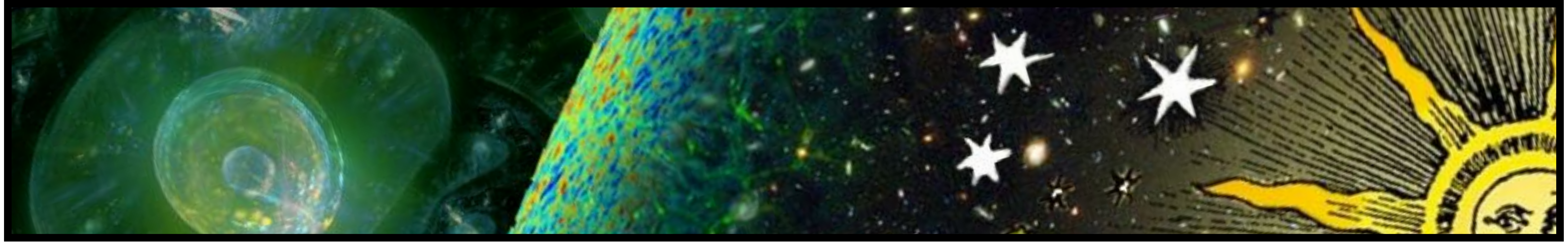
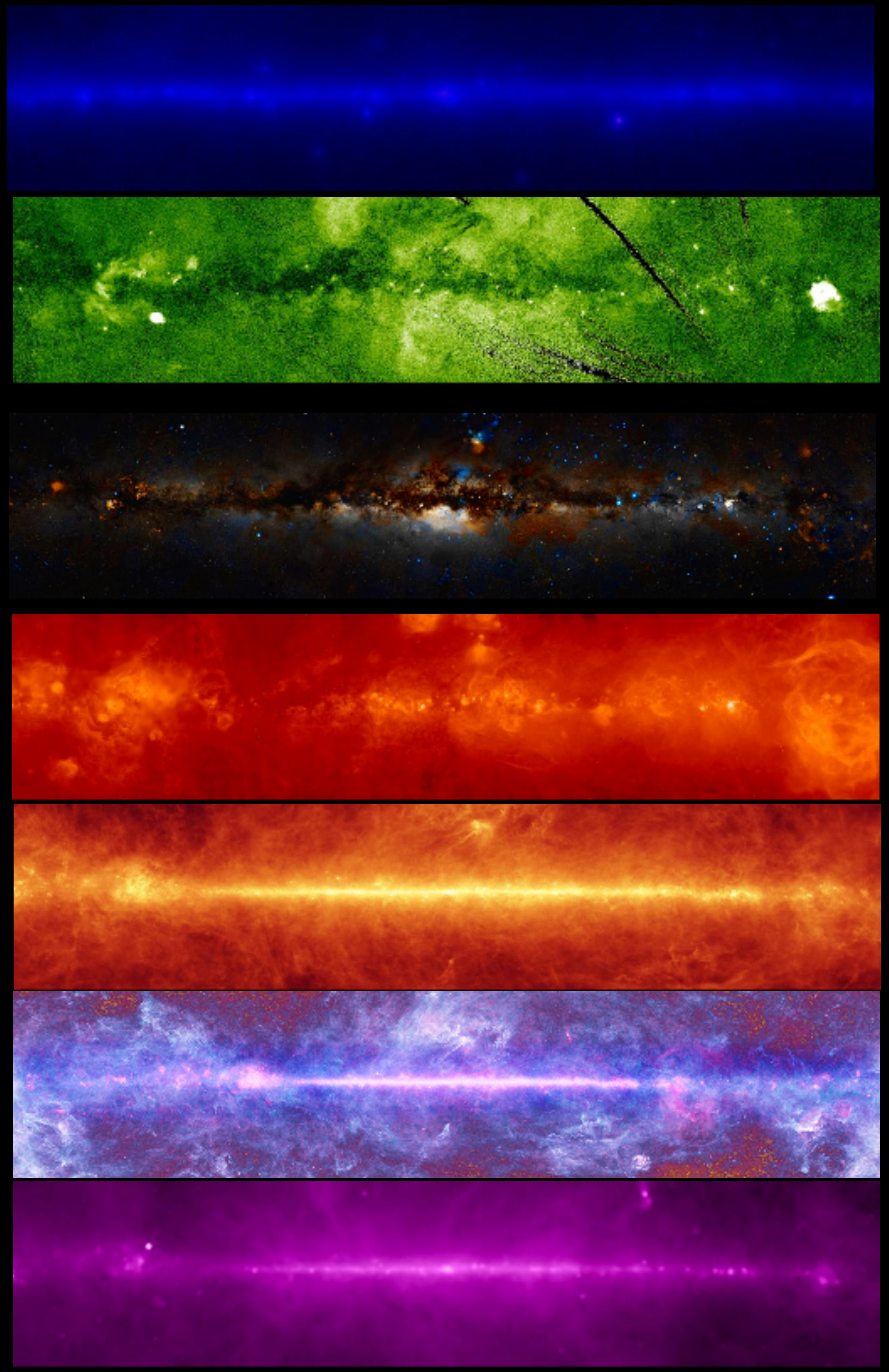


Prospects for understanding the physics of the Universe

Hiranya V. Peiris

UCL and Oskar Klein Centre Stockholm

The era of surveys



Gamma Ray (Fermi)

X Ray (ROSAT)

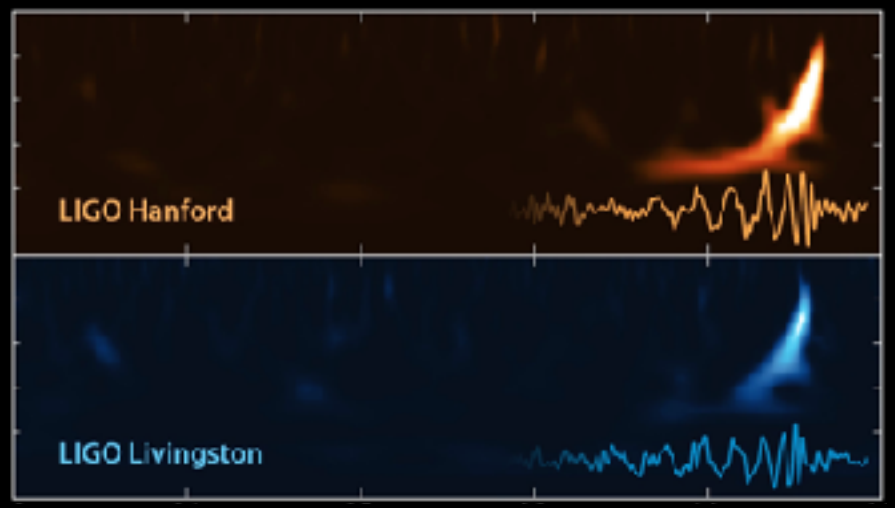
Optical (DSS)

H-alpha (WHAM/SHASSA/VTSS)

Far Infrared (IRAS)

Microwave (Planck)

Radio (Haslam)



Gravitational Waves (LIGO)

CREDIT: CHROMOSCOPE / CARDIFF

Highlights of era of precision cosmology

- *Determined the basic cosmological model (including measuring the age and composition of the Universe).*

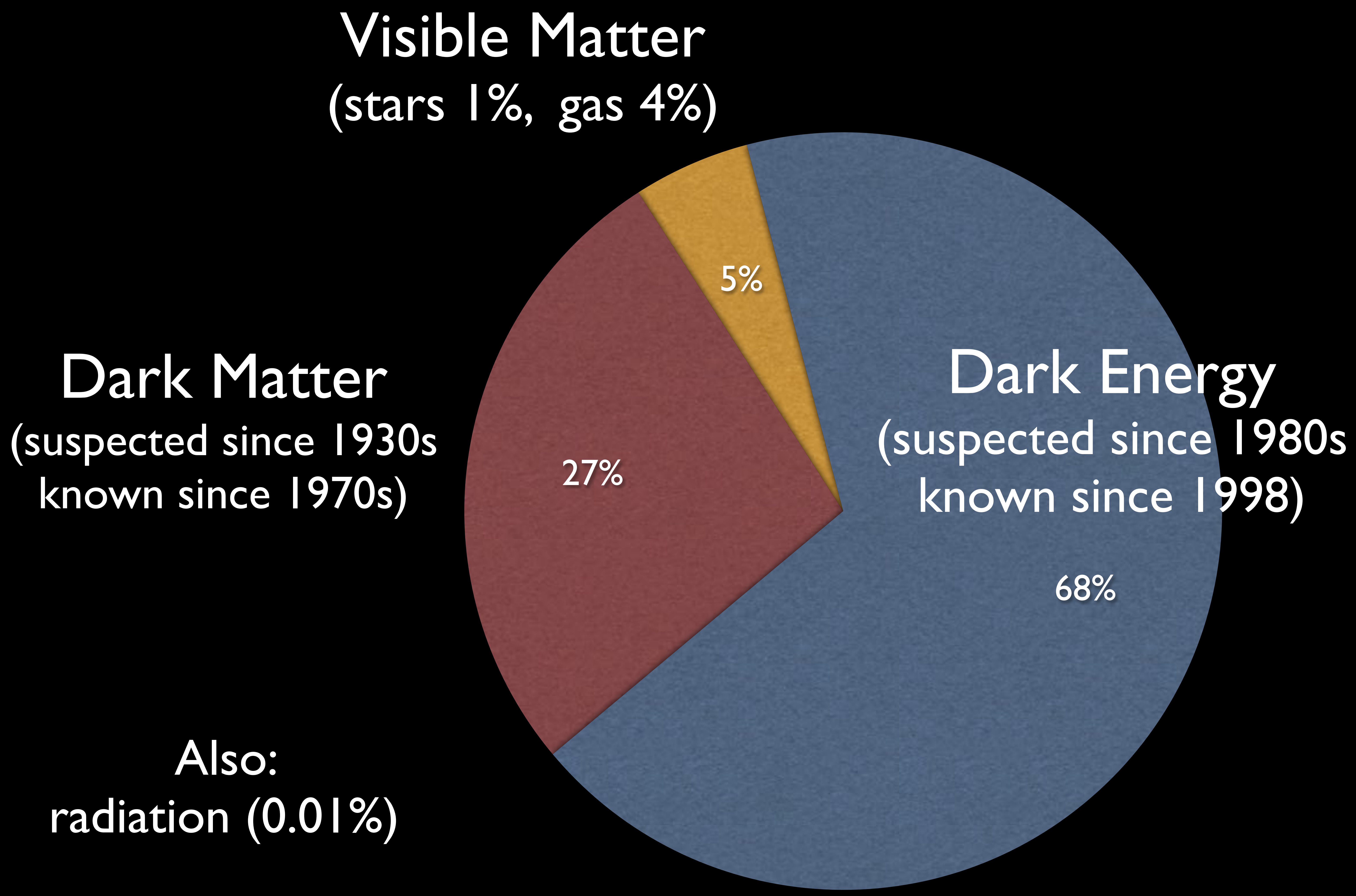
- *Found strong evidence for the quantum origin of cosmic structure.*

- *Measurements of* ***cosmic microwave background (CMB)*** *and* ***supernovae Ia*** *form cornerstones of this achievement.*

- ***Now + future: progress will come through multiple complementary probes.***

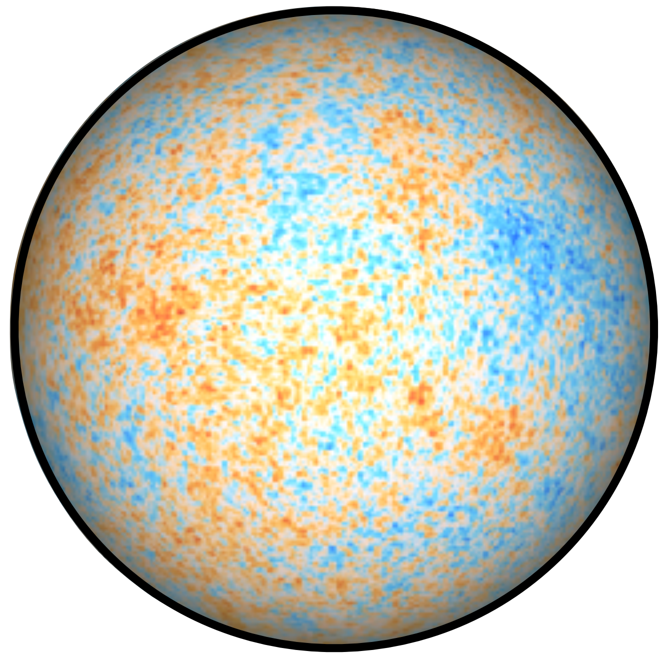
- ***Major theoretical questions remain unanswered.***

What is Dark Matter? Dark Energy?

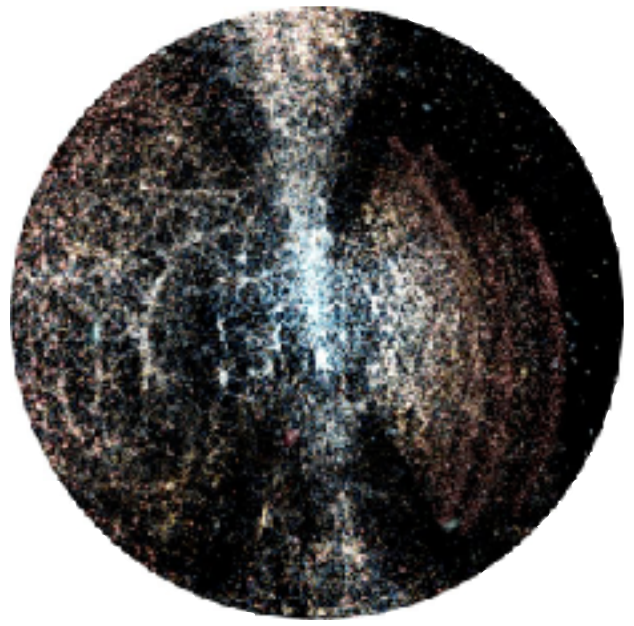


Also:
radiation (0.01%)

Electromagnetic cosmological probes in the next decade



Cosmic Microwave Background



Large Scale Structure

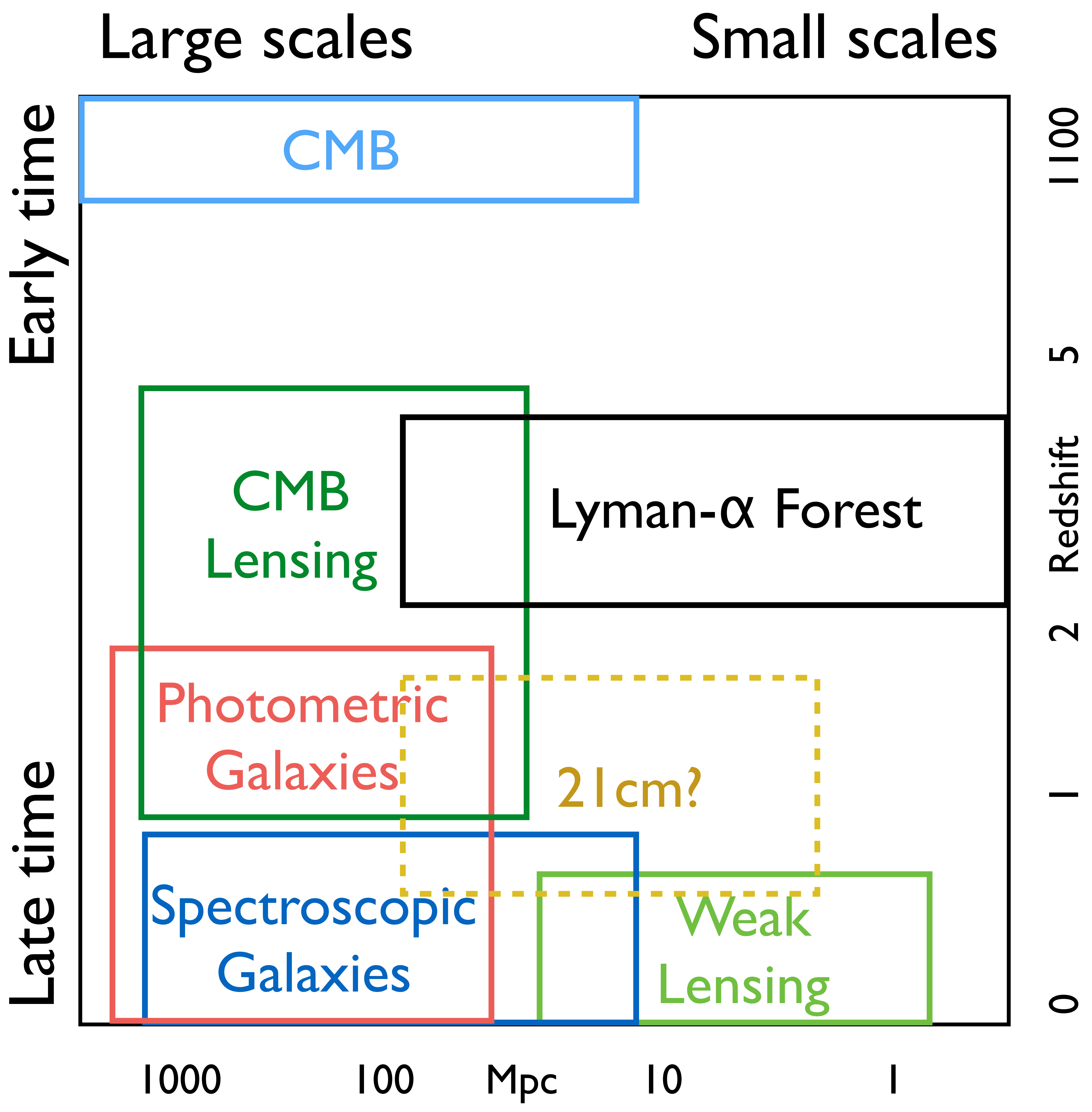


Figure: Andreu Font-Ribera

LSST
Legacy Survey of Space and Time

VERA C. RUBIN OBSERVATORY

Rubin's Legacy Survey of Space and Time (LSST)

