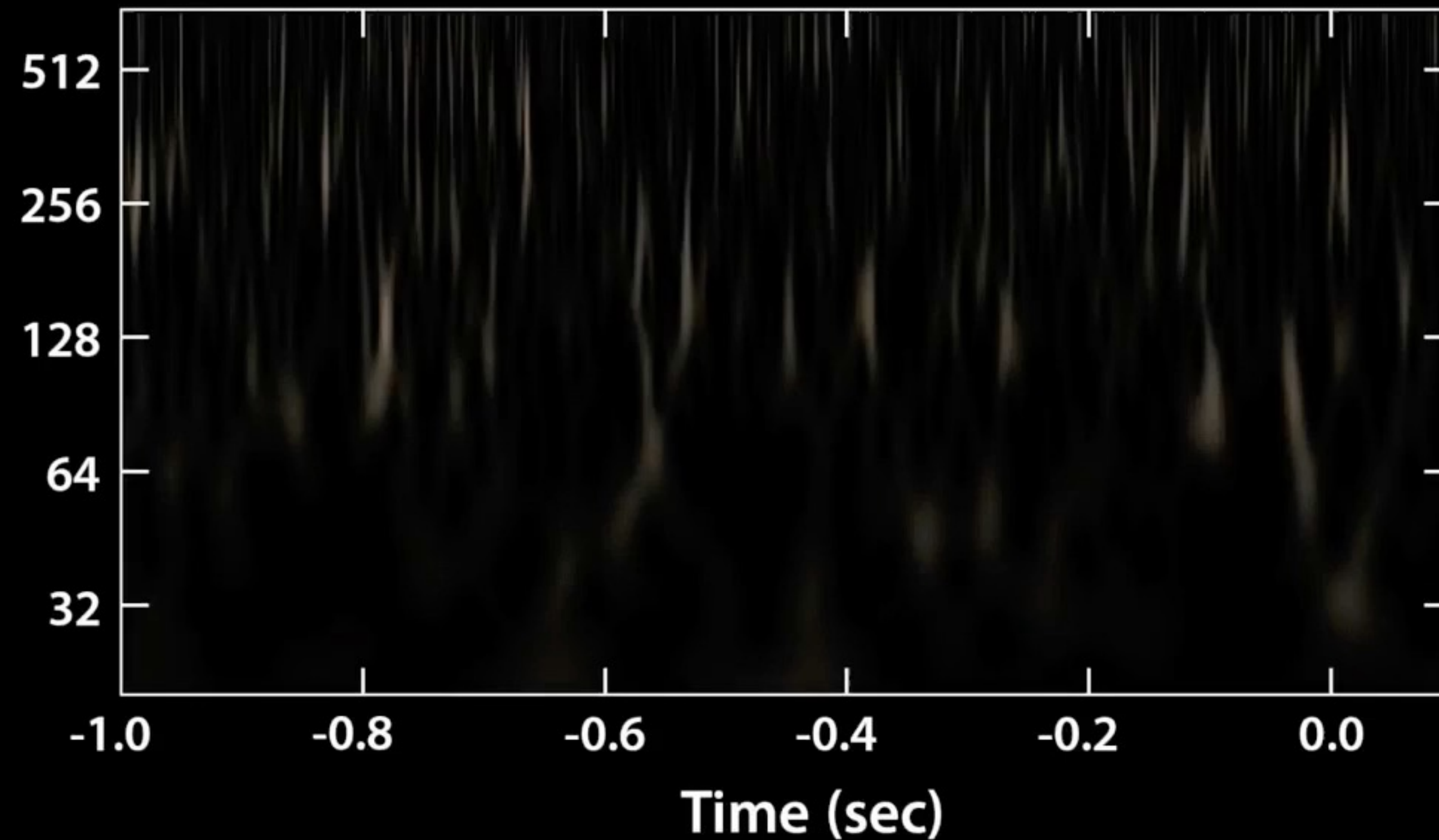
James Webb Space Telescope



New windows into the Universe:

