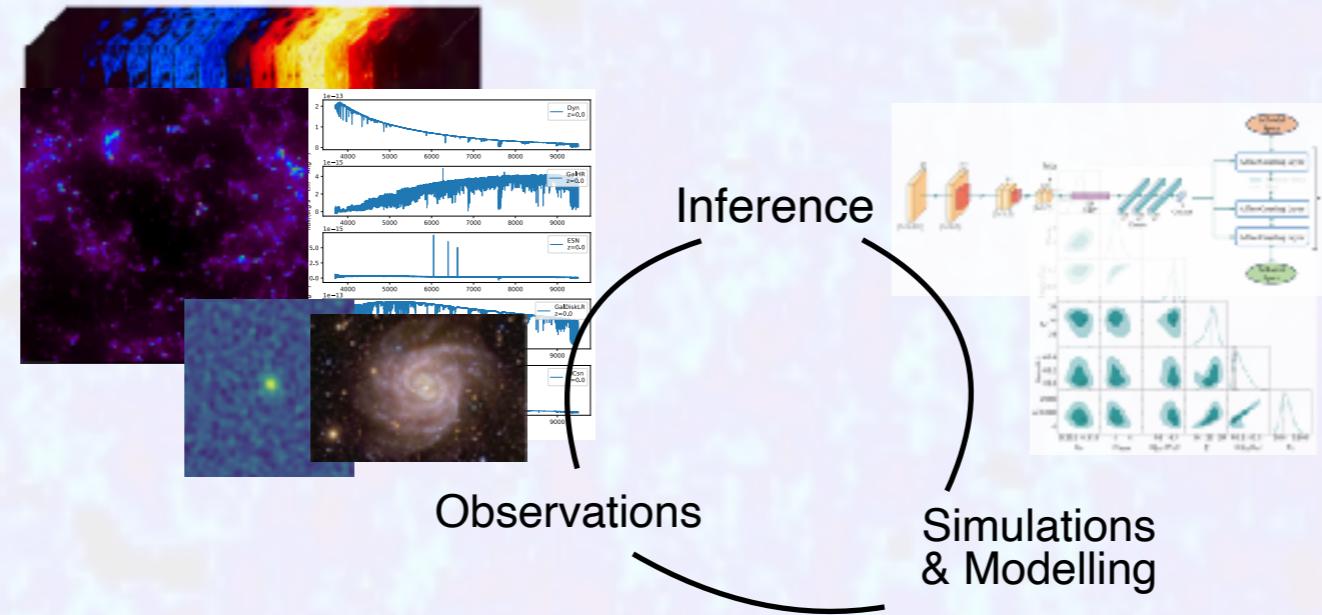


# Machine Learning for Astrophysics



Caroline Heneka, ITP Heidelberg

Group ‘Computer Vision Astrophysics and Cosmology’

Advanced School on Applied Machine Learning, ICTP Trieste, May 28th 2024

**Who am I? Caroline Heneka**  
**Institute for Theoretical Physics, Heidelberg University**



- B.Sc. and M.Sc. Physics in Heidelberg (+ Erasmus NPAC Paris)
- Ph.D. (2017) at Copenhagen University,  
DARK Cosmology Centre, Niels Bohr Institute
- 2017-2019: DFG Transregio 33 Fellowship (Heidelberg), Postdoc SNS Pisa
- ca. 1.5 yrs: DLR (German Aerospace Center) Headquarters Cologne,  
Executive Board Area Space, Programme Strategy Space
- 2020-2022: Senior Postdoc Hamburg University
  - Since Oct 2022: back in HD  
Junior Group Leader & Freigeist (Volkswagen Foundation) Fellow  
'Computer Vision Astrophysics and Cosmology'



## My Research Interests

- **Line Intensity Mapping**  
(also: radio galaxy clustering, cross-correlation studies, galaxy clusters, ..)



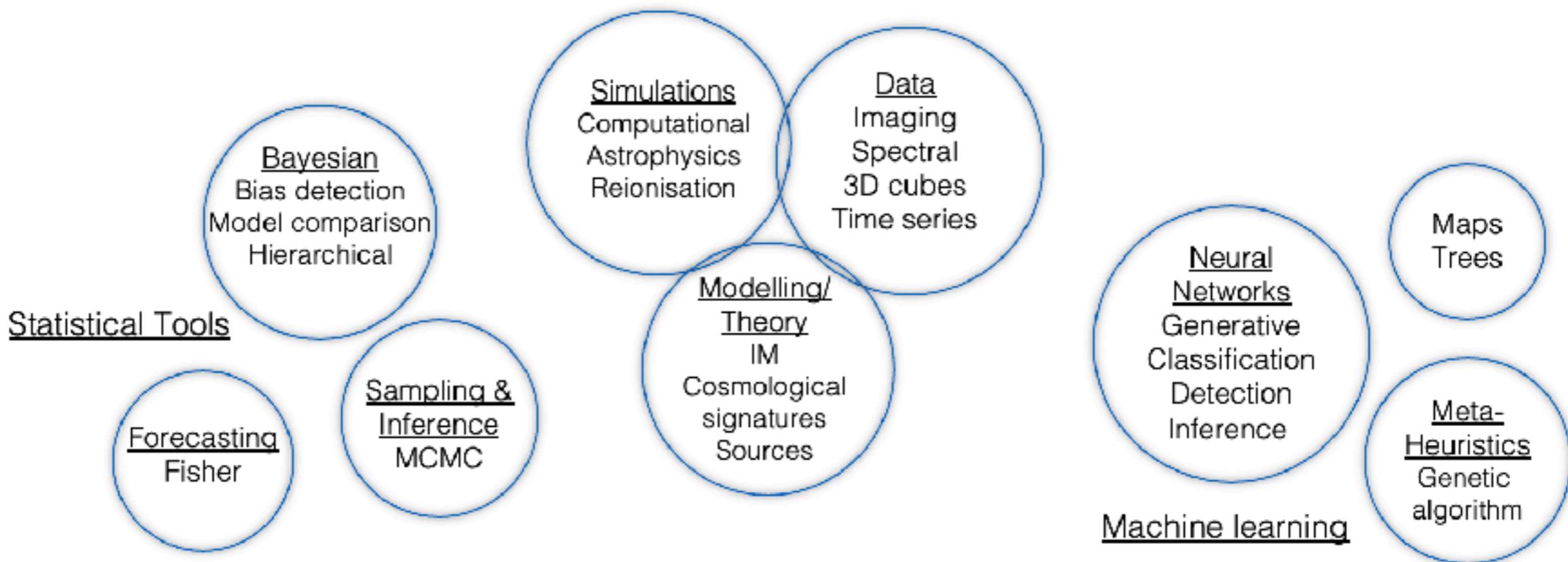
- **High-redshift astrophysics & Epoch of Reionization:**  
Modelling of 21cm background and further high-redshift lines (Lya, Ha, ..)

- The modern machine learning toolkit with '**Computer Vision Astrophysics + Cosmology**', specifically for intensity mapping of large-scale backgrounds:

- Emulation, generation
- Inference

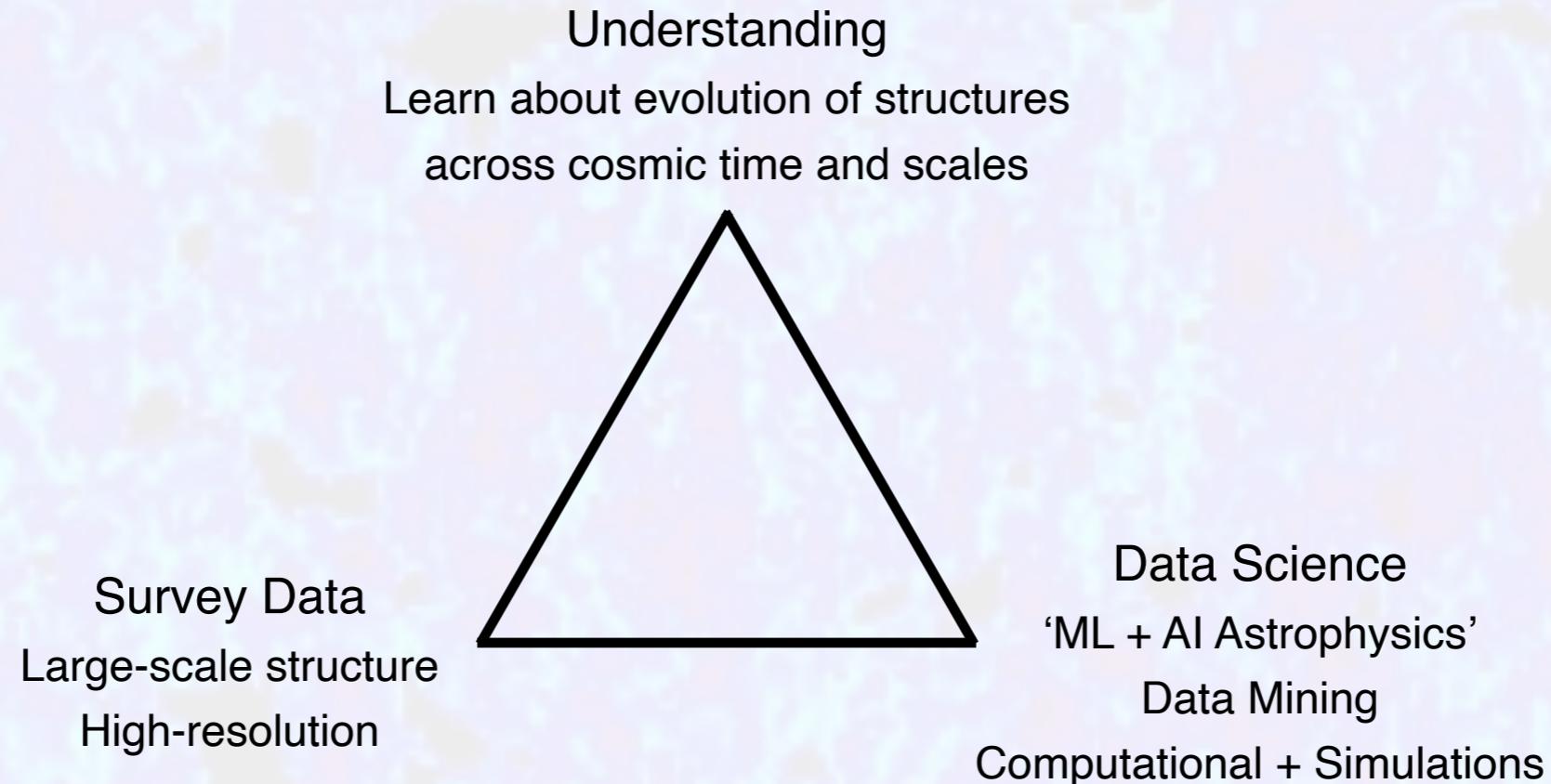
Also:

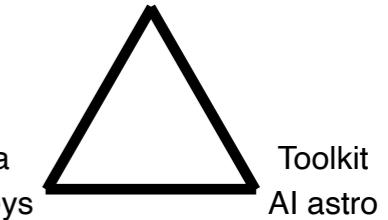
- Classification (e.g. 4MOST spectra)
- Detection (SKA preparation)



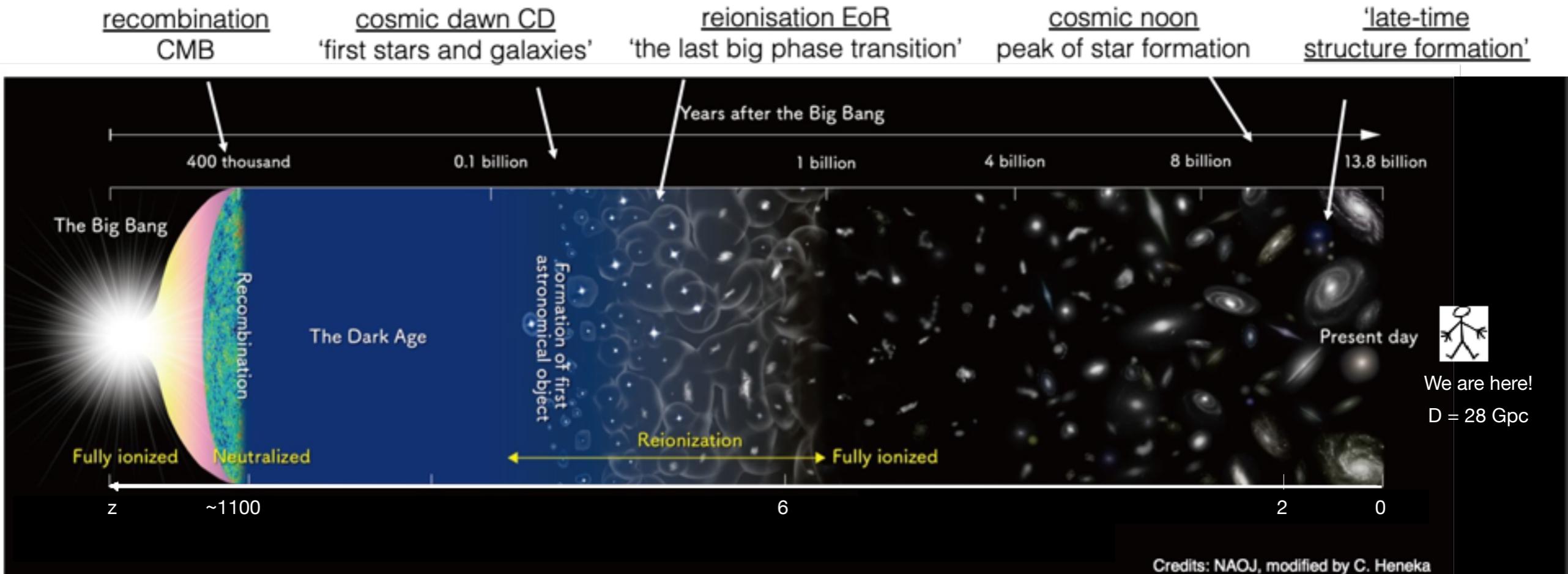
# How will Astronomy and Astrophysics advance in coming years?

---



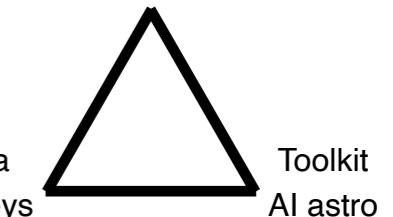


# Where we stand: Data revolution and cosmic evolution

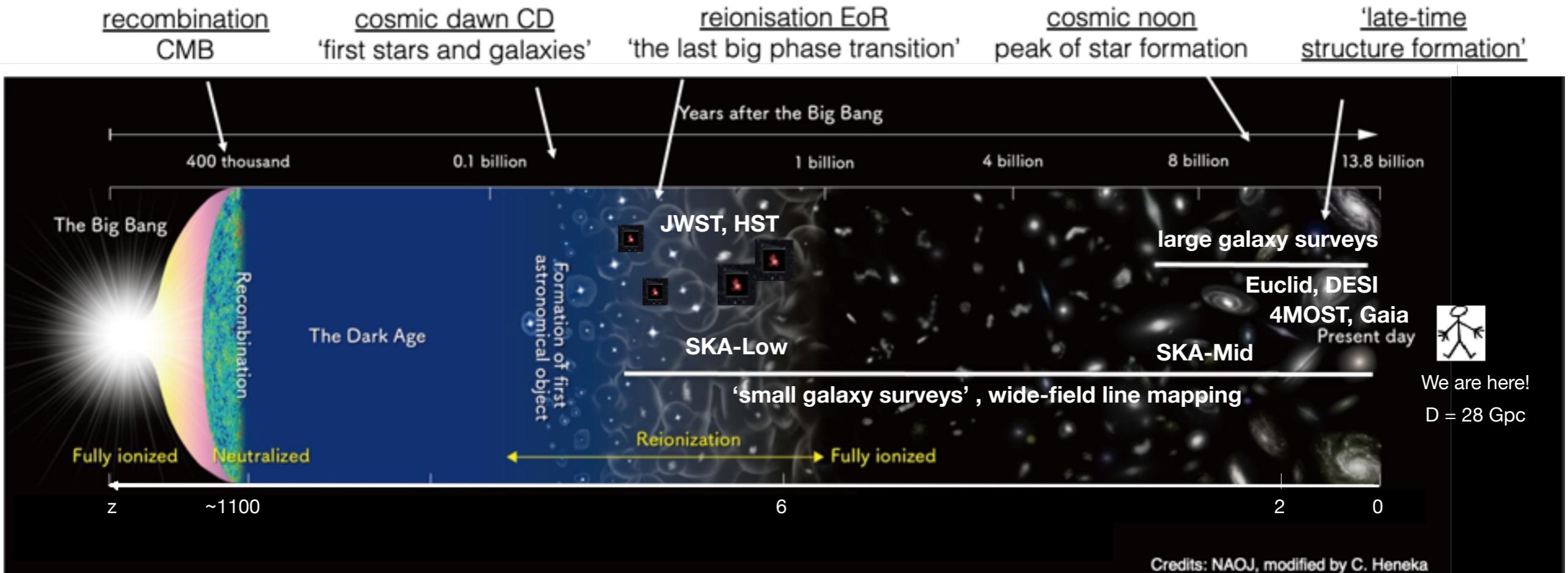


## Our goal:

Learn about astrophysical & cosmological evolution  
across cosmic time and scales



# Where we stand: Data revolution and cosmic evolution



## Our goal:

Learn about astrophysical & cosmological evolution  
across cosmic time and scales

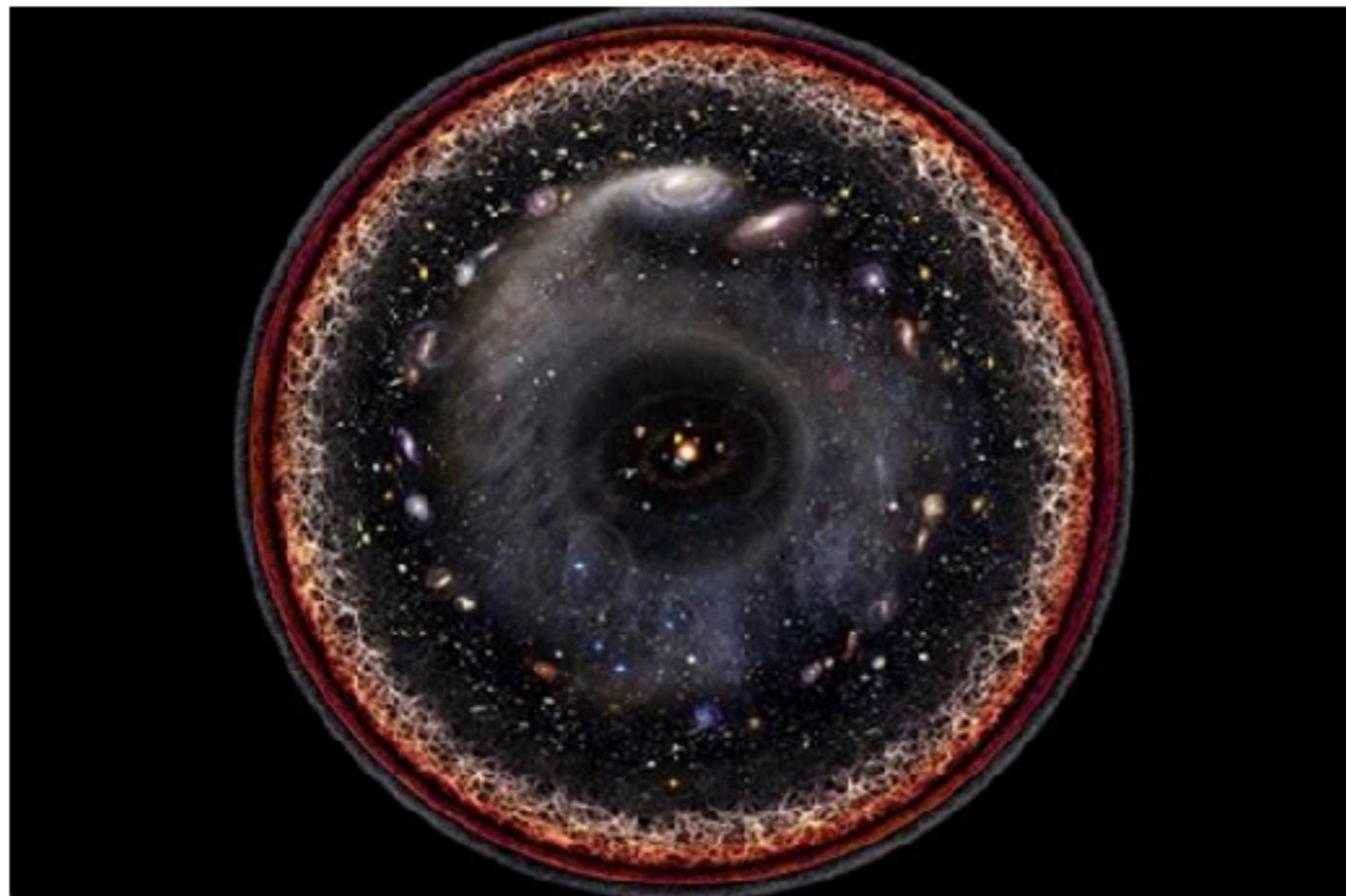
Coming decade: push to map up to **80% of the observable Universe**

... what does 80% of the observable Universe mean?

---

### Modelling challenges

True LSS probes → orders of magnitude of scales up to the ultra-large  
...what does 80% of the observable Universe even mean?



APOD, NASA, License & Credit: Wikipedia, Pablo Carlos Budassi

Observable Universe:  
 $d \sim 28 \text{ Gpc} (\times 3 \text{ Gyr})$

80% if this:  
 $d \sim 22 \text{ Gpc}$

Let's say we resolve (only)  $\sim \text{Mpc}$

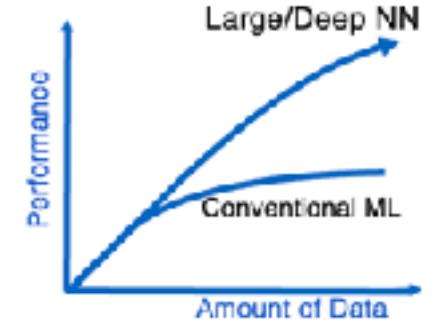
→ about 3-4 orders of magnitude

→ about  $10^9\text{-}10^{10}$  modes!

... at some point we sub-grid model and/or change modelling approach

# Advances in Data Science, for Science

Deep Learning  
Driven by ability to improve  
with large datasets



**One big  
goal?**

Learn about astrophysical & cosmological evolution  
across cosmic time and scales

**No, really - many goals, ...**

**... and instruments**

**... types of data**

**... datarates, scales, signal-to-noise**

ELT, Credit: ESO



Credit: SKAO

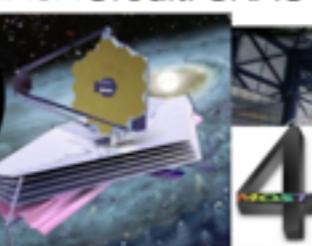
Credit: ESO

SPHEREx

Credit: JPL, NASA



Credit: ESA



Credit: NASA, ESA

MeerKAT, Credit: SRAO

**Large-scale surveys**

**High-resolution imaging and/or spectroscopy**



**Efficient data reduction  
Automation**

**Extract more & less biased information  
Data mining**

\* non-comprehensive list

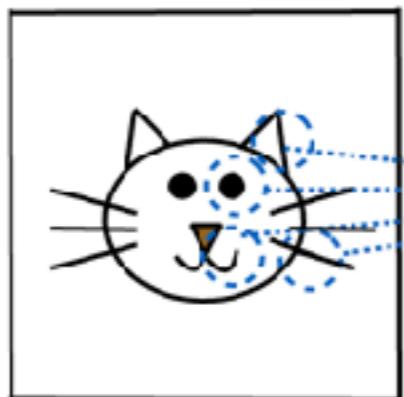
# Why ML/DL for Astrophysics?



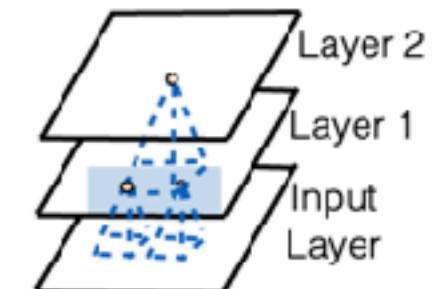
<https://braintour.harvard.edu/archives/portfolio-items/the-first-neurobiology-department>

Neuron response to visual stimuli

Nobel Prize in Physiology or Medicine 1981  
David Hubel and Torsten Wiesel



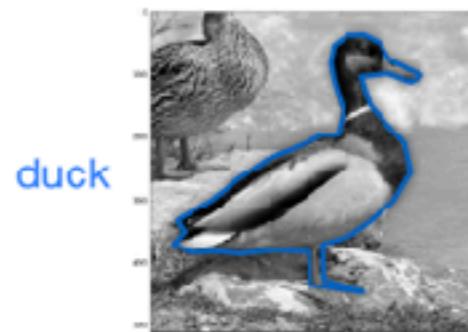
Representation learning



Convolutional neural network  
'Neocognitron' Kunihiko Fukushima 1979

Hierarchical learning

Non-linear, non-Gaussian

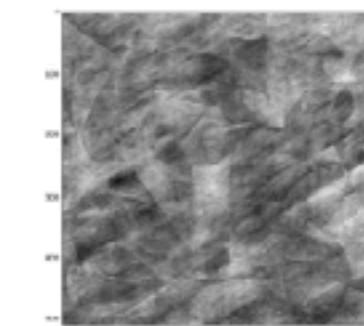


size  
color  
bkg



randomise  
phases

Same 2D  
power spectrum



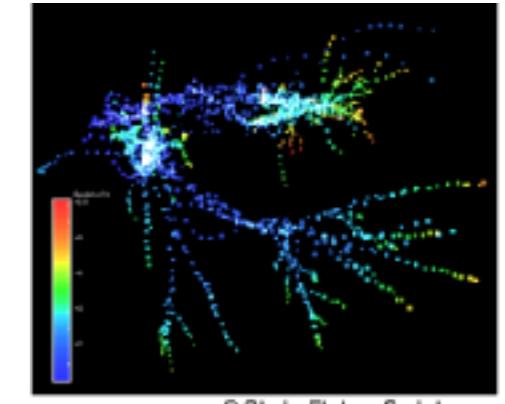
vs. "The famous  
Gaussian duck"

# Where we stand: ML and AI for Astronomy and Astrophysics

We need a versatile ML/AI toolkit, for:

- detection, segmentation
- classification
- regression, inference
- anomaly detection
- generation, emulation, ...

Hierarchical

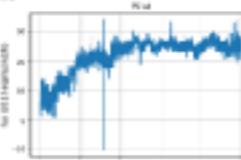
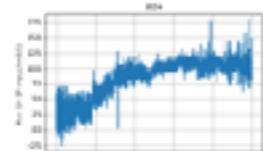


+ plenty of inverse problems

$$I^D(x, y) = R \times I(x, y) + n$$

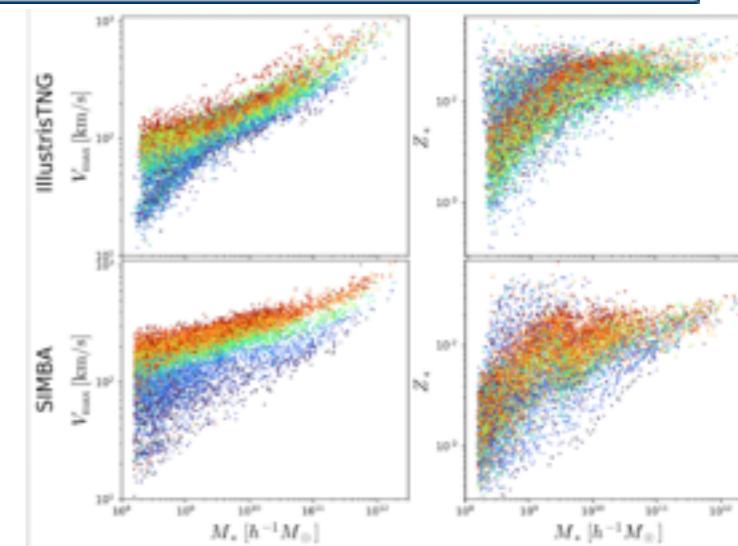


Representation learning

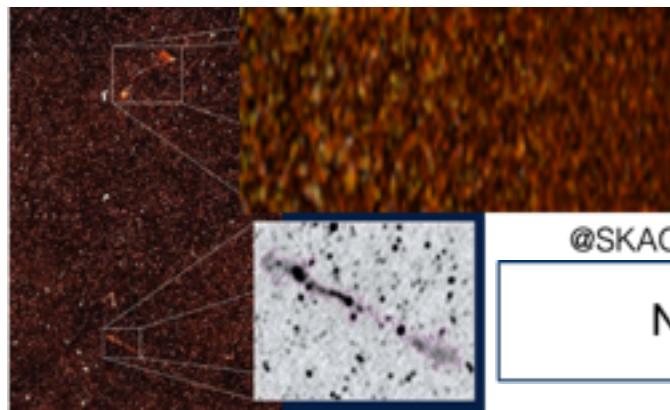


@SDSS

High-dim. correlations



arXiv:2201.02202

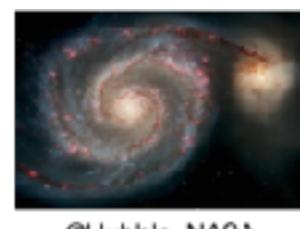


Non-linear, non-Gaussian

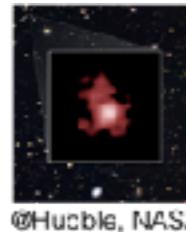
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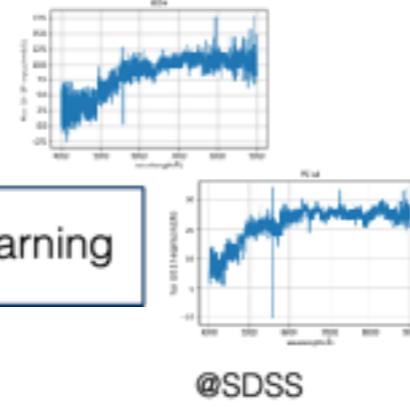
- detection, segmentation
- classification
- regression, inference
- anomaly detection
- generation, emulation, ...