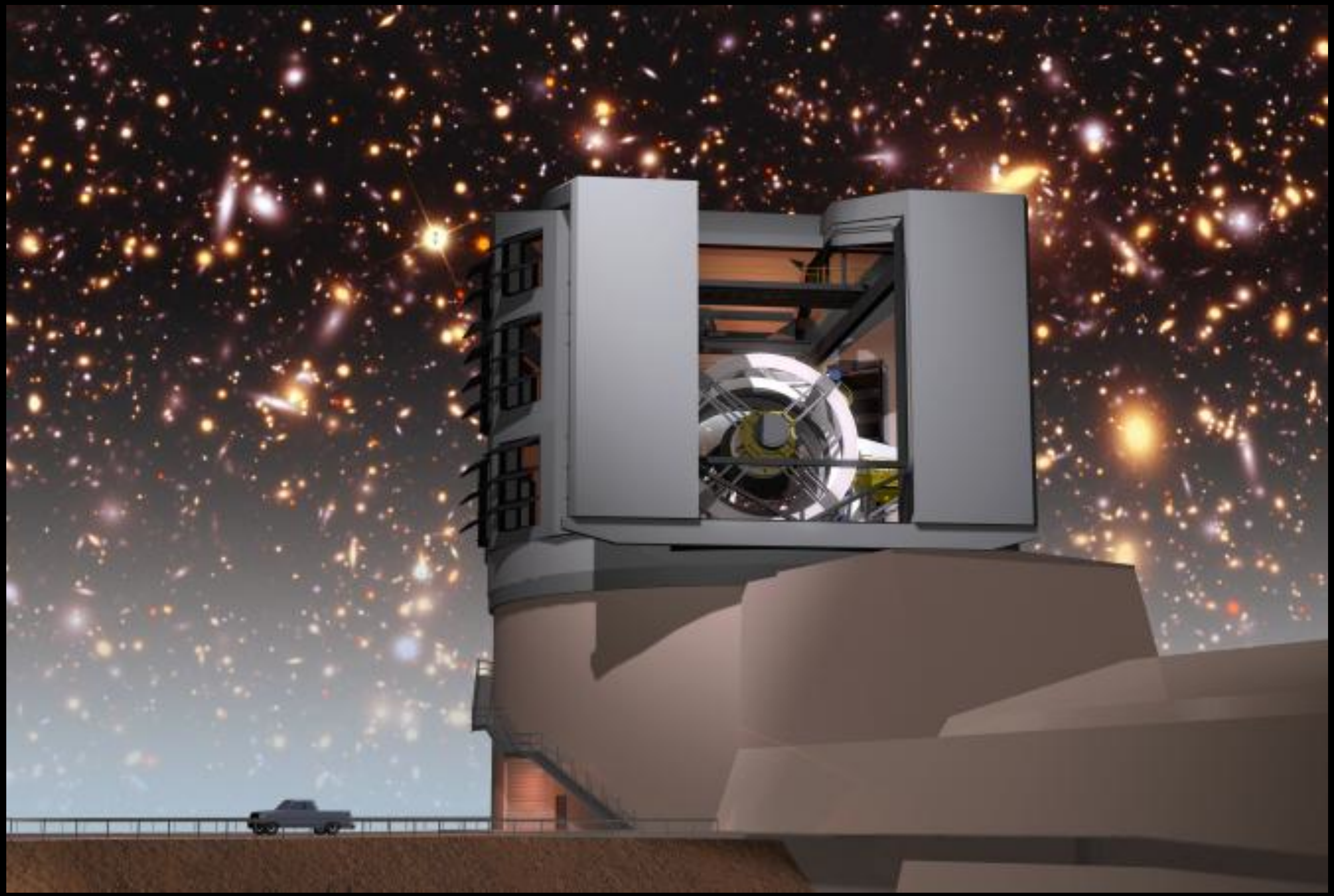
- Wide (half-sky), deep (24-27 mag), fast (every ~3 days) images
- Beginning in 2024, LSST will survey the Southern sky for 10 years
- Expand space-time volume 1000 times over current surveys

VERA C. RUBIN
OBSERVATORY

LSST
Legacy Survey of Space and Time

LSST: survey of 18,000 sq deg

(half the sky)



37 billion objects in space and time

30 trillion measurements

60 PB raw data (20 TB/night)

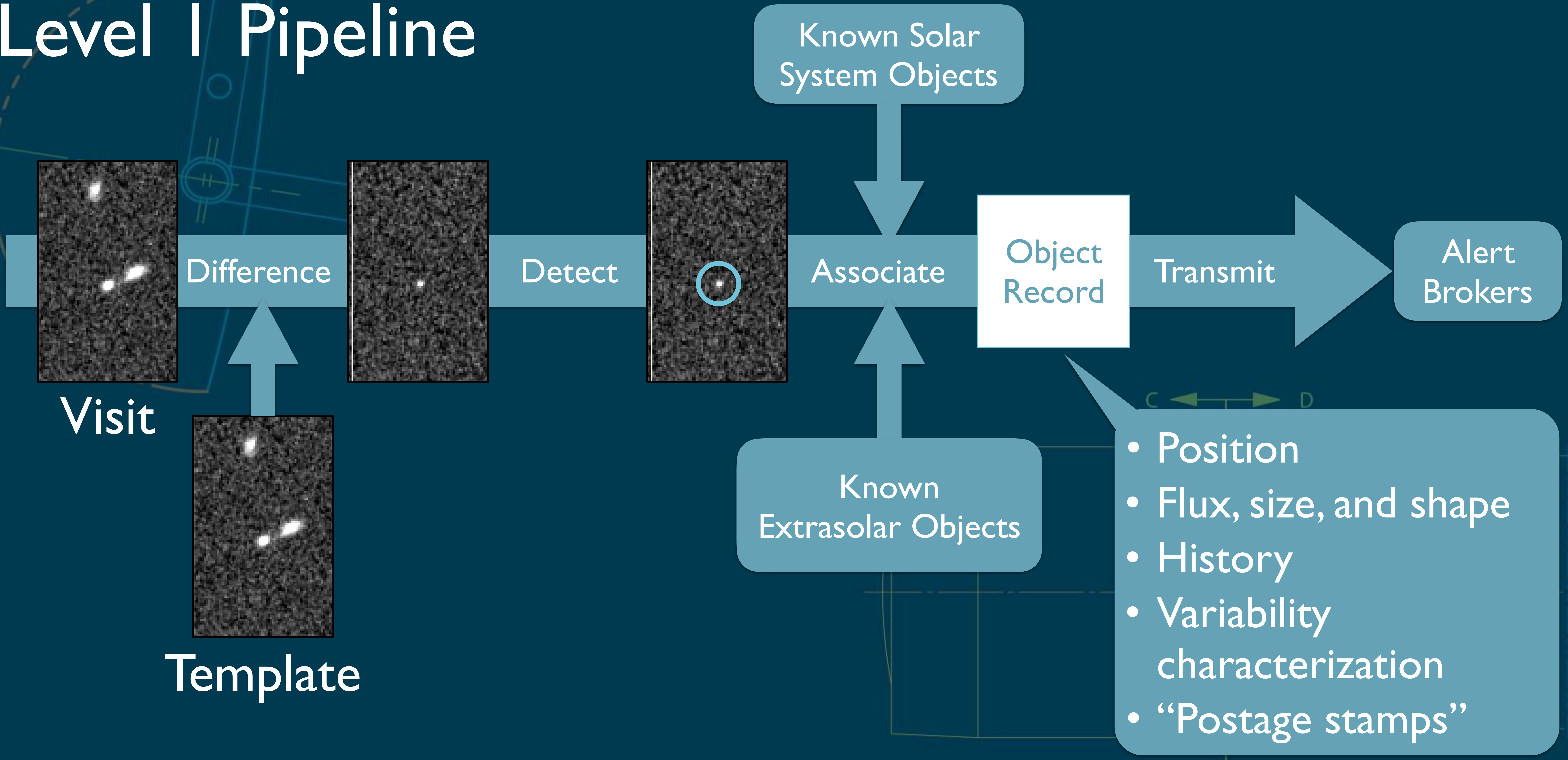
Dark matter-Dark energy

Solar system inventory

“Movie of the Universe”