September 14, 2015

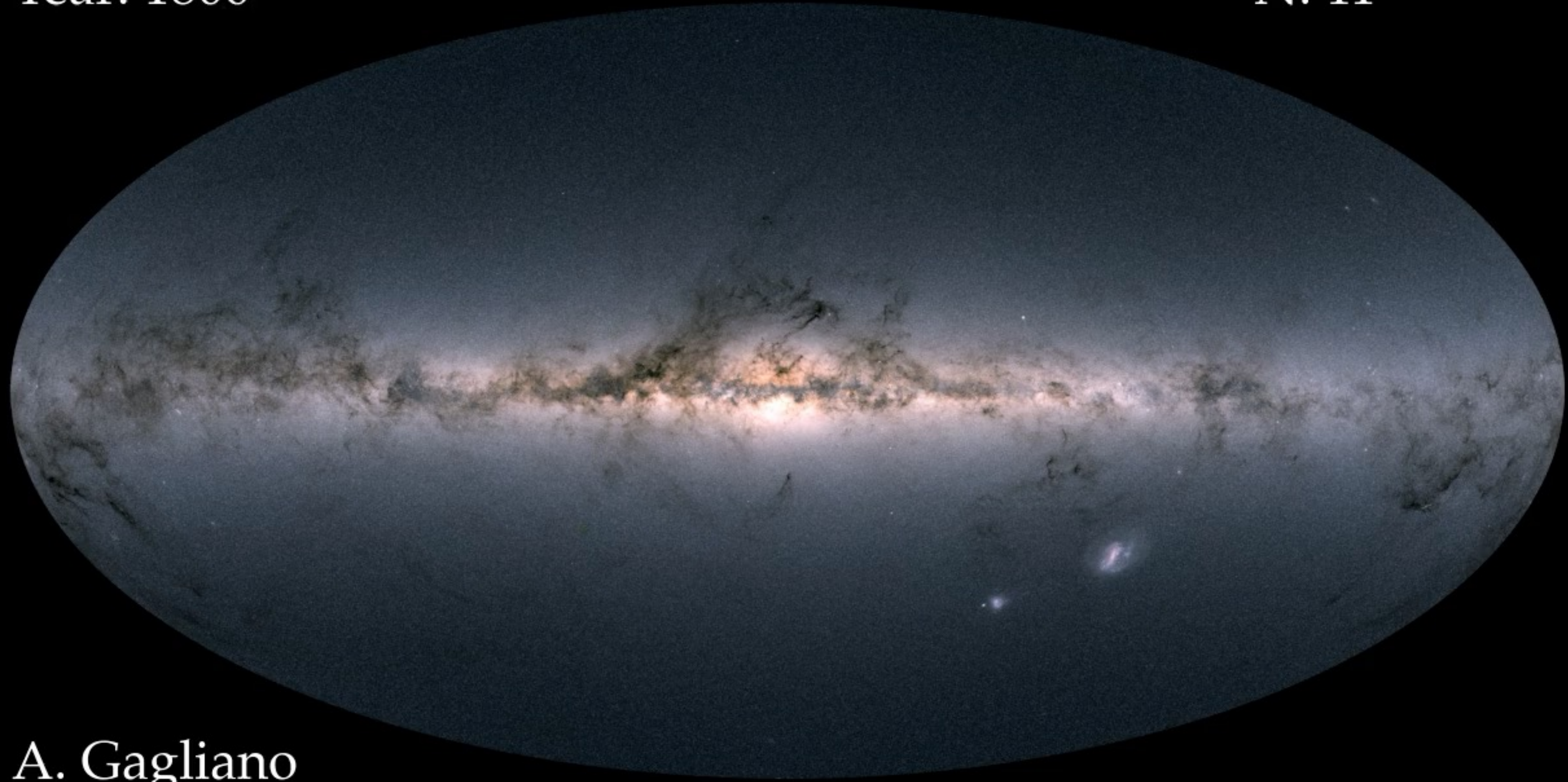
Hanford Observatory
Natural Pitch



Radio/Gravitational Waves

Year: 1800

N: 11



A. Gagliano

Observing more data in 1 year, than all observations so far

New eyes



Big Data

How do we make discoveries in this new era?

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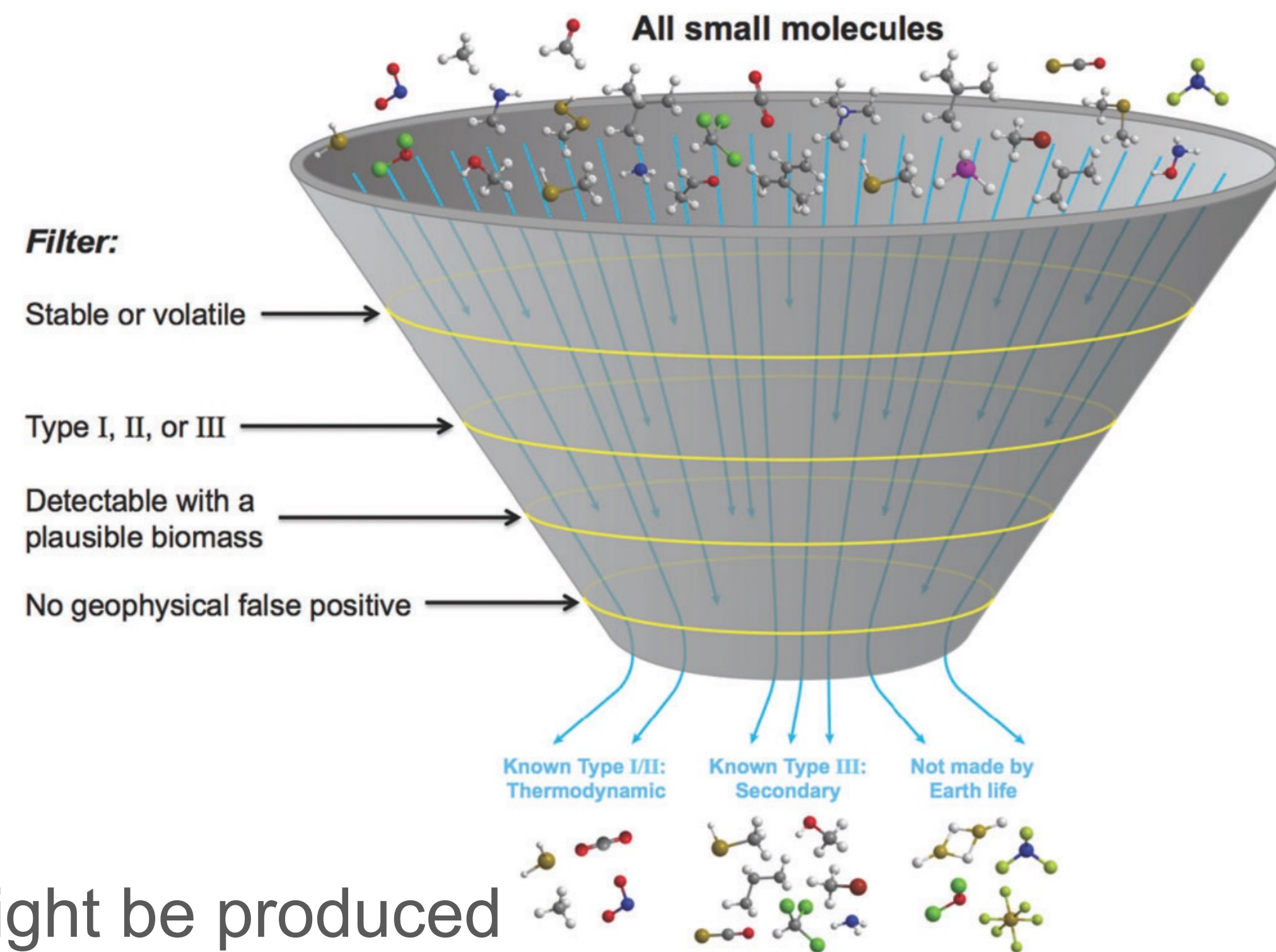
Exoplanet Atmospheres and Biosignatures