@Hubble, NASA

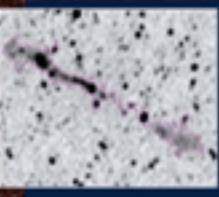
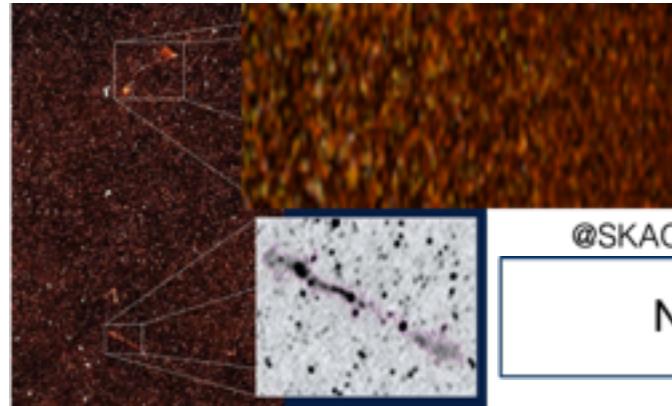


@Hubble, NASA



@SDSS

Representation learning



@SKAO

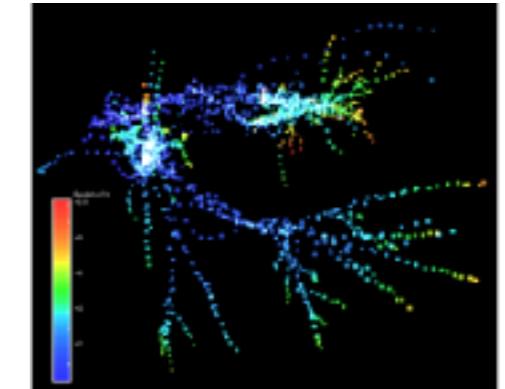
Non-linear, non-Gaussian

Examples:  
Few sec: Classification 40.000 spectra  
Few sec: 7-parameter inference ~100MB cube  
Few sec: detection, segmentation & flux measurement O(100-1000) sources

+ plenty of inverse problems

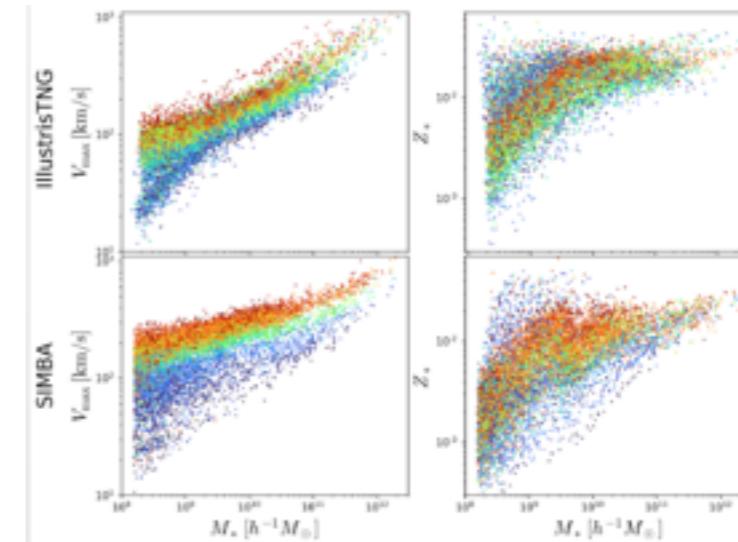
$$I^D(x, y) = R \times I(x, y) + n$$

Hierarchical



@Chris Fluke, Swinburne University of Technology

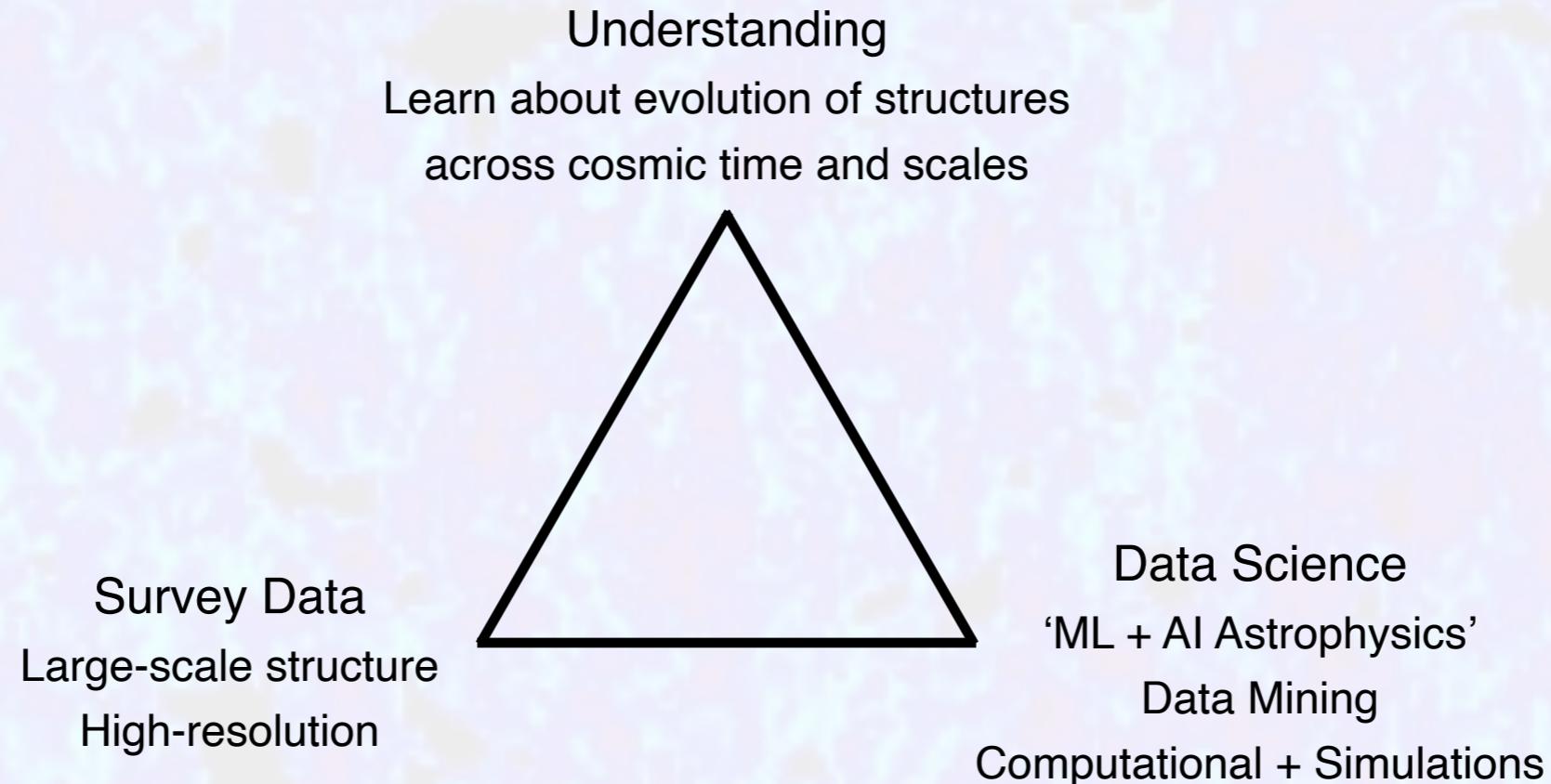
High-dim. correlations



arXiv:2201.02202

# How will Astronomy and Astrophysics advance in coming years?

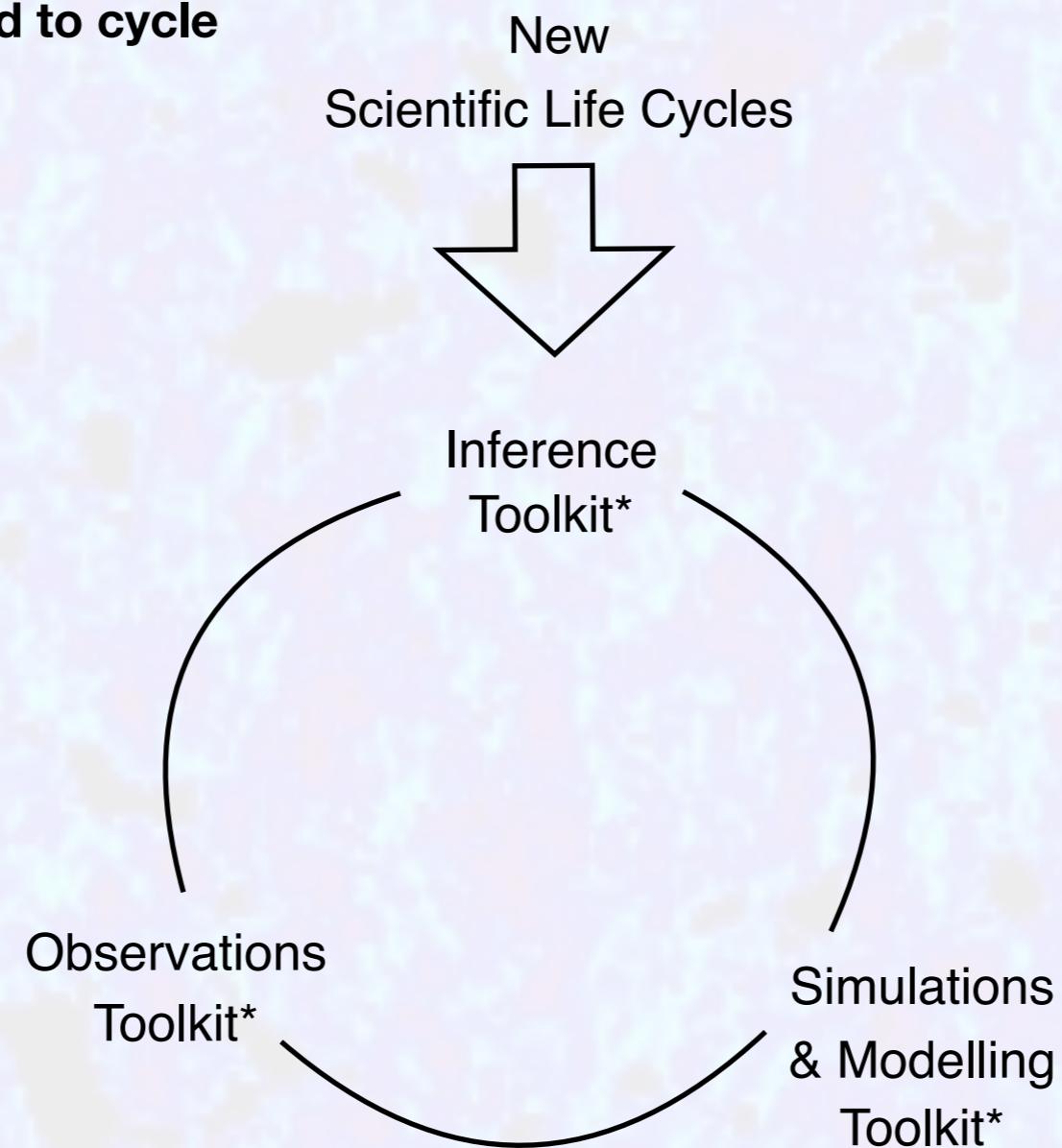
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# Astronomical and Astrophysical Machine Learning

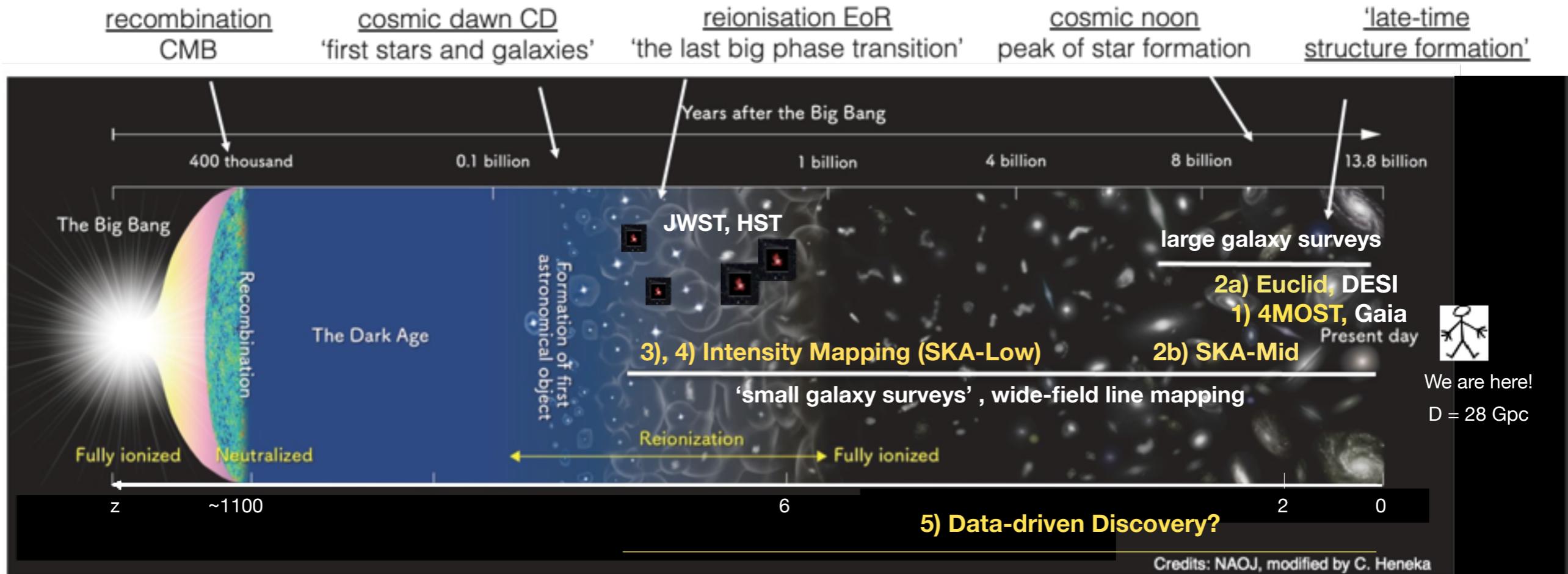
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In practice: From pyramid to cycle



\*The Toolkit: Statistics, Machine & Deep Learning, Data Mining

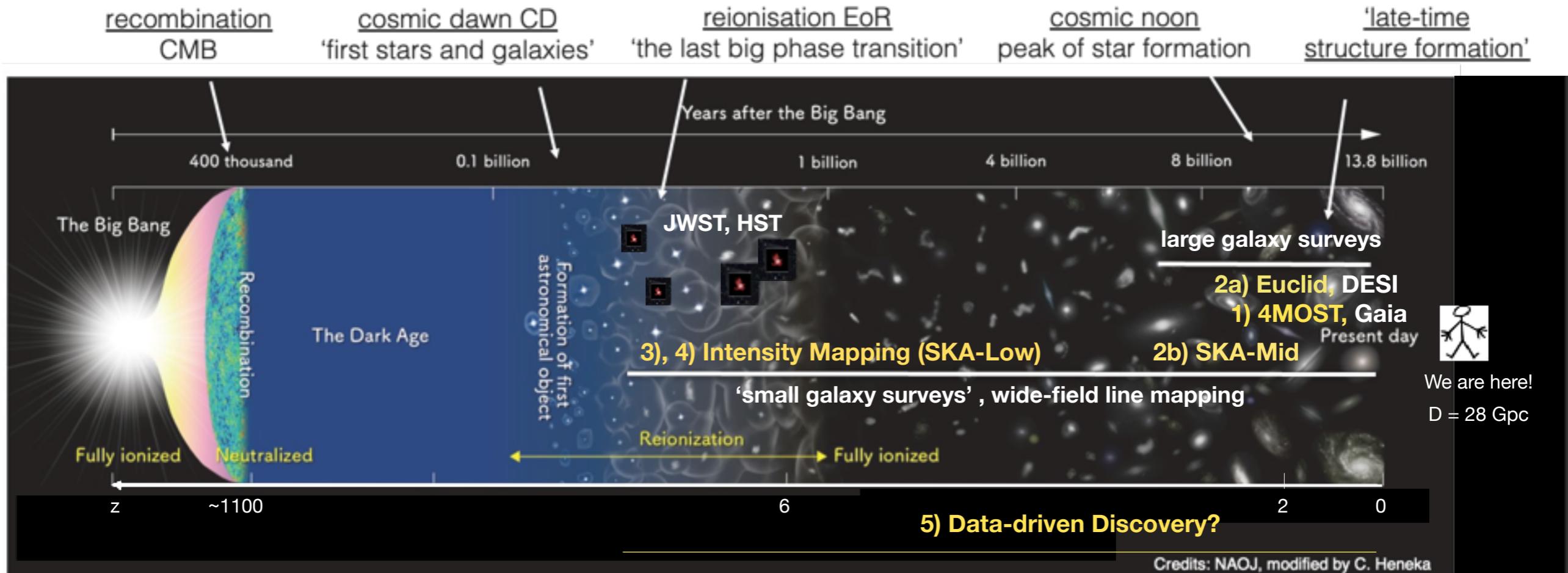
# Astronomical and Astrophysical Machine Learning



## Highlights in this Lecture

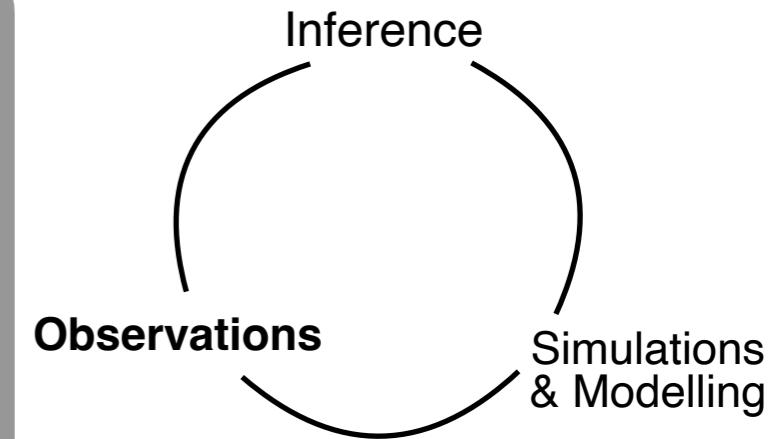
- 1) Classification / Triggering
- 2) Source detection & characterisation
- 3) Simulation-based inference (SBI) in 3D
- 4) Generative methods
- 5) Data-driven Discovery

# Astronomical and Astrophysical Machine Learning



## Highlights in this Lecture

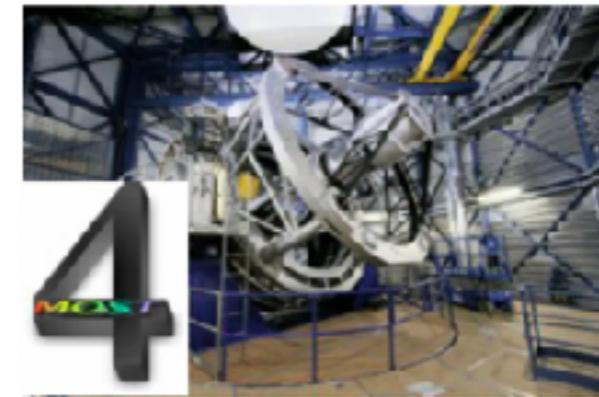
- 1) Classification / Triggering
- 2) Source detection & characterisation
- 3) Simulation-based inference (SBI) in 3D
- 4) Generative methods
- 5) Data-driven Discovery



# 1) Classification and triggering for large astronomical surveys

4MOST: On-the-fly classification of spectra (1D)

- 5-year survey
- wide-field, fibre-fed, optical spectroscopy
- on ESO's 4-m-class telescope VISTA
- 2.5-degree diameter field-of-view, 2436 fibres
- HRS R  $\approx$  18000 – 21000, LRS R  $\approx$  4000 – 7500
- 20mio. (LRS), 3mio. (HRS) sources



<https://www.4most.eu> Credit: ESO

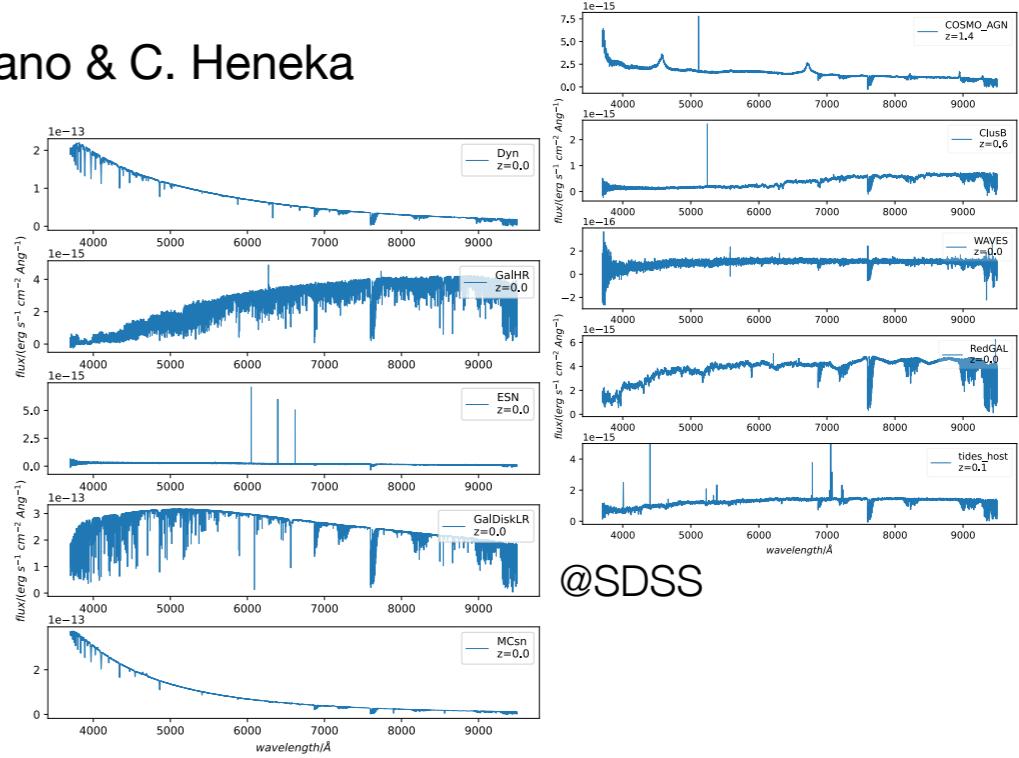
## Goal: Data-driven classification pipeline layer (galactic & extragalactic sources)

Classification infrastructure working group, led by: N. Napolitano & C. Heneka



*Benchmark with  
SDSS archival spectra:*

*See also our tutorial!*



@SDSS

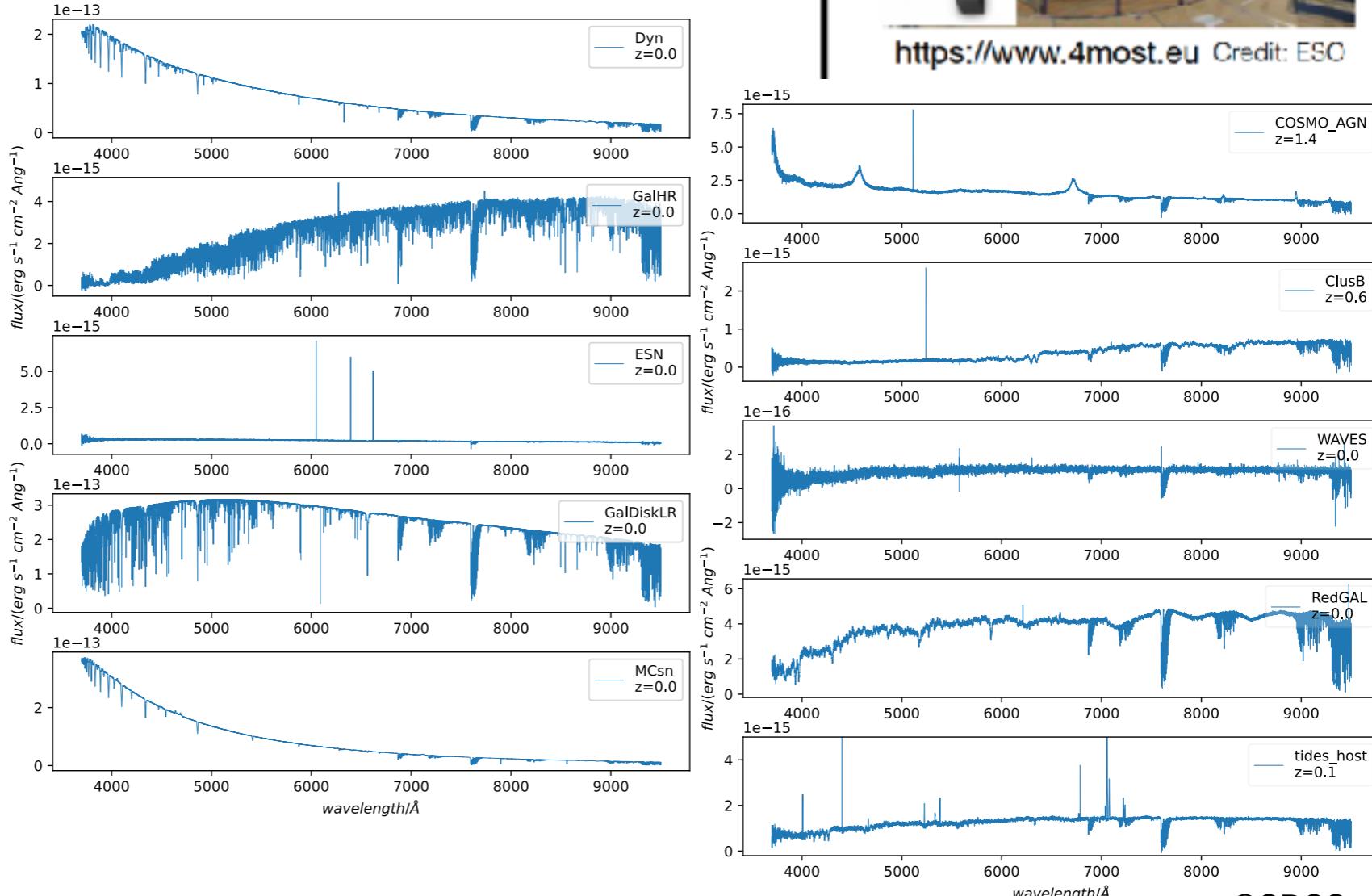
# 1) Classification and triggering for large astronomical surveys

4MOST: On-the-fly classification of spectra (1D)



<https://www.4most.eu> Credit: ESO

- 5-y
- wid
- on
- 2.5
- HR
- 20r



**Goal:** Data-driven classi

Classification infrastructu

*Galactic vs. Extragalactic  
See also our tutorial!*

@SDSS

# 1) Classification and triggering for large astronomical surveys

4MOST: On-the-fly classification of spectra (1D)



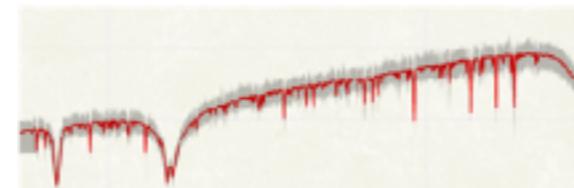
<https://www.4most.eu> Credit: ESO

**Goal: Data-driven classification pipeline layer (galactic & extragalactic sources)**

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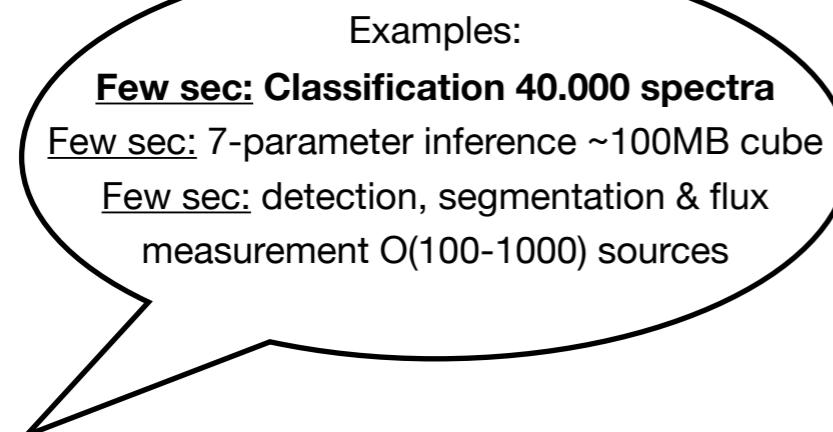
→ Probabilistic multi-classifier