Mapping the Milky Way

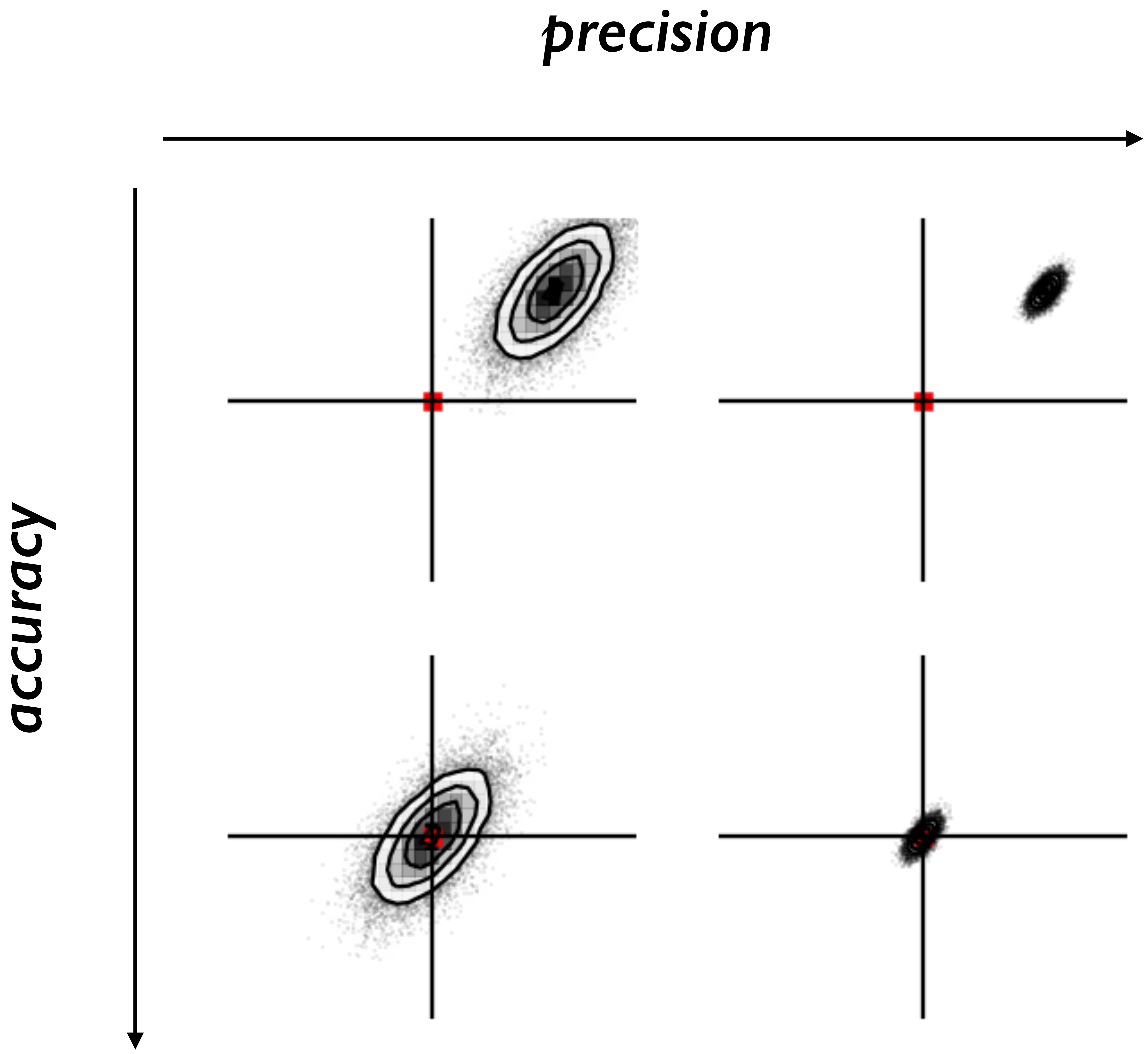
Level 1 Pipeline



0 seconds

60 seconds

Meredith Rawls • @merrdiff

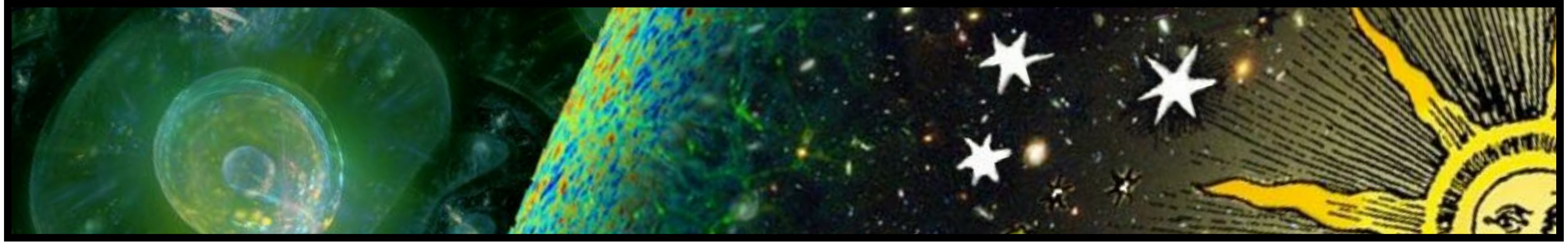

precision
accuracy

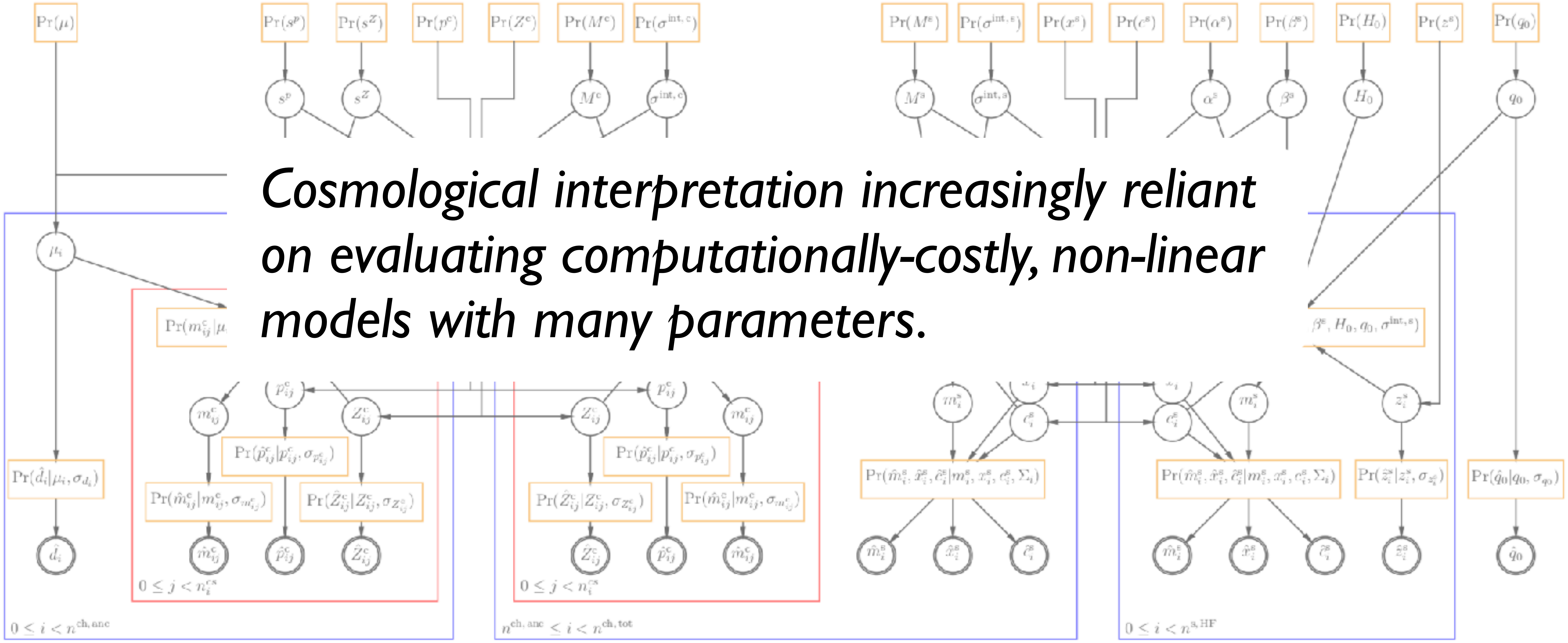
How should we compare

vs

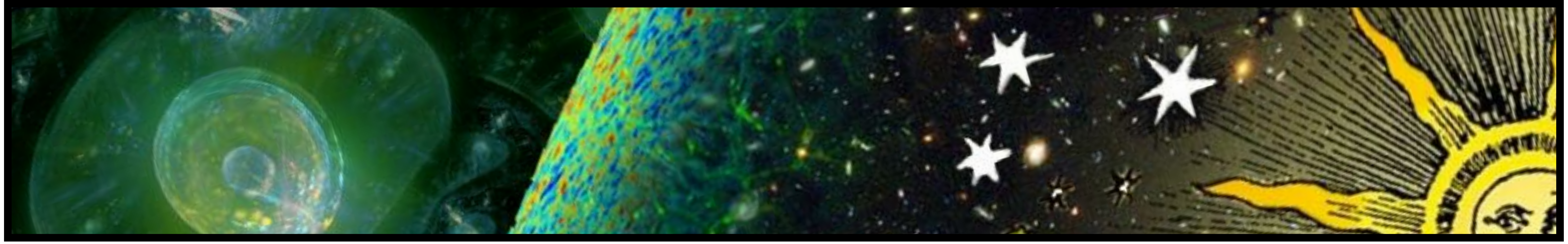
Theory

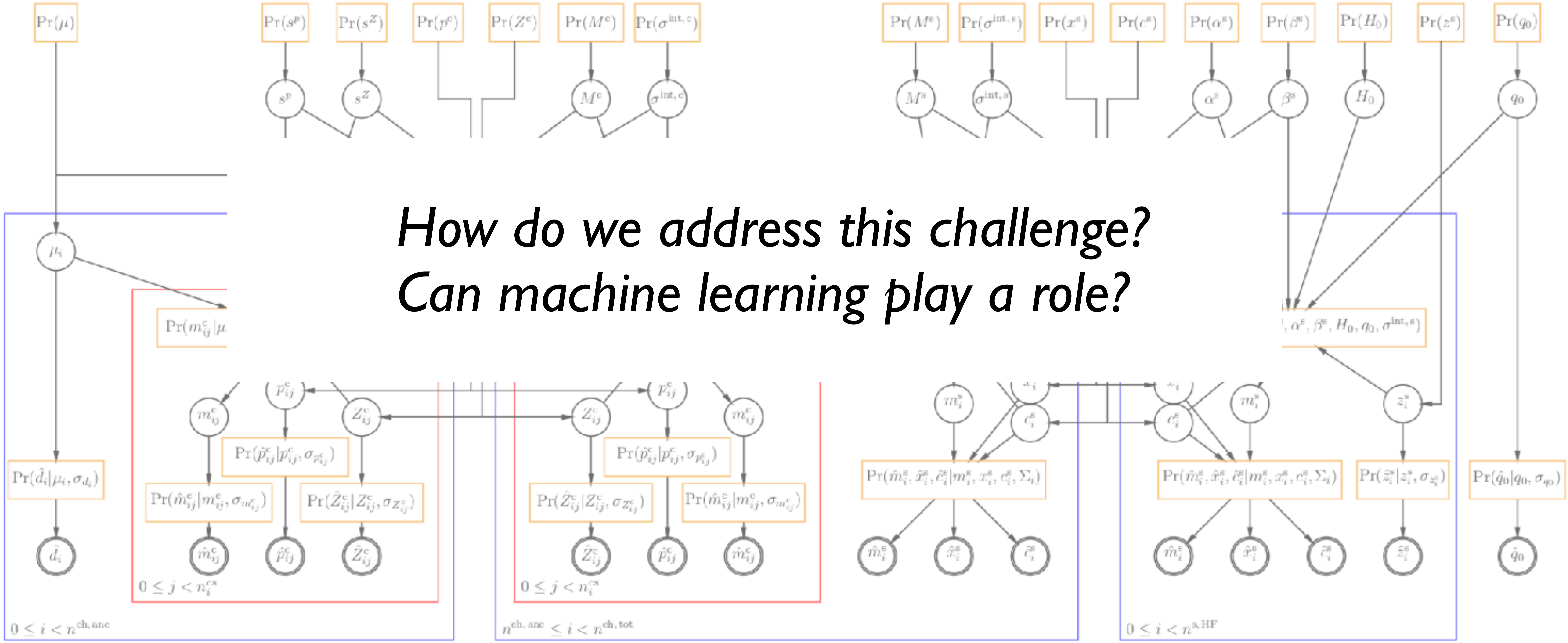
Data?





Cosmological interpretation increasingly reliant on evaluating computationally-costly, non-linear models with many parameters.





How do we address this challenge?
Can machine learning play a role?

What are ML models good at? (in astronomy)

- *providing fast, flexible models for mapping between complex, very high-dimensional datasets, e.g. for classification.*

- *accurately speeding up forward-modelling / data emulation.*

- *many applications where physical models are simply not available or tractable, e.g. anomaly-detection or automated discovery in very large datasets.*

Characteristics of (good) physical models

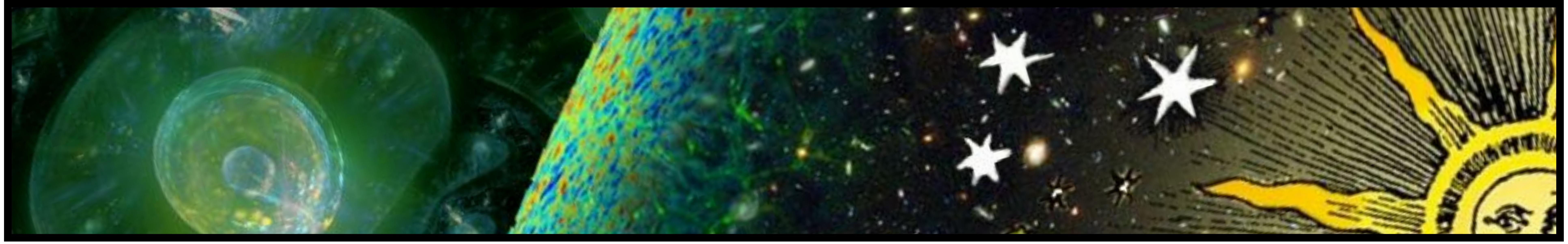
- *Follow from explicitly enumerable set of assumptions and physical principles*
- *Leads to mathematical models that can be solved (analytically/numerically) to yield useful* ***predictions*** *(deterministically/probabilistically).*
- ***Explainable*** *(rooted in cause-effect relationships grounded in domain knowledge.)*
- ***Generalises*** *beyond initial domain to explain wider range of phenomena.*
- ***Compresses*** *information: explains wide range of phenomena from minimal set of ingredients (~Occam's razor.)*
- ***Domain of validity*** *can be quantified explicitly.*

Desiderata towards a common footing

(i) ***interpretability****: account for why ML system reaches particular decision or prediction;*

(ii) ***explainability:*** *map this account onto existing knowledge in relevant science domain.*

- *Currently challenging because of "black box" nature of ML architectures.*
- *Many physical models satisfy my list of characteristics only partially, e.g. systems exhibiting emergent phenomena, chaotic systems.*



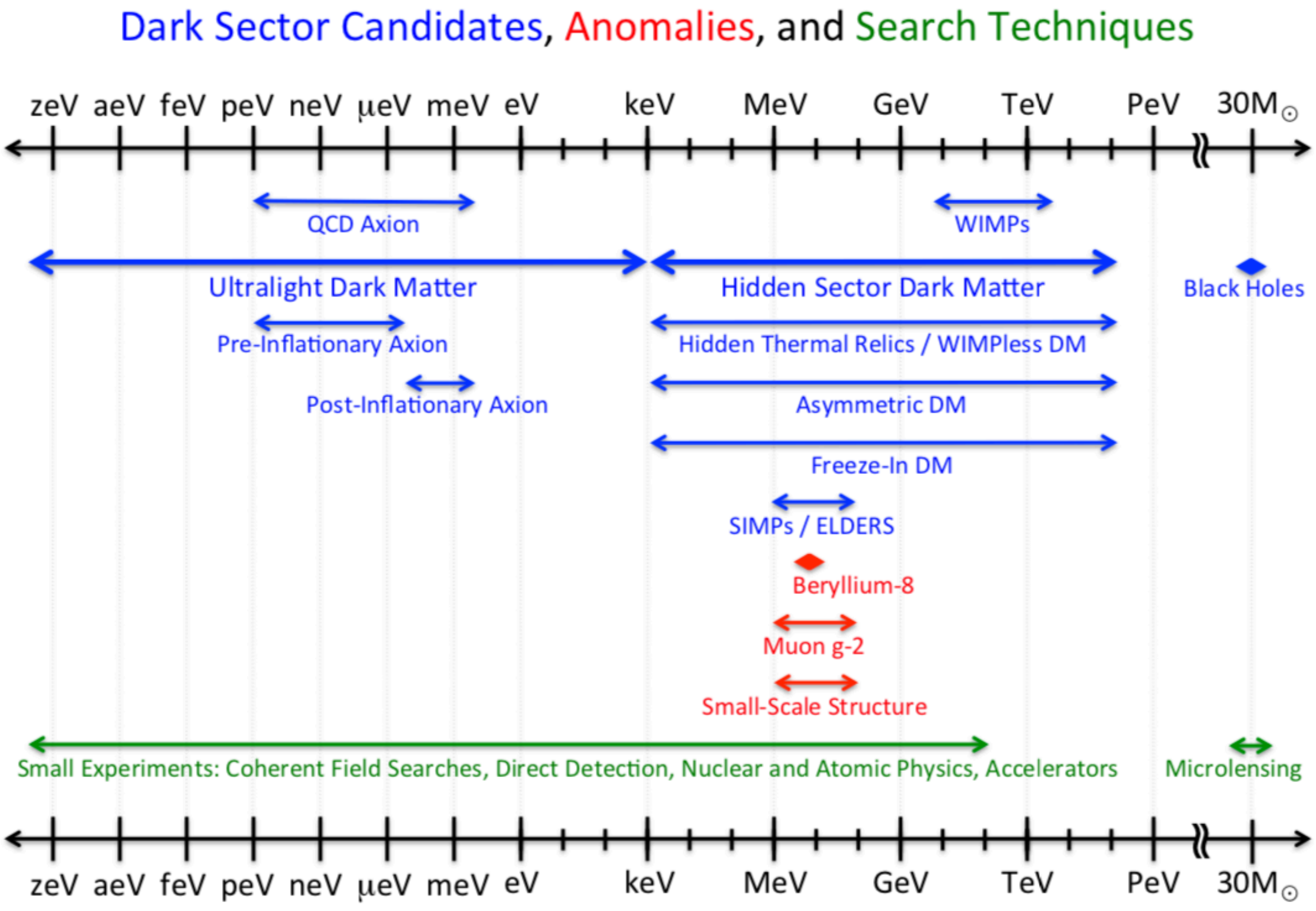
Efficient emulation of cosmological simulations

Keir Rogers
(Dunlap/Toronto)

Cora Dvorkin
(Harvard)

With: Andrew Pontzen, Simeon Bird, Andreu Font-Ribera, Licia Verde

What does the dark matter consist of?



Constraining dark matter with cosmology

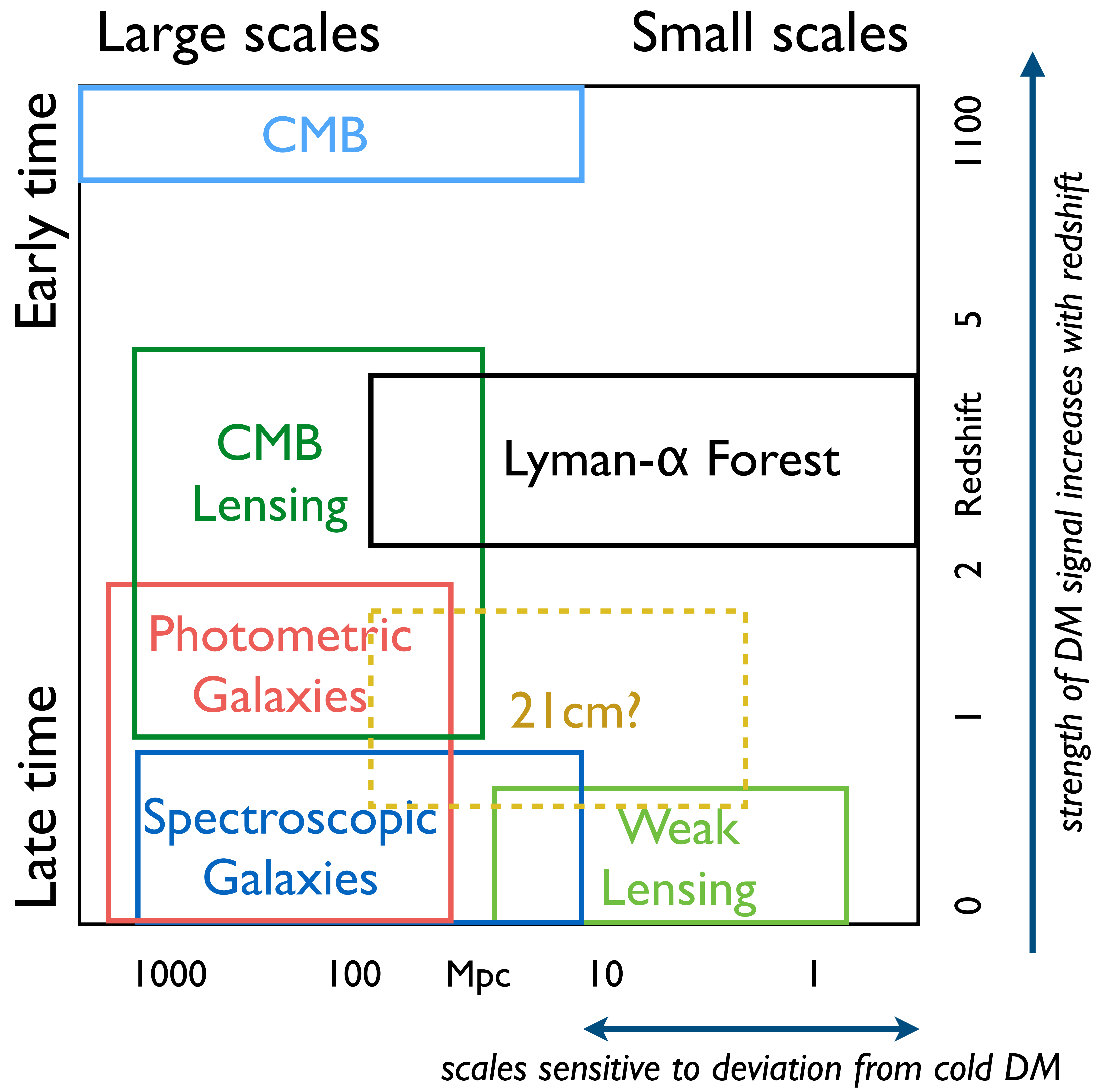
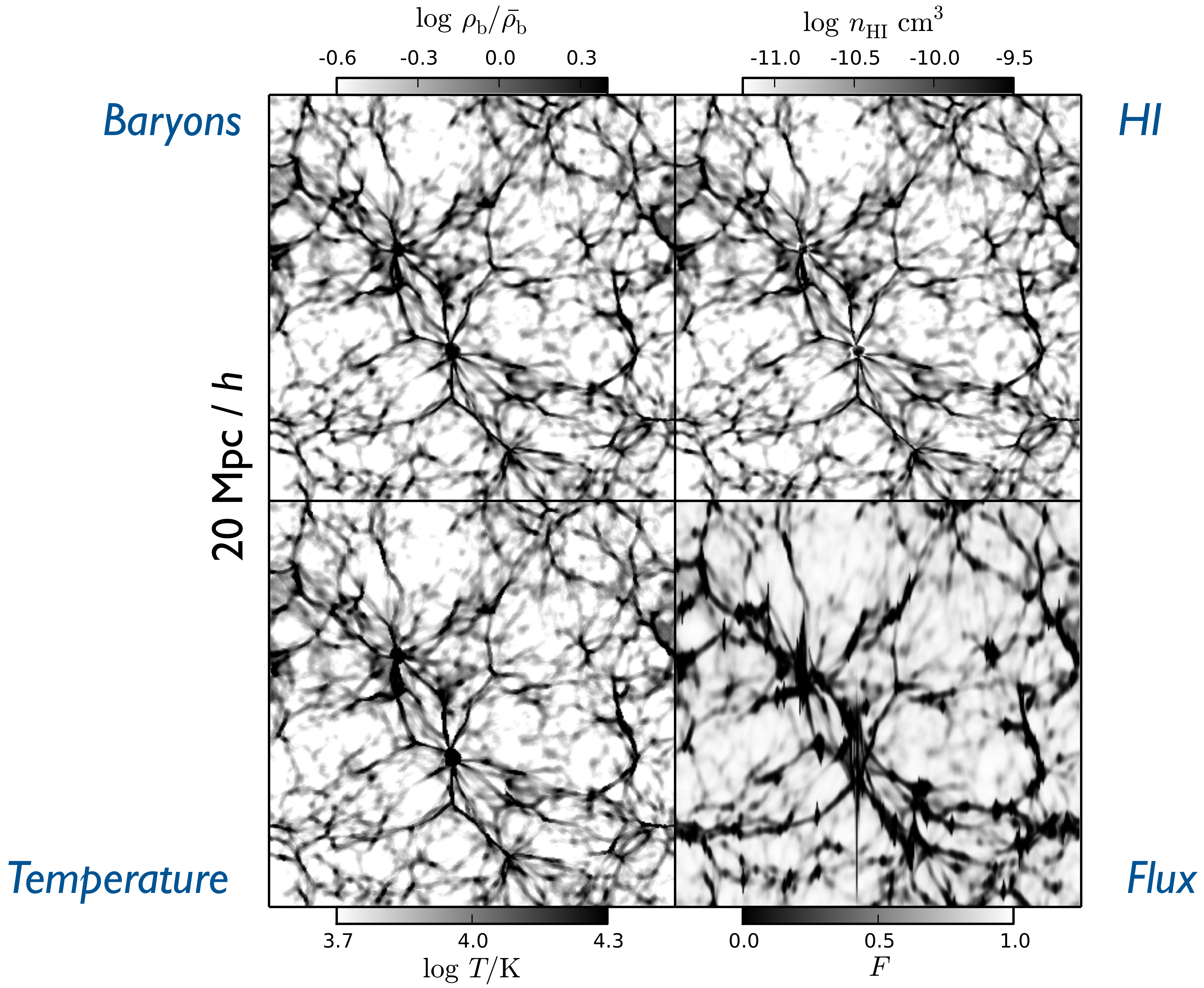