What is the big Science Question?

- Is there life elsewhere in the universe?

How will our work answer it?

- Classic Molecules: H₂O, CH₄, NH₃, O₂, CO₂, CO
- Seager+2016 proposed a list of 14,000 molecules that might be produced by life



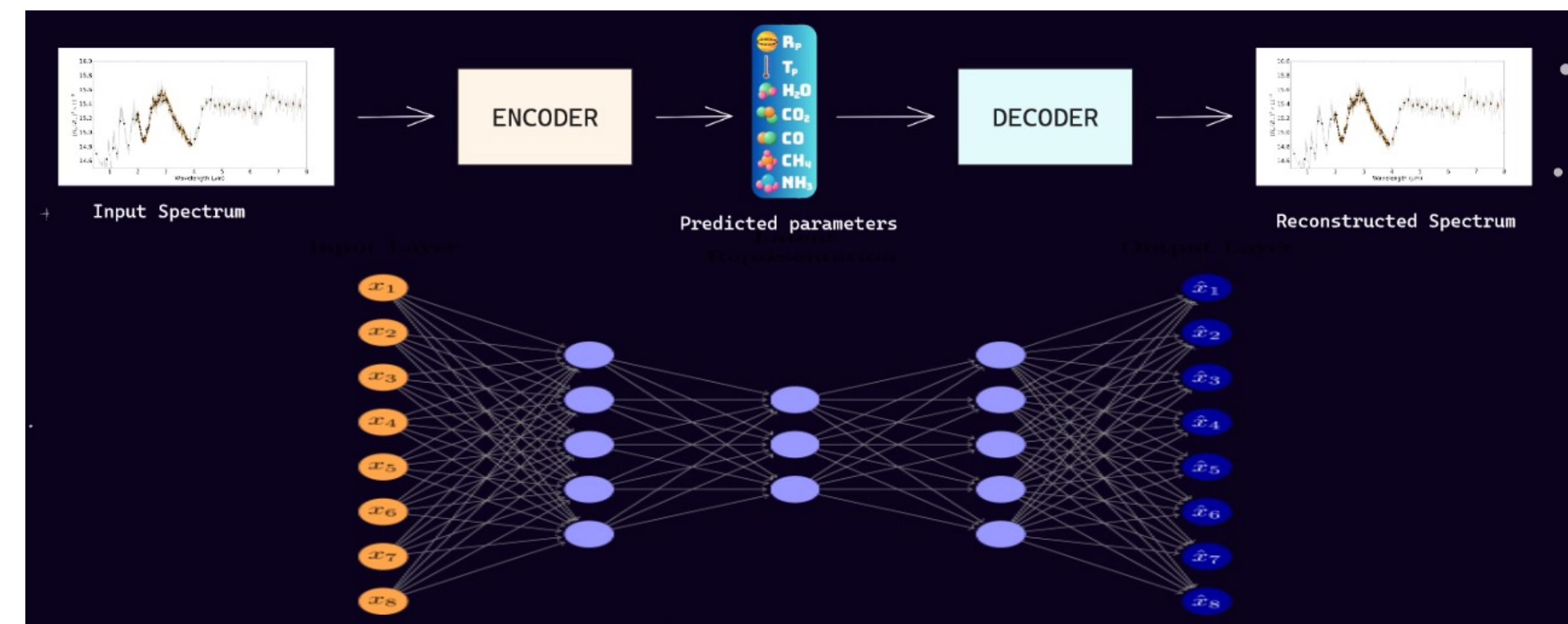
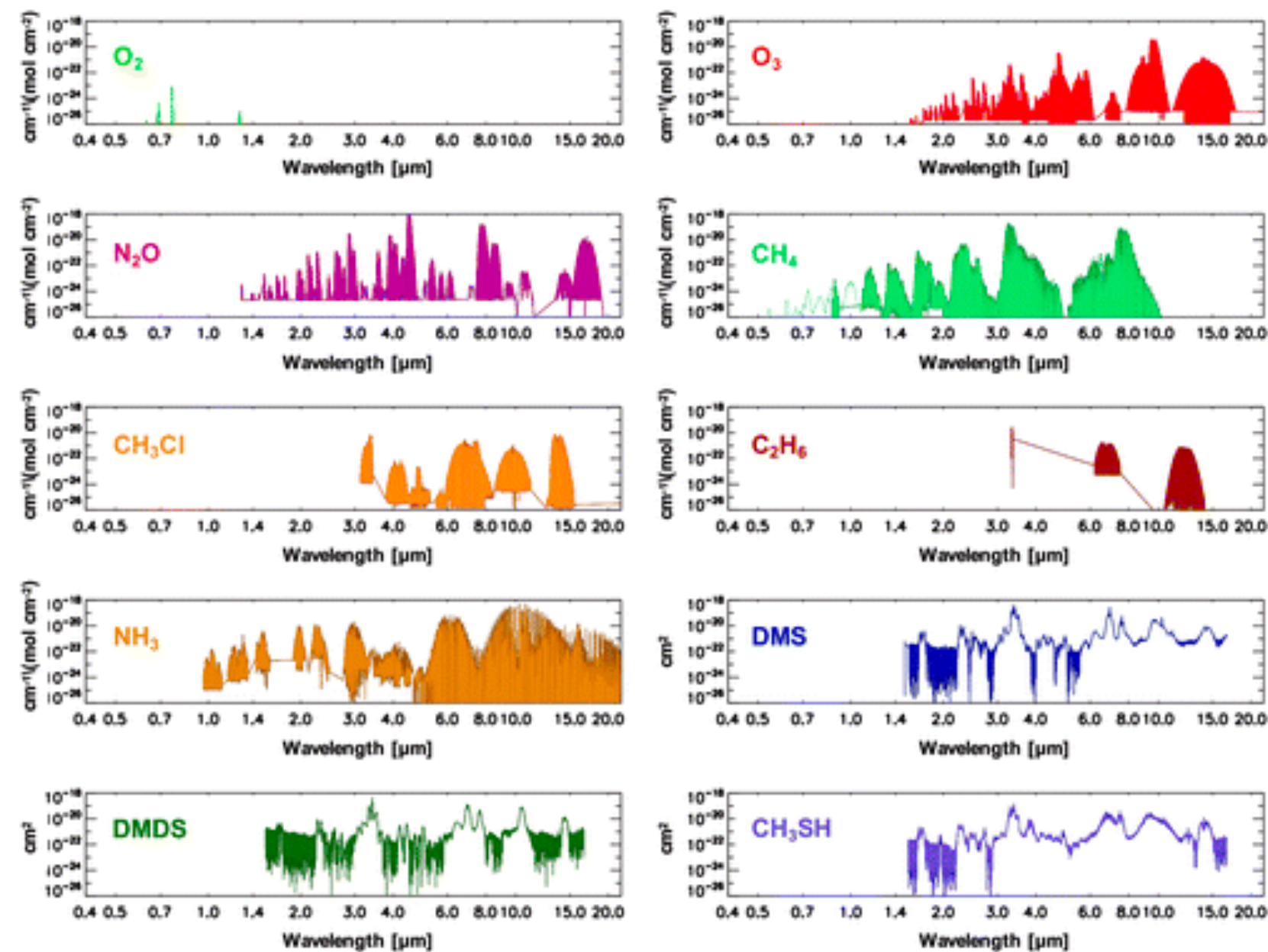
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Next Big Steps: Do this for 14K molecules