For class:  
*Convolutional  
network variants*



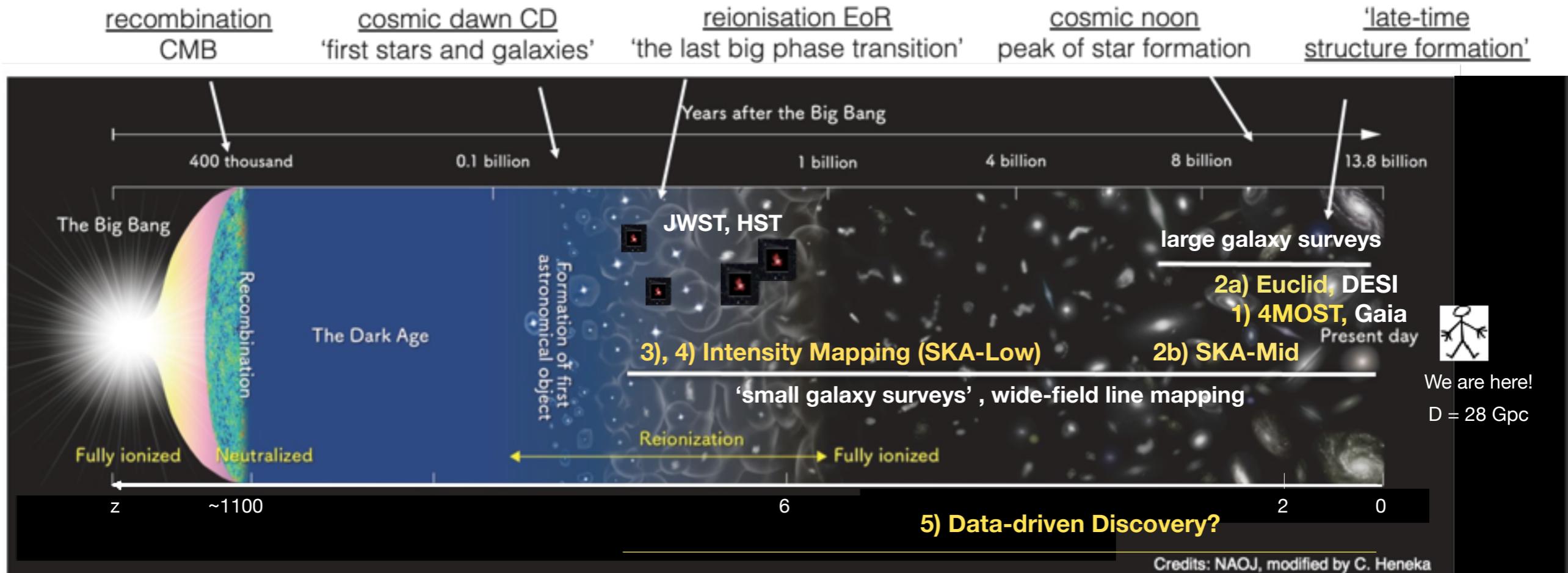
For class uncertainties:  
*Bayesian neural networks  
and contrastive learning*

*++ competitive with template fitting*



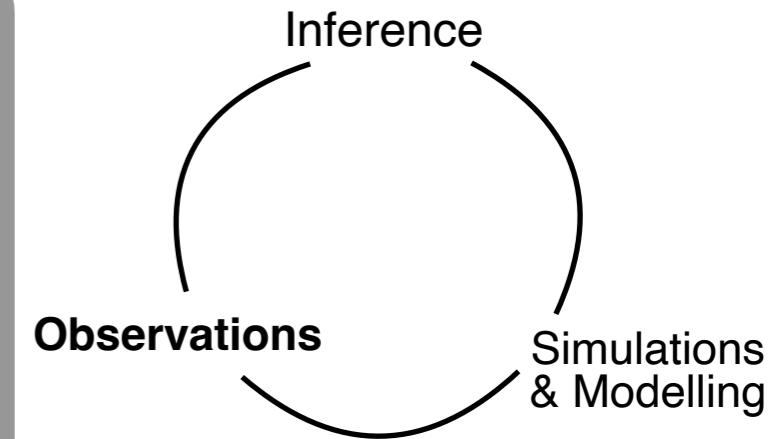
		Zhong, Napolitano, Heneka+ arXiv:2311.04146																					
		Predicted																					
		STAR_K5 -	STAR_K3 -	STAR_K1 -	STAR_G2 -	STAR_F9 -	STAR_F5 -	STAR_A0 -	QSO_nan -	QSO_BROADLINE -	GALAXY_nan -	GALAXY_STARFORMING -	GALAXY_STARBURST -	GALAXY_agn -	STAR_A0 -	STAR_F5 -	STAR_F9 -	STAR_G2 -	STAR_K1 -	STAR_K3 -	STAR_K5 -		
STAR_K5 -	1 0.00	3 0.00	1 0.00	1 0.00	3 0.00	1 0.00	1 0.00	2725 0.91	95 0.03	64 0.02	9 0.00	2 0.00	1 0.00	1 0.00	186 0.06	2719 0.91	75 0.03	1 0.00	142 0.05	2920 0.97			
STAR_K3 -		2 0.00													8 0.00								
STAR_K1 -			1 0.00												126 0.04								
STAR_G2 -				1 0.00	1 0.00										14 0.00	139 0.05	2882 0.96						
STAR_F9 -						3 0.00																	
STAR_F5 -							1 0.00								1 0.00	165 0.06	2899 0.97						
STAR_A0 -								2 0.00							2 0.00	2832 0.94	87 0.03						
QSO_nan -	9 0.00	6 0.00	4 0.00	32 0.01	284 0.09	2716 0.91	2 0.00								2 0.00								
QSO_BROADLINE -		3 0.00		1 0.00			2703 0.90	187 0.06															
GALAXY_nan -	103 0.03	19 0.01	100 0.03	2716 0.91	2 0.00	65 0.02	1 0.00								1 0.00								
GALAXY_STARFORMING -	87 0.03	163 0.05	2608 0.87	126 0.04			3 0.00																
GALAXY_STARBURST -	17 0.01	2794 0.93	135 0.04	21 0.01																			
GALAXY_agn -	2780 0.93	17 0.01	150 0.05	98 0.03	11 0.00	17 0.01																	

# Astronomical and Astrophysical Machine Learning



## Highlights in this Lecture

- 1) Classification / Triggering
- 2) Source detection & characterisation
- 3) Simulation-based inference (SBI) in 3D
- 4) Generative methods
- 5) Data-driven Discovery



## 2a) The deblending problem

Example: Optical source detection & characterisation

**Goal:** 'Good' photometry for surveys with high blended fraction  
- avoid bias!

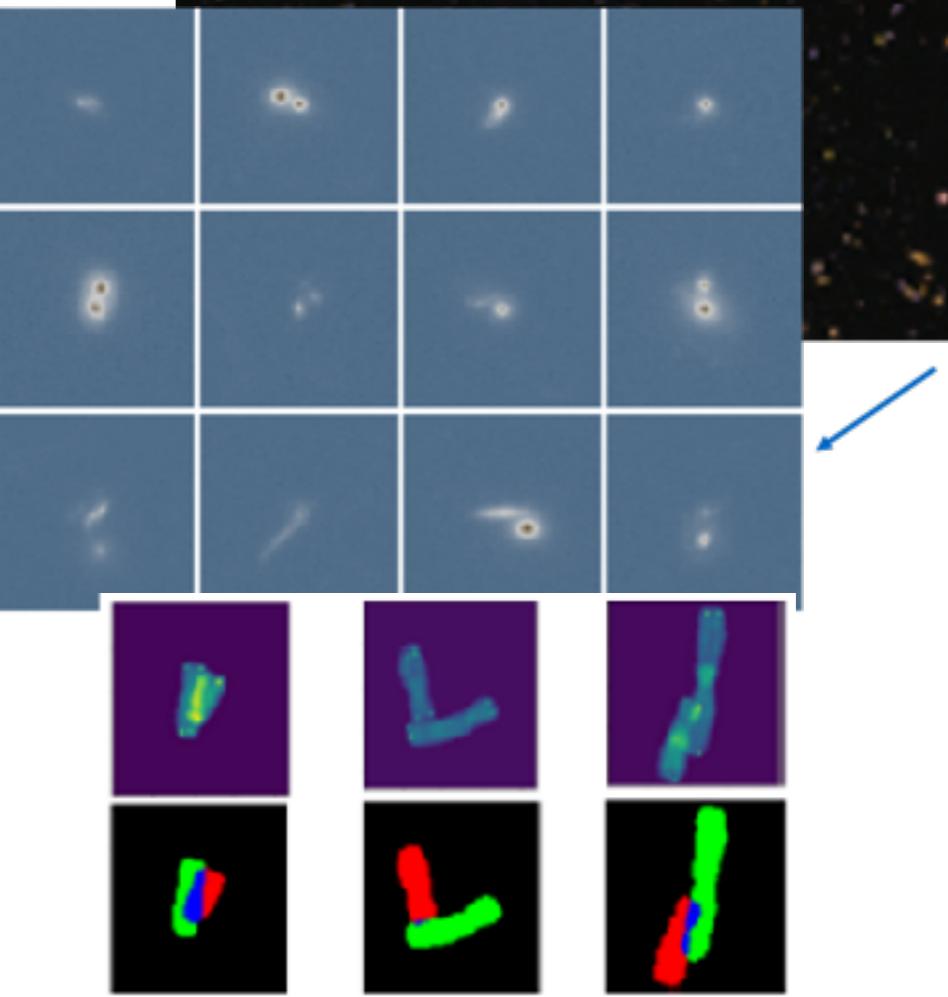
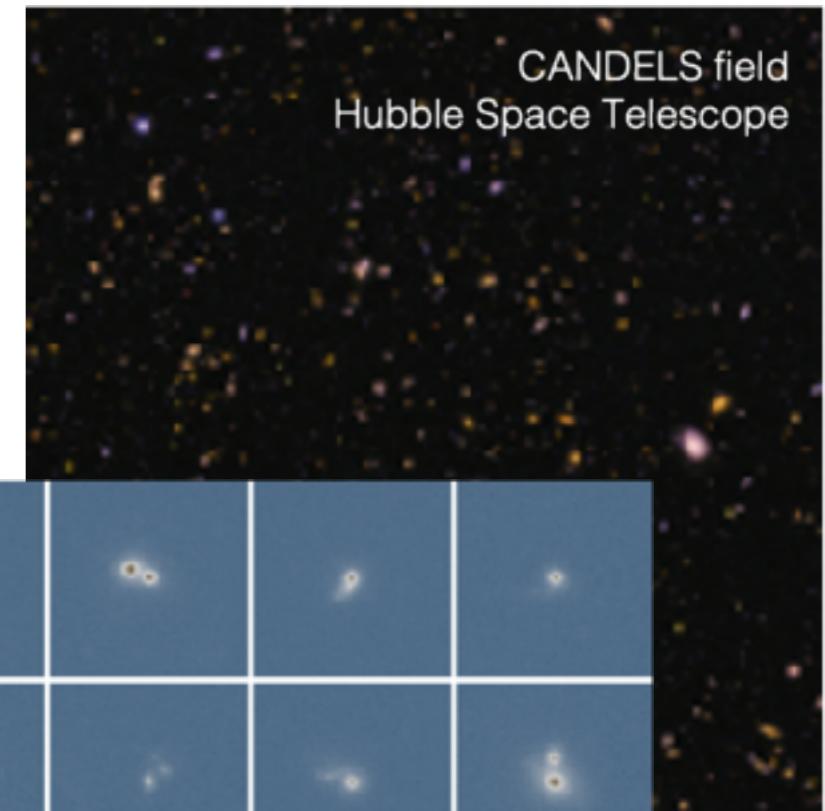
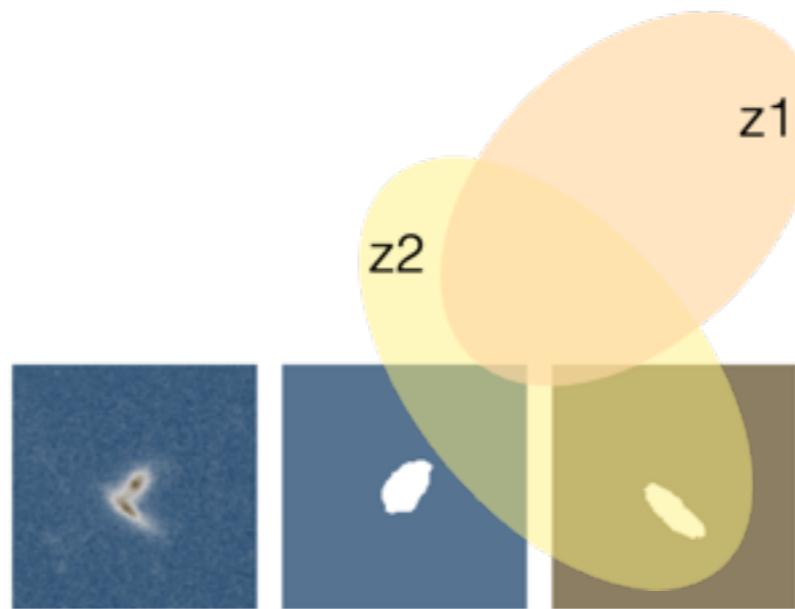
Galaxy morphology

**Challenge:** Galaxies are 'transparent'



coindeblend

Boucaud, Huertas-Company, Heneka+ 20,  
arXiv:1905.01324



Lily Hu+ 2017

Similar challenge:  
Overlapping chromosomes

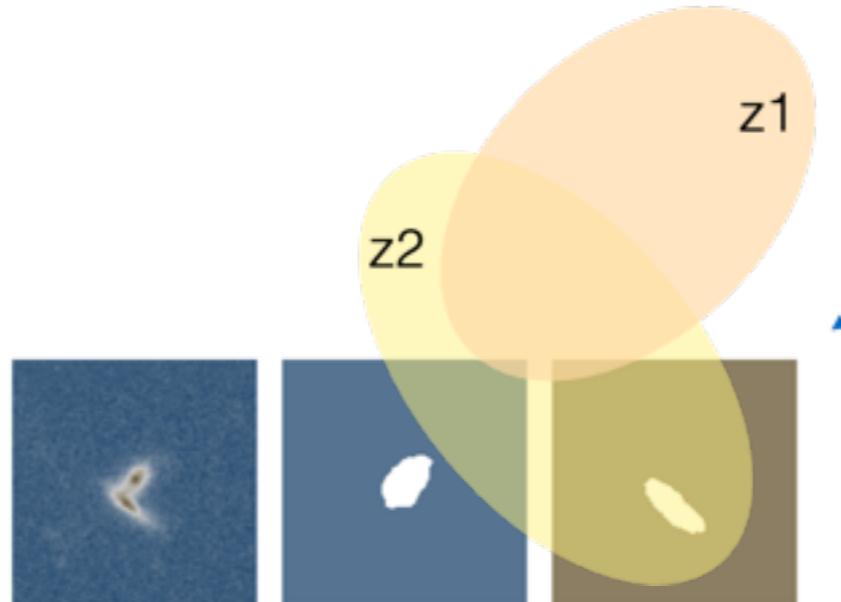
## 2a) The deblending problem

Example: Optical source detection & characterisation

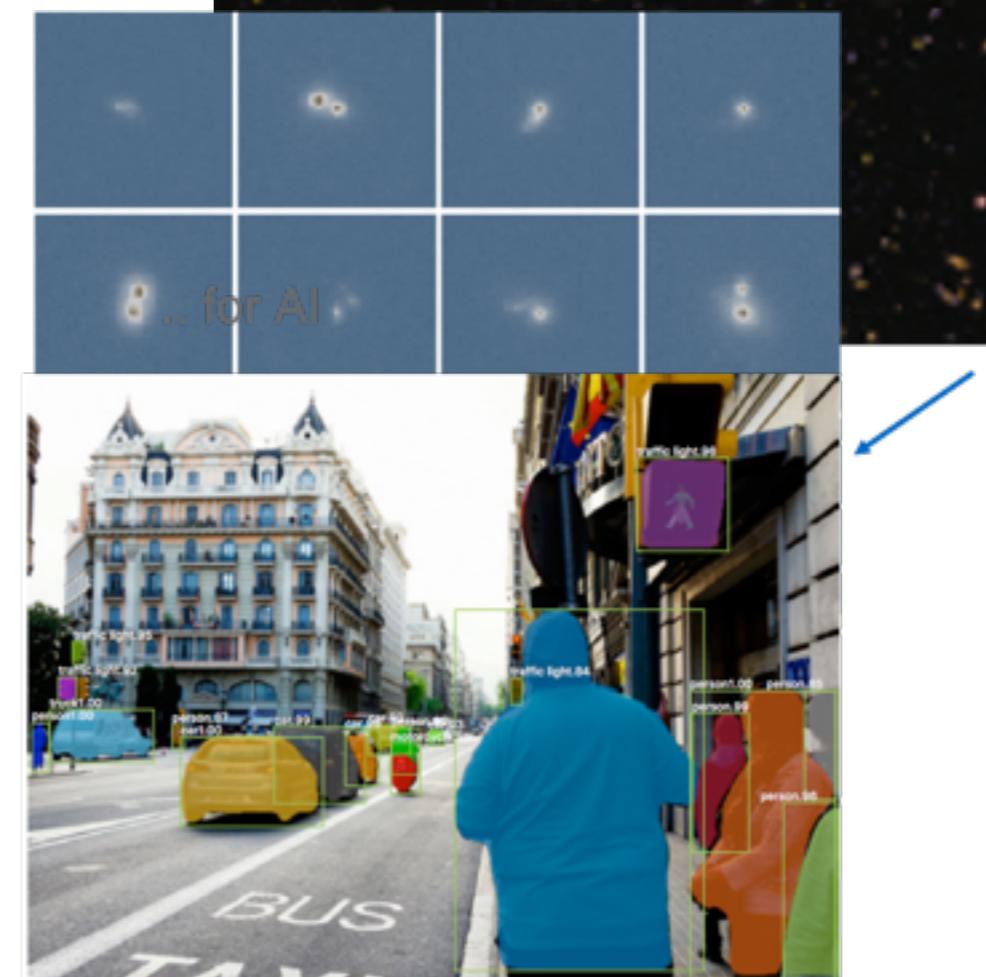
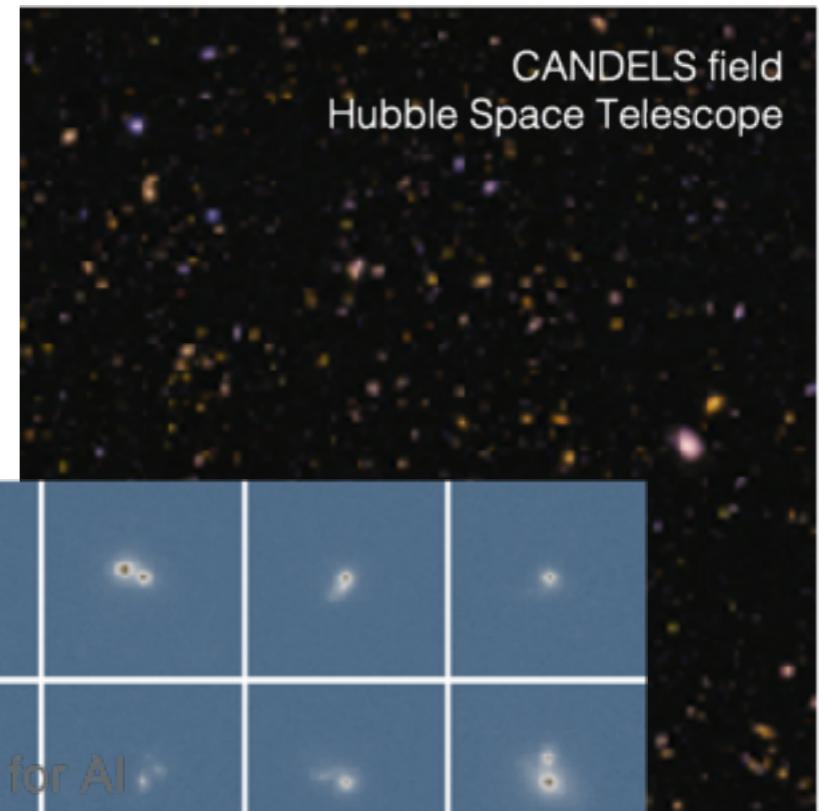
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Boucaud, Huertas-Company, Heneka+ 20,  
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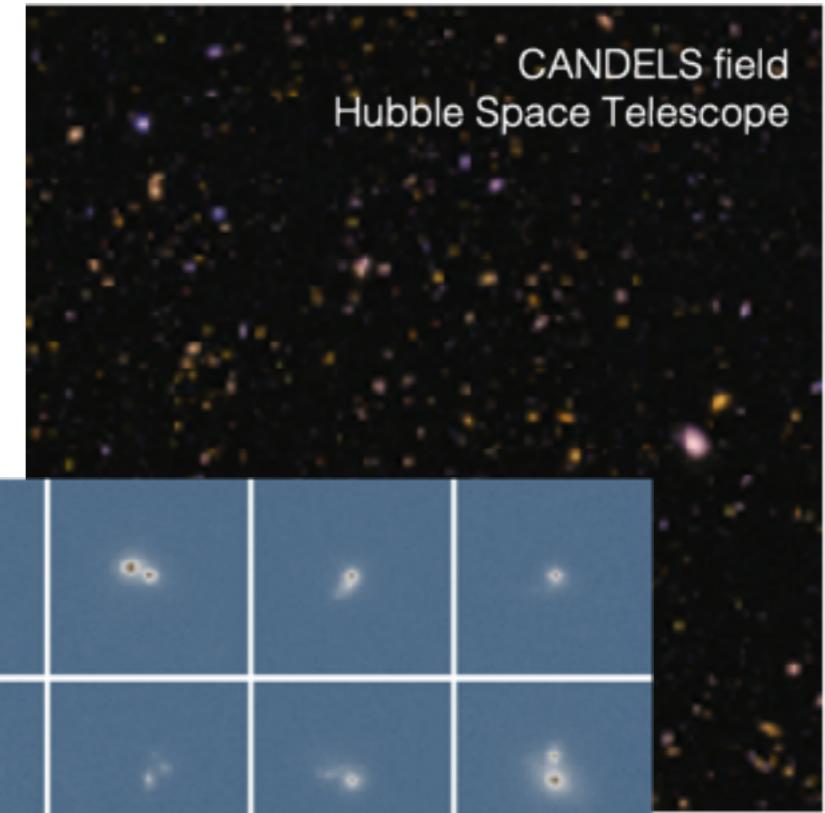


[https://medium.com/@umerfarooq\\_26378/from-r-cnn-to-mask-r-cnn-d6367b196cf](https://medium.com/@umerfarooq_26378/from-r-cnn-to-mask-r-cnn-d6367b196cf)

Another challenge: Object detection

## 2a) The deblending problem

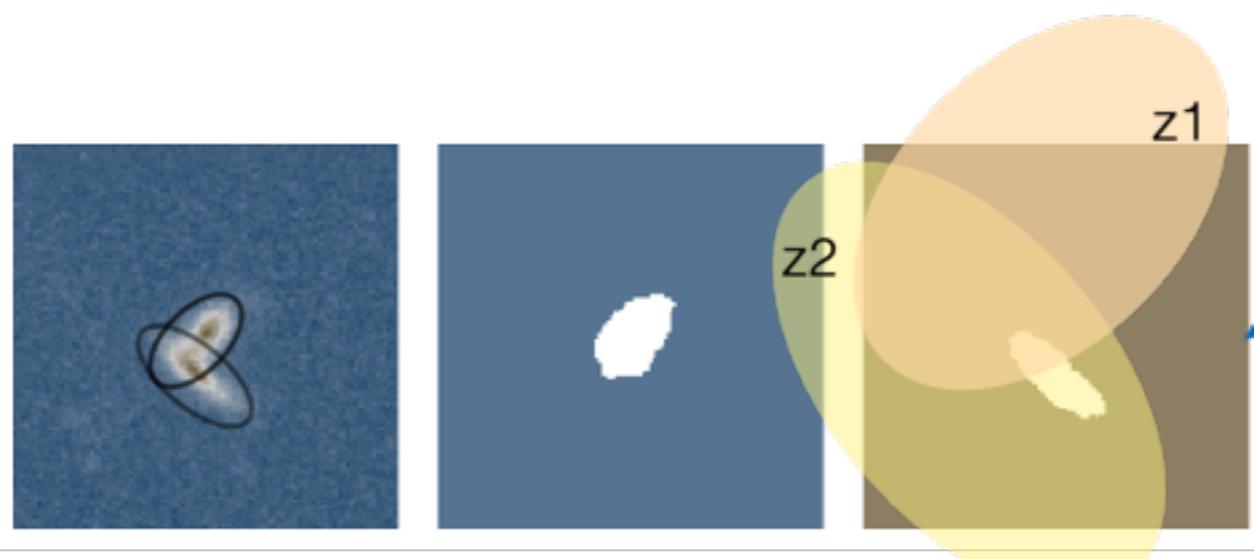
Example: Optical source detection & characterisation



**Goal:** 'Good' photometry for surveys with high blended fraction  
- avoid bias!

Galaxy morphology

**Challenge:** Galaxies are 'transparent'



**'Classic':**  
Fit ellipse(s)  
and profile(s)

e.g. Einasto ('65):