Figure: Andreu Font-Ribera

Lyman-alpha forest flux: biased, redshift-space distorted tracer of cosmic density field



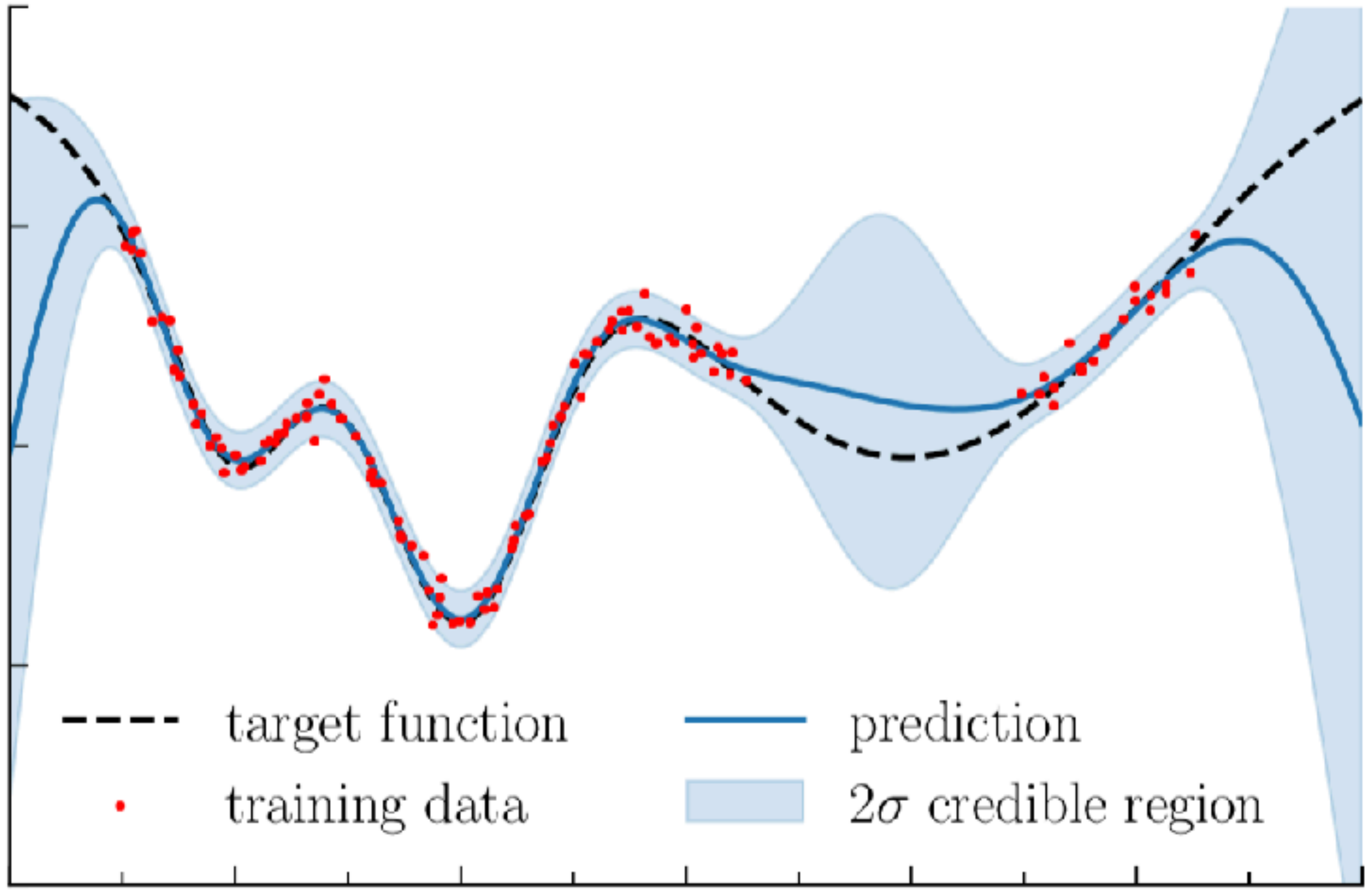
Accurate modelling requires intensive simulations:

~3000 CPU-hrs per parameter combination in 12-D parameter space

Figure: Lukić et al. (2015)

Gaussian process for emulating high-dimensional models

- *Smooth interpolation scheme that gives tight constraints where there are training points and broad constraints where there are none*



$$f(\mathbf{x}) \sim \mathcal{N}(0, K(\mathbf{x}, \mathbf{x}'; \theta))$$

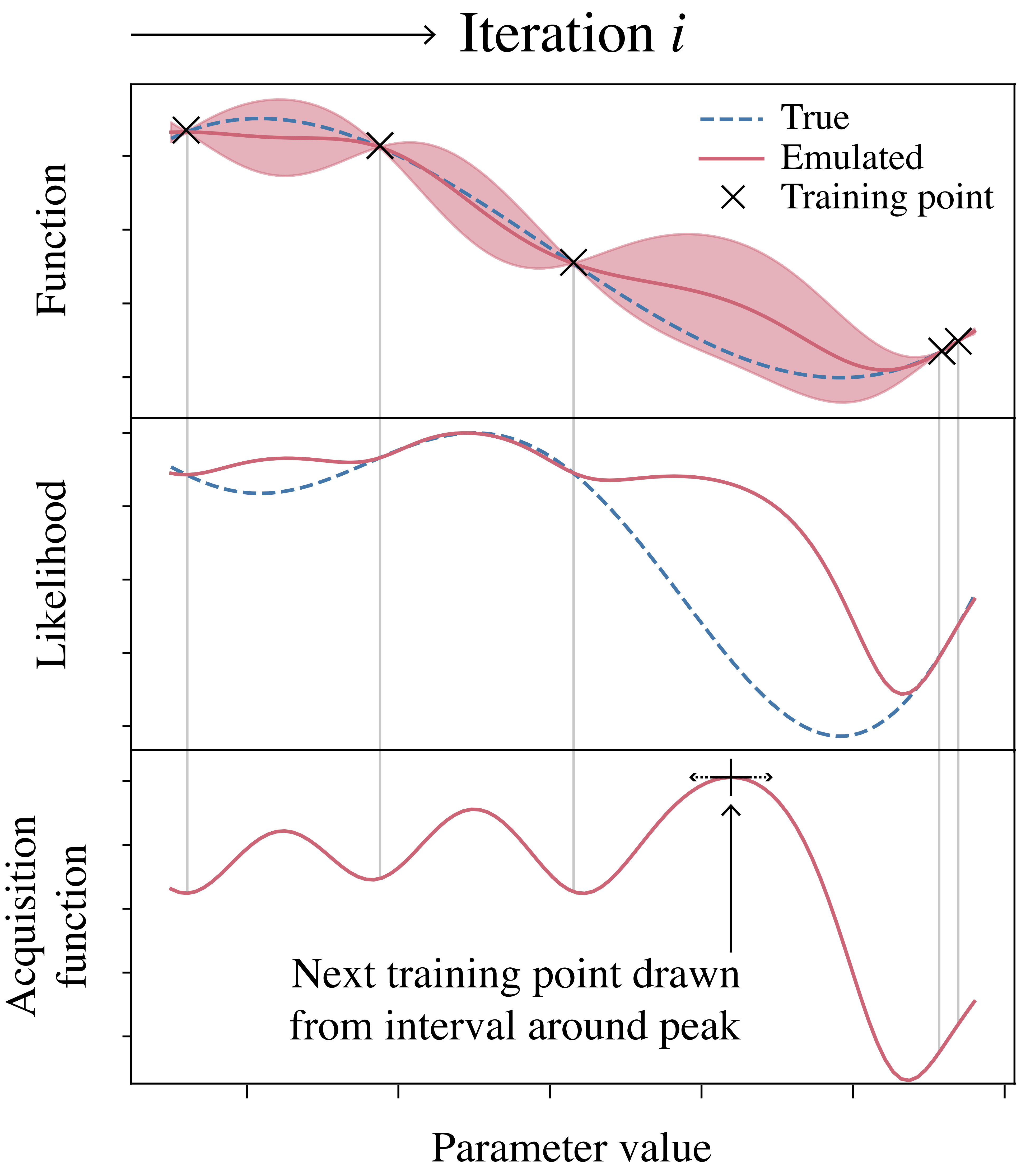
Simulation output

Simulation parameters

Kernel hyperparameters (covariance model)

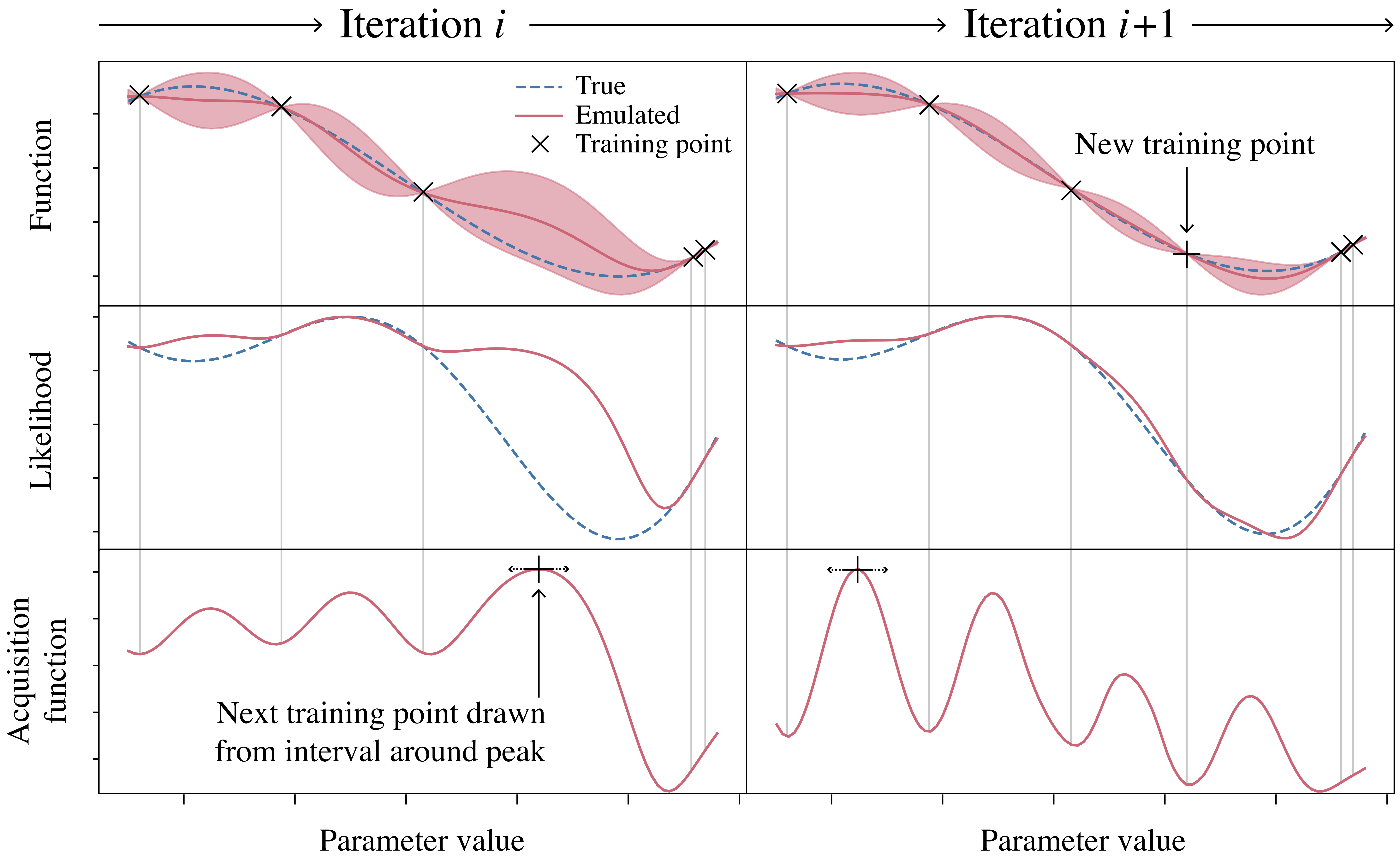
Figure: Leclercq (2018)