1- Detection of Biosignature Gases

2- Exoplanet Atmospheric Retrievals with AI



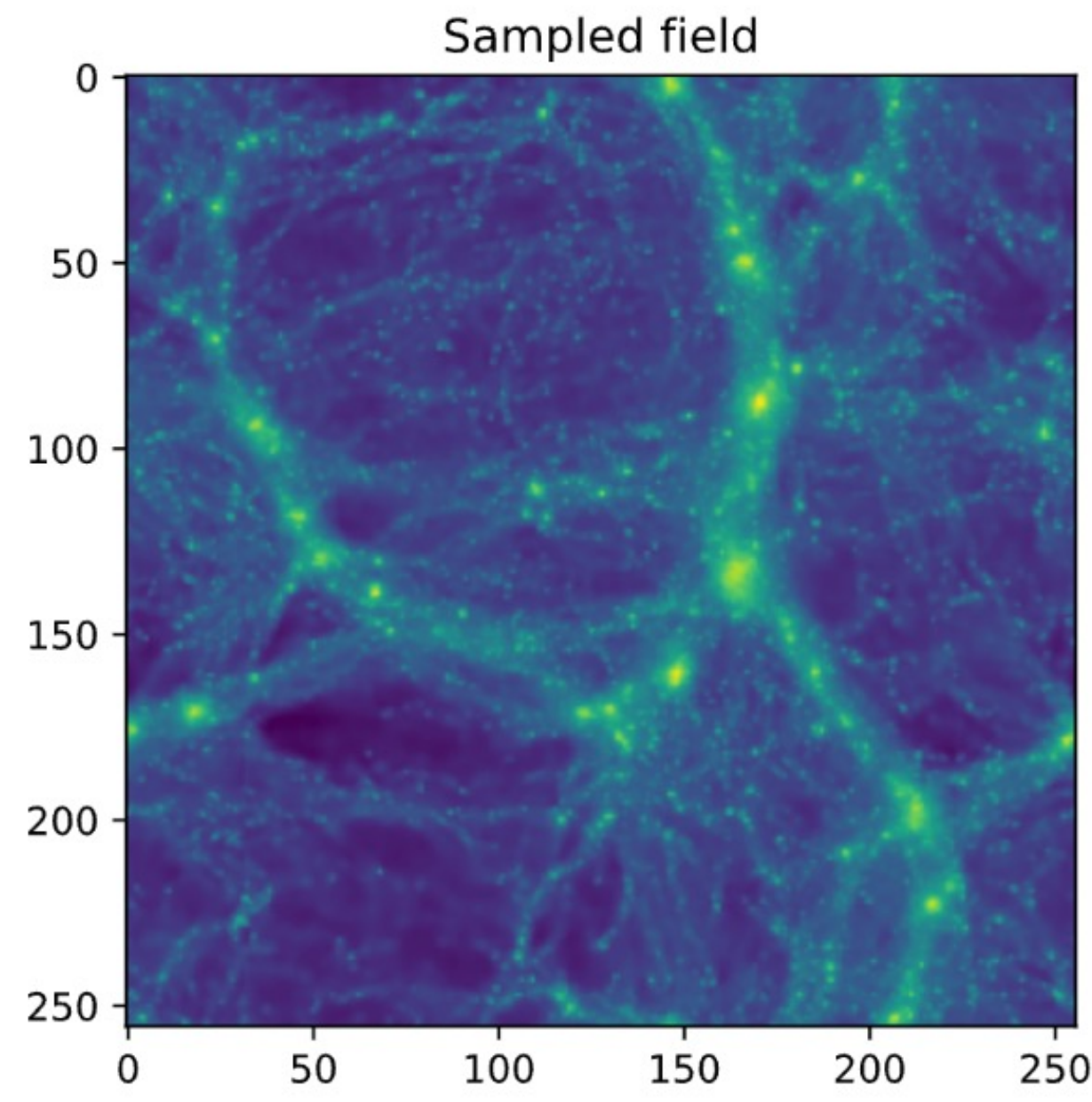