$$\frac{d \log(\rho)}{d \log(r)} = -2 \left( \frac{r}{r_s} \right)^\alpha$$



## 2a) The deblending problem

Example: Optical source detection & characterisation

**Goal:** 'Good' photometry for surveys with high blended fraction  
- avoid bias!

Galaxy morphology



Credit: Euclid, ESA

## 2a) The deblending problem

Example: Optical source detection & characterisation

CANDELS field  
Hubble Space Telescope

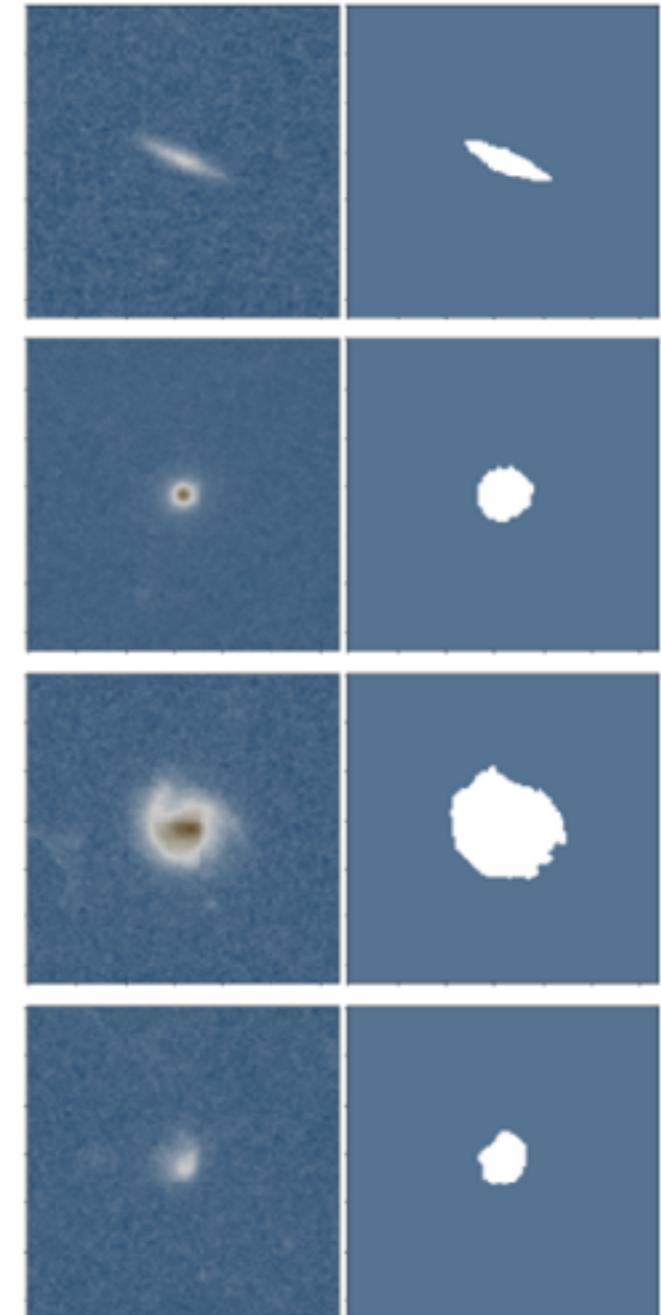


Get precise  
Photometry

..and do so bias-free

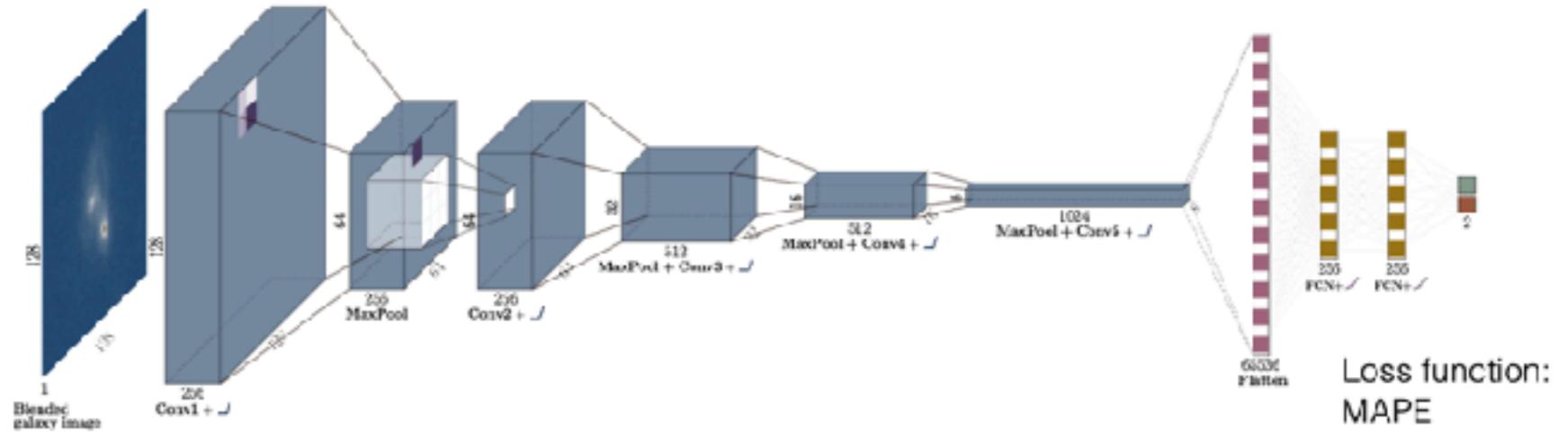


Derive masks

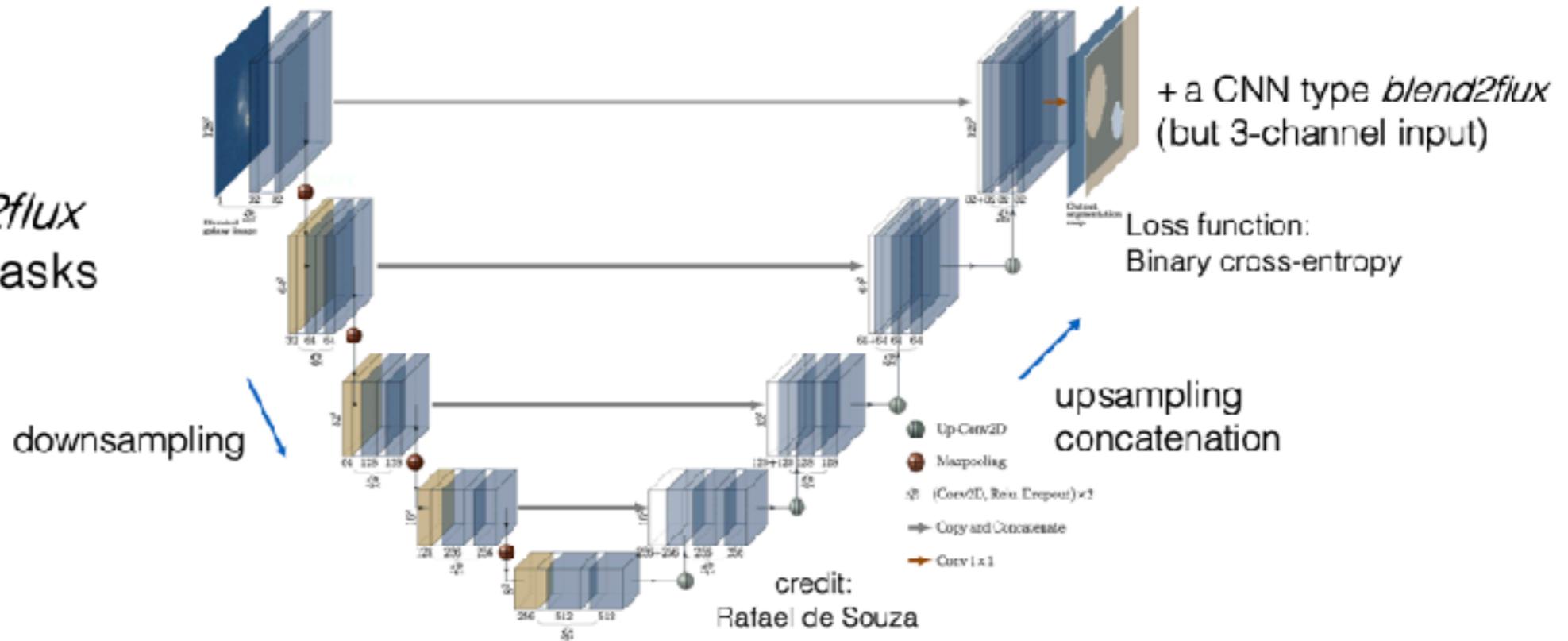


## 2a) The deblending problem

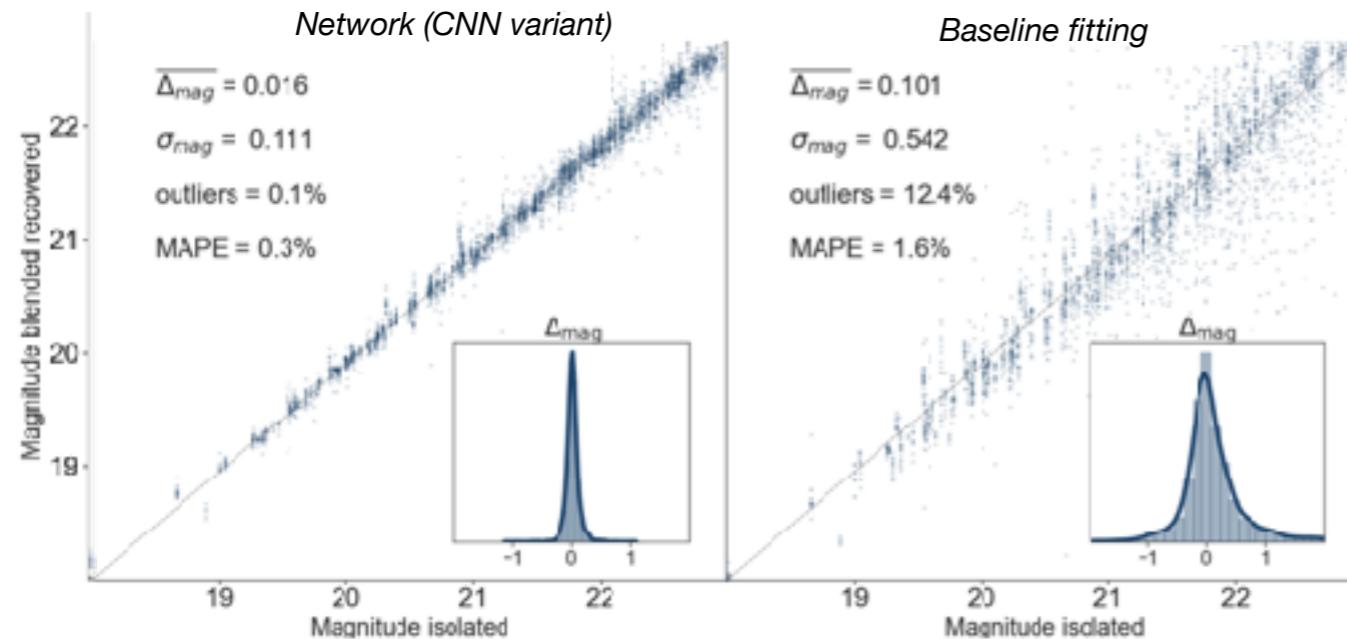
1) *blend2flux*  
a CNN for photometry



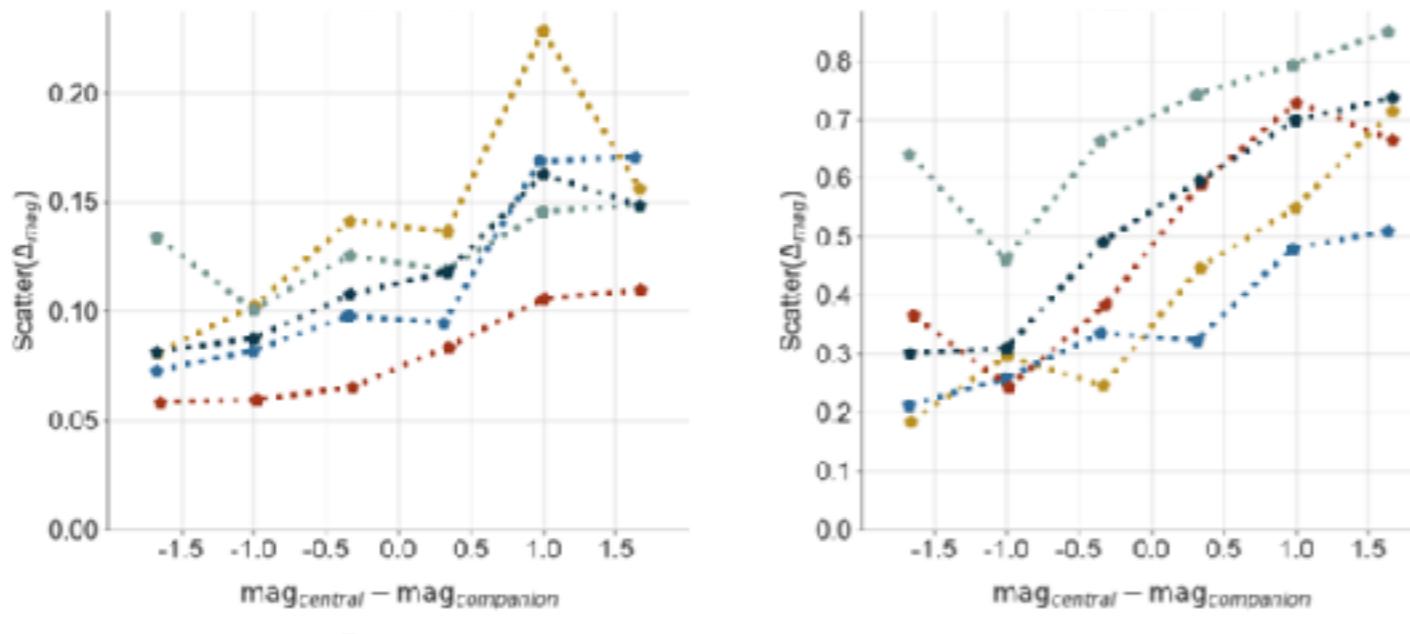
2) *blend2mask2flux*  
photometry + masks



## 2a) Optical source detection and characterisation



Get precise  
Photometry



For irregular  
shapes

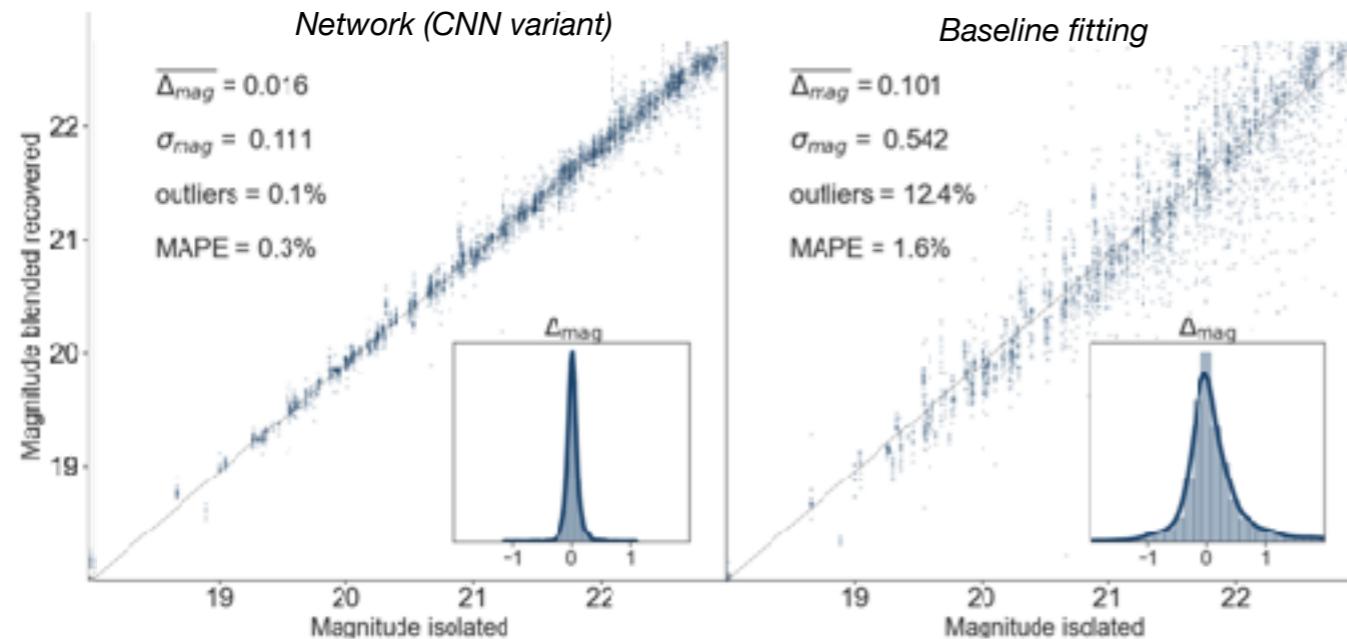


Spheroids      Bulge + Disk      Disks      Irregular      All

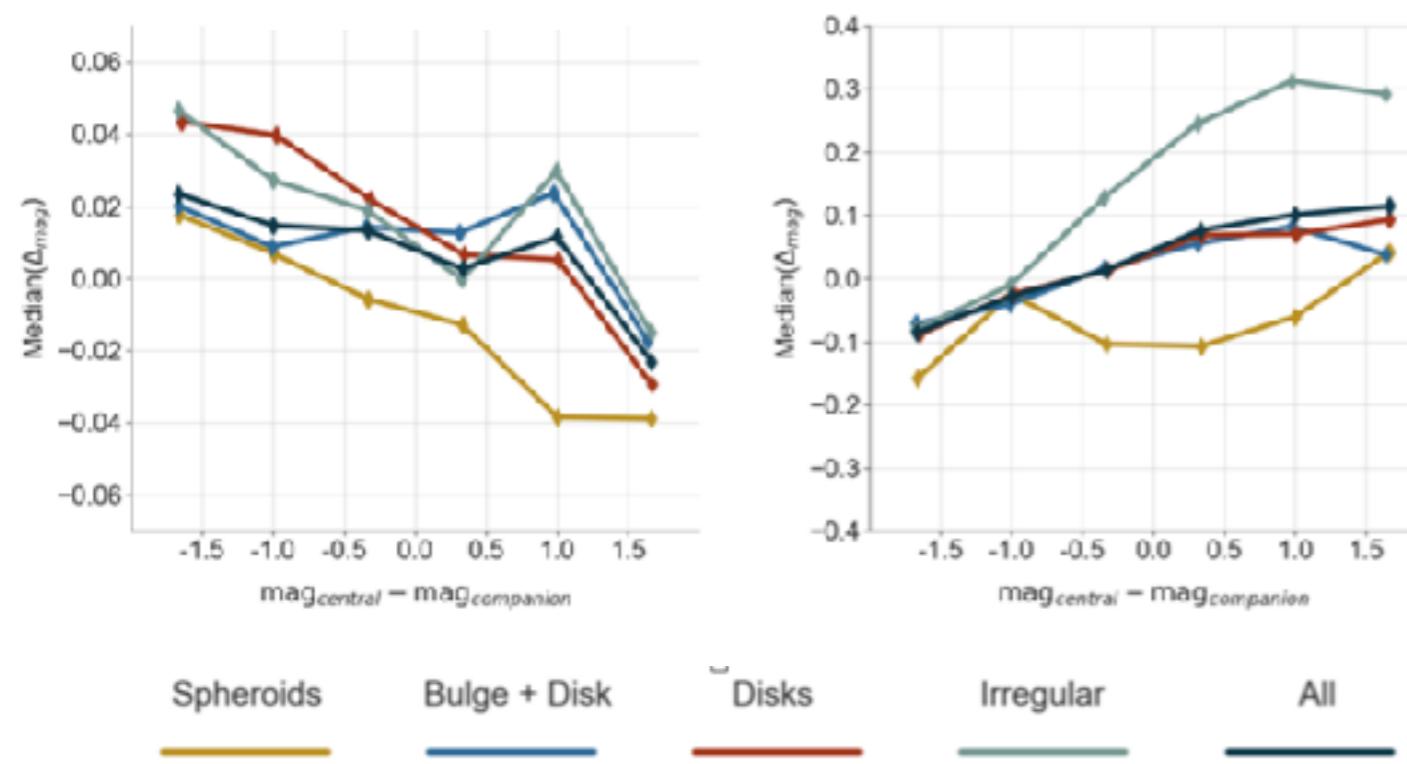
 coindeblend

Boucaud, Huertas-Company, Heneka+ 20

## 2a) Optical source detection and characterisation



Get precise  
Photometry



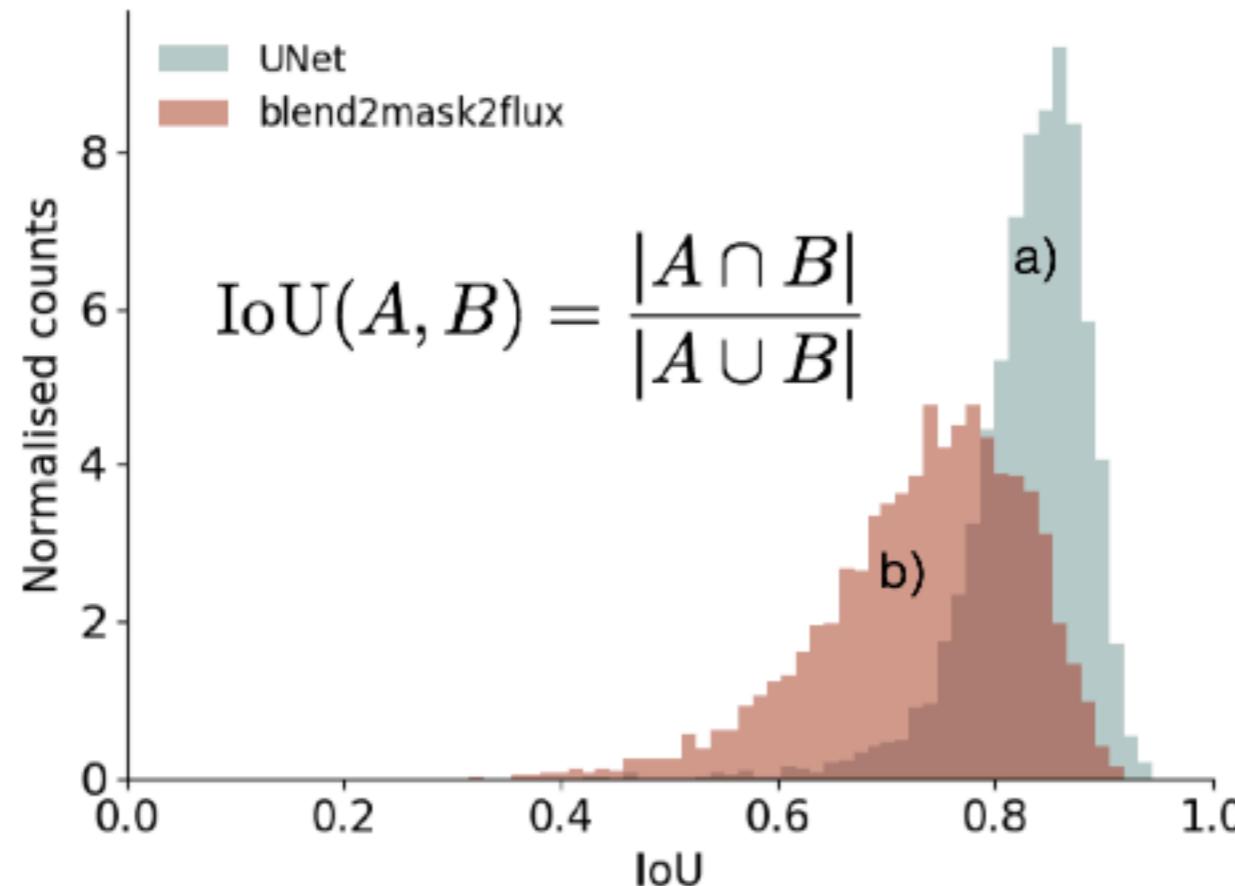
..and do so  
bias-free



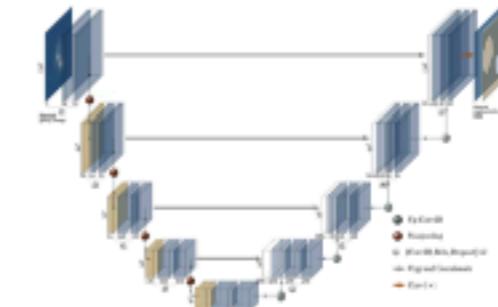
Boucaud, Huertas-Company, Heneka+ 20

## 2a) Optical source detection and characterisation

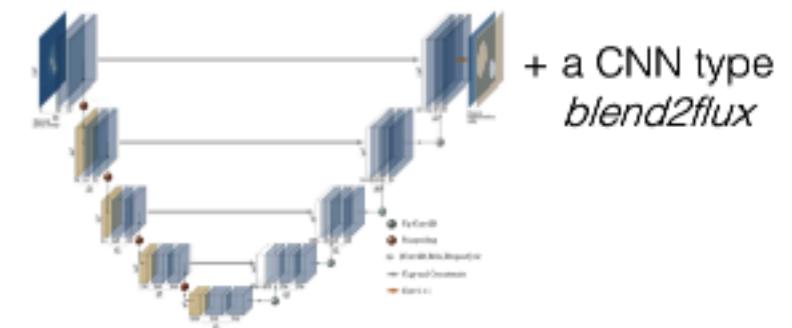
Optimal design is goal-dependent



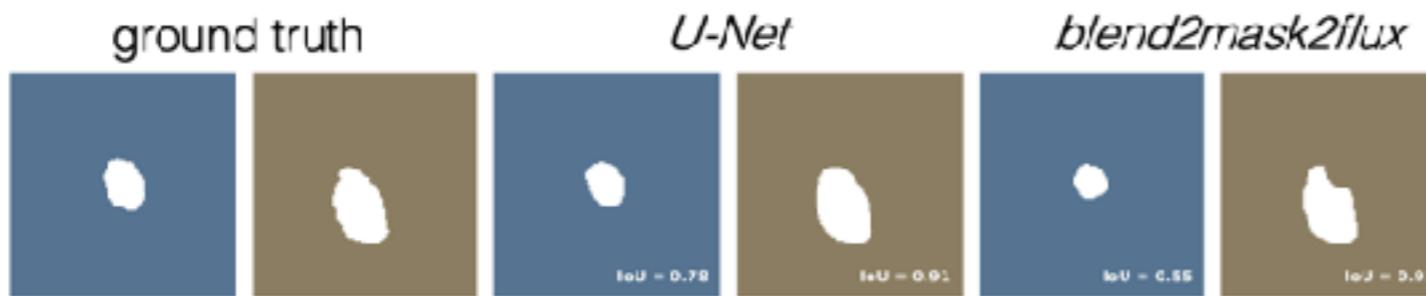
a) *U-net*  
masks, no photometry



b) *blend2mask2flux*  
photometry + masks

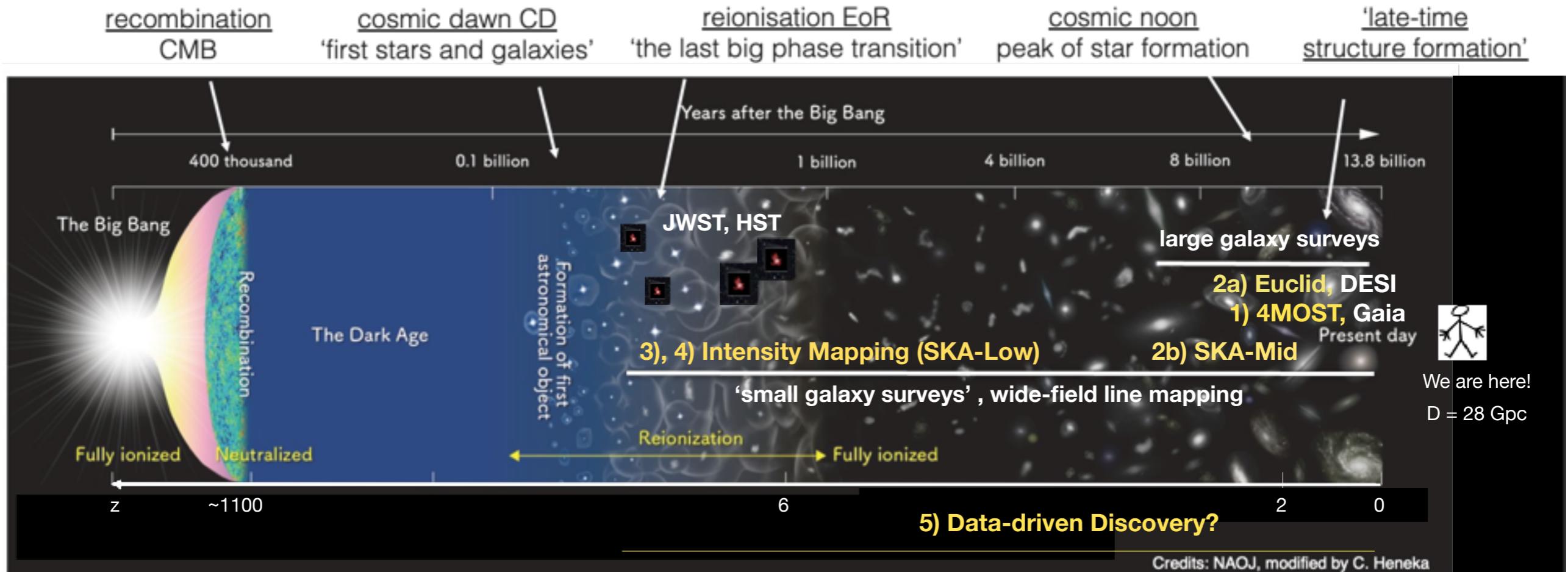


+ a CNN type  
*blend2flux*



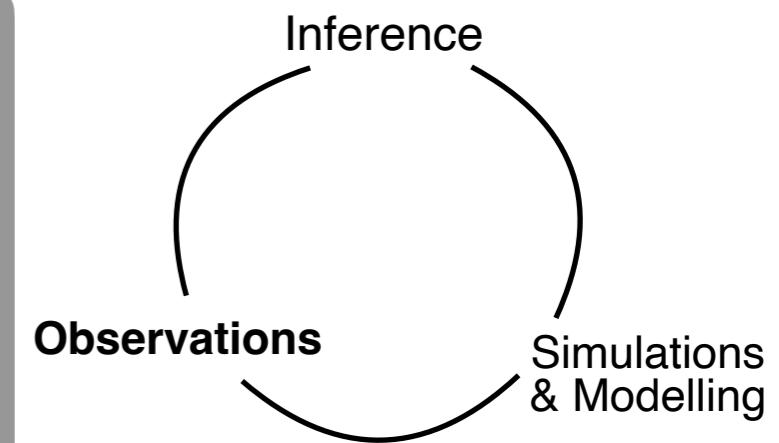
- Dispersion broadens when optimised for photometry
- Tailor to your research question

# Astronomical and Astrophysical Machine Learning



## Highlights in this Lecture

- 1) Classification / Triggering
- 2) Source detection & characterisation
- 3) Simulation-based inference (SBI) in 3D
- 4) Generative methods
- 5) Data-driven Discovery



# The Square Kilometre Array (SKA) in one slide

## SKA in numbers

- Currently 16 member countries, >100 member organisations
- Routine science observations are expected to start in the late 2020s
- Consists of thousands of dishes and up to 1 million antennas, >1km<sup>2</sup> collecting area
- Expected data rate in full operation: 1 TB/s



SKA-LOW

SKA-MID

Credits: SKAO

## SKA1-mid

the SKA's mid-frequency instrument



Location:  
South Africa



Frequency range:  
**350 MHz**  
to  
**15.3 GHz**  
with a goal of 24 GHz



**197 dishes**  
(including 84 MeerKAT dishes)



Maximum baseline:  
**150km**

## SKA1-low

the SKA's low-frequency instrument



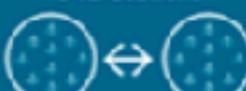
Location: Australia



Frequency range:  
**50 MHz**  
to  
**350 MHz**



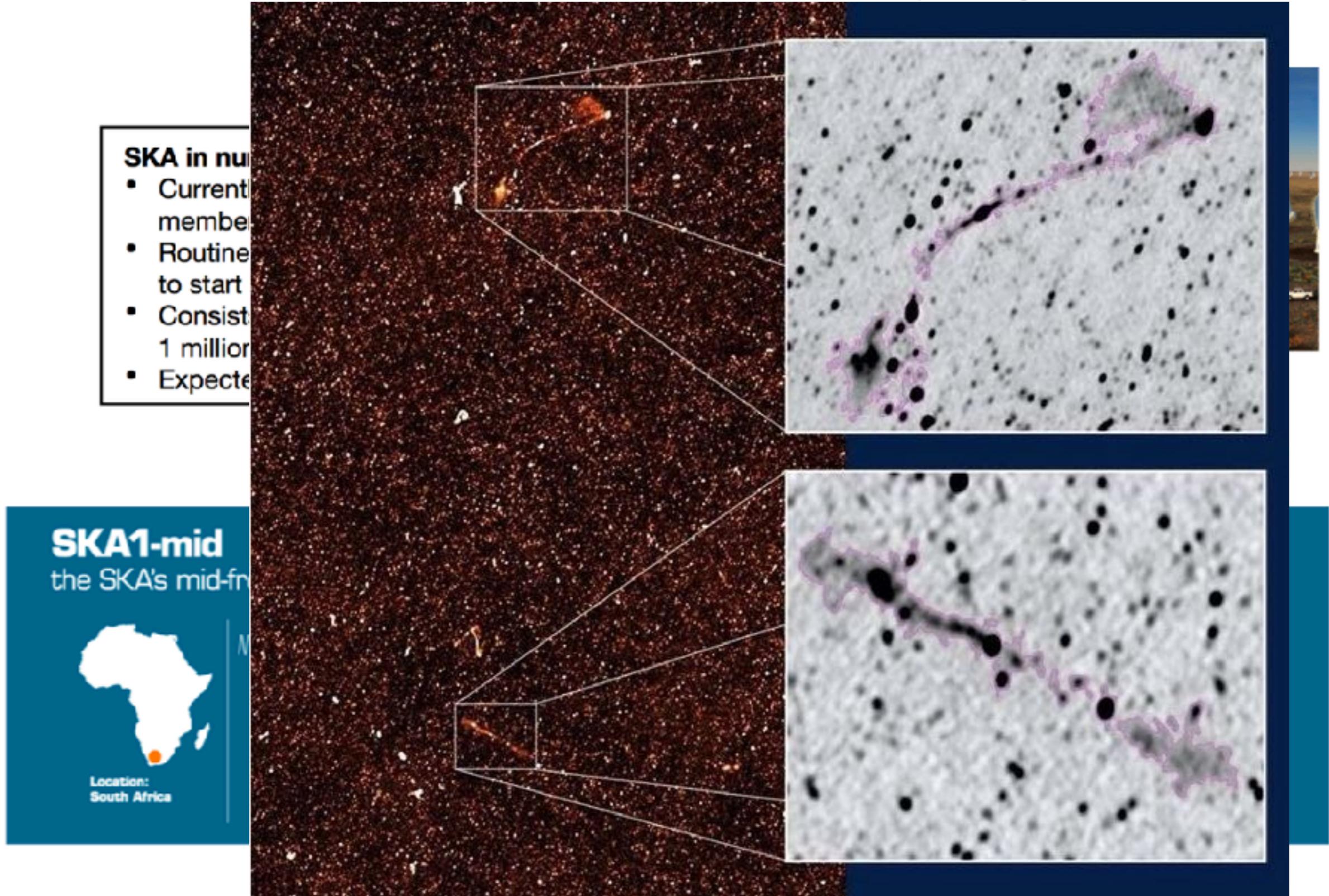
**~131,000**  
antennas spread between  
512 stations