Key idea: active learning via Bayesian optimisation



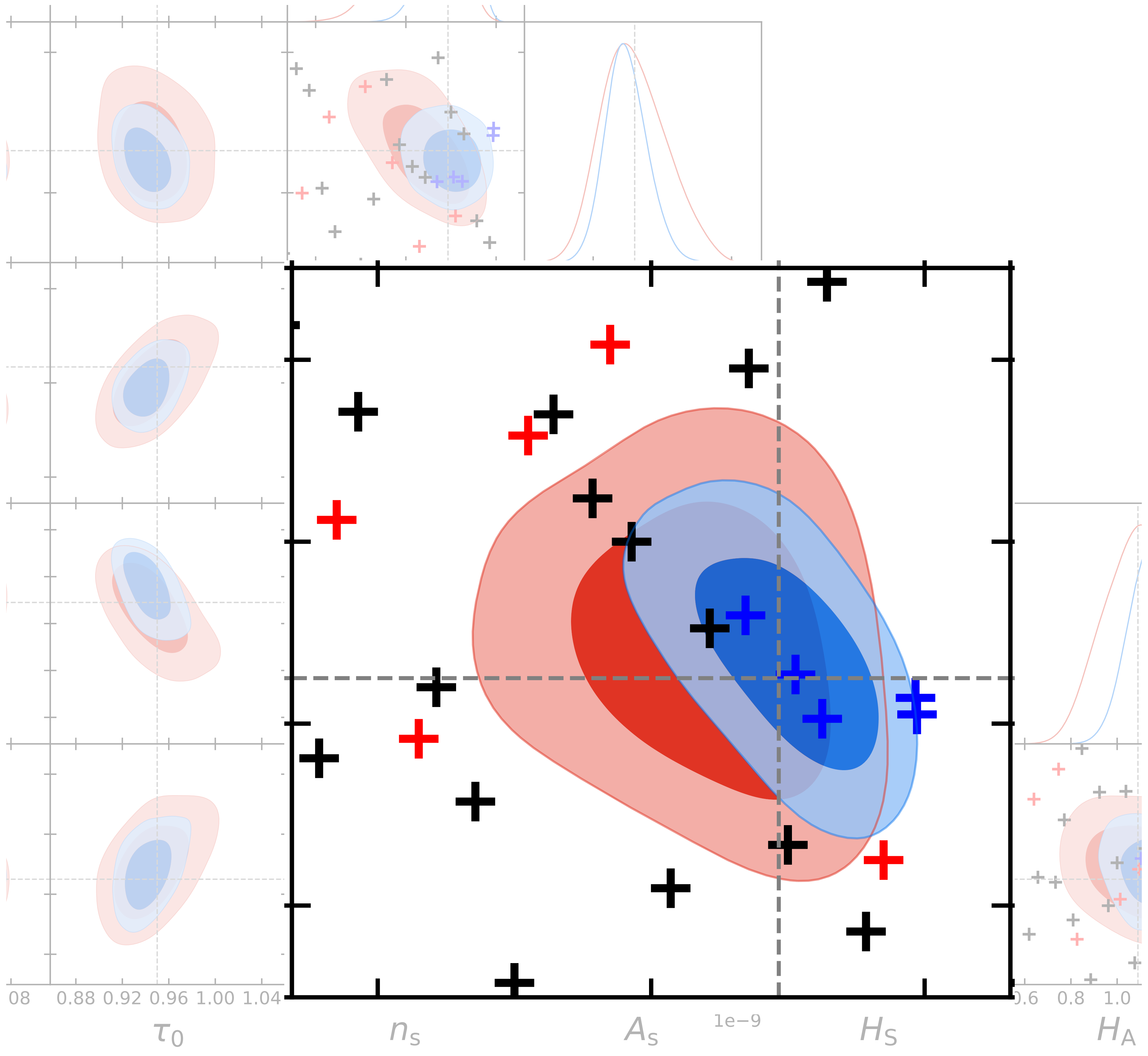
ROGERS & PEIRIS (PRL, PRD, 2021A,B), ROGERS, PEIRIS, PONTZEN, BIRD, VERDE & FONT-RIBERA (JCAP, 2019), LECLERCQ (PRD, 2018)

Key idea: active learning via Bayesian optimisation



Rogers & Peiris (PRL, PRD, 2021a,b), Rogers, Peiris, Pontzen, Bird, Verde & Font-Ribera (JCAP, 2019), Leclercq (PRD, 2018)

Key idea: active learning via Bayesian optimisation

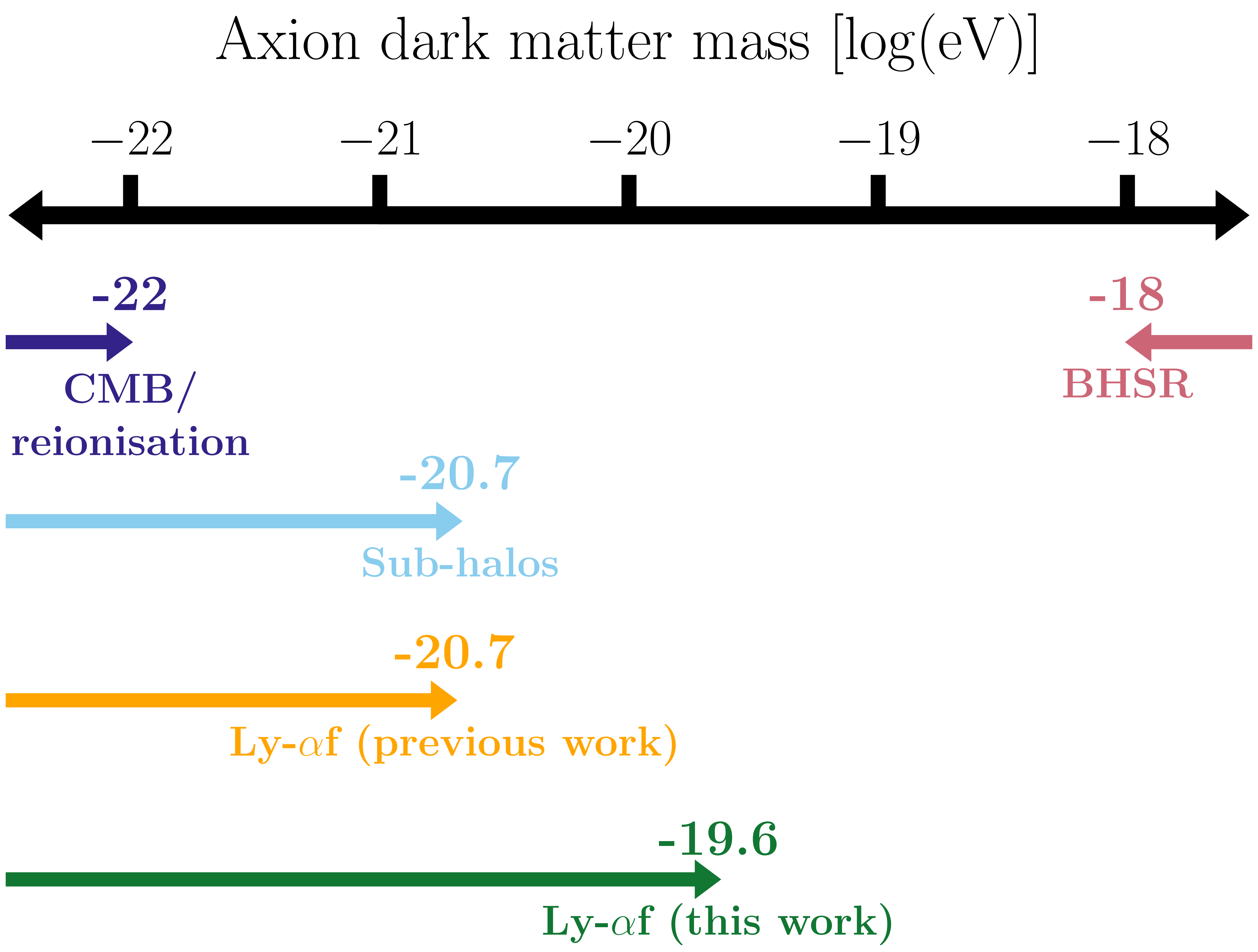


Large Latin hypercube (30 simulations)
Bayesian optimisation (26 simulations)

+ Initial Latin hypercube
+ Extra Latin hypercube simulations
+ Optimisation simulations

Rogers & Peiris (PRL, PRD, 2021a,b), Rogers, Peiris, Pontzen, Bird, Verde & Font-Ribera (JCAP, 2019), Leclercq (PRD, 2018)

"Canonical" 10^{-22} - 10^{-21} eV ULA dark matter strongly disfavoured

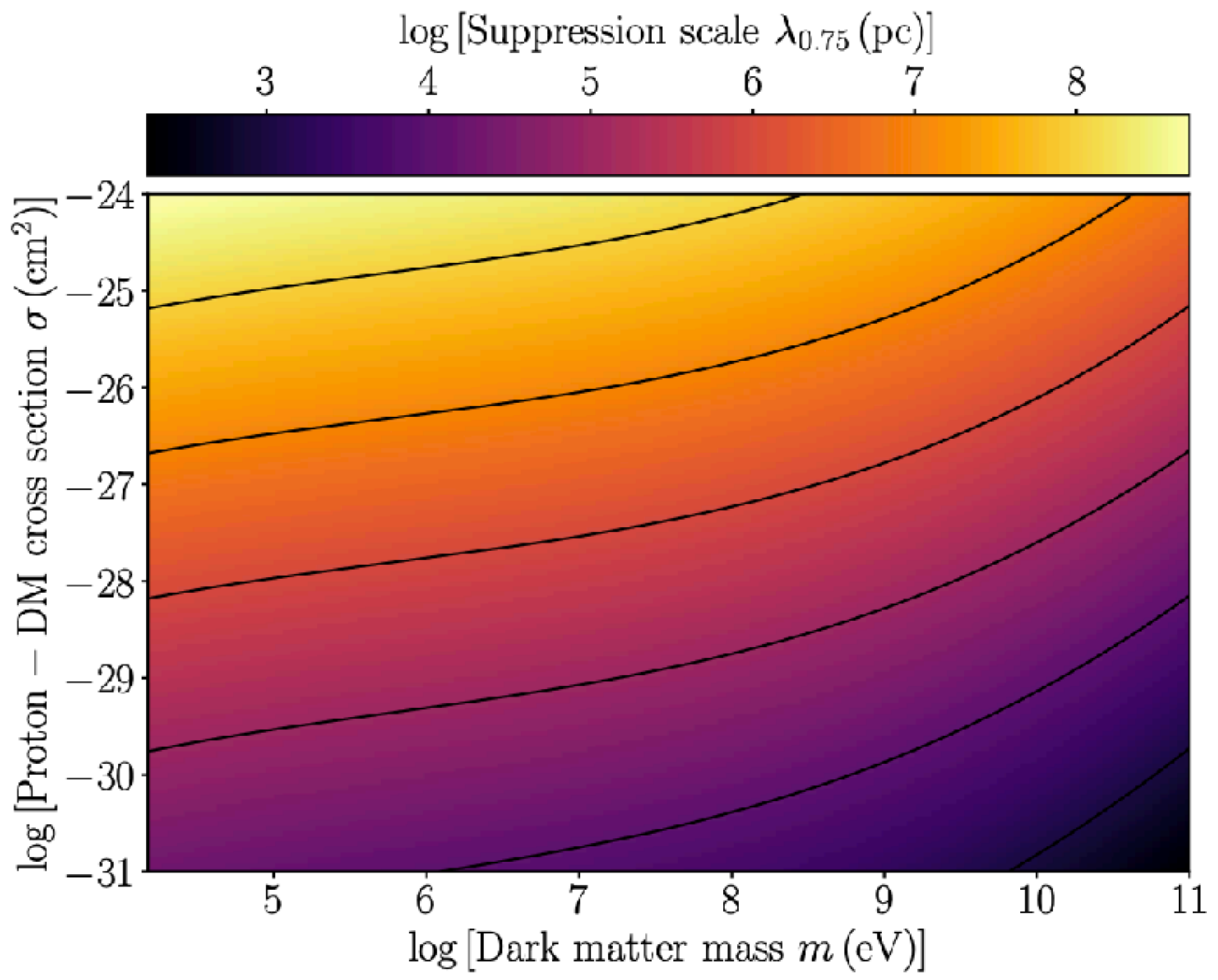


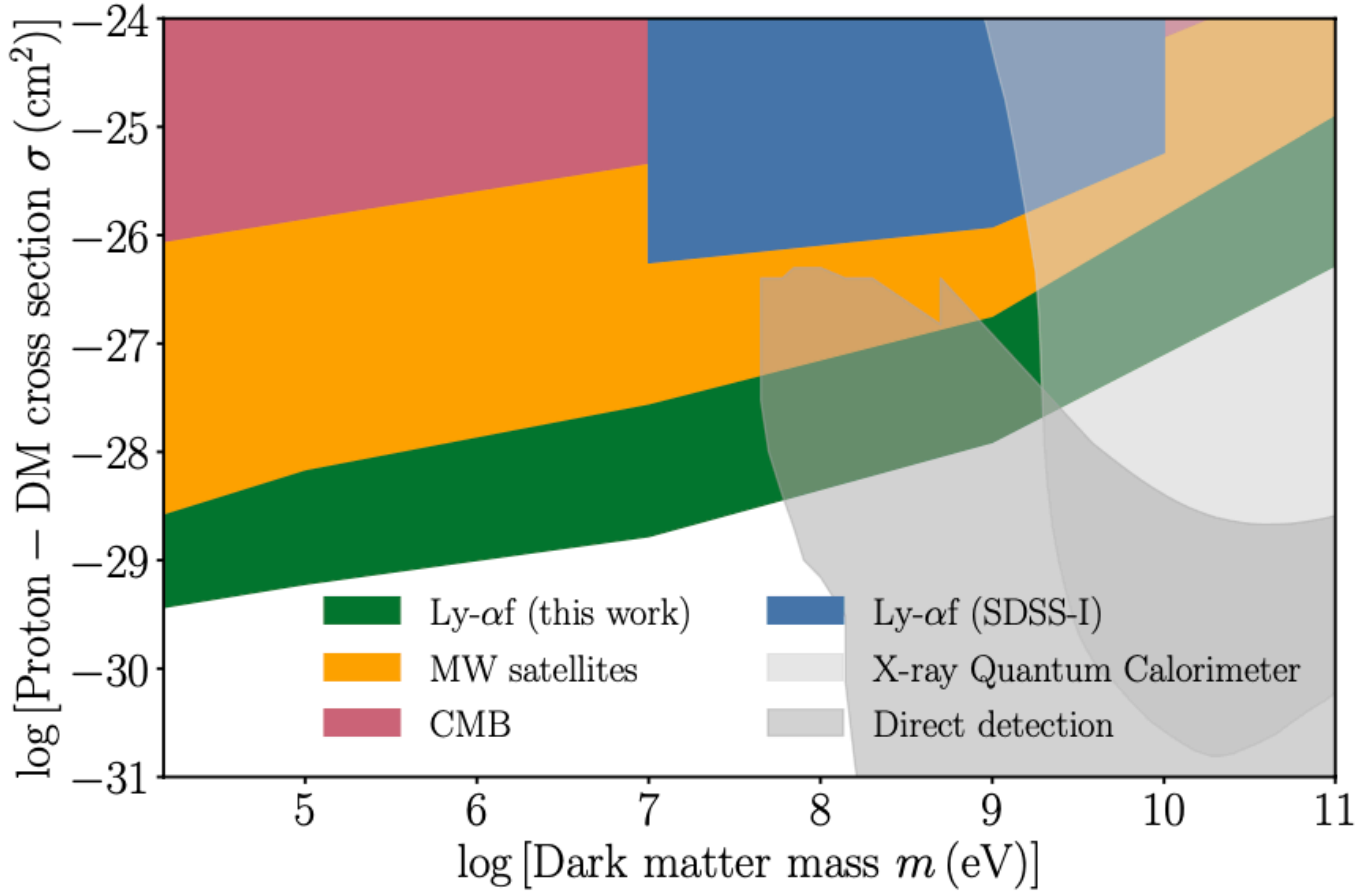
$$m_{\mathrm{a}} > 2 \times 10^{-20}\,\mathrm{eV}$$

Improved bound by ~ order of magnitude

Rogers & Peiris (2021a,b, Phys. Rev. Lett; Phys. Rev. D)

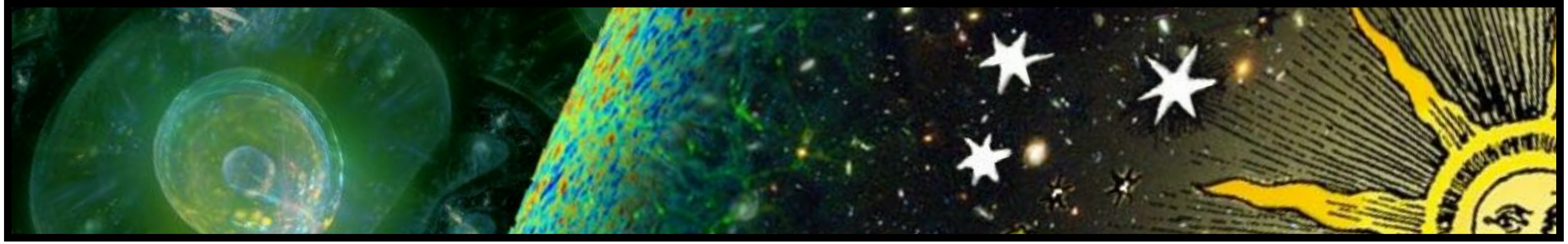
New Lya limits on light dark matter – proton cross section





Strongest limits to-date on velocity-independent dark matter (DM) – proton cross section σ for DM masses m = 10 keV to 100 GeV

ROGERS, DVORKIN & PEIRIS (PRL ACCEPTED, 2111.10386)