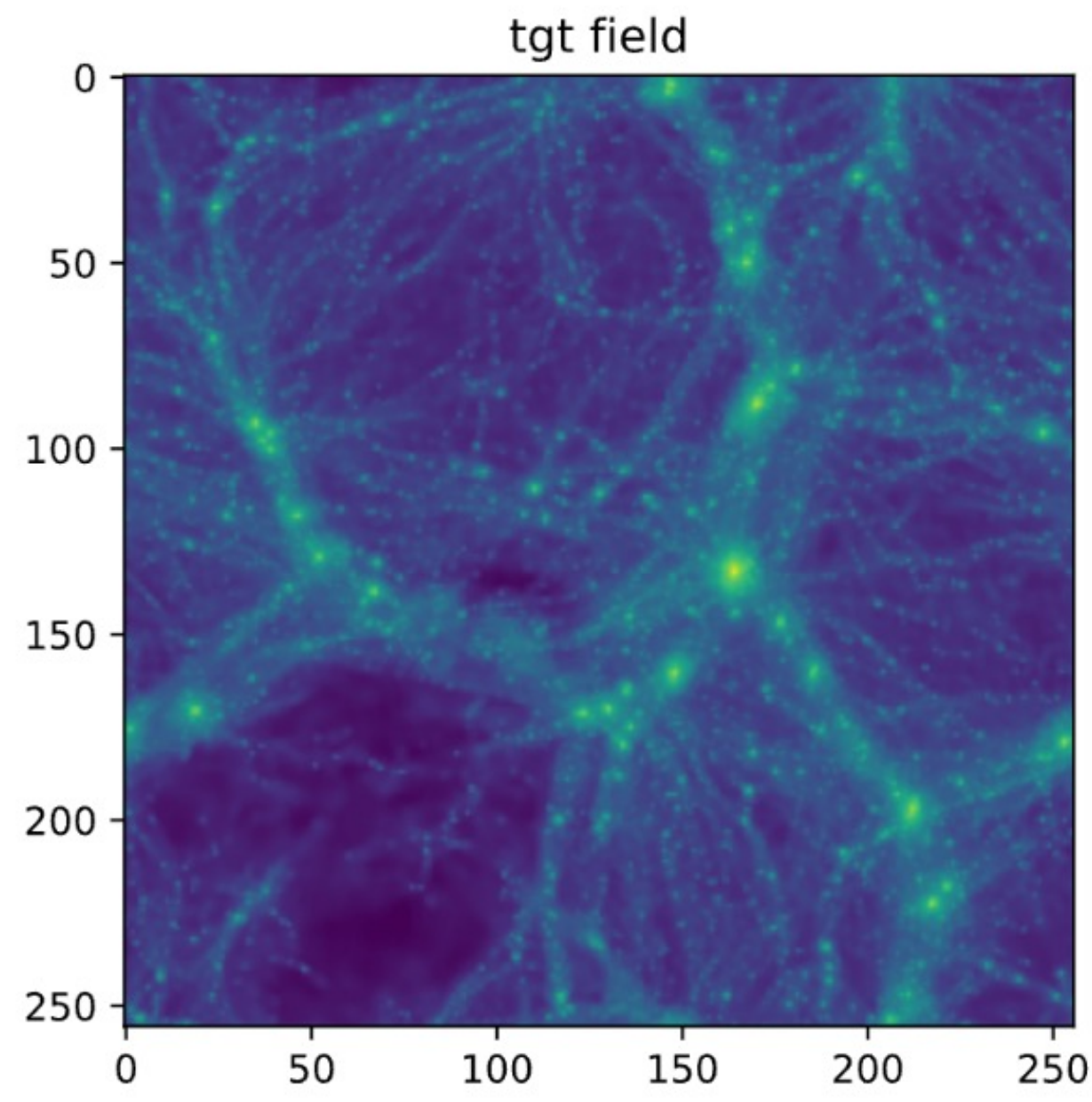
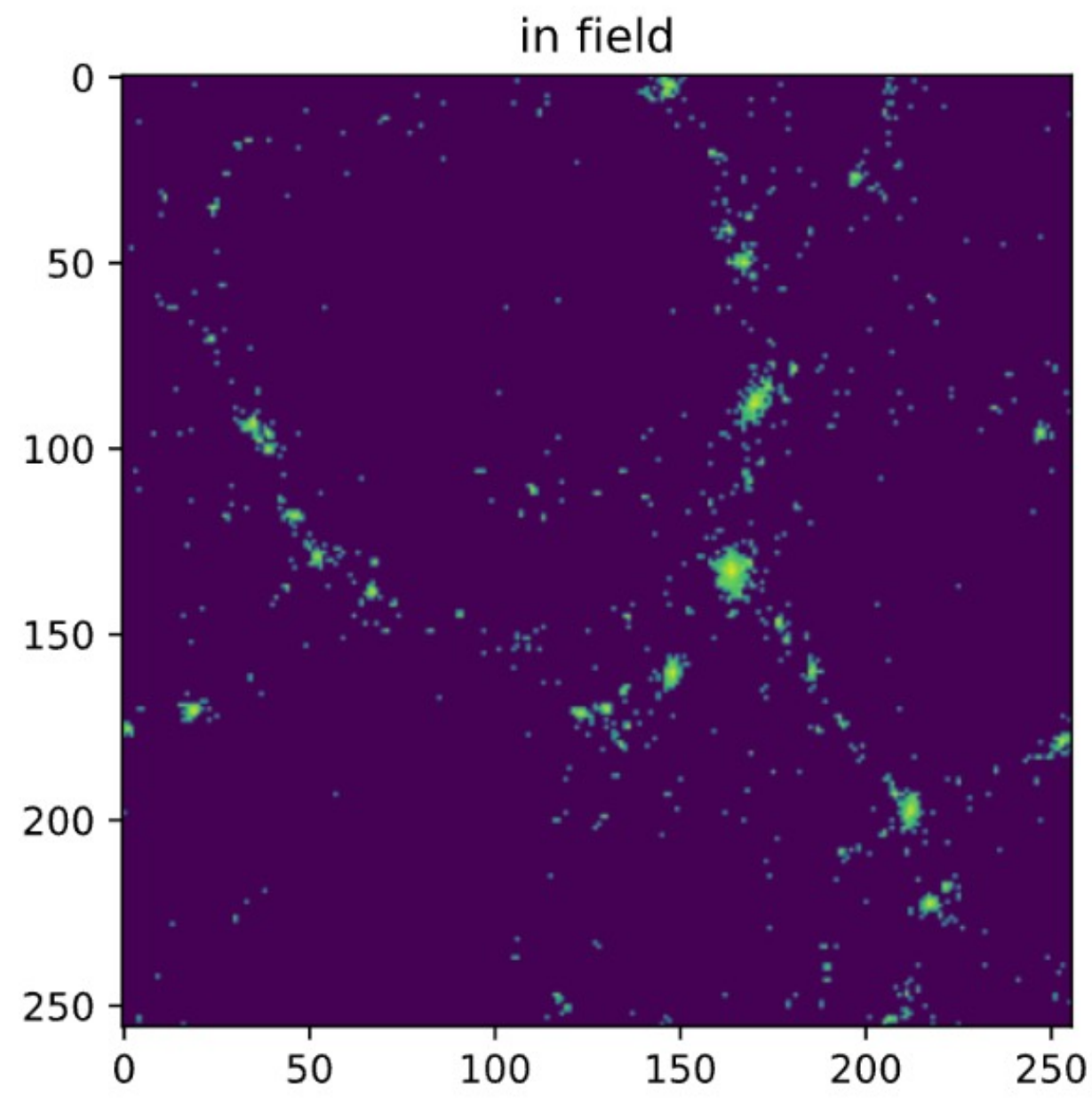
Breakthrough: Find Life Elsewhere in the Universe!