Maximum baseline:  
**~65km**

# The Square Kilometre Array (SKA) in one slide

<https://doi.org/10.1093/mnras/staa3837>



## 2b) Radio source detection and characterisation

Example: Source detection in 3D tomographic data

Source finding

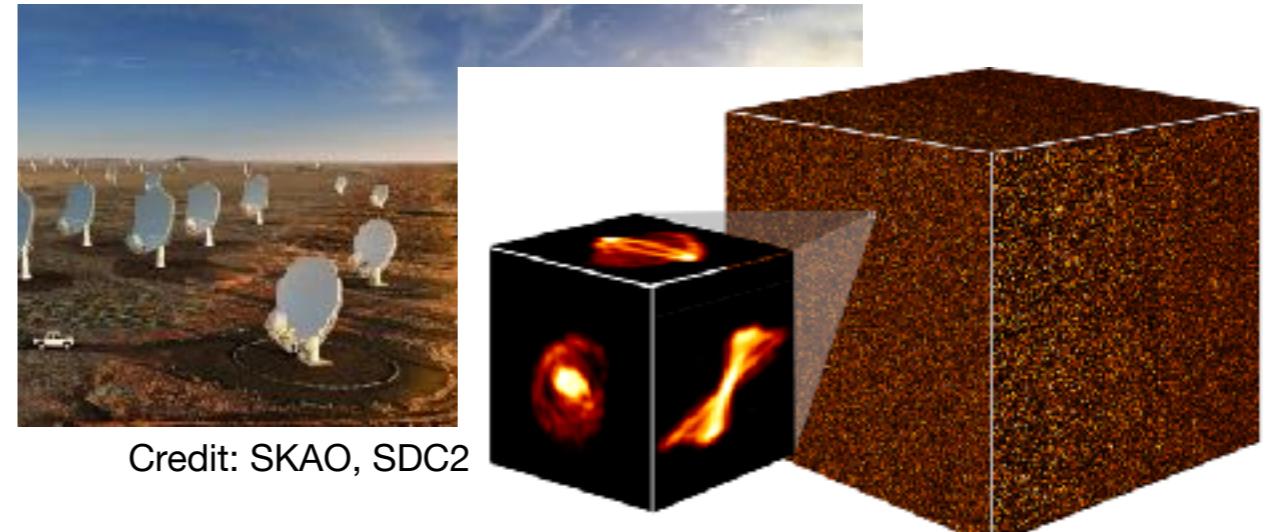
Location in RA, Dec,  
central frequency (Hz)

Characterisation

- Integrated line flux (Jy Hz)
- Line width (km/s)
- HI major axis diameter (arcsec)
- Position angle (degrees)
- Inclination angle (degrees)



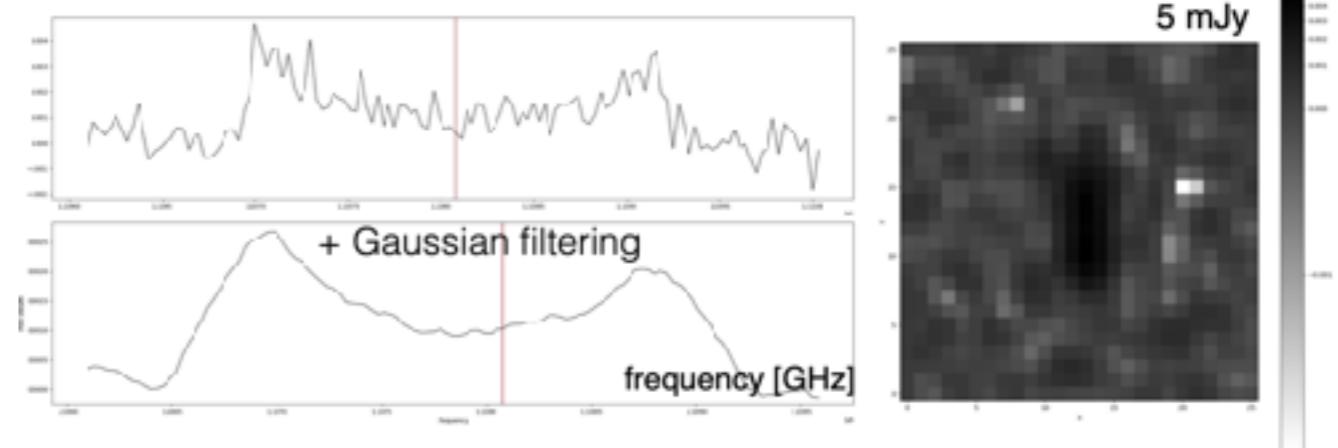
Credit: SKAO, SDC2



Total dimensions: (25,714 x 25,714 x 6,667) vox

The challenging HI sources:

- low S/N
- small spatial size
- systematics



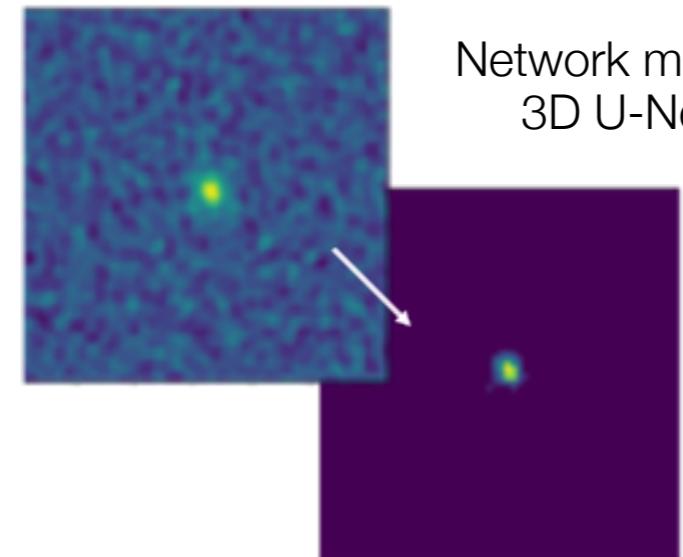
Hartley+ 23 (incl. Heneka), arXiv:2303.07943

Heneka 23, arXiv:2311.17553

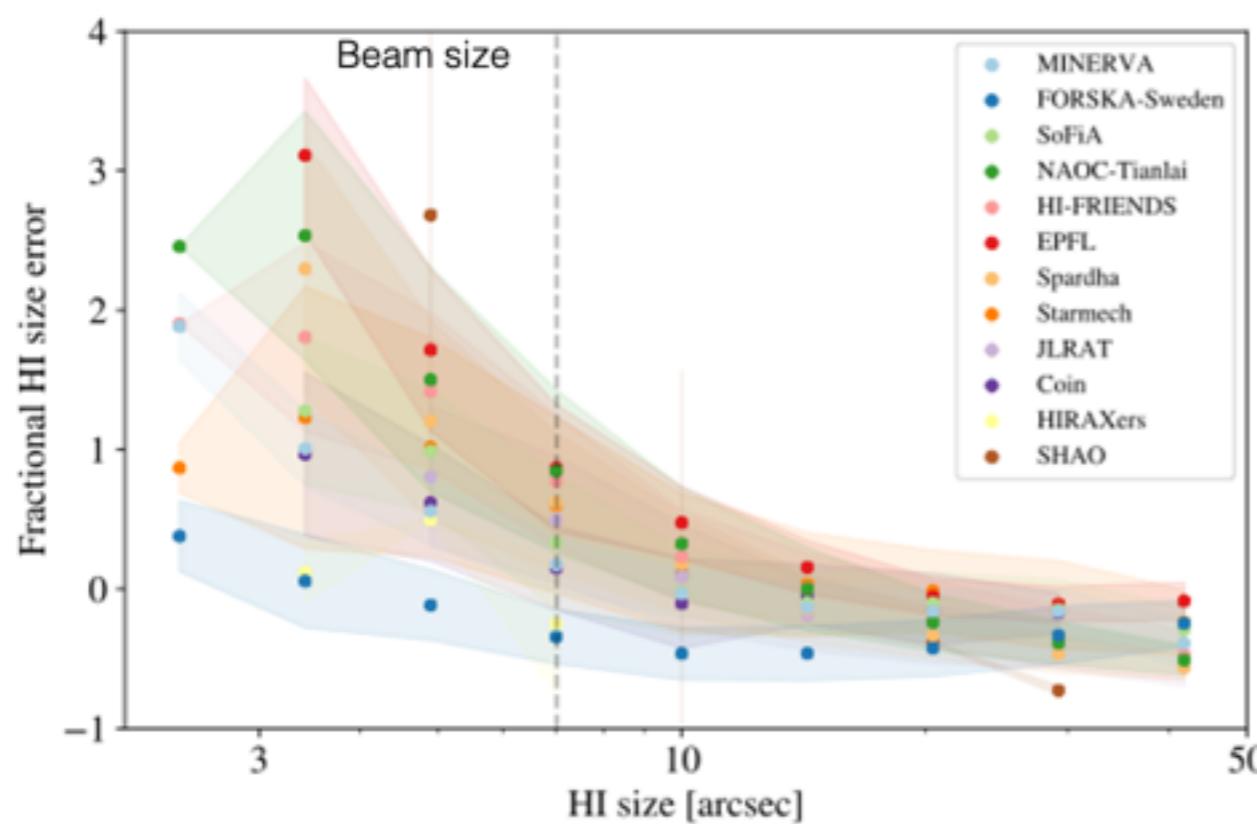
## 2b) Radio source detection and characterisation

Example: Source detection in 3D tomographic data

- 3D better than stitching of 2D + 1D
- High-fidelity 3D reconstructions
- **Good prior for characterisation tasks via nets:**



Network model:  
3D U-Net

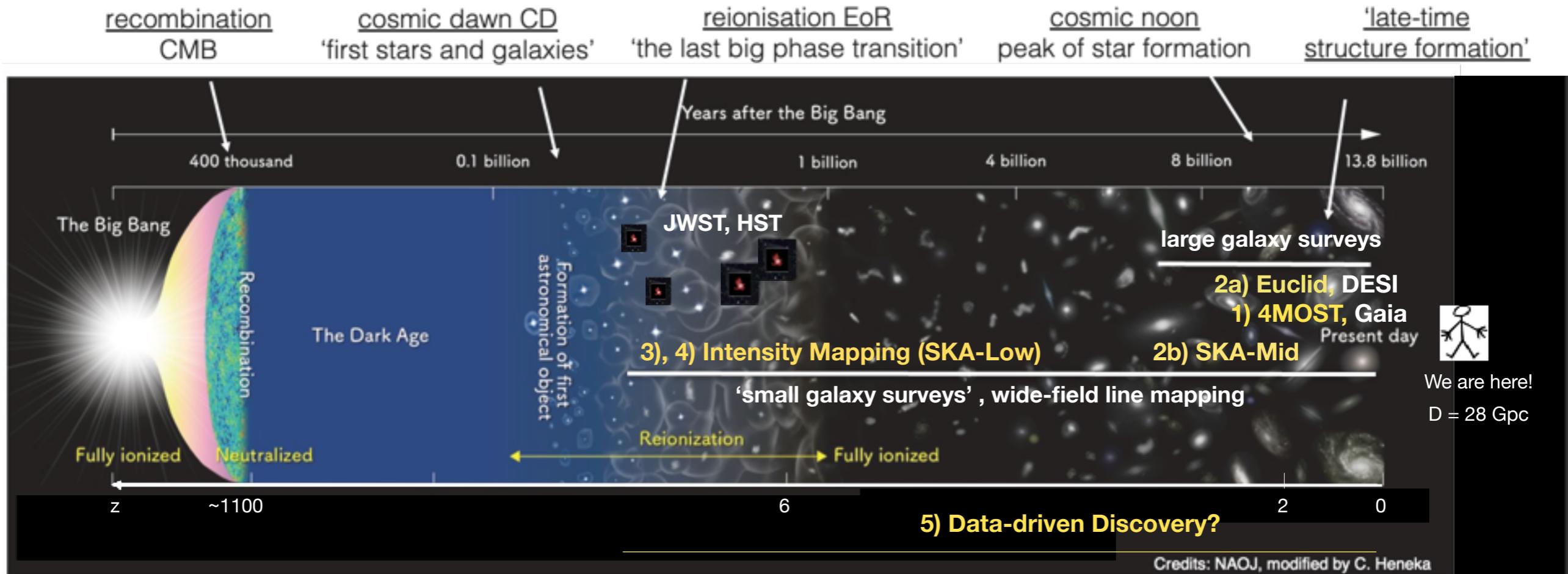


Recovery across wide range in HI flux and size  
Pushing to low S/N recovery came at a cost (FPs)

Uncertainty?

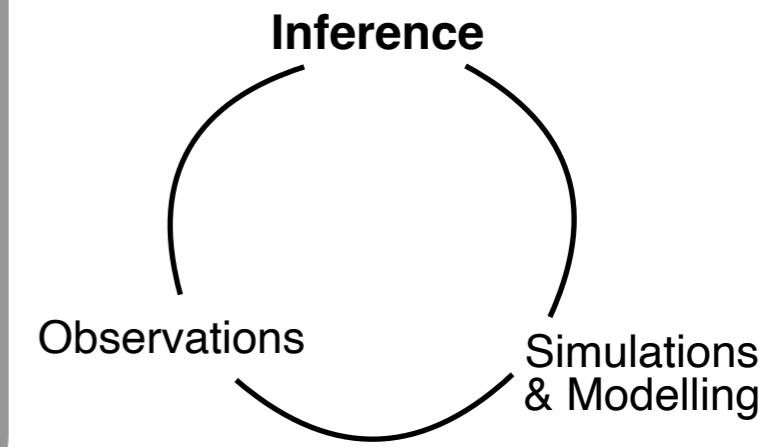
Hartley+ 23 (incl. Heneka), arXiv:2303.07943  
Heneka 23, arXiv:2311.17553

# Astronomical and Astrophysical Machine Learning



## Highlights in this Lecture

- 1) Classification / Triggering
- 2) Source detection & characterisation
- 3) **Simulation-based inference (SBI) in 3D**
- 4) Generative methods
- 5) Data-driven Discovery



### 3) Simulation-based inference (SBI) for intensity mapping (3D)

21cm signal

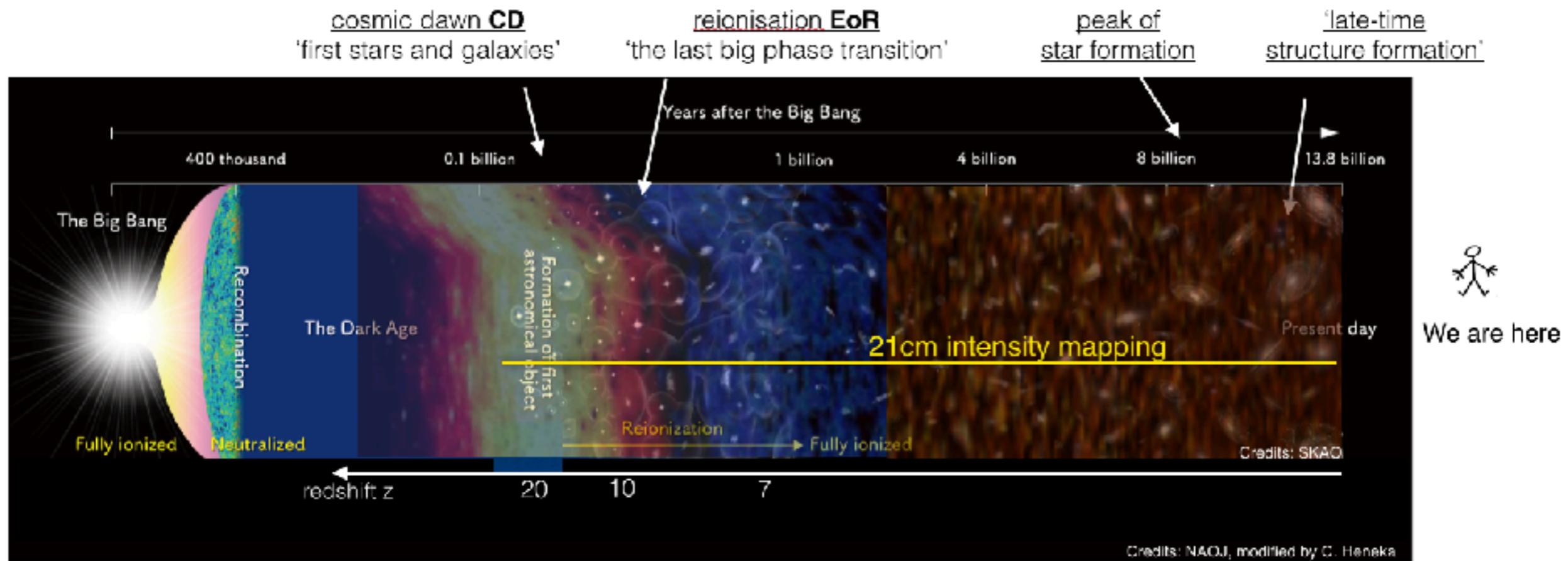
a tracer of neutral hydrogen:

$$\delta T_b(\nu) = \frac{T_S - T_\gamma}{1+z} (1 - e^{-\tau_{\nu_0}})$$

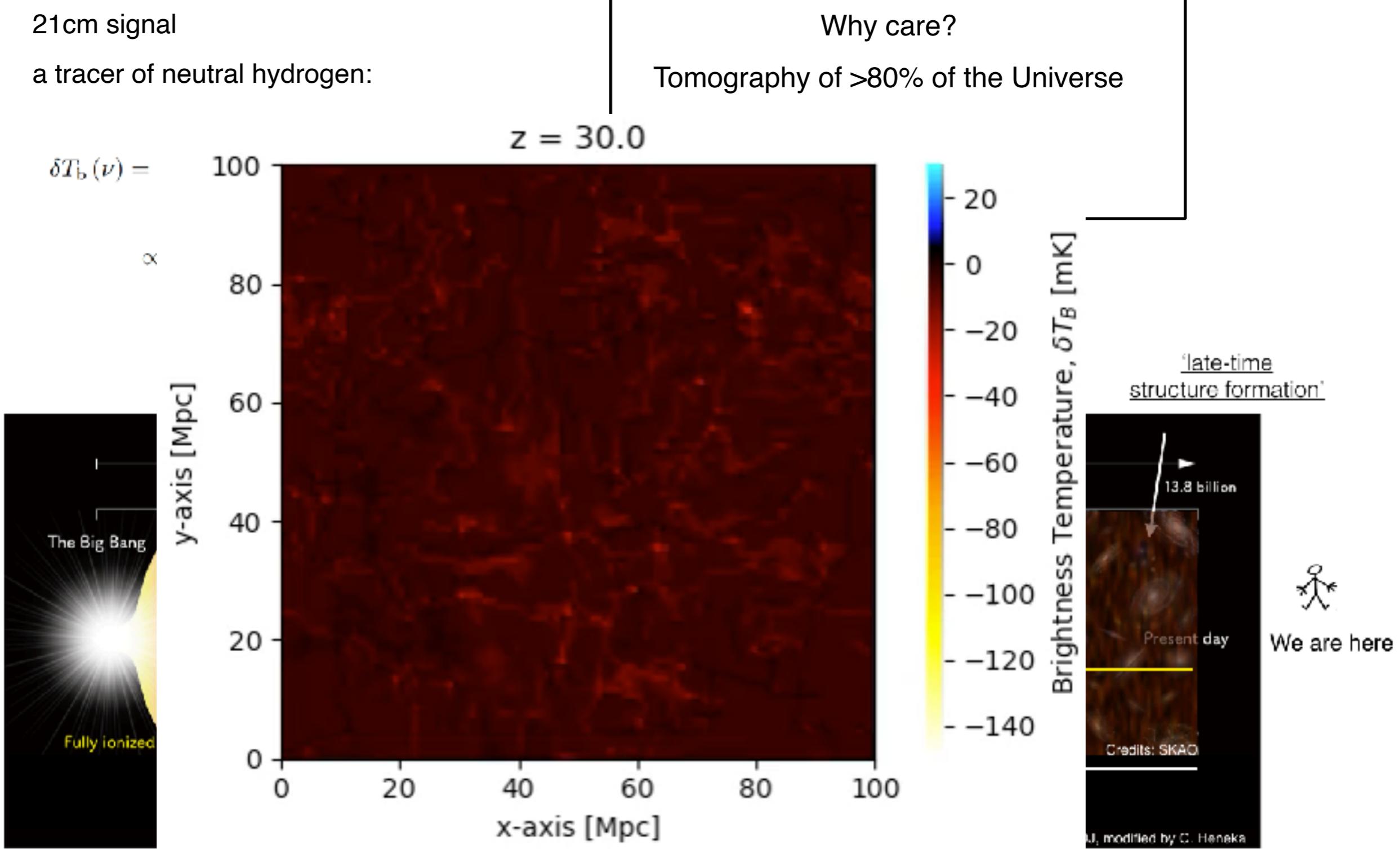
$$\propto x_{\text{HI}} (1 + \delta_{\text{nl}}) \left( \frac{H}{dv_r/dr + H} \right)$$

Why care?

Tomography of >80% of the Universe



### 3) Simulation-based inference (SBI) for intensity mapping (3D)



### 3) Simulation-based inference (SBI) for intensity mapping (3D)



@SKAO

Why care?

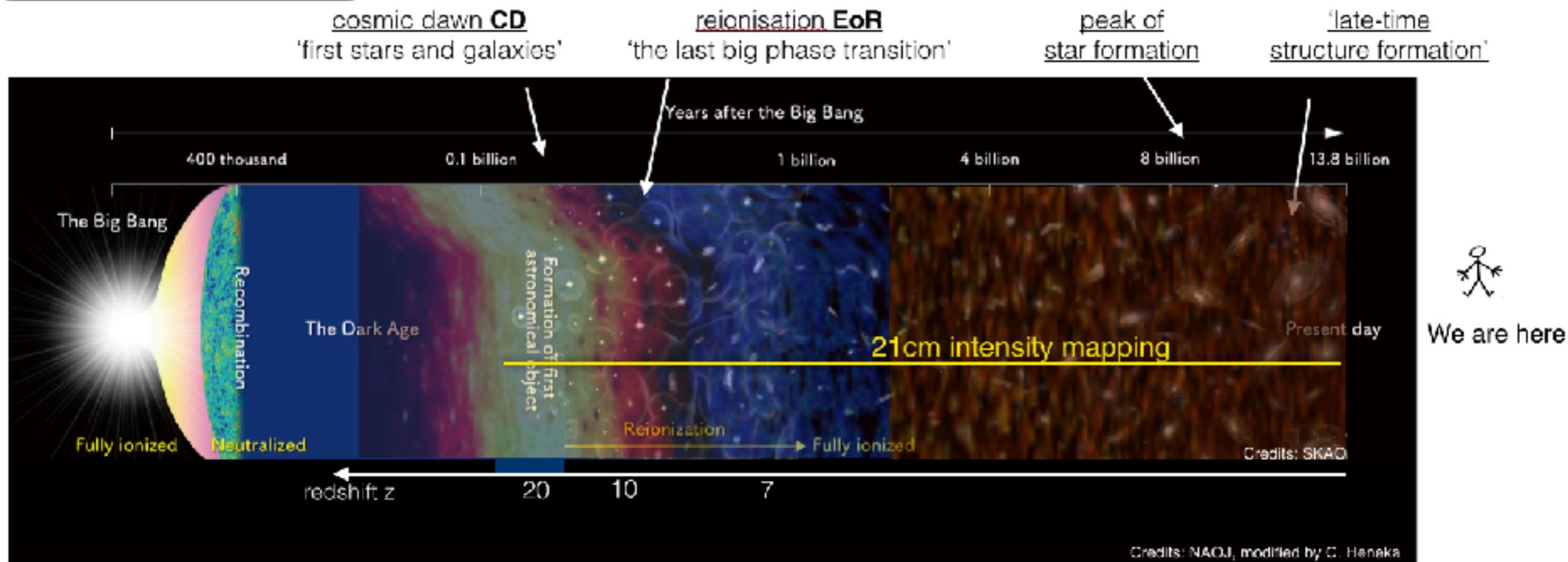
Tomography of >80% of the Universe

Square Kilometre Array - true 'Big Data'

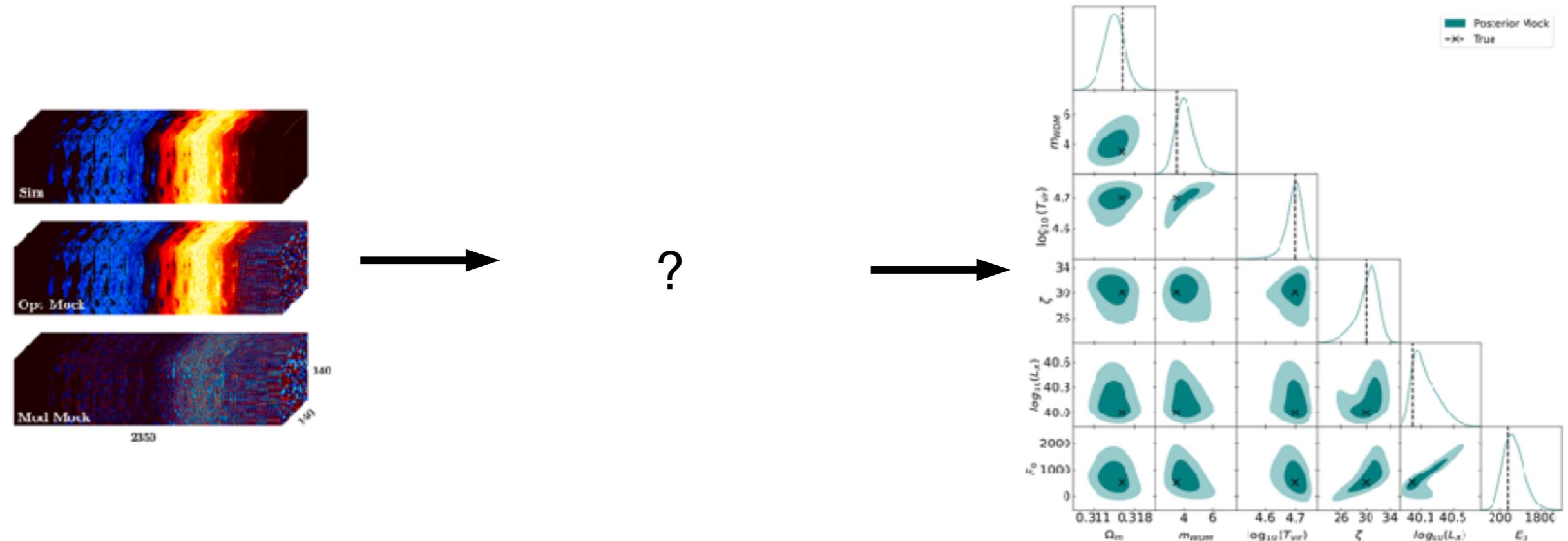
non-linear, non-Gaussian signal

Expected data SKA rate:  
TB/s, few EB/day  
Archive: ~700 PB/yr

→ Move to full likelihood inference with networks



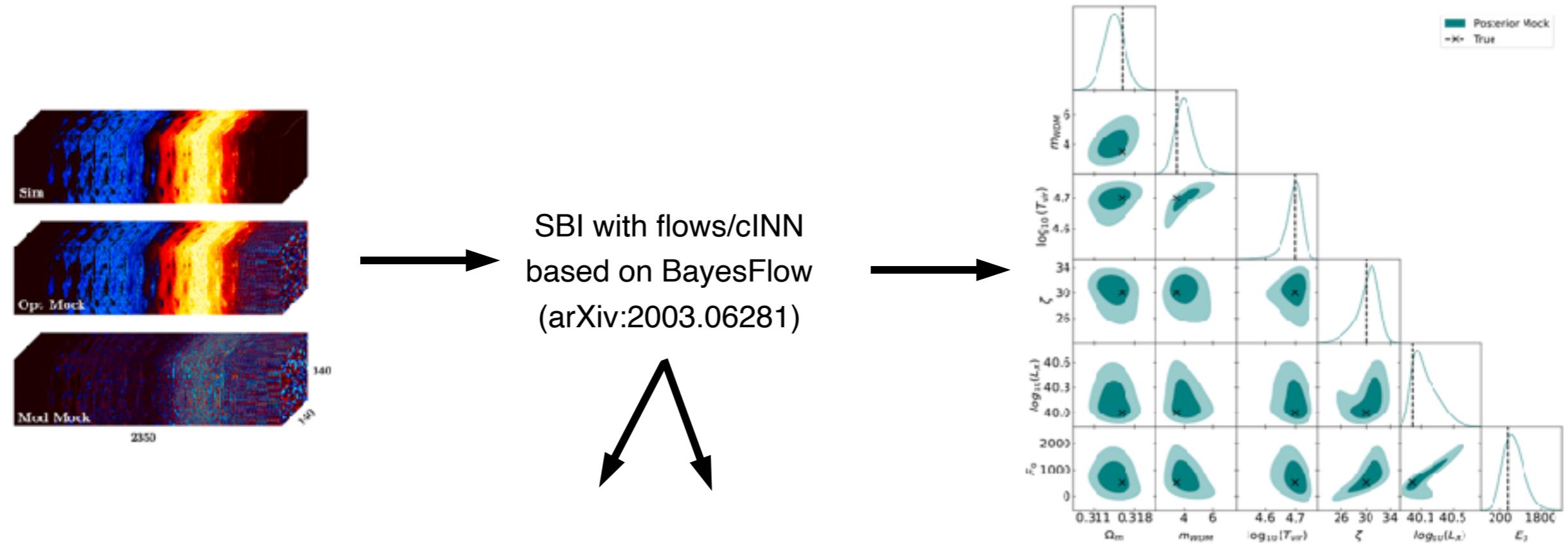
### 3) Simulation-based inference (SBI) for intensity mapping (3D)