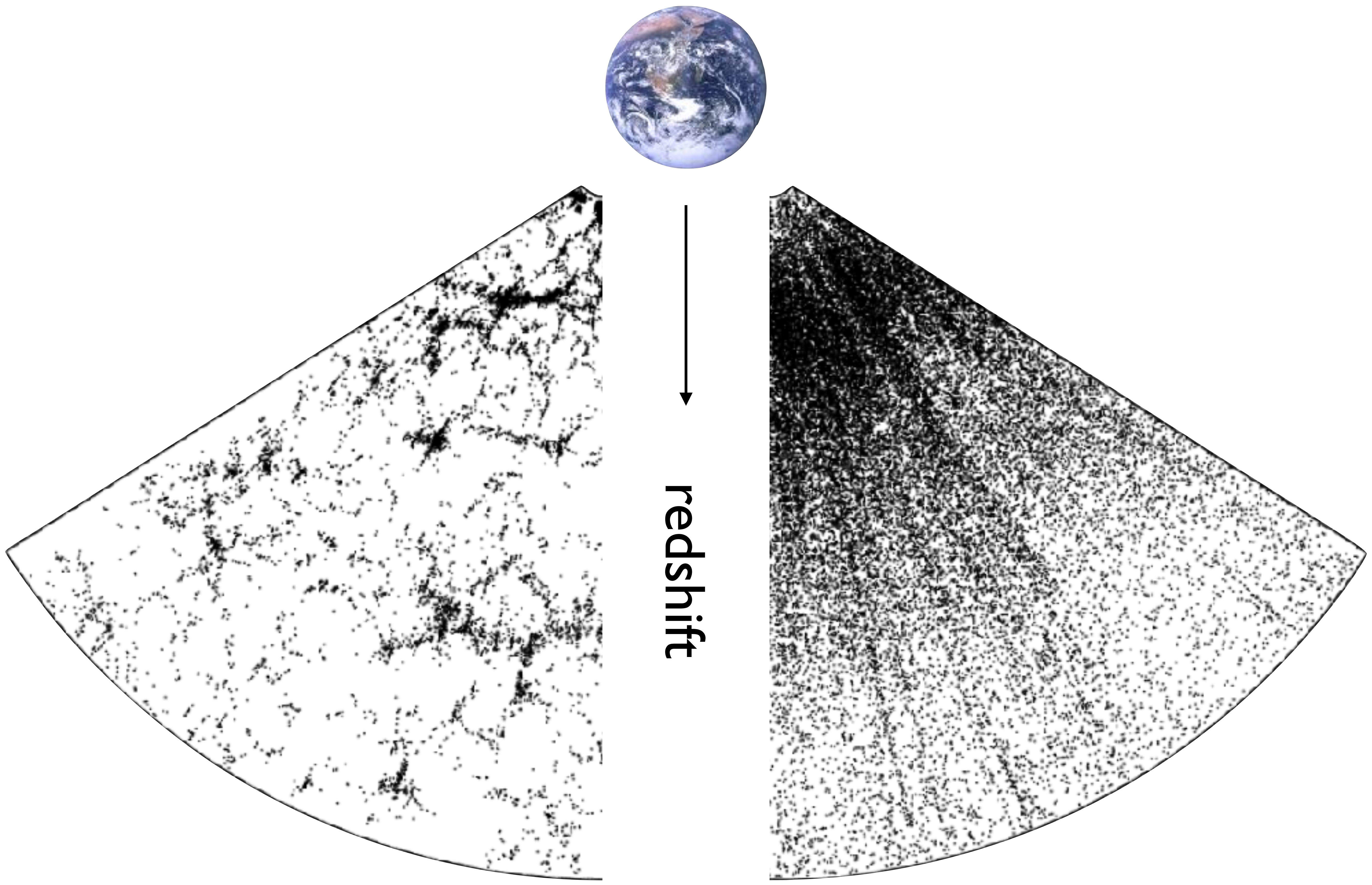
Bayesian hierarchical models with machine learning components

Justin Alsing
(OKC/Stockholm)

Boris Leistedt
(Imperial College London)

With: Joel Leja, Daniel Mortlock, George Efstathiou

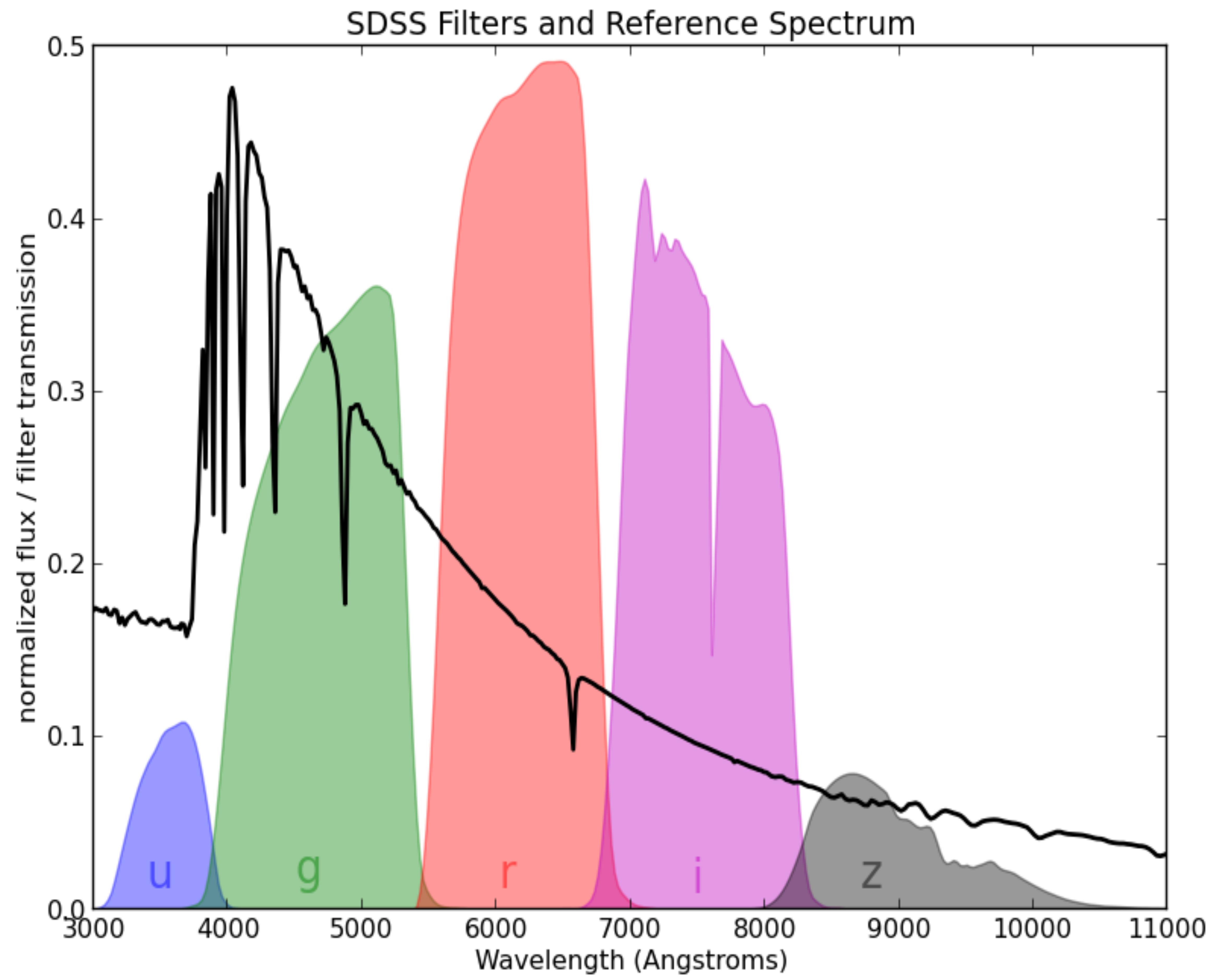
Observational frontier with galaxy surveys



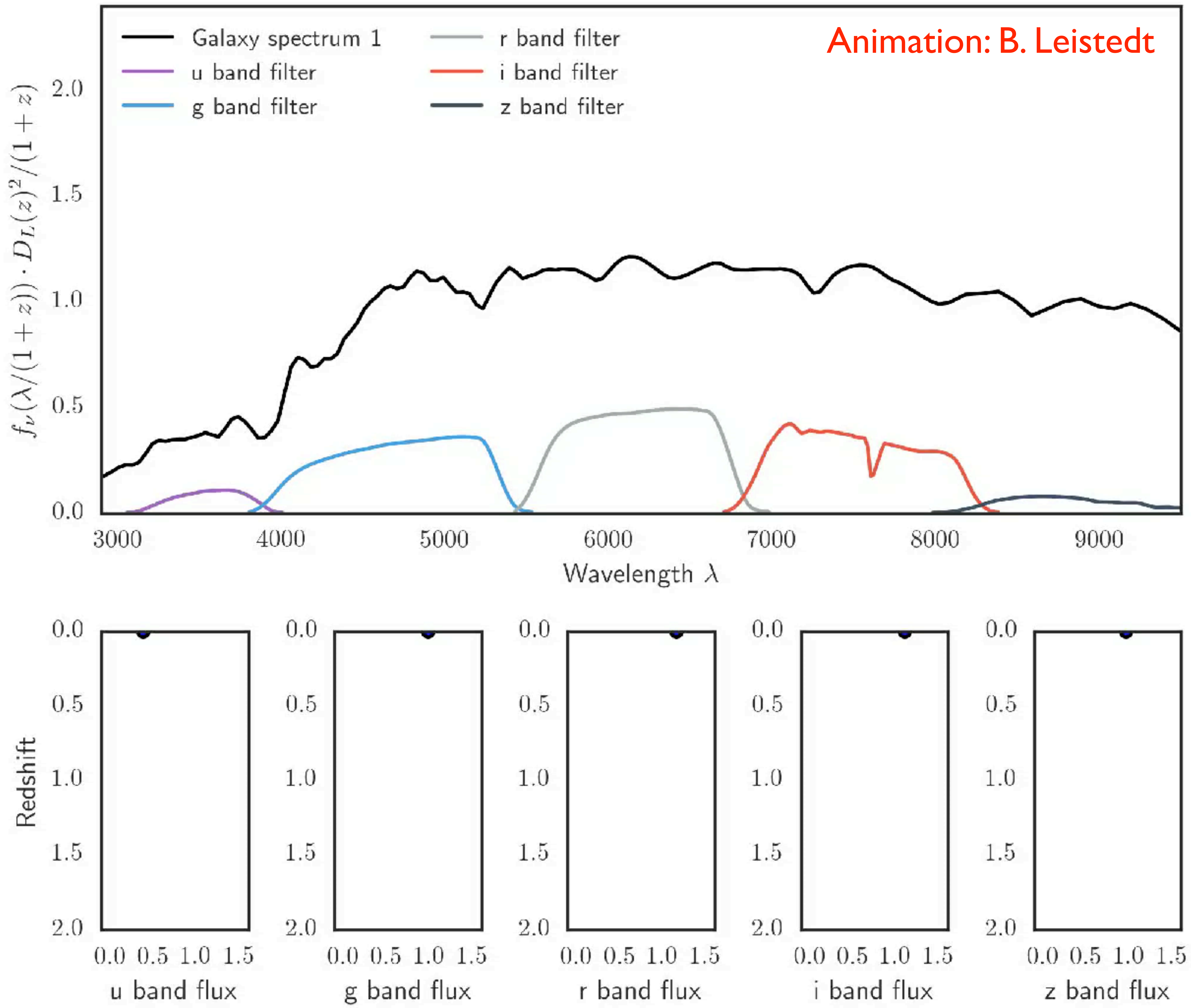
<u>Spectroscopic</u>
DESI (ground)

<u>Photometric</u>
LSST (ground), Euclid (space), Roman (space)

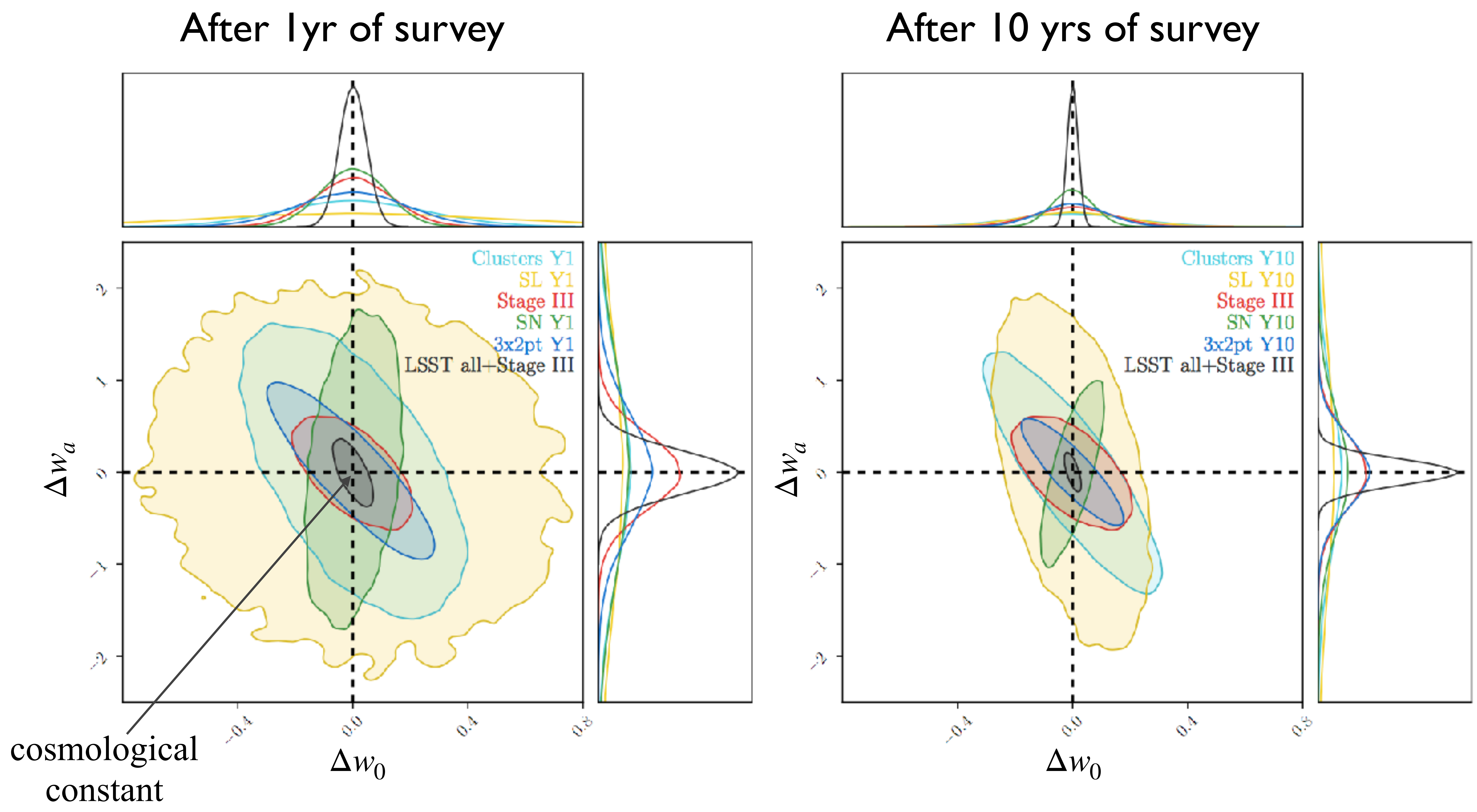
Spectroscopic vs photometric samples



Photometric catalogues require ***redshift estimation***


Animation: B. Leistedt
Galaxy spectrum 1
u band filter
g band filter
r band filter
i band filter
z band filter
$f_\nu(\lambda/(1+z)) \cdot D_L(z)^2/(1+z)$
Wavelength λ
Redshift
u band flux
g band flux
r band flux
i band flux
z band flux