Carolina Cuesta-Lázaro

Modeling the Universe

Inferring Dark Matter



First dedicated center for
Astrophysical AI

ASTROAI

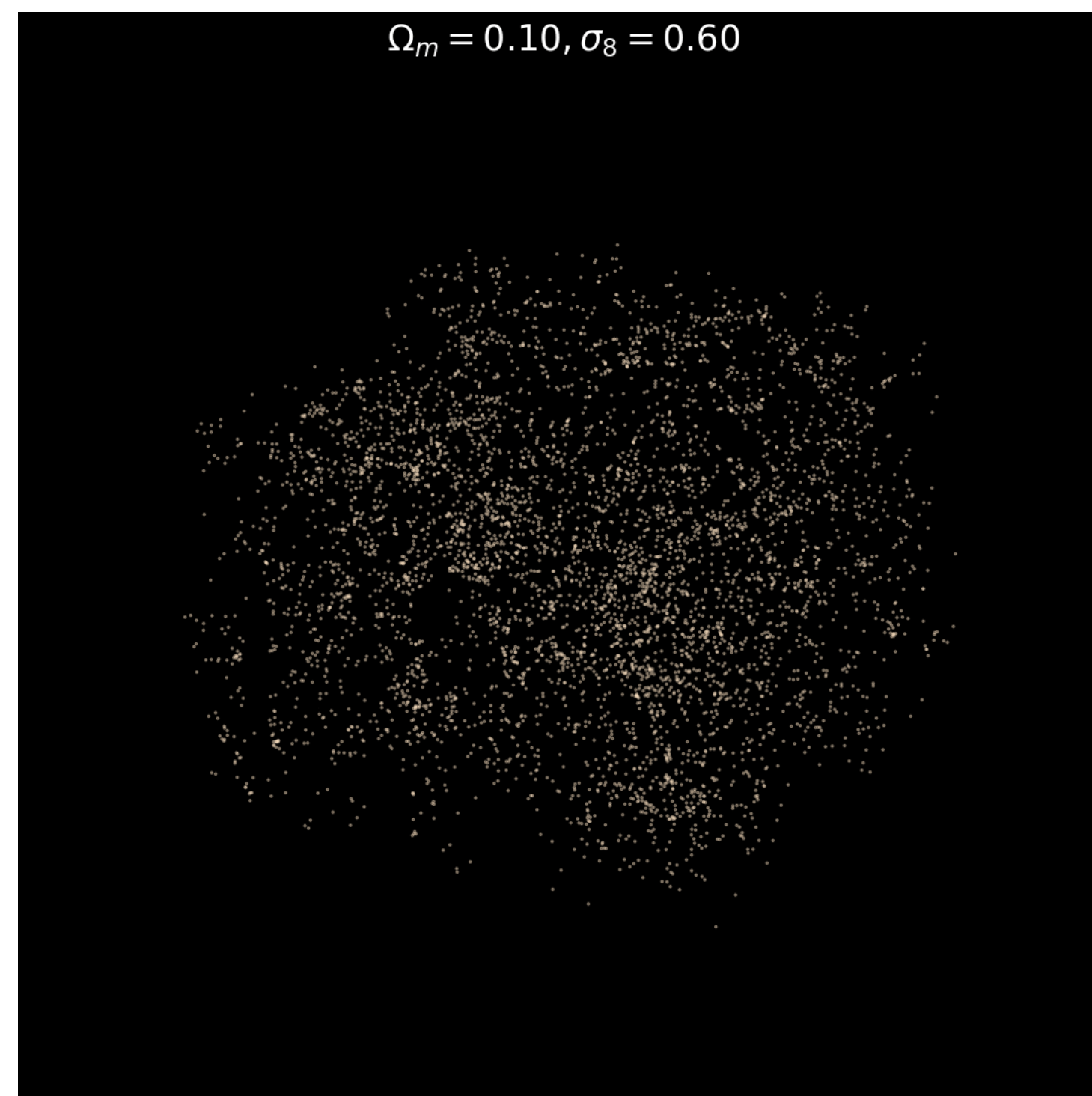