Neutsch, Heneka, Brüggen (2022), arXiv:2201.07587

Schosser, Heneka, Plehn, arXiv:2401.04174

### 3) Simulation-based inference (SBI) for intensity mapping (3D)



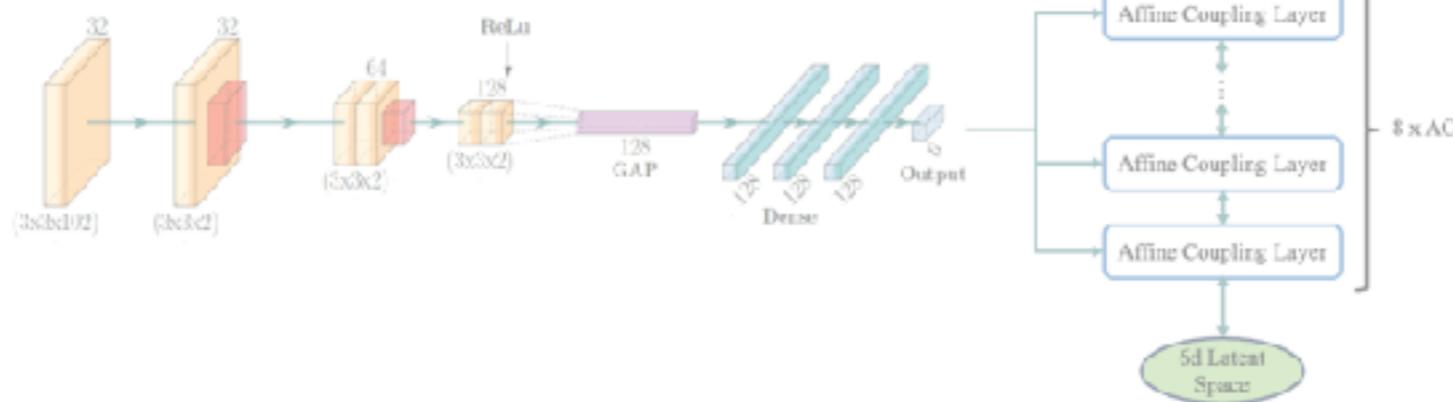
3D-21cmPIE-Net (public)

Neutsch, Heneka, Brüggen (2022)  
arXiv:2201.07587

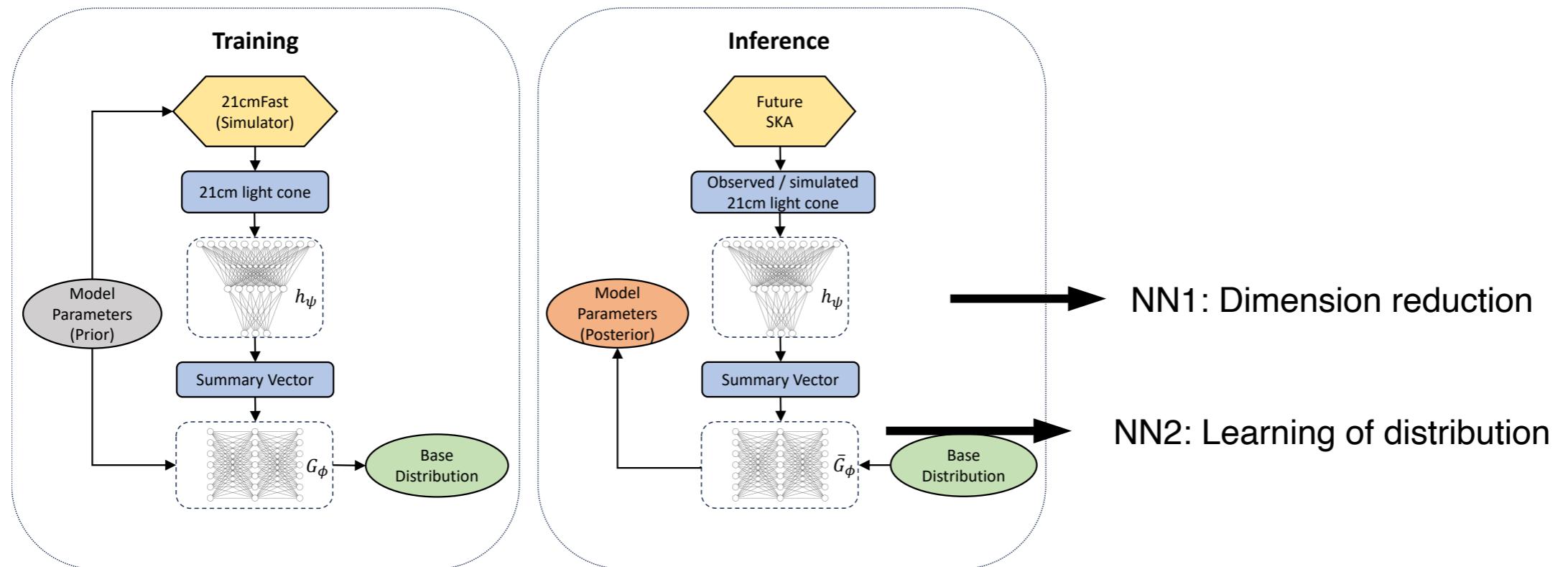


21cm-cINN (public when published)

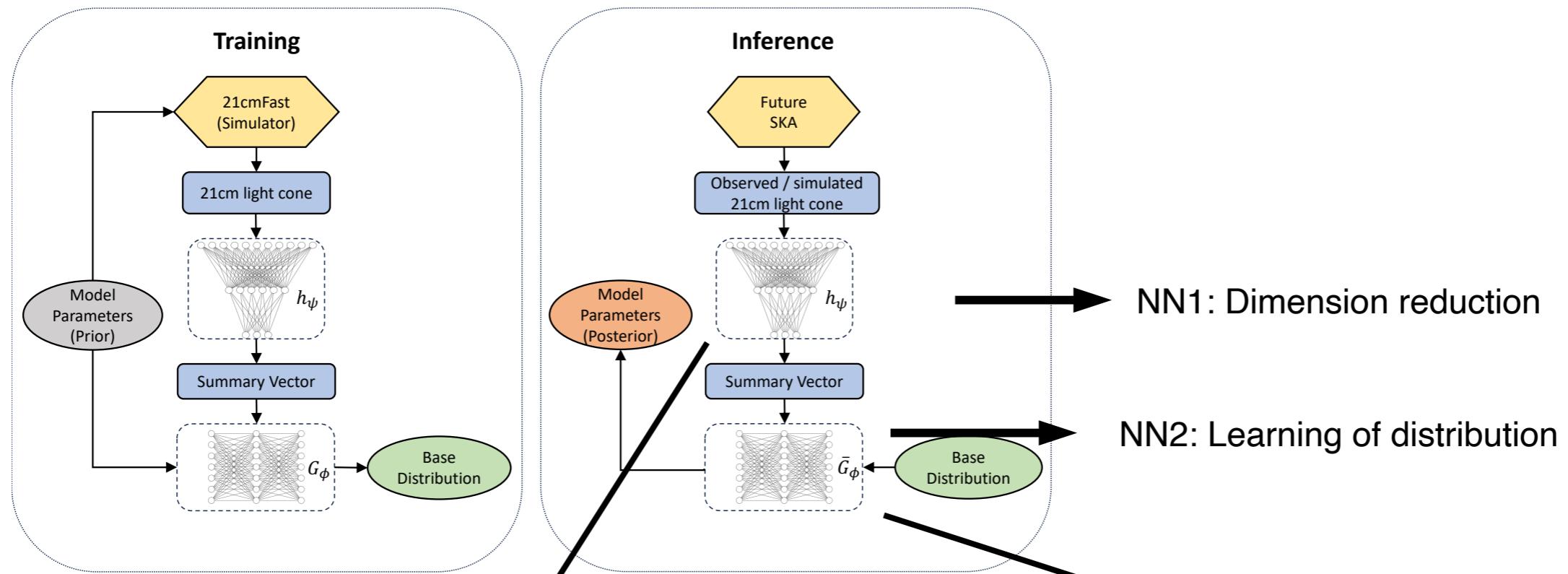
Schosser, Heneka, Plehn, arXiv:2401.04174



### 3) Simulation-based inference (SBI) for intensity mapping (3D)

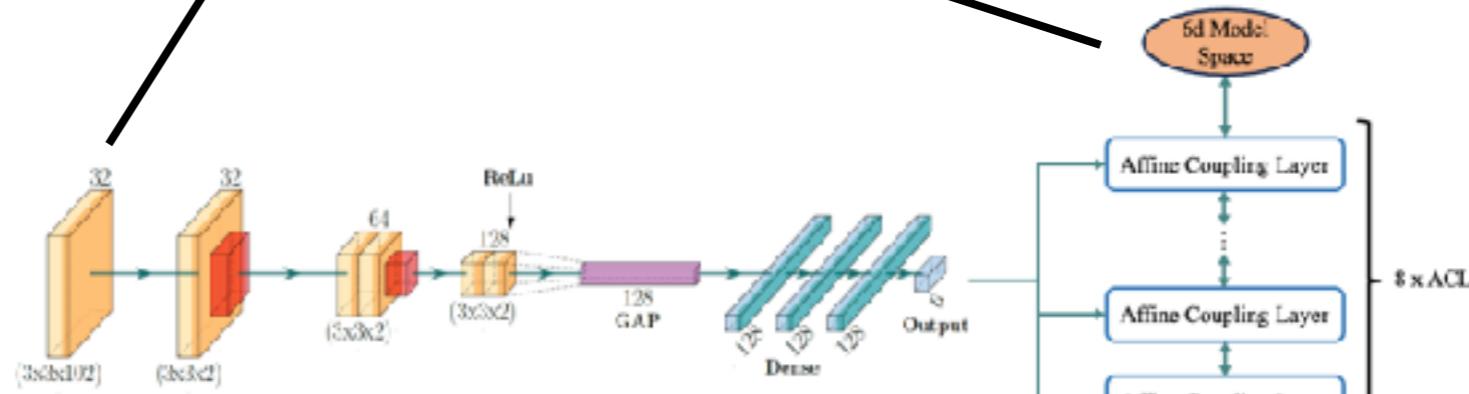


### 3) Simulation-based inference (SBI) for intensity mapping (3D)



Network Model:

Small networks,  
comparably few parameters  
= fast training and convergence

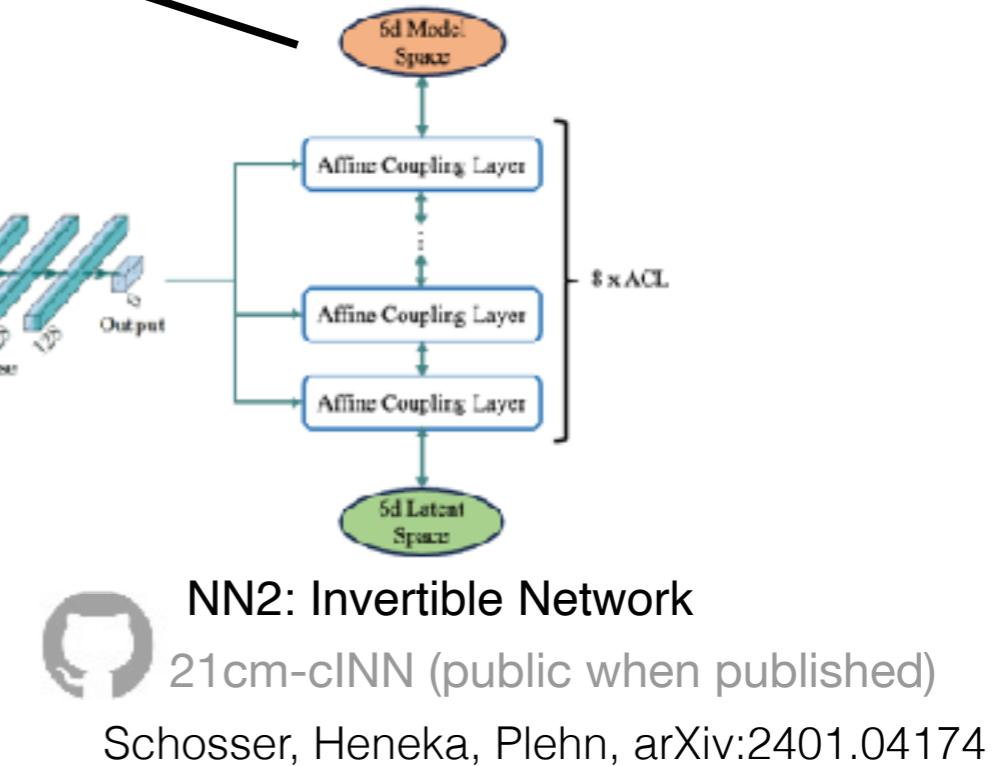


NN1: 3D-CNN



3D-21cmPIE-Net (public)

Neutsch, Heneka, Brüggen (2022)  
arXiv:2201.07587

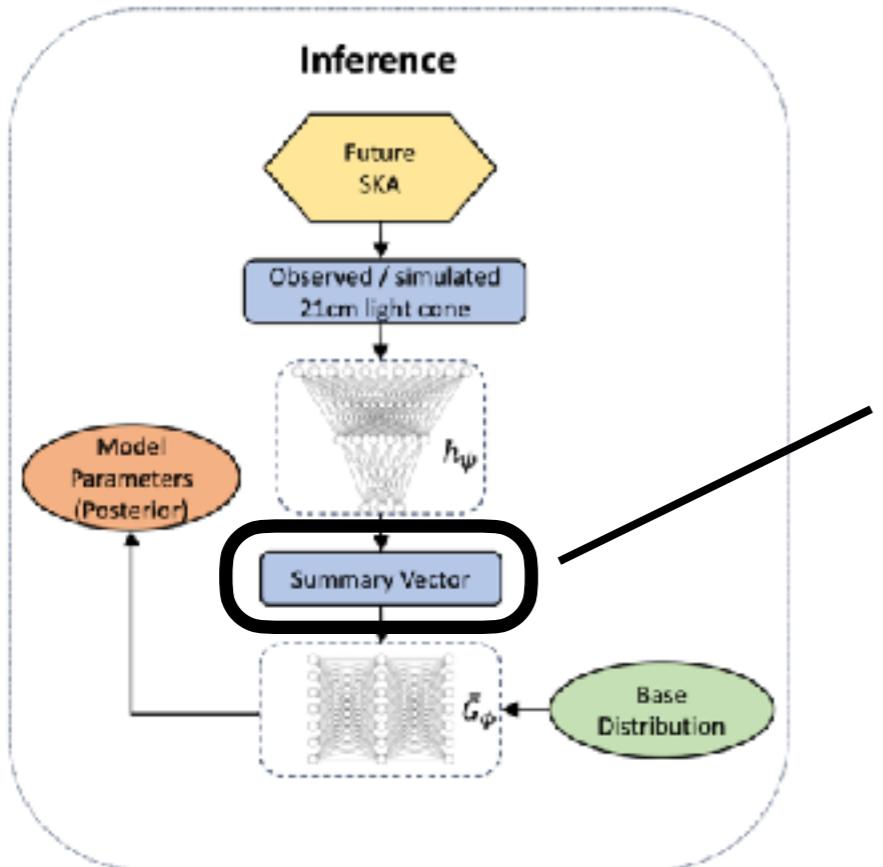


NN2: Invertible Network



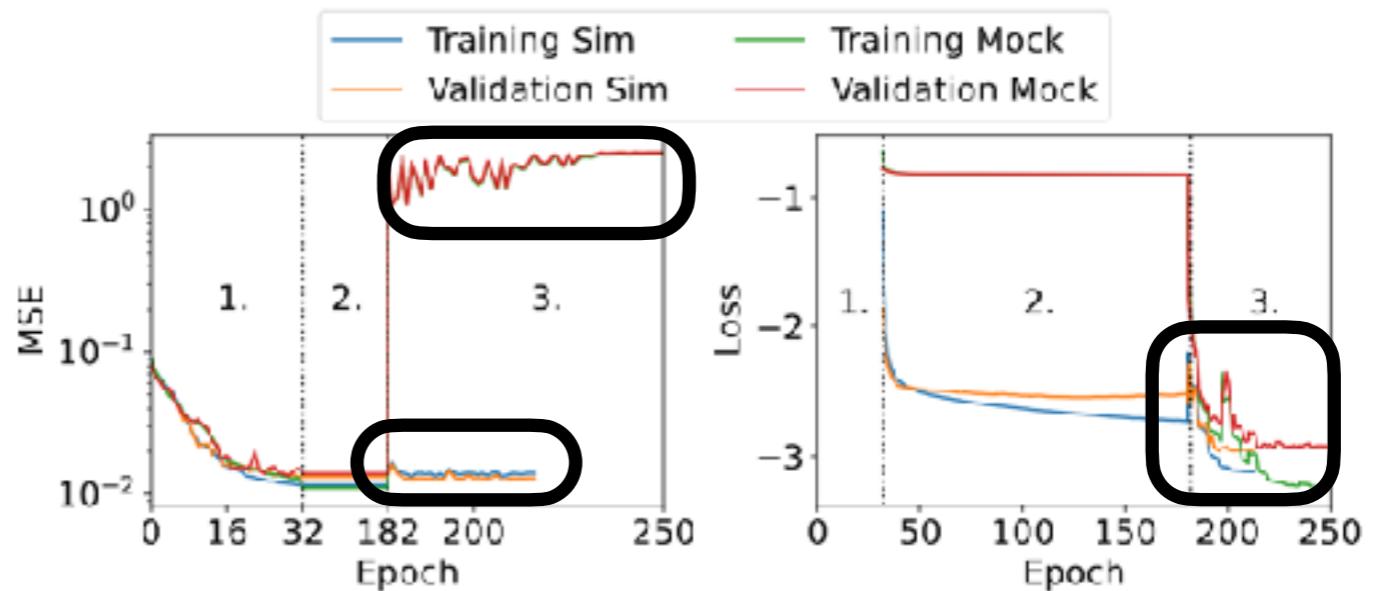
21cm-cINN (public when published)  
Schosser, Heneka, Plehn, arXiv:2401.04174

### 3) Simulation-based inference (SBI) for intensity mapping (3D)



Summary vector versus summary statistics:  
Free adjustment with scheduled training  
= move away from 'parameter interpretation' of vector

Key difference between Sim and Mock:



We profit from learned summary  
in presence of noise (more).

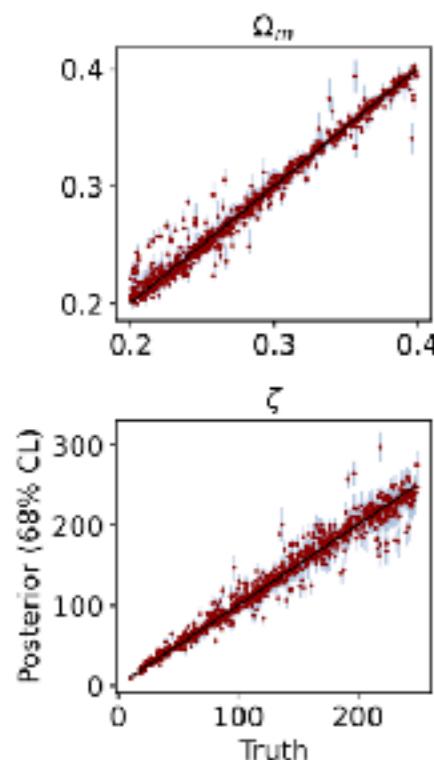
Sim: Summary stays close to original  
Mock: Heavy adjustment of summary vector

Schosser, Heneka, Plehn, arXiv:2401.04174

### 3) Simulation-based inference (SBI) for intensity mapping (3D)

Performance validation via:

- Distribution of latent variables
- Simulation-based calibration
- Parameter recovery



Check Posterior vs. True label

Schosser, Heneka, Plehn, arXiv:2401.04174

### 3) Simulation-based inference (SBI) for intensity mapping (3D)

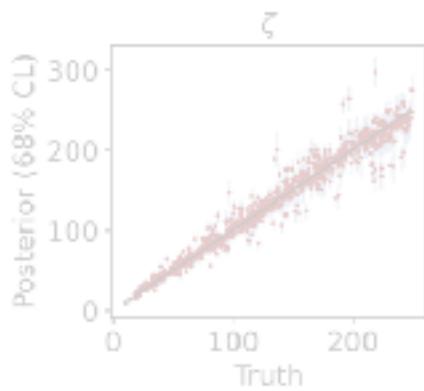
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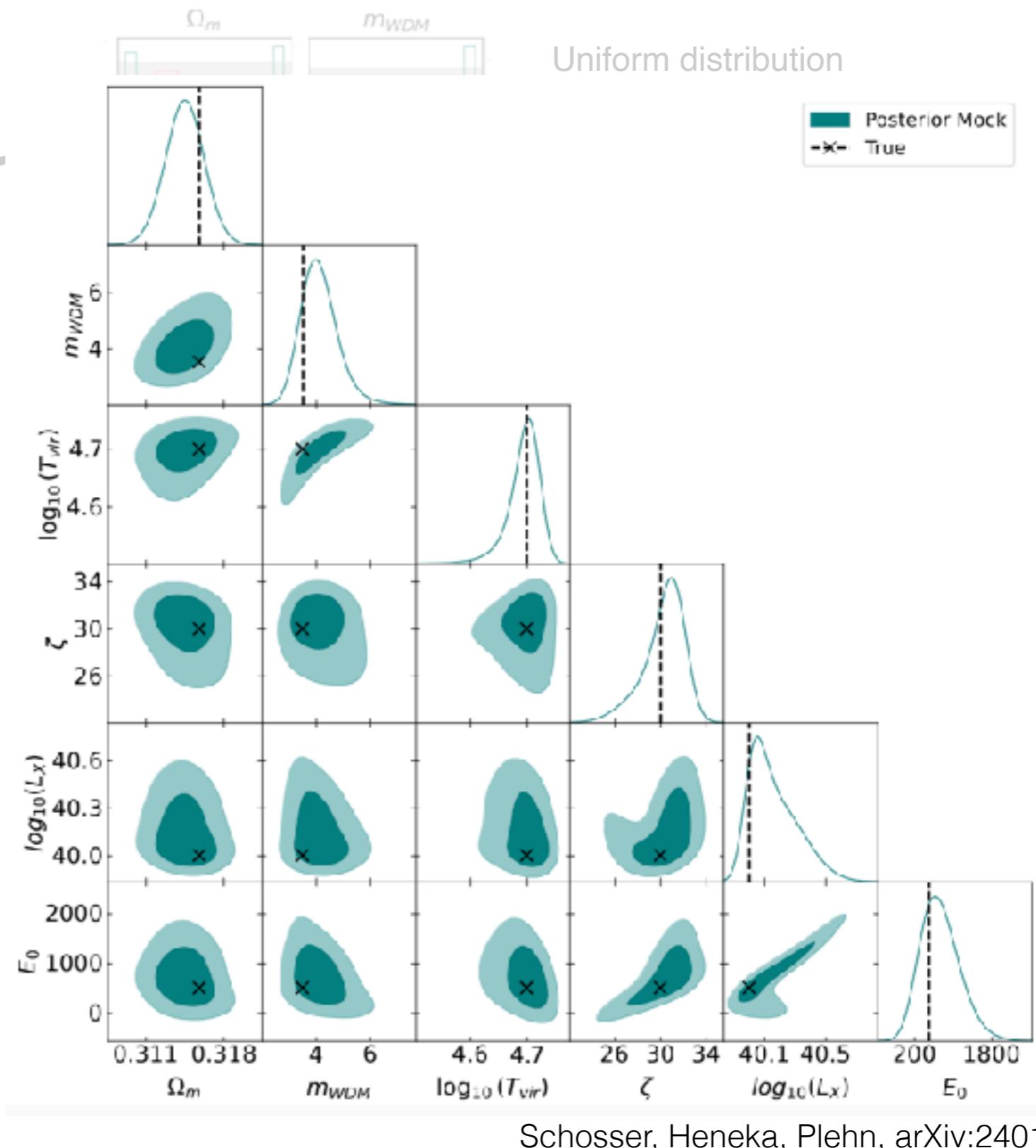
Likelihood contours:

Explore any model in prior range!

+ similar performance  
Mock vs. Sim  
(except for  $E_0$ )



Check Posterior vs. True label



Schosser, Heneka, Plehn, arXiv:2401.04174

### 3) Simulation-based inference (SBI) for intensity mapping (3D)

Performance validation via:

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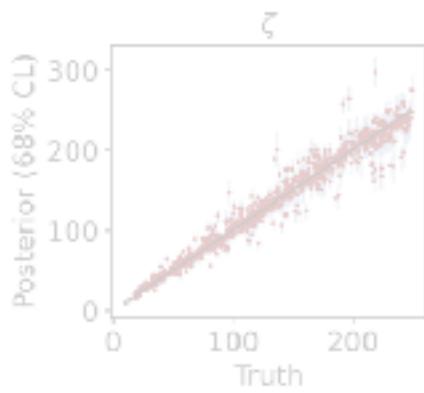
Likelihood contours:

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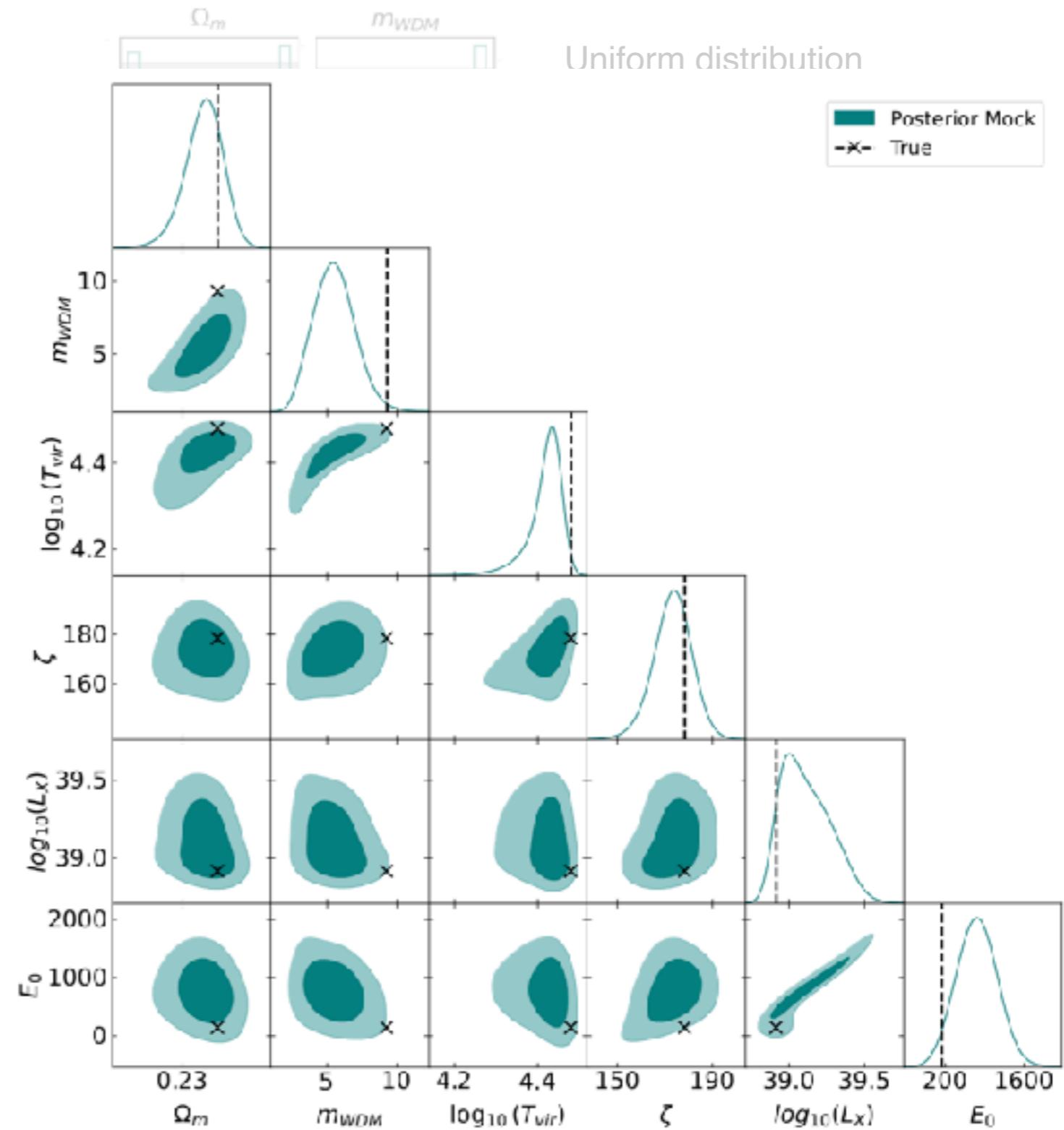
+ similar performance