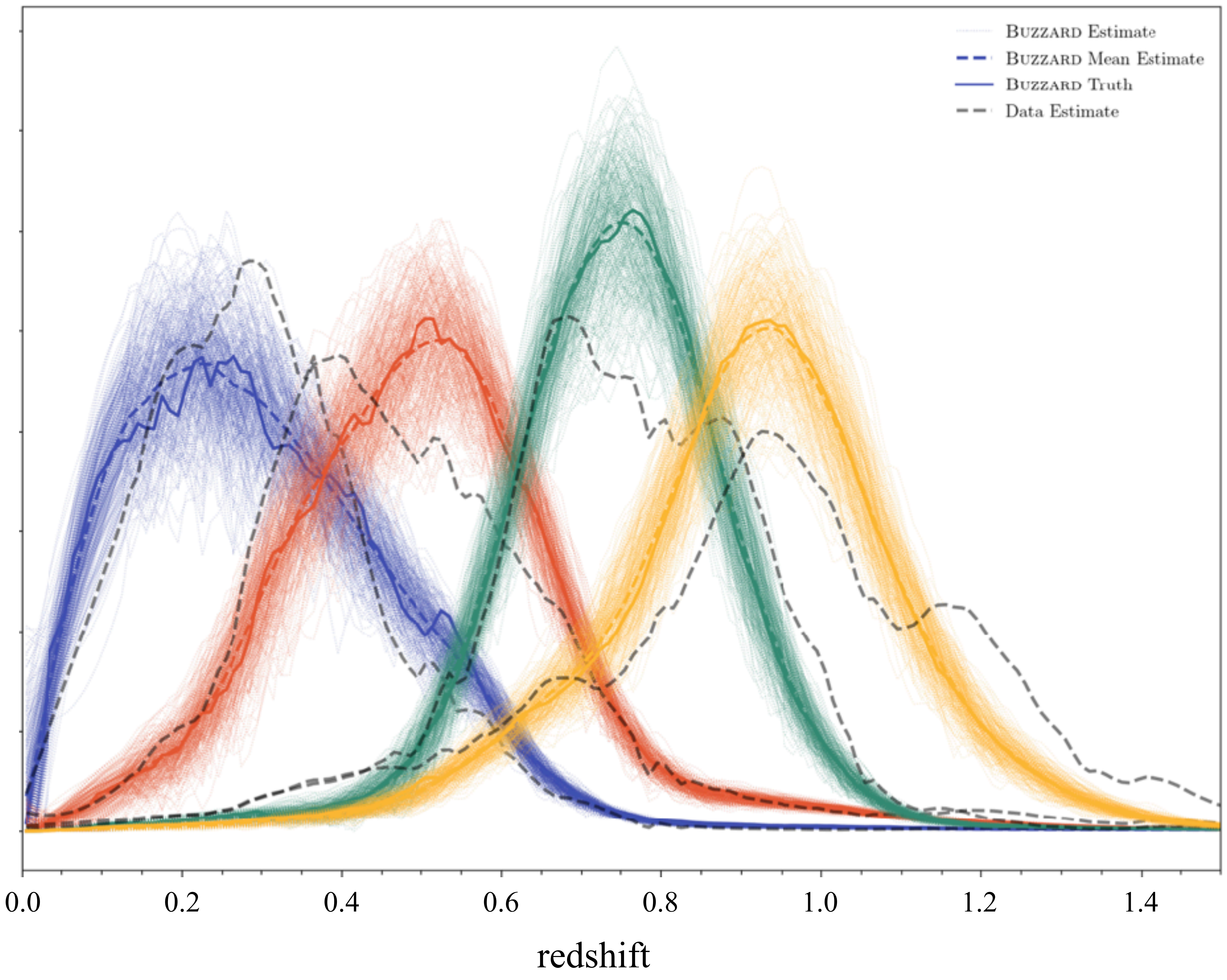
LSST and Dark Energy Science



Measuring if / how dark energy evolves with time

Forecasts: LSST DESC Collaboration

N(z) inference is challenging

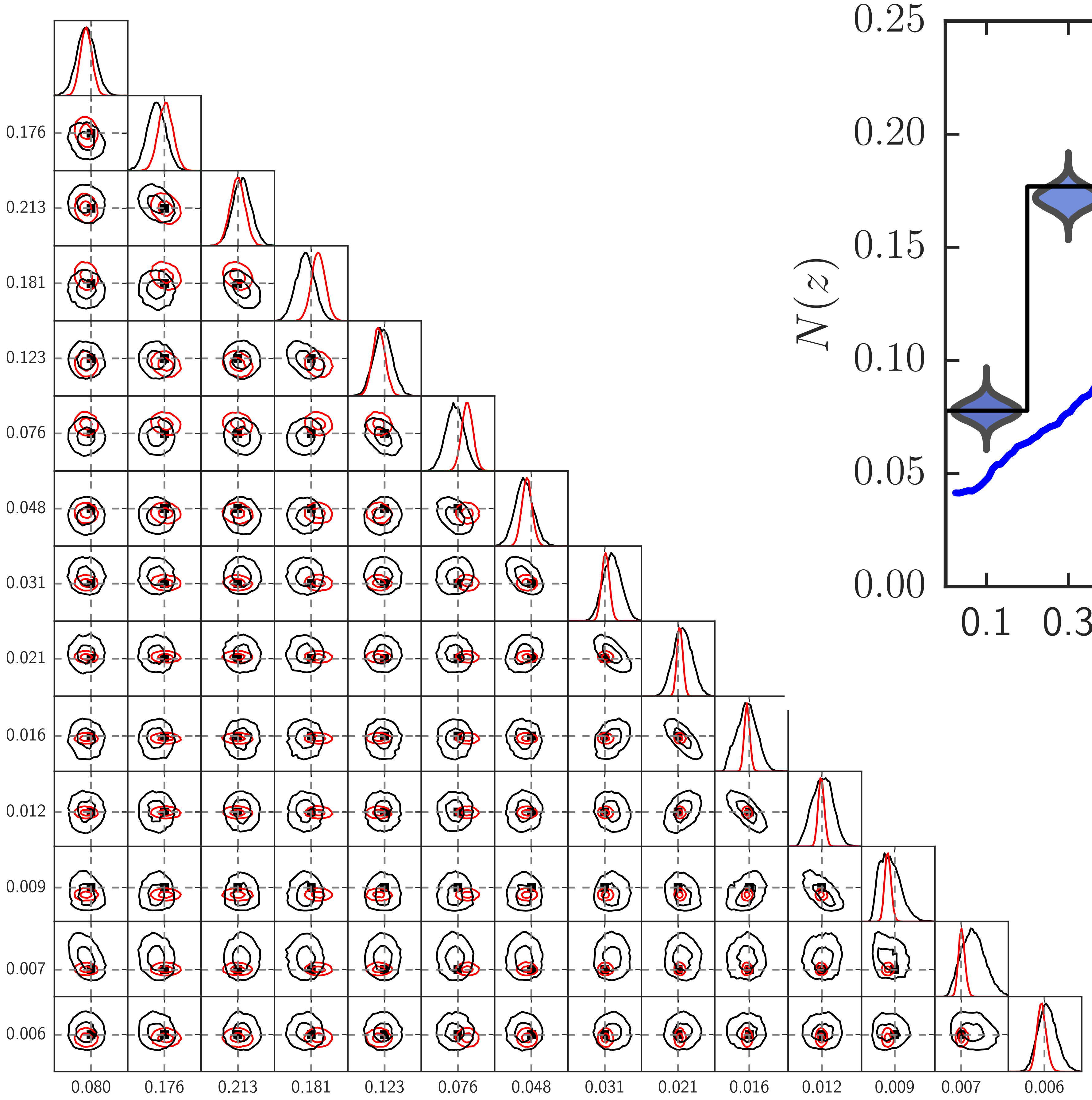


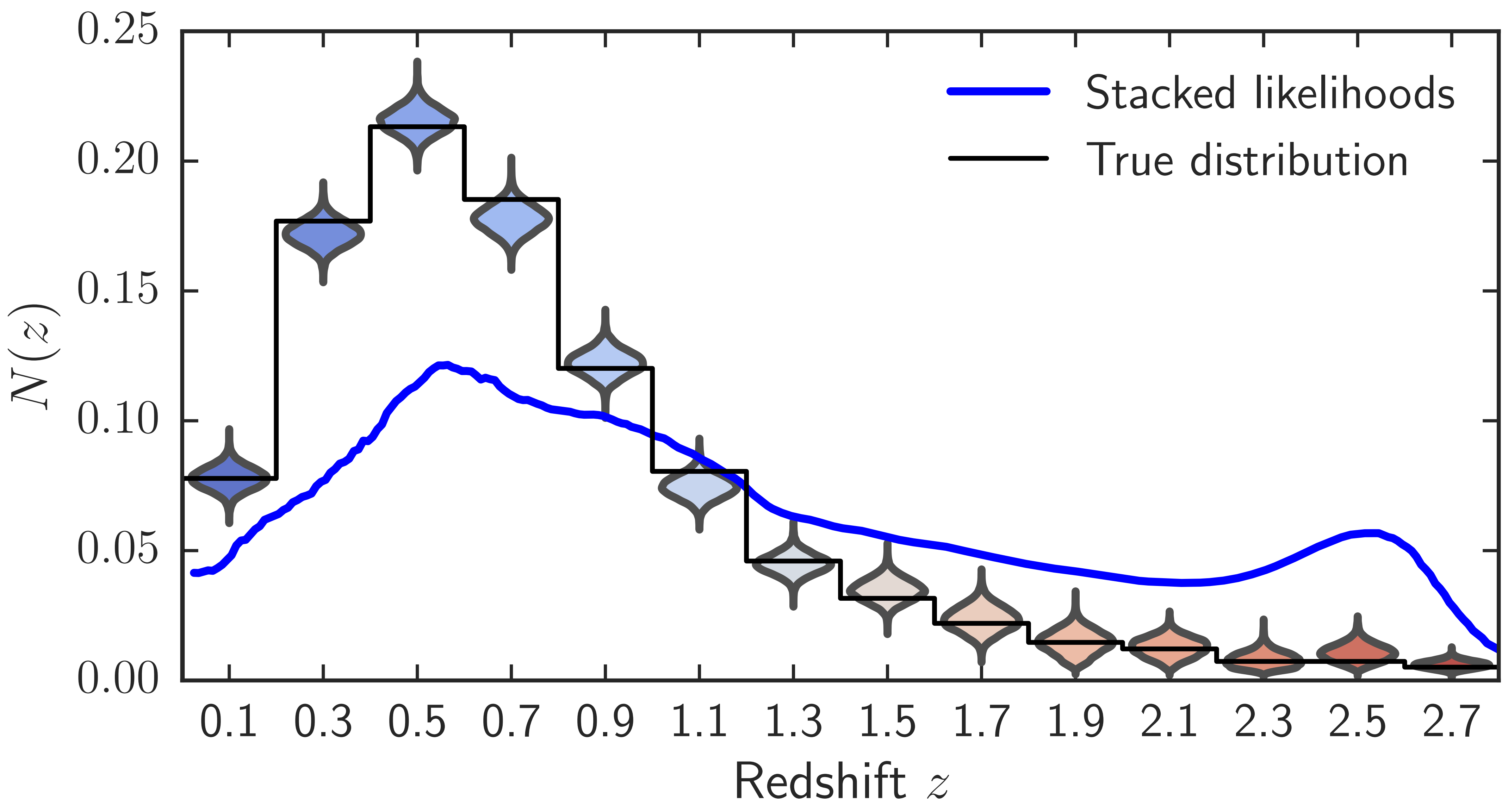
- *Spectroscopic training / calibration samples are:*
  - *not representative of photometric catalogues (due to brighter flux limits and population evolution)*
  - *heterogeneous and contain difficult-to-model selection effects*
- *Introduces biases which are difficult to mitigate at required precision*

Figure: Myles et al (DES Collaboration 2021)

Hierarchical Bayesian Model for N(z) inference

- **Sources:** p(fluxes | z,t,m) likelihood based on spectral energy distribution (SED) templates
- **Population:** Histogram representation of p(z,t,m) parameterized by {fijk}
- Jointly infer {z,t,m} per source and {fijk} using Gibbs sampler



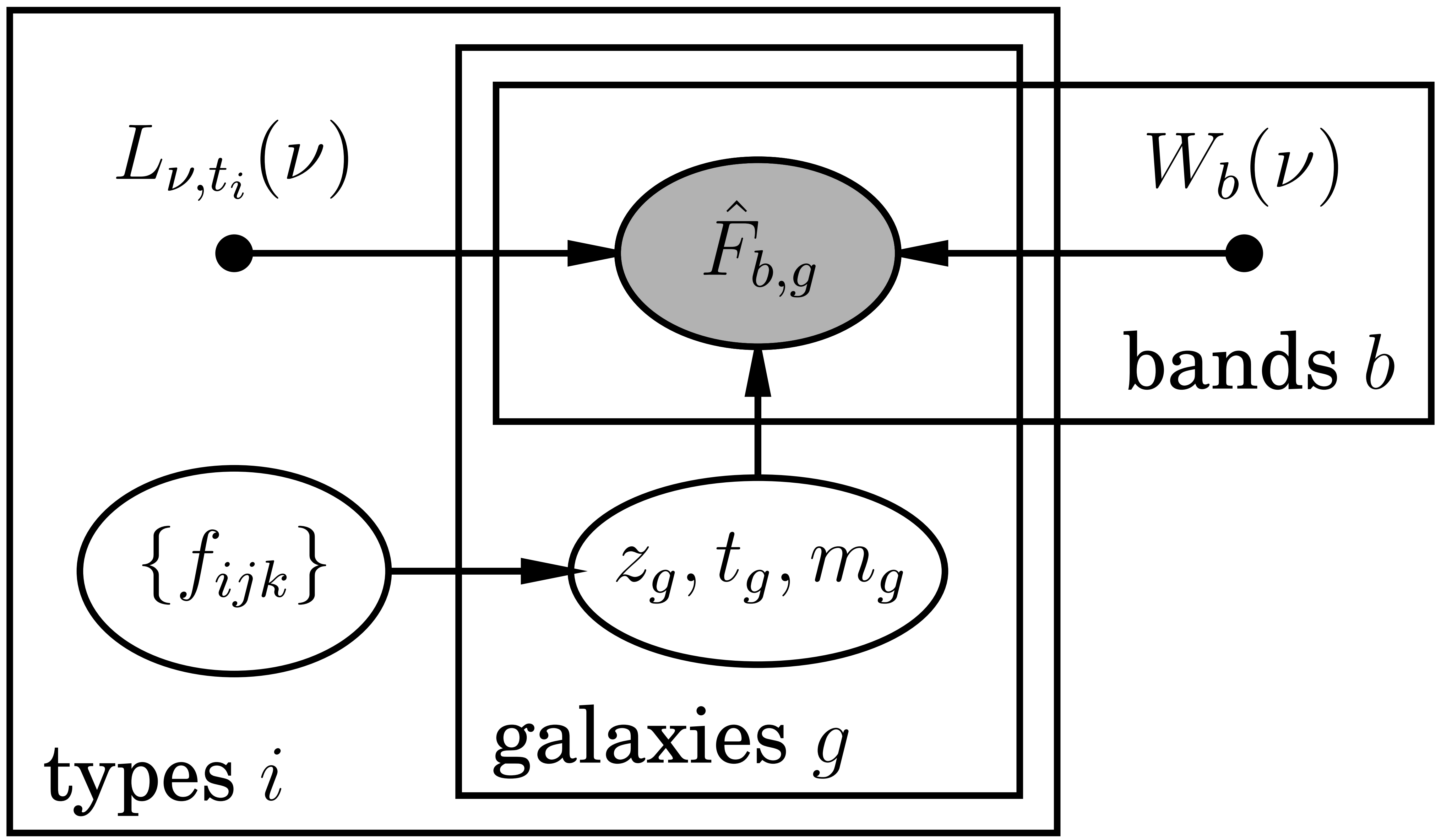


Full posterior distribution for N(z)

cosmological likelihoods

LEISTEDT, MORTLOCK & PEIRIS (MNRAS, 2016)