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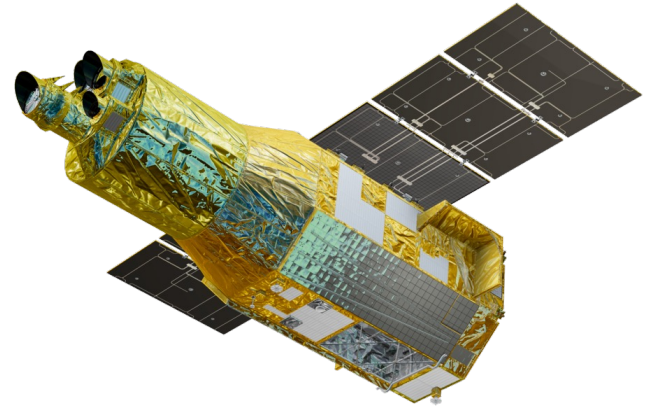
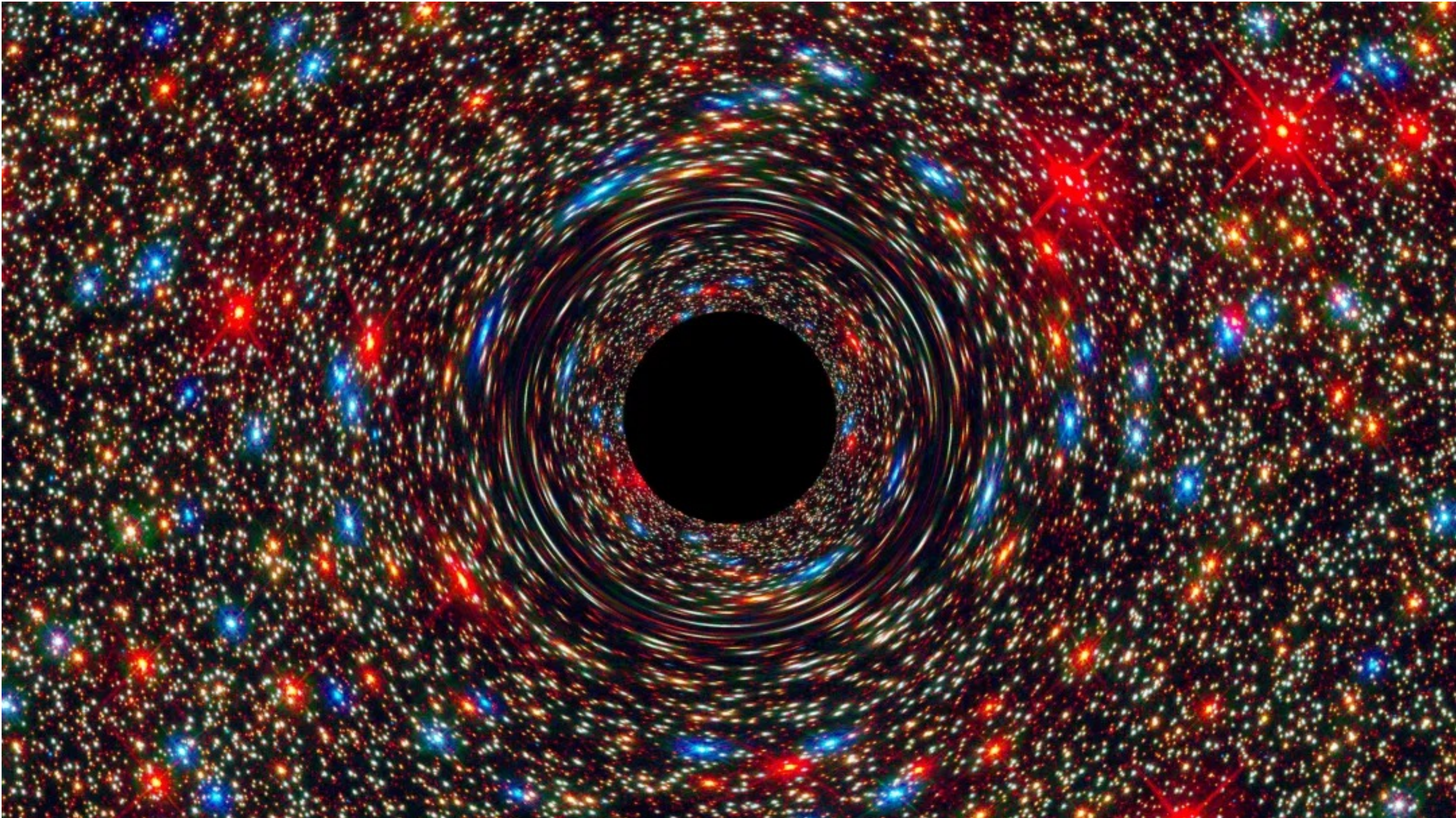
Carolina
Cuesta-Lázaro