Mock vs. Sim

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Schosser, Heneka, Plehn, arXiv:2401.04174

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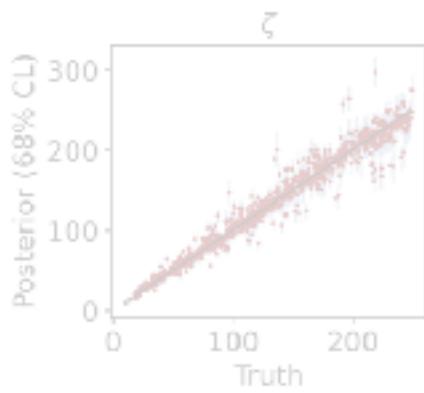
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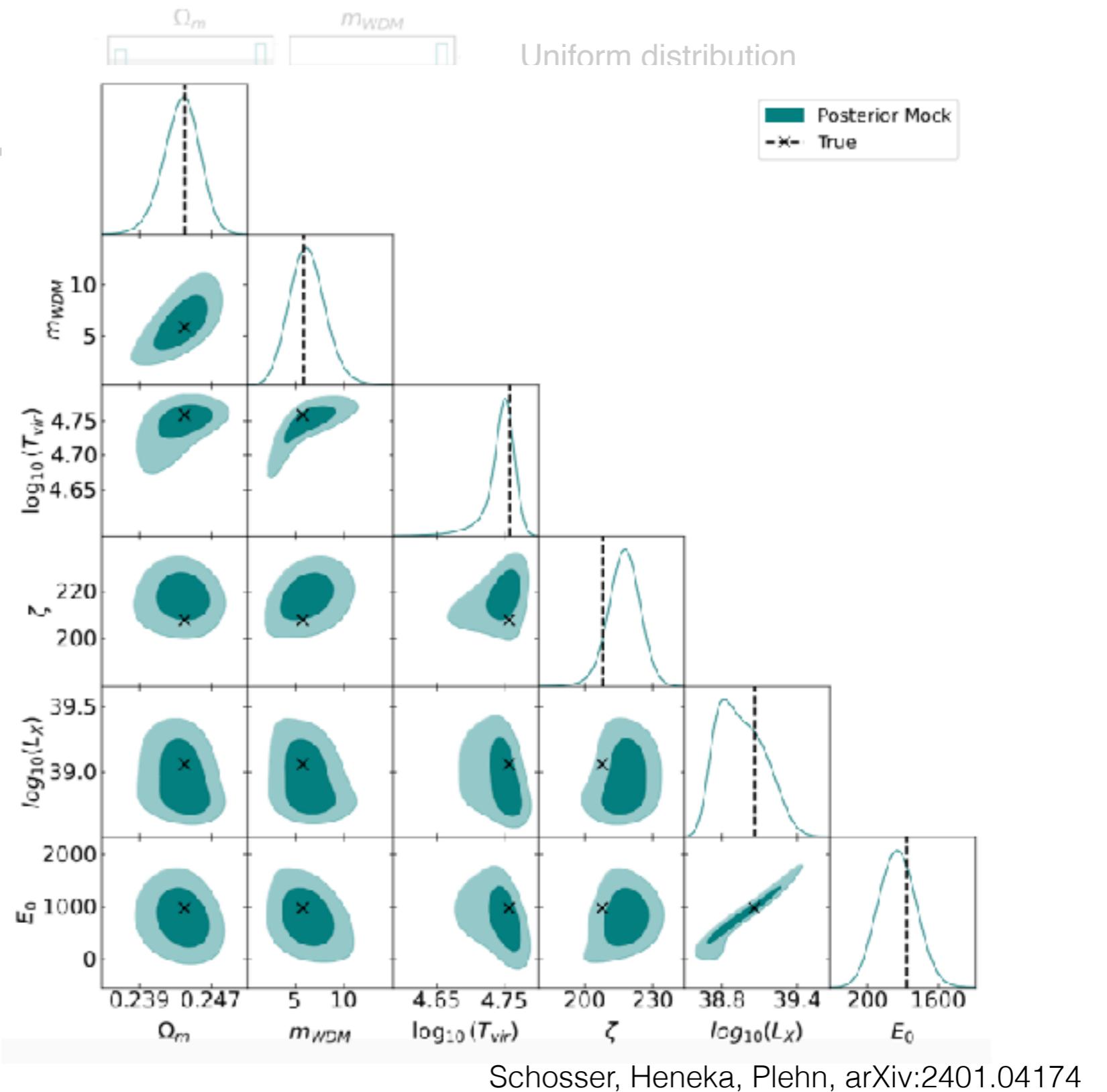
+ similar performance

Mock vs. Sim

(except for  $E_0$ )

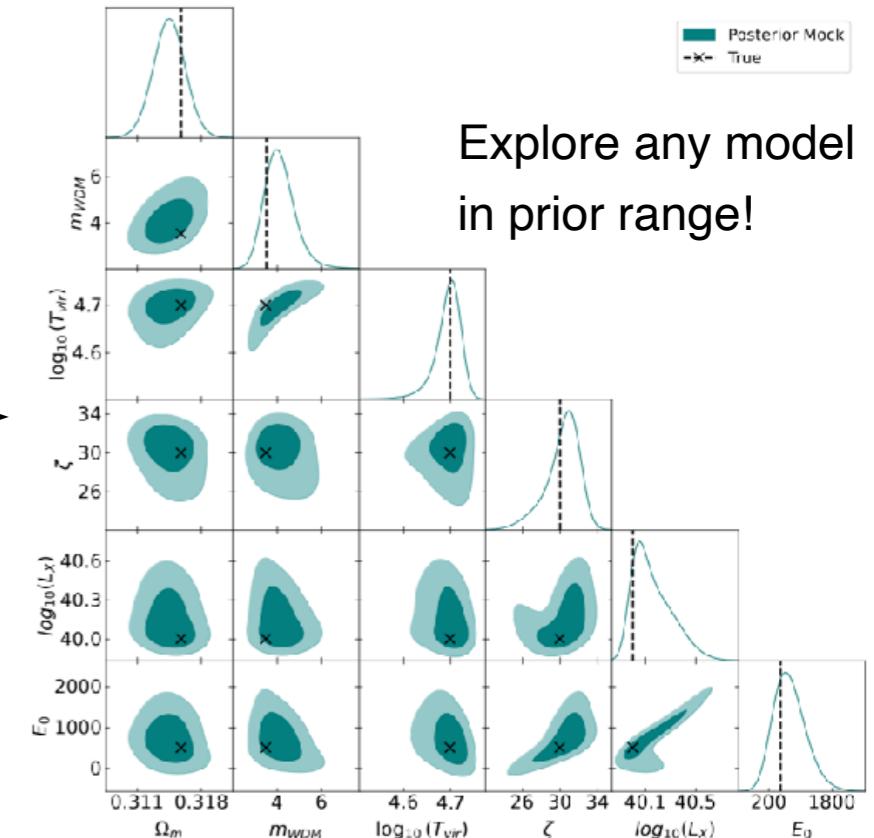
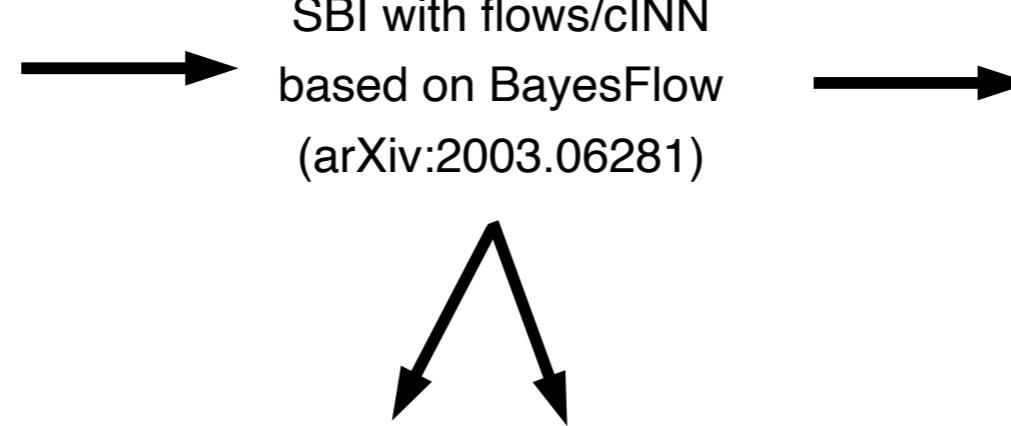
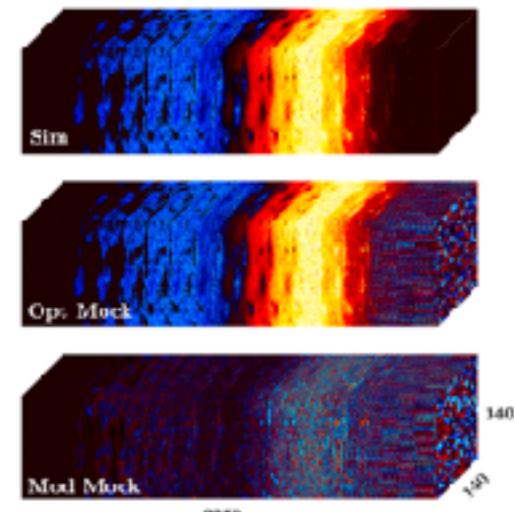


Check Posterior vs. True label



Schosser, Heneka, Plehn, arXiv:2401.04174

### 3) Simulation-based inference (SBI) for intensity mapping (3D)



3D-21cmPIE-Net (public)

Neutsch, Heneka, Brüggen (2022)  
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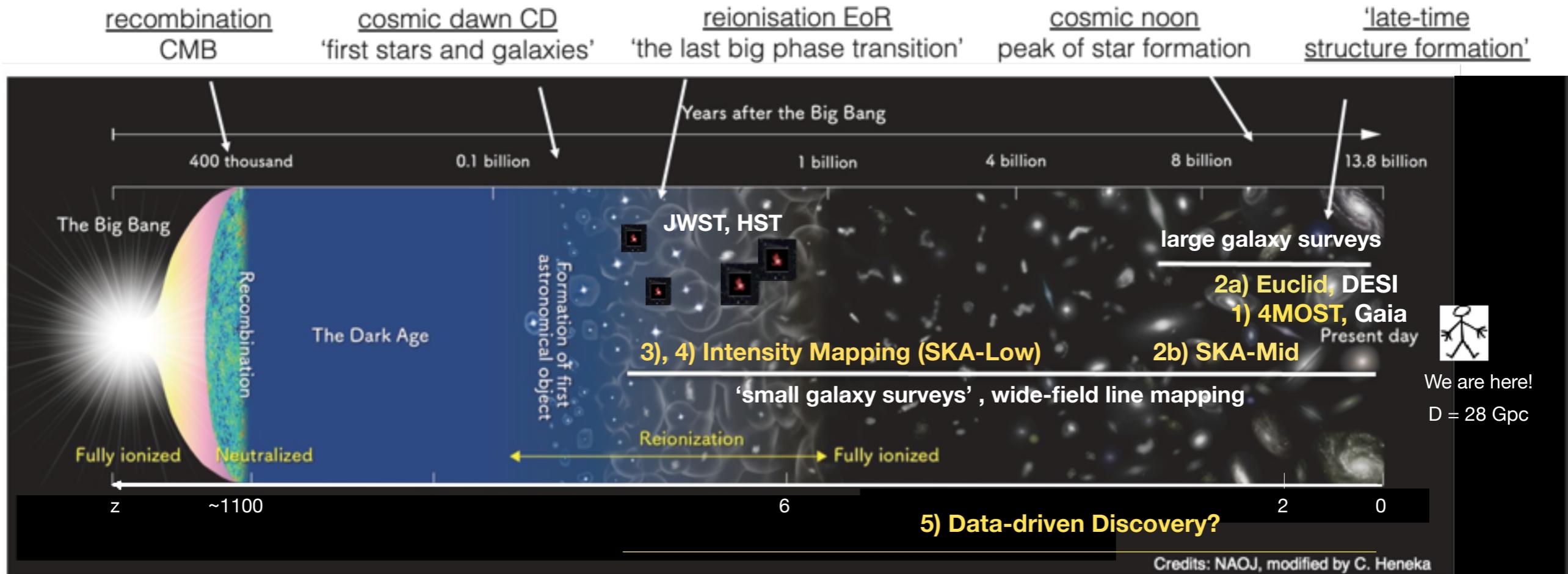


21cm-cINN (public when published)

Schosser, Heneka, Plehn (2024), arXiv:2401.04174

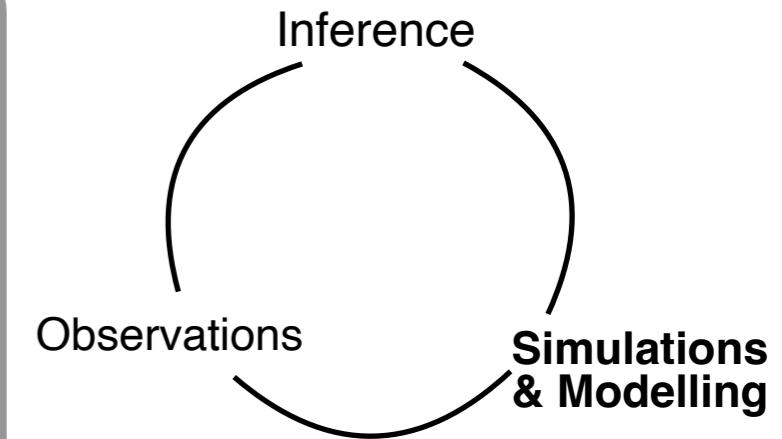
**'Optimal, fast, and robust inference of reionization-era cosmology with the 21cmPIE-INN'**

# Astronomical and Astrophysical Machine Learning



## Highlights in this Lecture

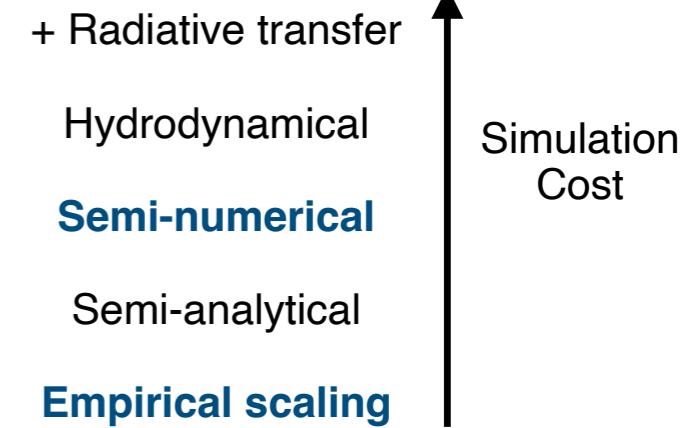
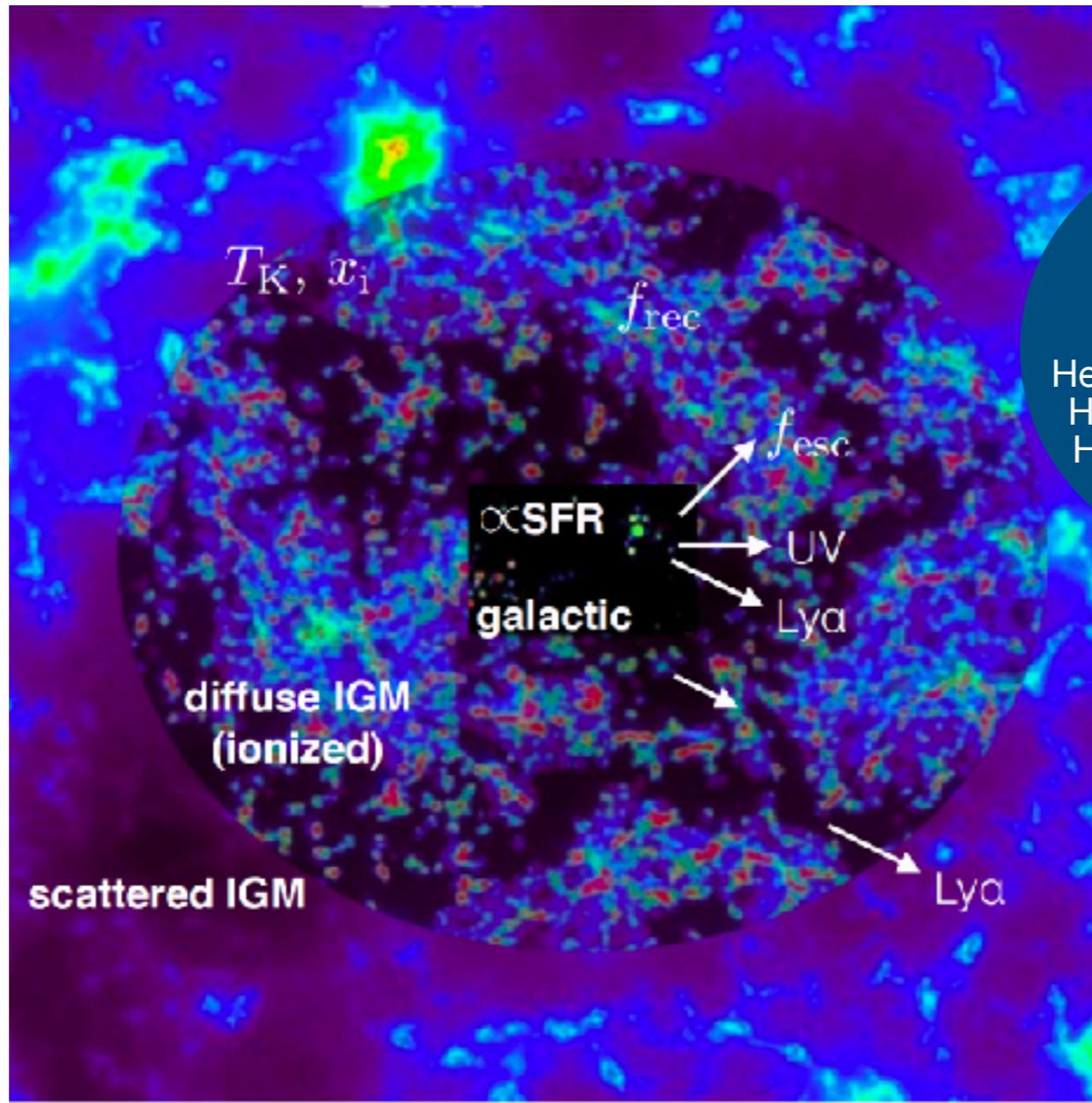
- 1) Classification / Triggering
- 2) Source detection & characterisation
- 3) Simulation-based inference (SBI) in 3D
- 4) Generative methods
- 5) Data-driven Discovery



### 3) Generative methods for simulation

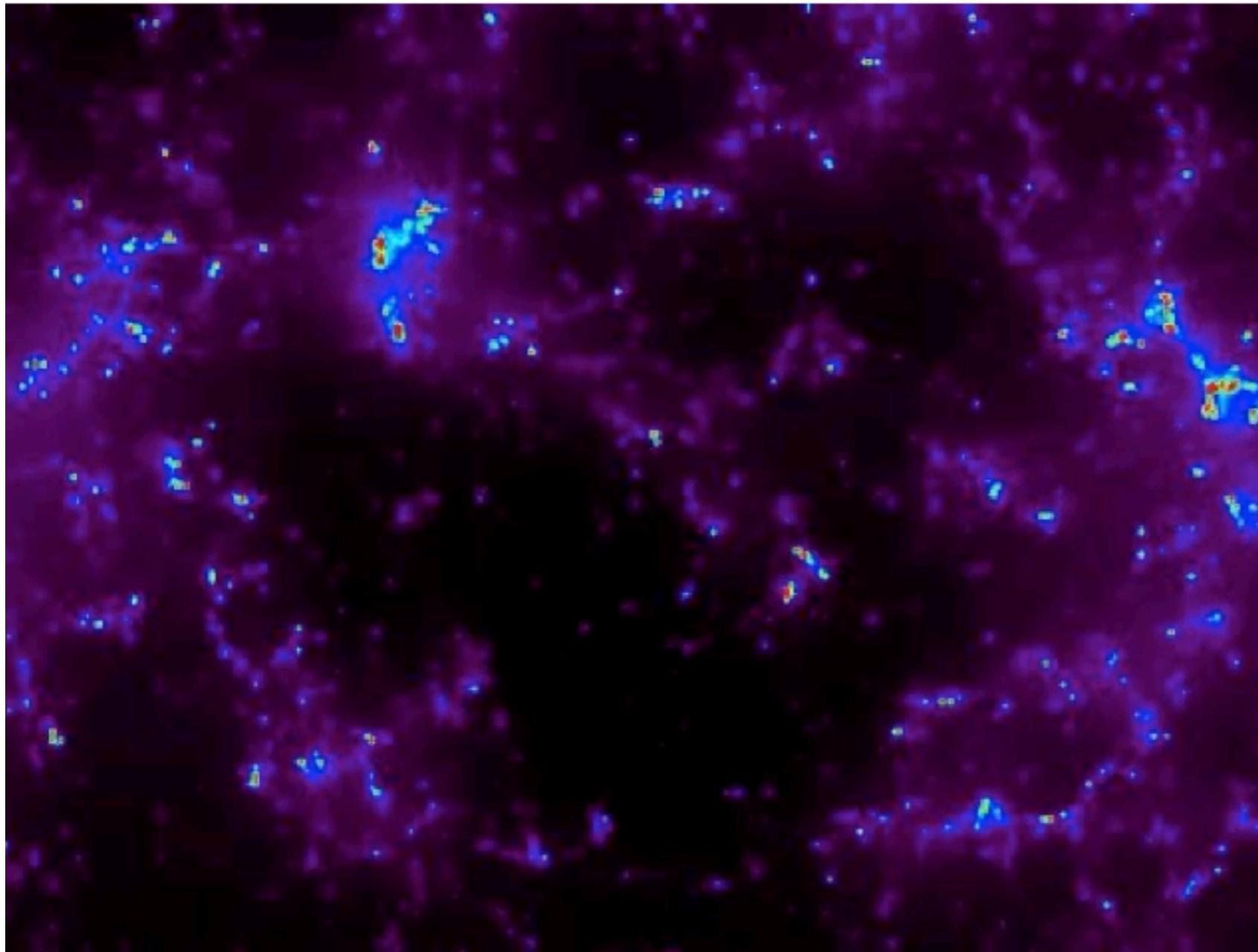
Reionization simulations are costly

Is there a fast way to emulate whole simulations?

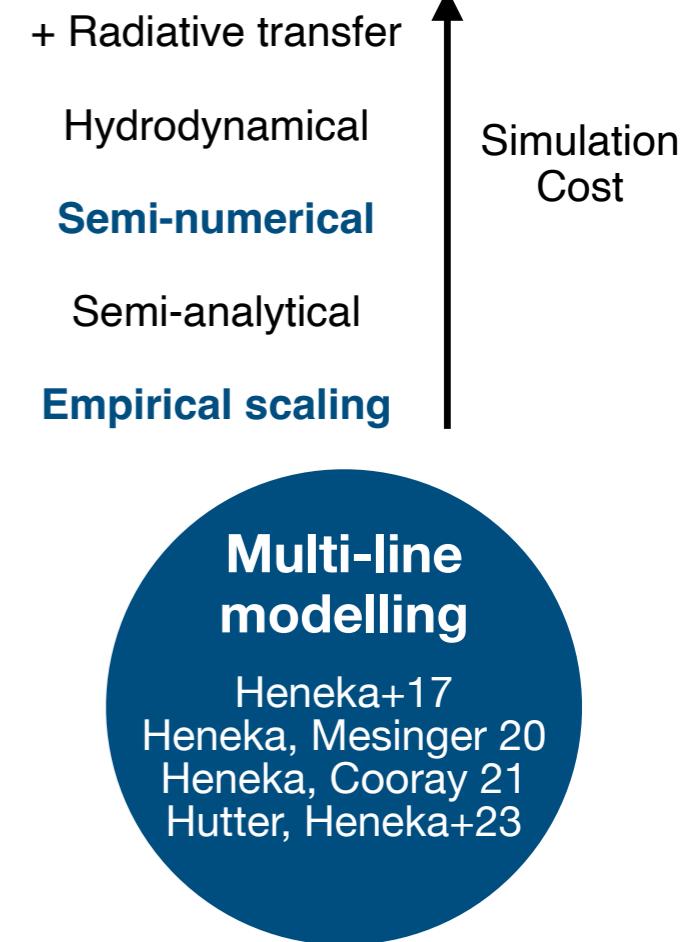


### 3) Generative methods for simulation

Reionization simulations are costly ... and model a rich signal  
Is there a fast way to emulate whole simulations?



Example: Lyman-alpha to 21cm

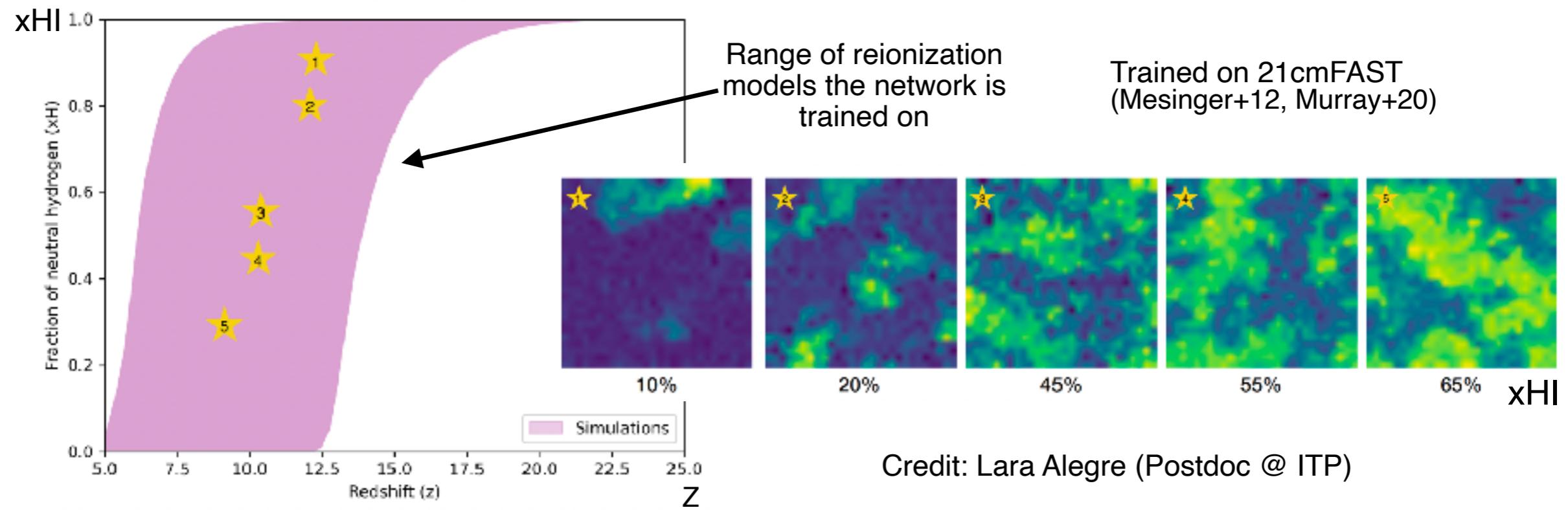
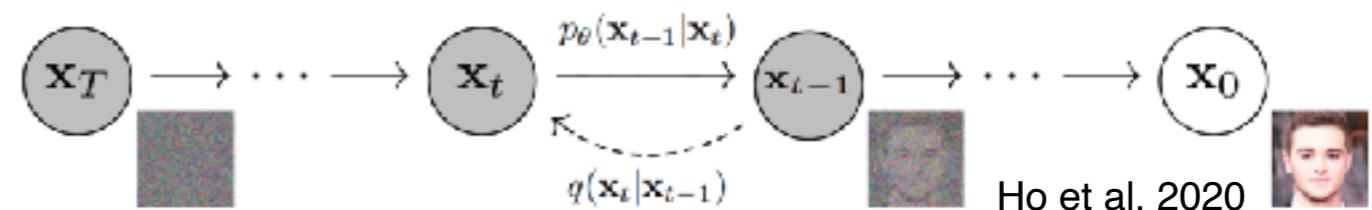


### 3) Generative methods for simulation (of the 21cm signal)

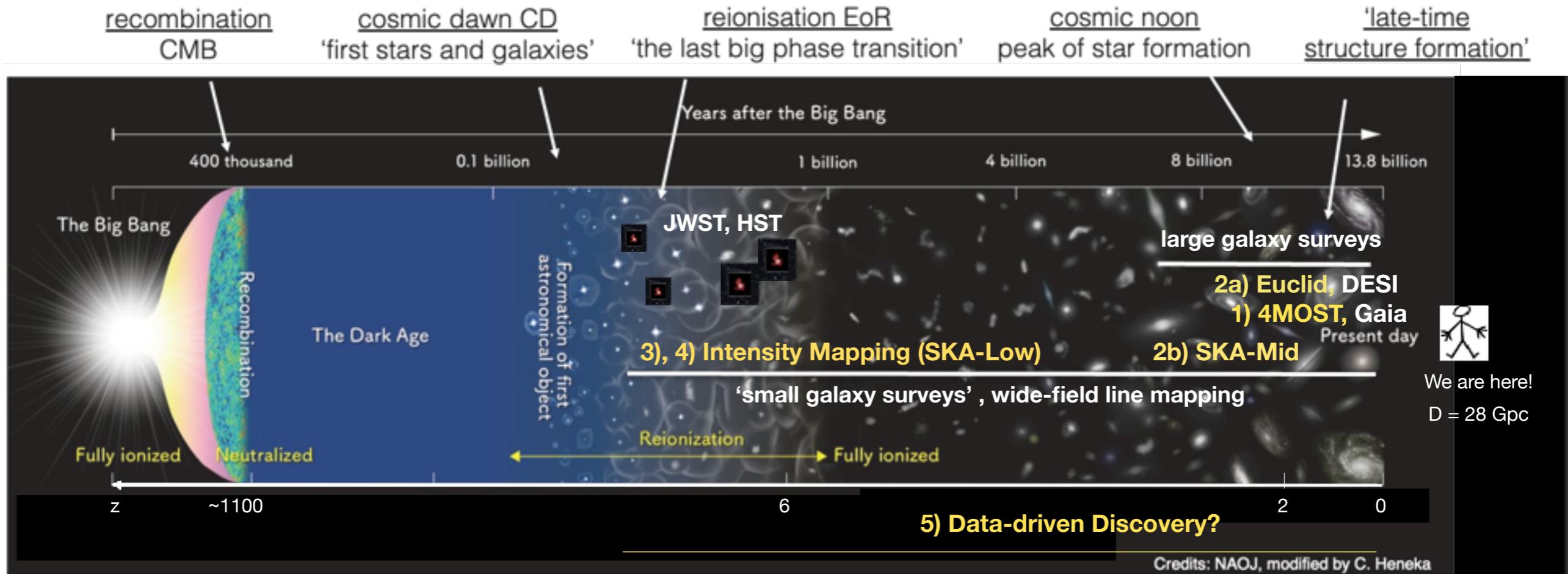
Reionization simulations are costly

Is there a fast way to emulate whole simulations?

Our DL solution: Generation of slices of the 21cm brightness temperature using diffusion models



# Astronomical and Astrophysical Machine Learning



## Highlights in this Lecture

- 1) Classification / Triggering
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- 5) Data-driven Discovery

## Inference

Observations

Simulations & Modelling

## 5) Already now: Data-driven discovery

### CAMELS

= Cosmology and Astrophysics with MachinE Learning Simulations

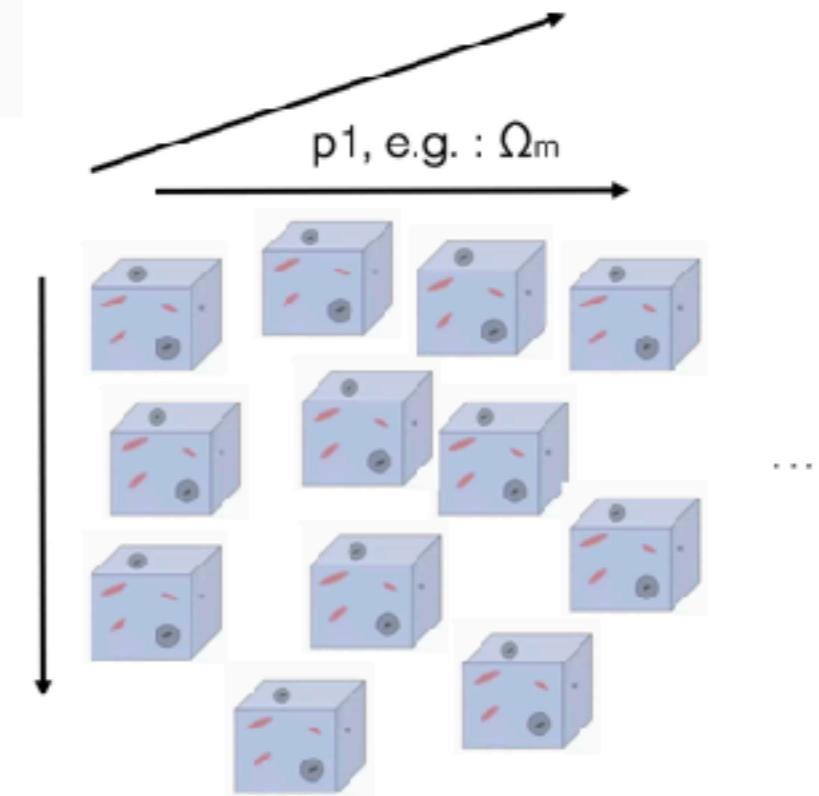
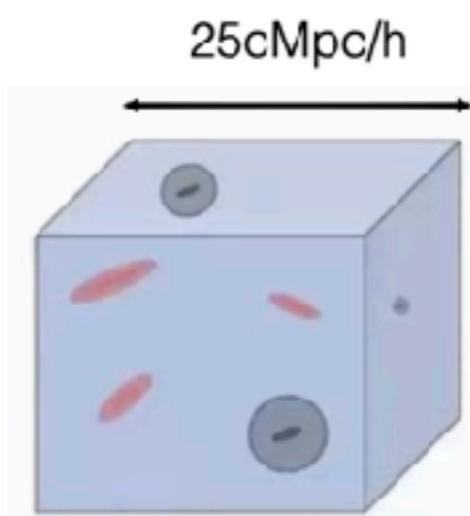
Type	Code	Subgrid model	Simulations
Hydrodynamic	Arepo	IllustrisTNG	1,092
Hydrodynamic	Gizmo	SIMBA	1,092
Hydrodynamic	MP-Gadget	Astrid	1,092
N-body	Gadget-III	—	3,049



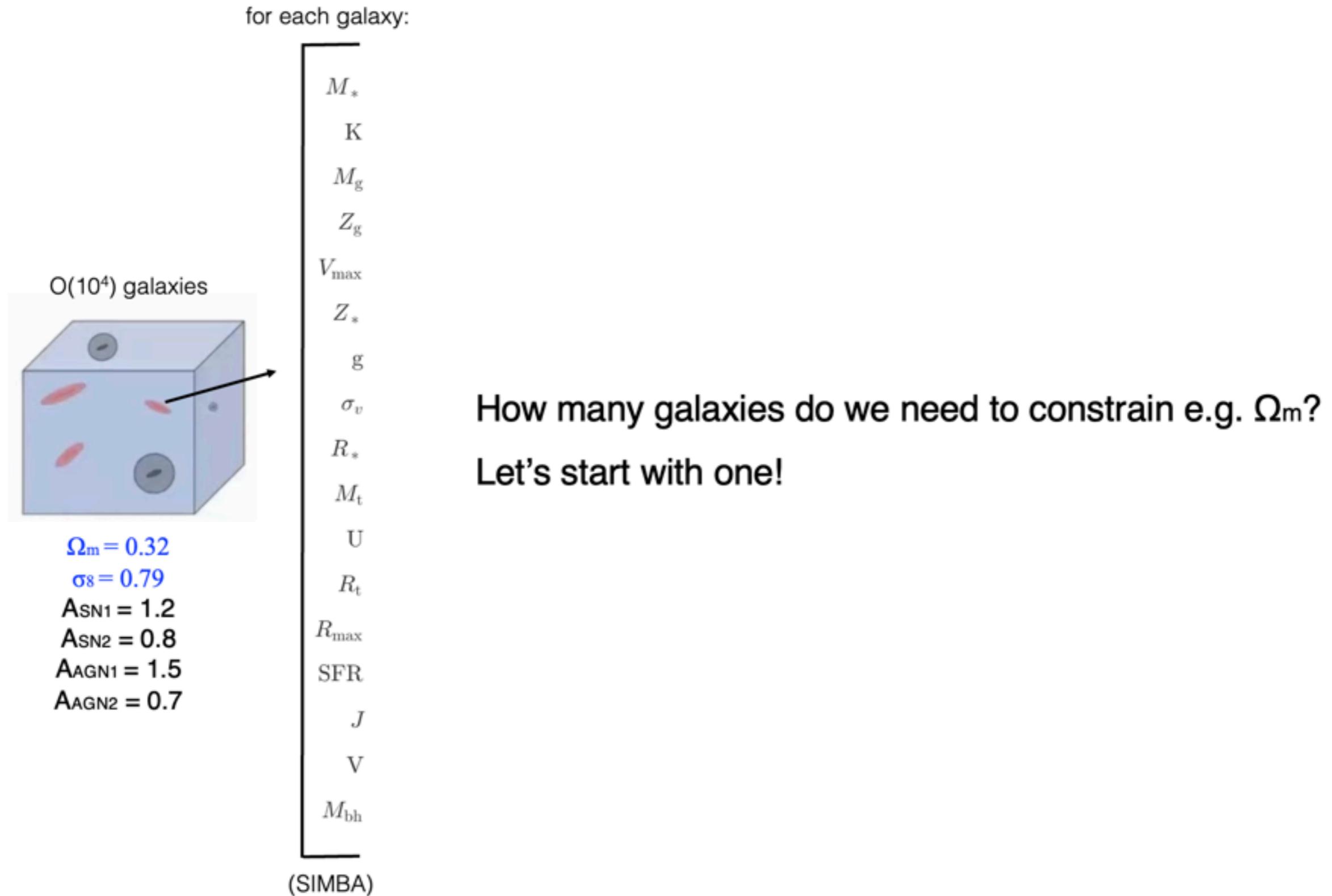
<https://camels.readthedocs.io>

Parameter set:

$$\begin{array}{ll} 0.1 \leq \Omega_m & \leq 0.5 \\ 0.6 \leq \sigma_8 & \leq 1.0 \\ 0.25 \leq A_{SN1} & \leq 4.0 \\ 0.50 \leq A_{SN2} & \leq 2.0 \\ 0.25 \leq A_{AGN1} & \leq 4.0 \\ 0.50 \leq A_{AGN2} & \leq 2.0 \end{array}$$

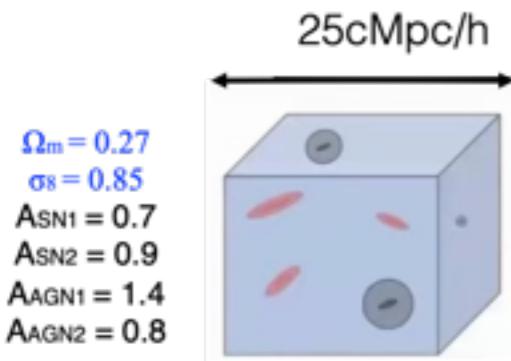


## 5) Already now: Data-driven discovery



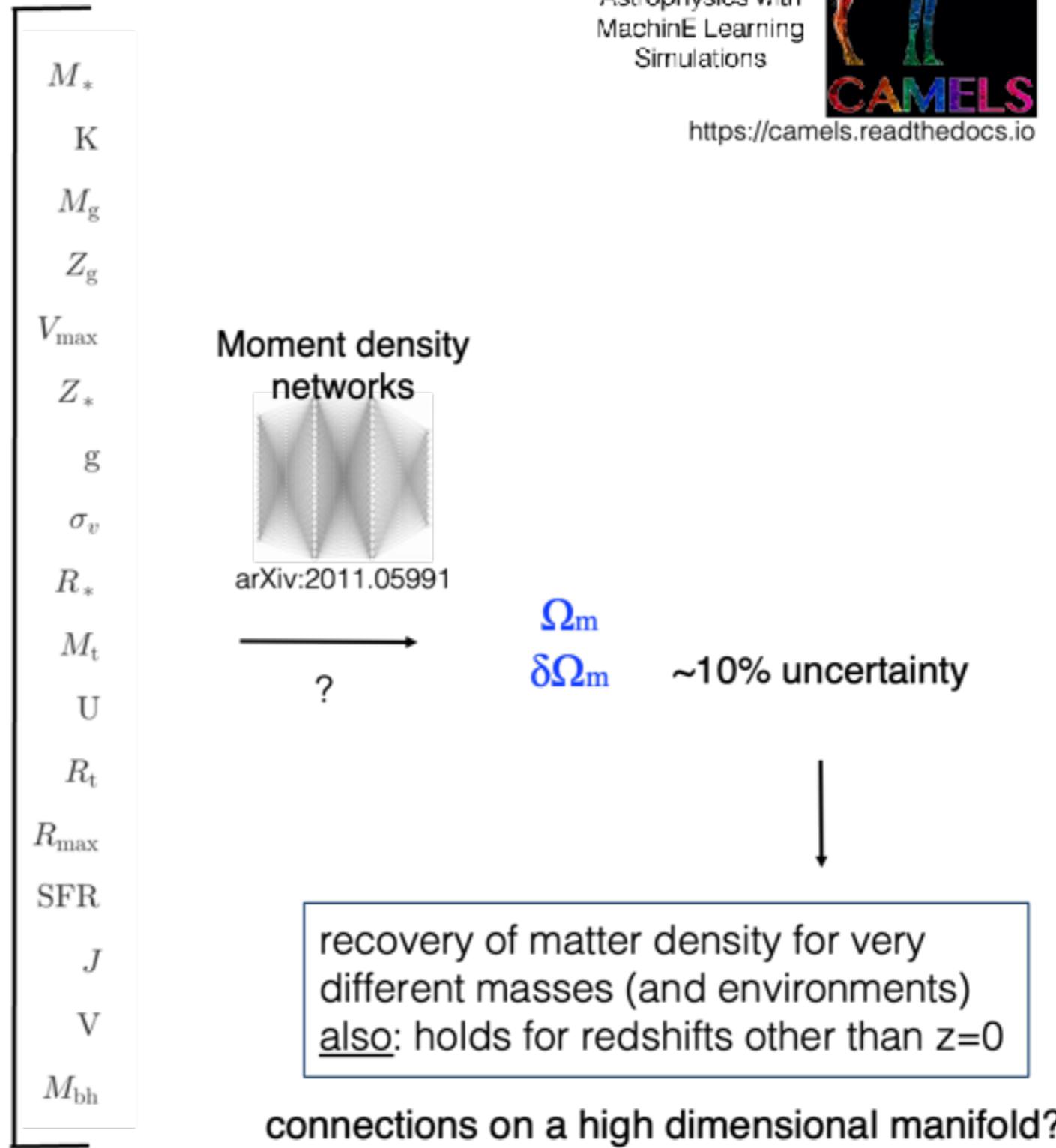
## 5) Already now: Data-driven discovery

How many galaxies do we need  
to constrain e.g.  $\Omega_m$ ?

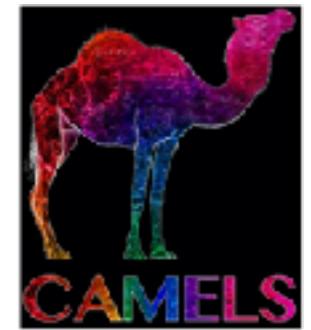


$O(10^4)$  galaxies  
per cube

random galaxy:  
→  
galaxy properties



= Cosmology and  
Astrophysics with  
Machine Learning  
Simulations



<https://camels.readthedocs.io>

## 5) Already now: Data-driven discovery

---

Loss based on moment density networks (MDN) Jeffrey & Wandelt 2011  
arXiv:2011.05991

**MDN idea:** hierarchy of neural regression models (mean  $\rightarrow$  variance  $\rightarrow$  skewness  $\rightarrow \dots$ )

We begin by noting that if we find some function of our data  $\mathcal{F}(x)$  that minimizes an  $L_2$  loss over the distribution of possible training examples  $\{x_i, \theta_i\}$ ,

$$J_0 = \int \|\theta - \mathcal{F}(x)\|^2 p(x, \theta) dx d\theta , \quad (4)$$

then  $\mathcal{F}$ , which we represent as a neural network, evaluated for the observed data is the mean of the posterior distribution  $\mathcal{F}(x_{obs}) = \langle \theta \rangle_{\theta|x_{obs}}$ . It is therefore possible to create a hierarchy of networks

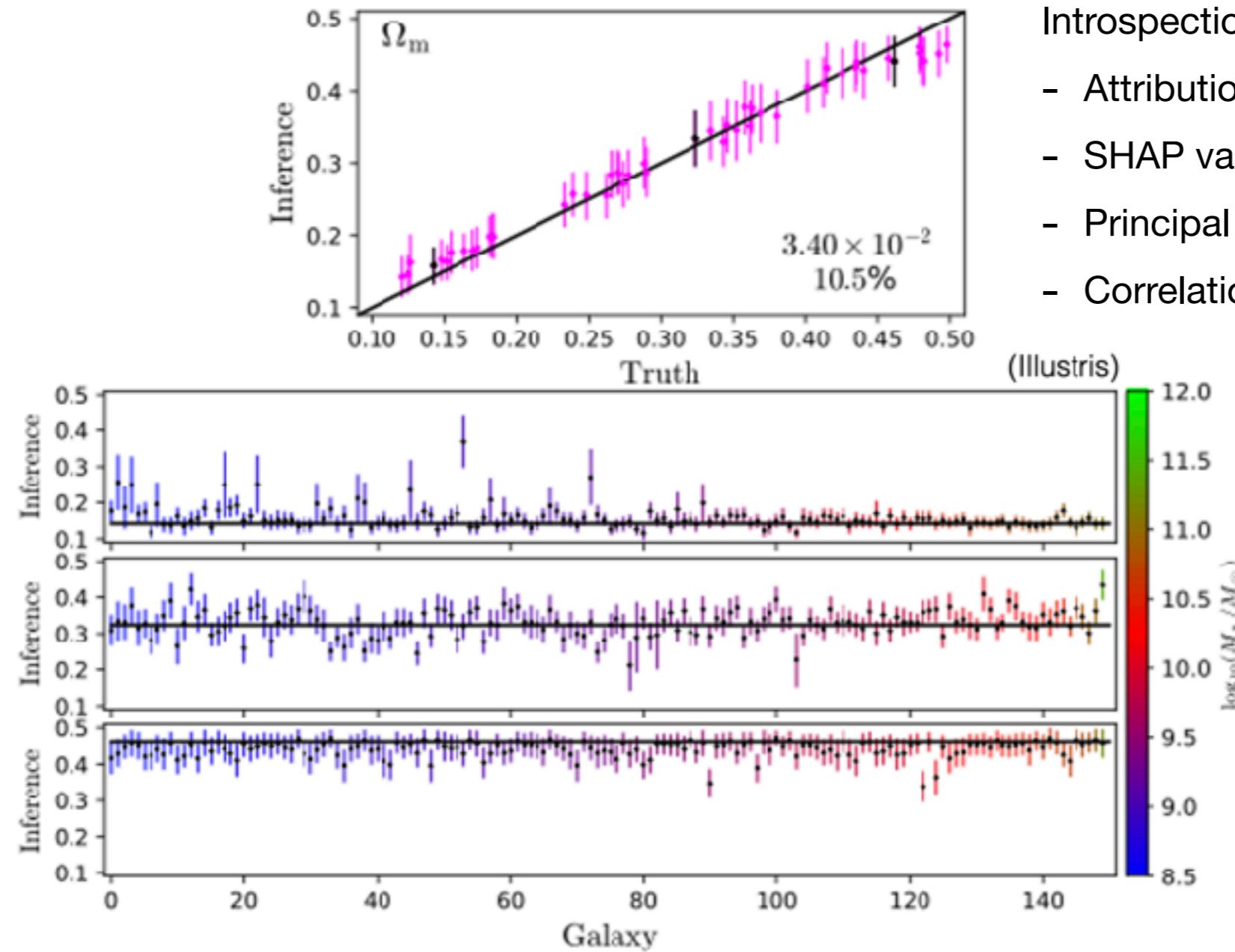
In practice we minimise the following loss function:

$$\begin{aligned} \mathcal{L} = & \sum_{i=1}^6 \log \left( \sum_{j \in \text{batch}} (\theta_{i,j} - \mu_{i,j})^2 \right) \\ & + \sum_{i=1}^6 \log \left( \sum_{j \in \text{batch}} \left( (\theta_{i,j} - \mu_{i,j})^2 - \sigma_{i,j}^2 \right)^2 \right) \end{aligned}$$

Our model  $F(x)$ :  
CNN layers (19)  
+ dense (2)

Villaescusa-Navarro+  
arXiv:2109.10915

## 5) Already now: Data-driven discovery



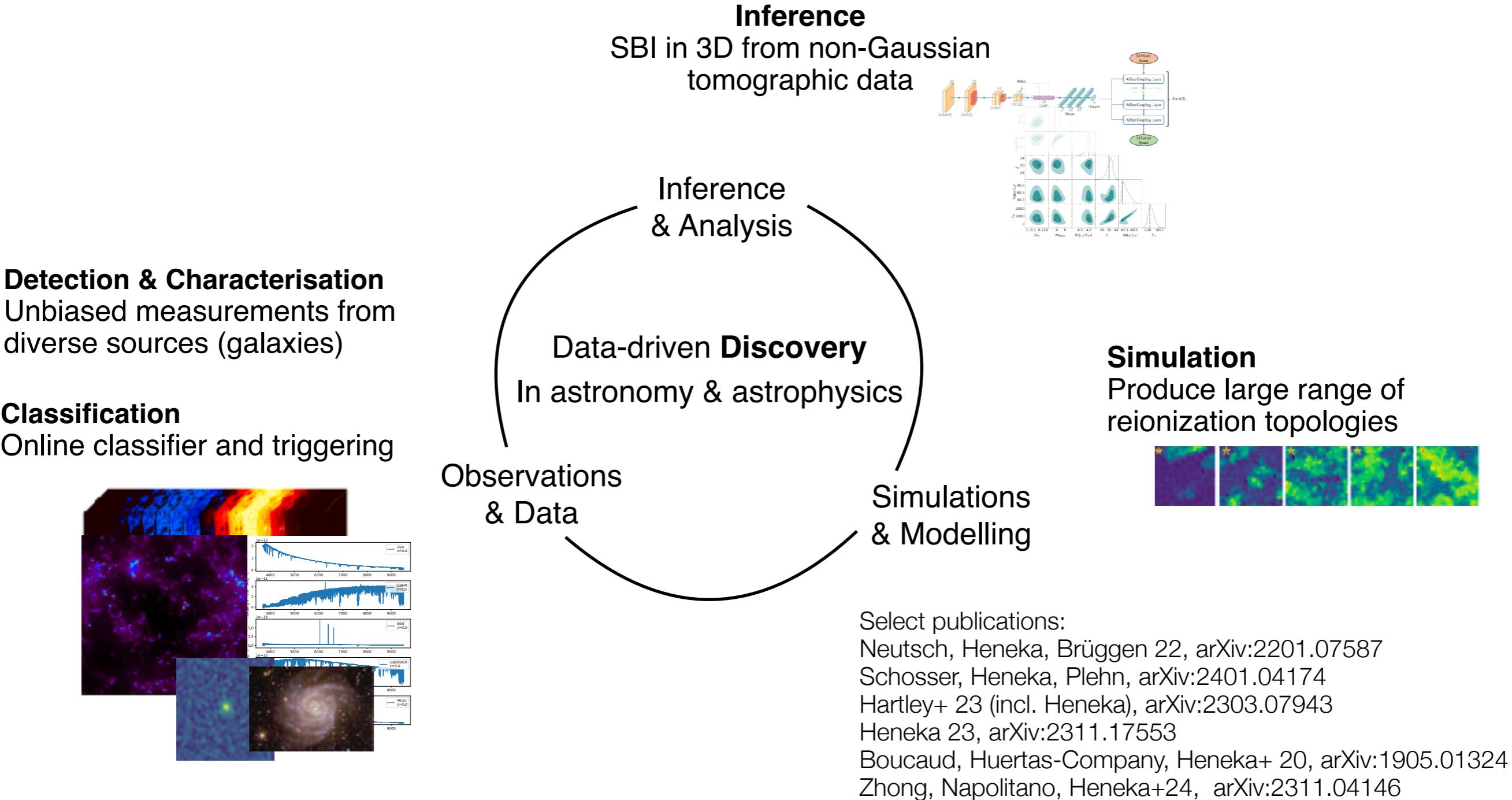
Introspection via:

- Attribution, one-by-one retraining
- SHAP values (Shapley Additive exPlanations)
- Principal Component Analysis (PCA)
- Correlation strengths

→ recovery of matter density for very different masses (and environments)  
also: holds for redshifts other than  $z=0$

# Summary: Where we stand

## Goal: Understanding & discovery

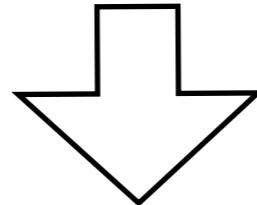


# Research plans: Where we are going

## Goal: Understanding & discovery

'What will bring our community forward'

Novel  
Scientific Life Cycles



Inference  
& Analysis

Representation  
Learning

Online  
Triggering

Data-driven discovery  
In astronomy & astrophysics

Observations  
& Data

Active  
Learning

Simulations  
& Modelling

eXplainable  
AI

Foundational

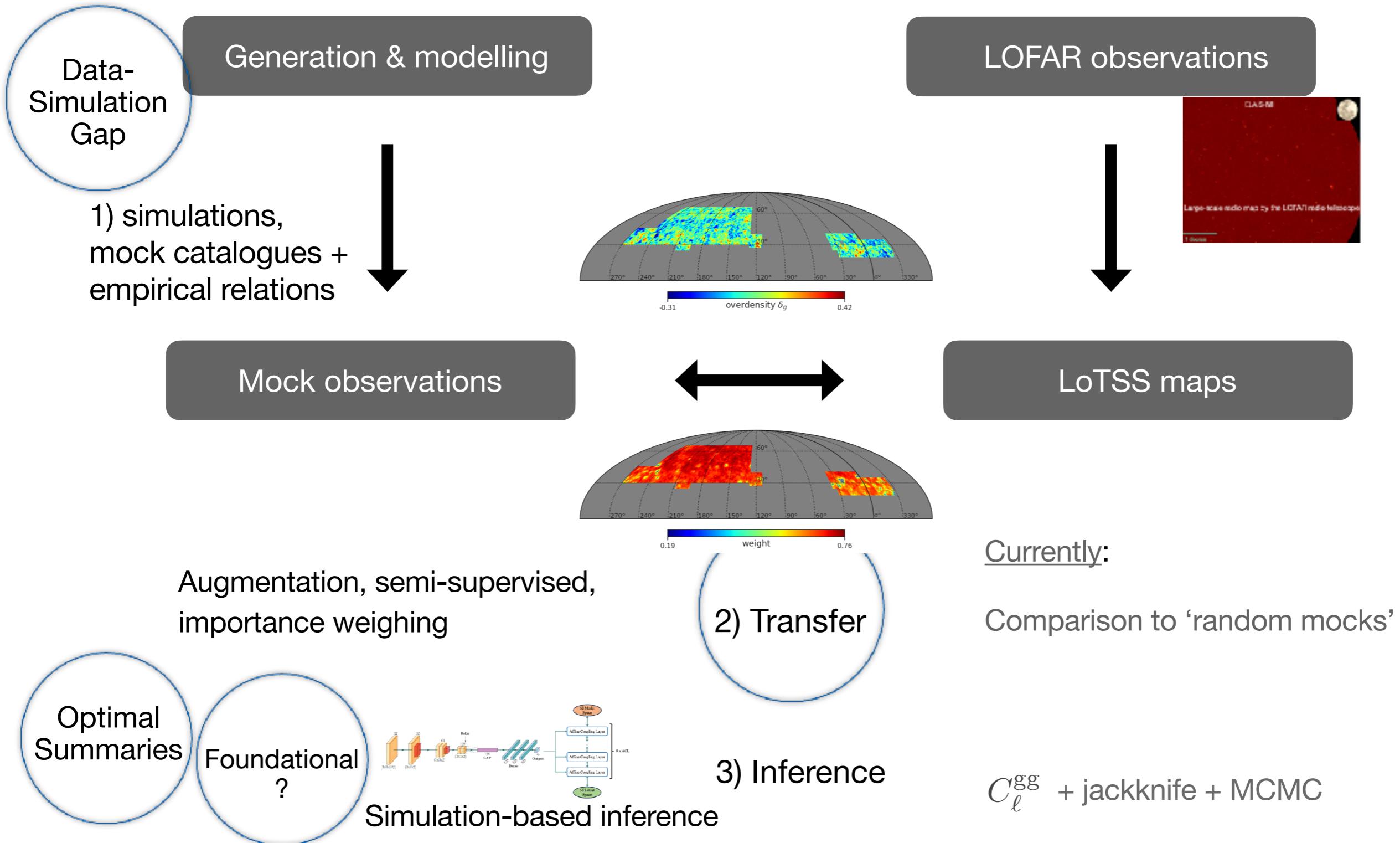
Optimal  
Summaries

Transfer

Self-supervised  
(Masked,  
Contrastive, ..)

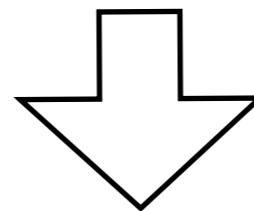
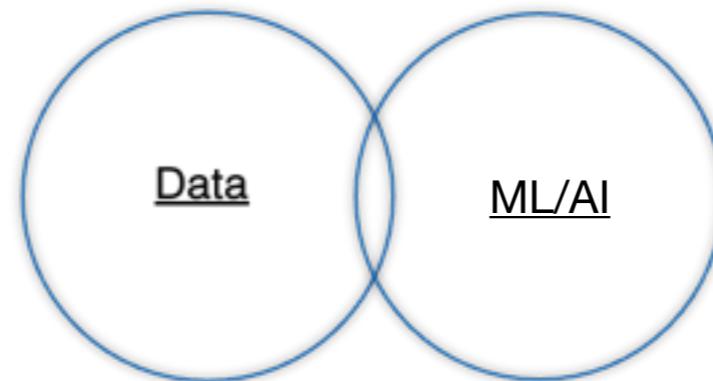
Data-  
Simulation  
Gap

# Example: Robust Foundational models for inference



# Research plans: where we are moving towards

Use data from astronomical surveys for **data-driven discovery**.



## Goals:

Map-based, multi-channel, '3D'  
approach to astrophysics  
Representation learning, beyond summaries  
Automated data mining, anomaly search  
New signatures & discovery

## Outcomes:

Fast and expressive simulators  
Reliable error estimates & inference  
Interpretability  
Active interaction and learning  
'human in the loop'  
New signatures & discovery

Based on  
foundational models

ML/DL/AI has come to stay when dealing with astronomical data.