Modeling the Universe

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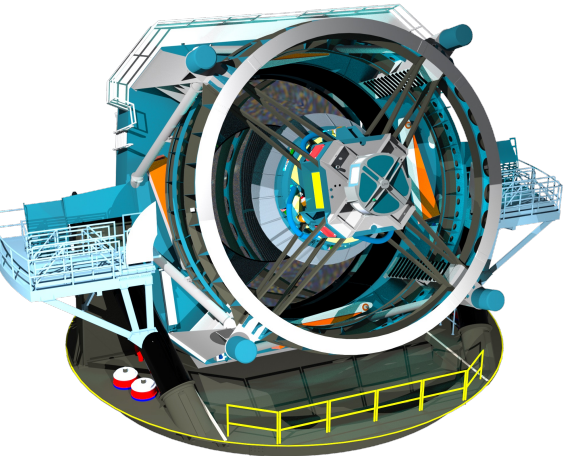
Big Data Revolution in *Astrophysics*



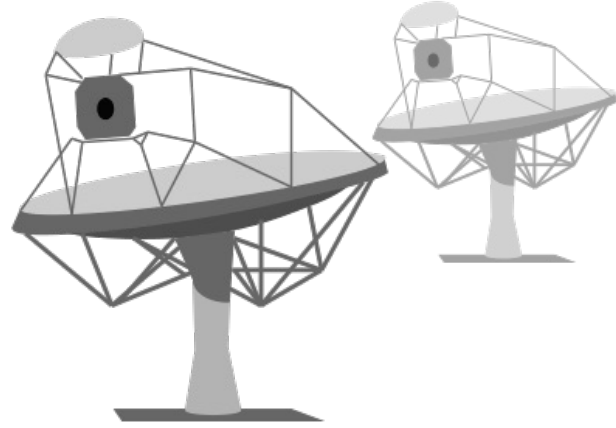
Next Gen X-ray Observatories



NASA Roman Space Telescope



Vera Rubin Observatory



Square Kilometer Array (SKA)

Chandra X-ray Observatory