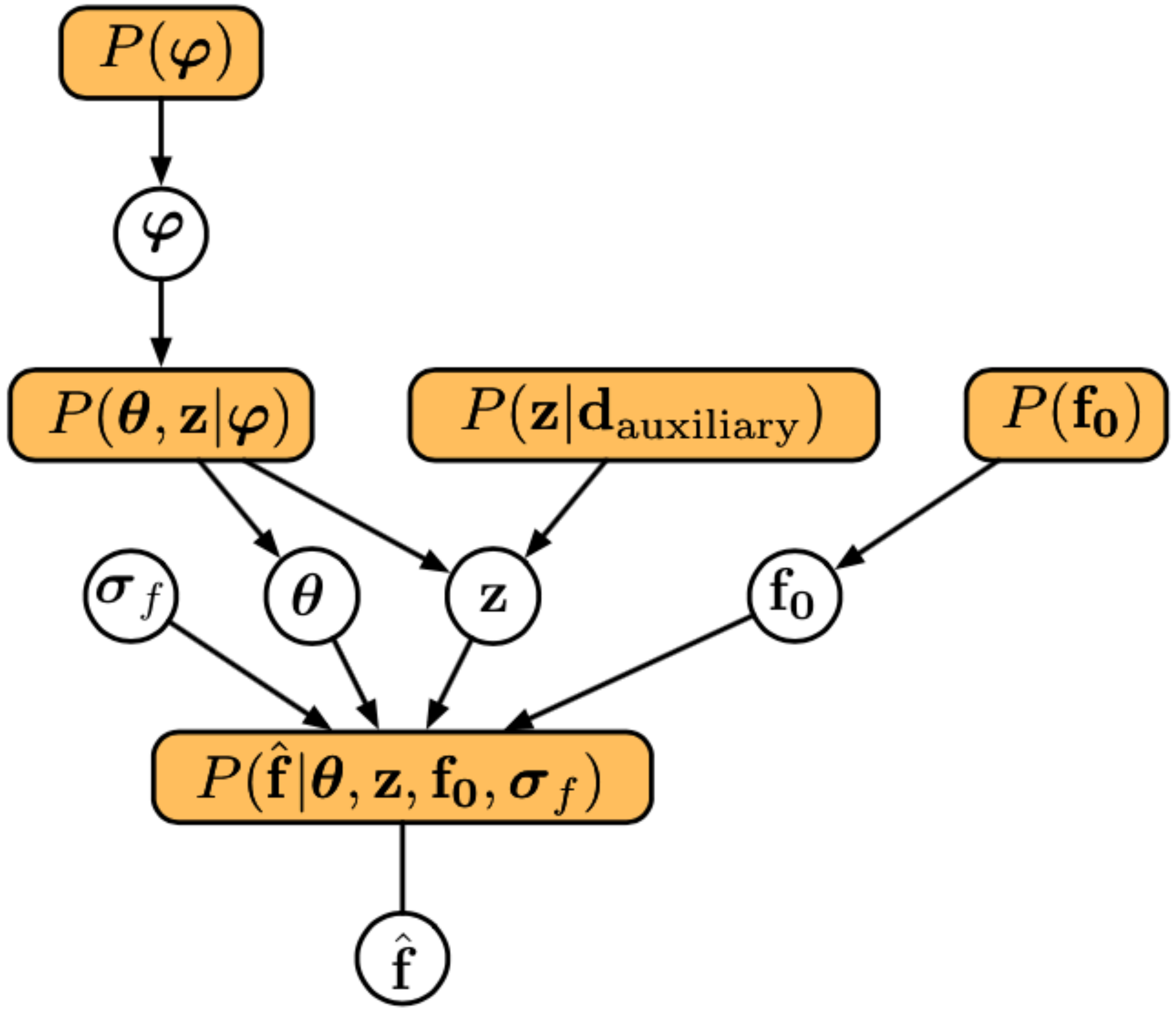
Challenges



- *Bayesian hierarchical inference based on selection of SED templates and simple population assumptions are limited*
- *Discrete templates do not characterise full diversity of galaxy SEDs*

Redshift distribution inference for static cosmology

- **Key idea:** *high-dimensional Bayesian hierarchical model with machine-learned parts.*



- *Neural network emulation of FSPS population synthesis model, describing realistic galaxy populations (replace templates).*

- *Flexible NN-parameterised probability density models (e.g. normalising flows) to describe population prior and selection effects.*

ALSING, PEIRIS, LEJA, HAHN, TOJEIRO, MORTLOCK, LEISTEDT, JOHNSON, CONROY (APJS, 2020) + WIP;
LEISTEDT, MORTLOCK AND PEIRIS (MNRAS, 2016)

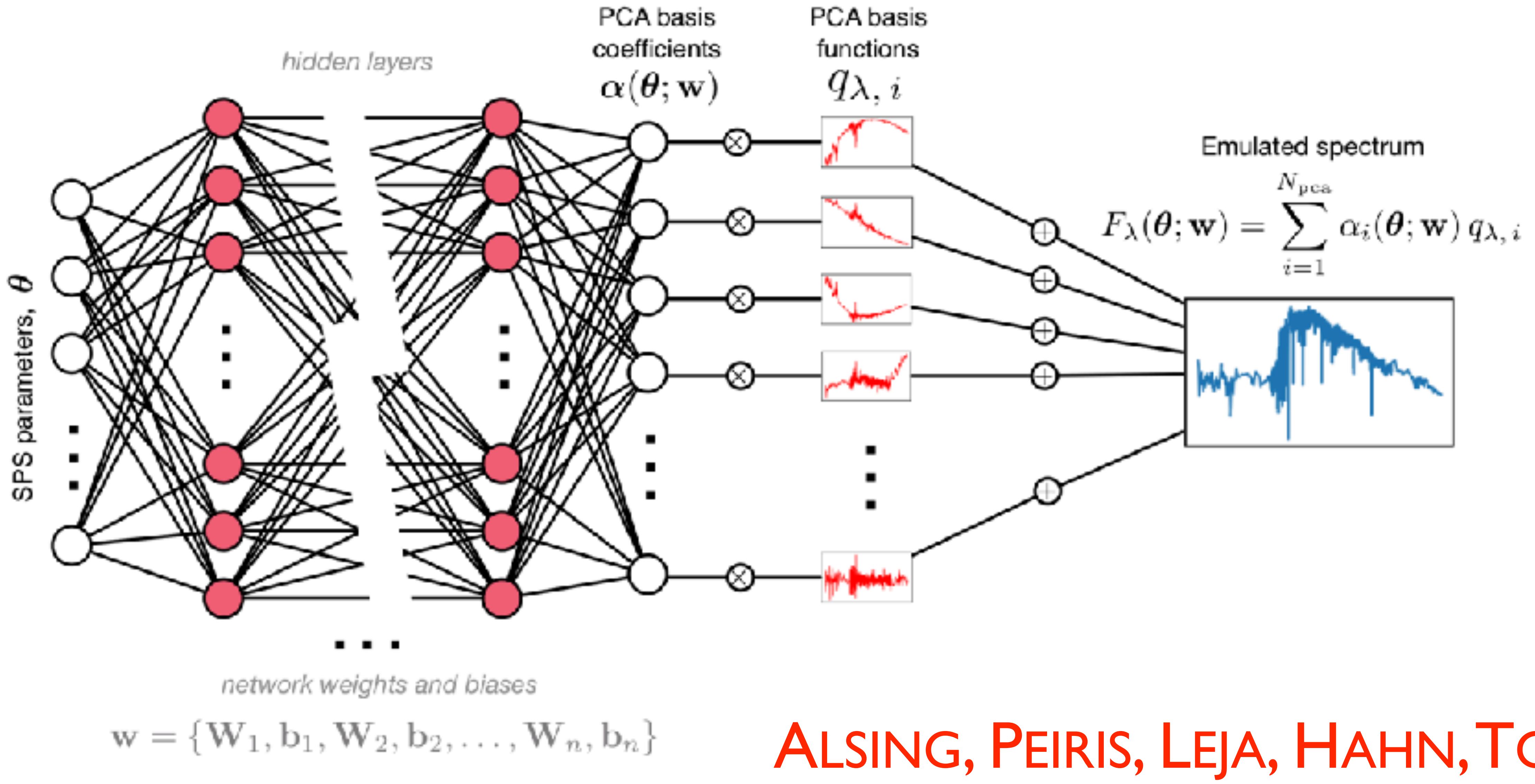
Emulating stellar population synthesis (SPS) models

- *SPS models (e.g. FSPS, Charlie Conroy and collaborators) are fast (<1 sec) but use cases require* ***large numbers of model evaluations****.*

  - *Stage IV galaxy survey catalog sim ~ 10^{10} SPS evaluations*

  - *Leja et al (2019) analysis of 60,000 galaxies under 14-parameter SPS model cost1.5 million CPU-hrs.*

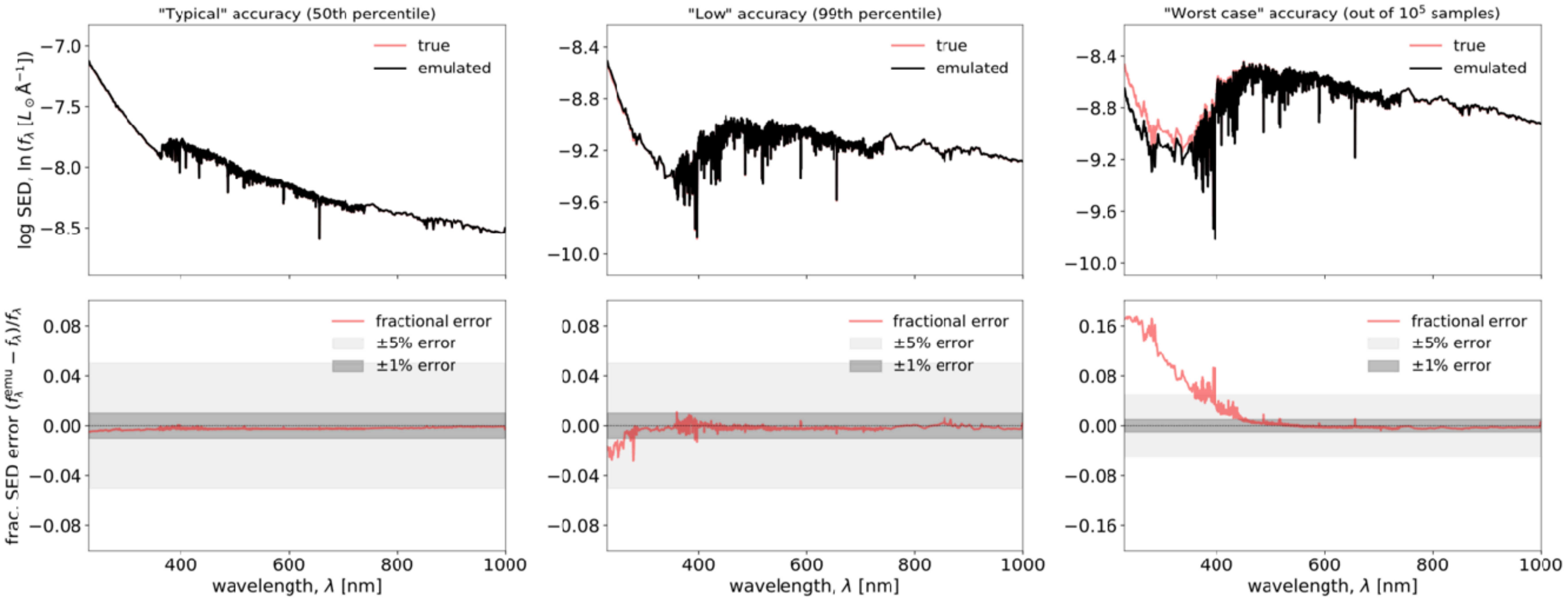
- *Can generate training sets of ~10^5* ***enabling neural network emulators.***



SPECULATOR SPS emulator

ALSING, PEIRIS, LEJA, HAHN, TOJEIRO, MORTLOCK, LEISTEDT, JOHNSON, CONROY (APJS, 2020)

Example: DESI Bright Galaxy Survey SEDs



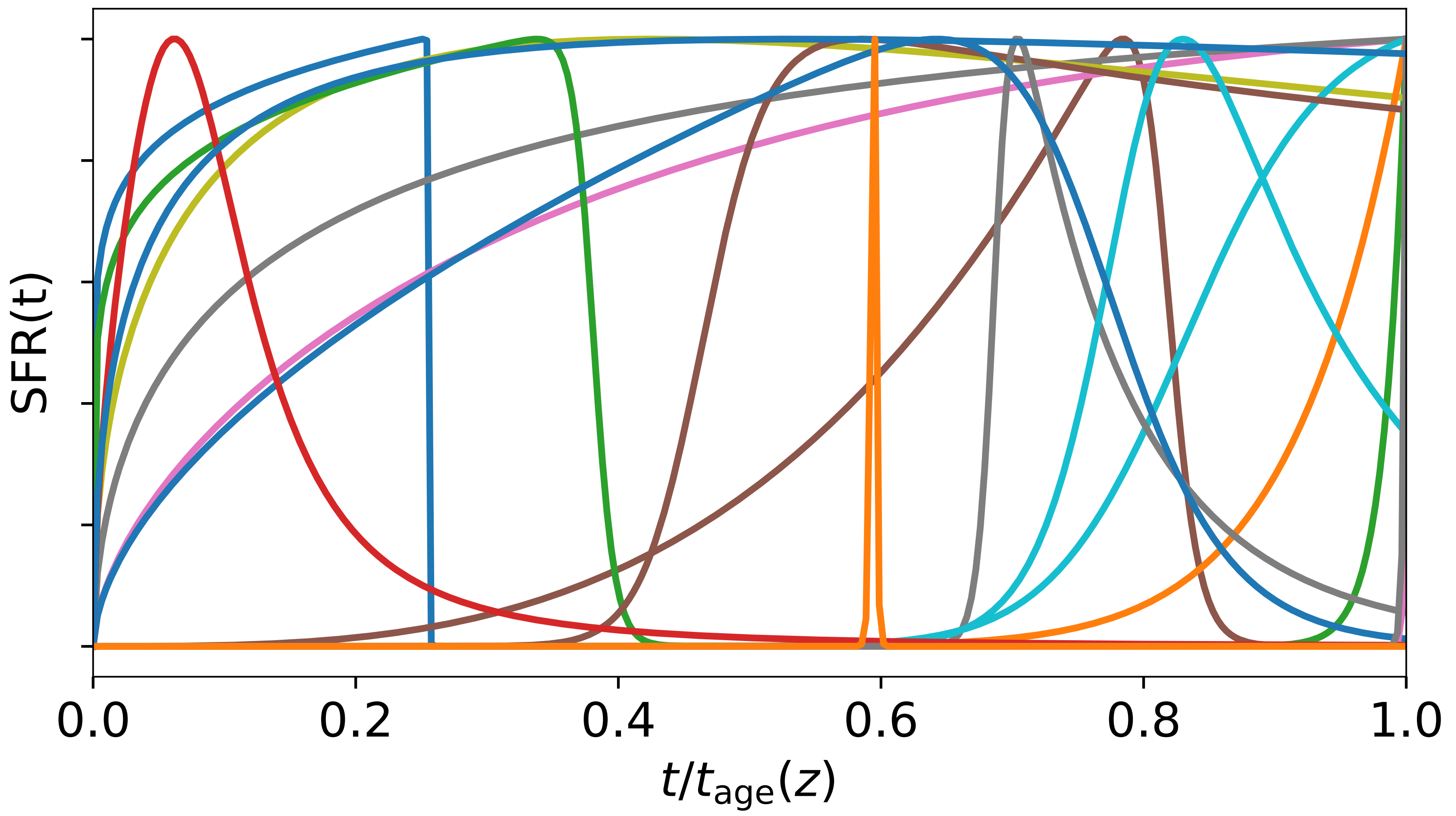
- *Accuracy <1% over the 8-parameter FSPS model for >99% of SEDs*

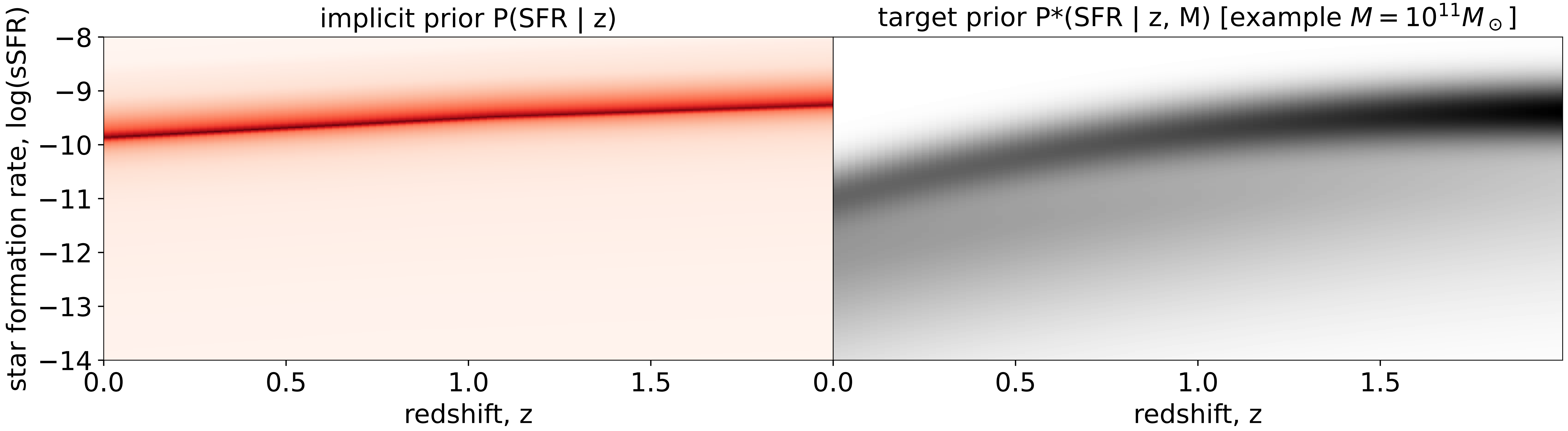
- *Generating 10^6 SEDs takes 2s on Tesla K80 GPU (Speedup 10^5 over FSPS on CPU); inference under SPS models can make use of gradients*

ALSING ET AL. (APJS, 2020)

Prior-matching example: double power-law star formation history

$$\mathrm{SFH}(t) \sim 1/\left[(t/\tau)^{\alpha} + (t/\tau)^{-\beta}\right]$$





Uniform prior on SFH parameters, gives good coverage of plausible SFHs.

Very specific (bad) prior on current star formation rate

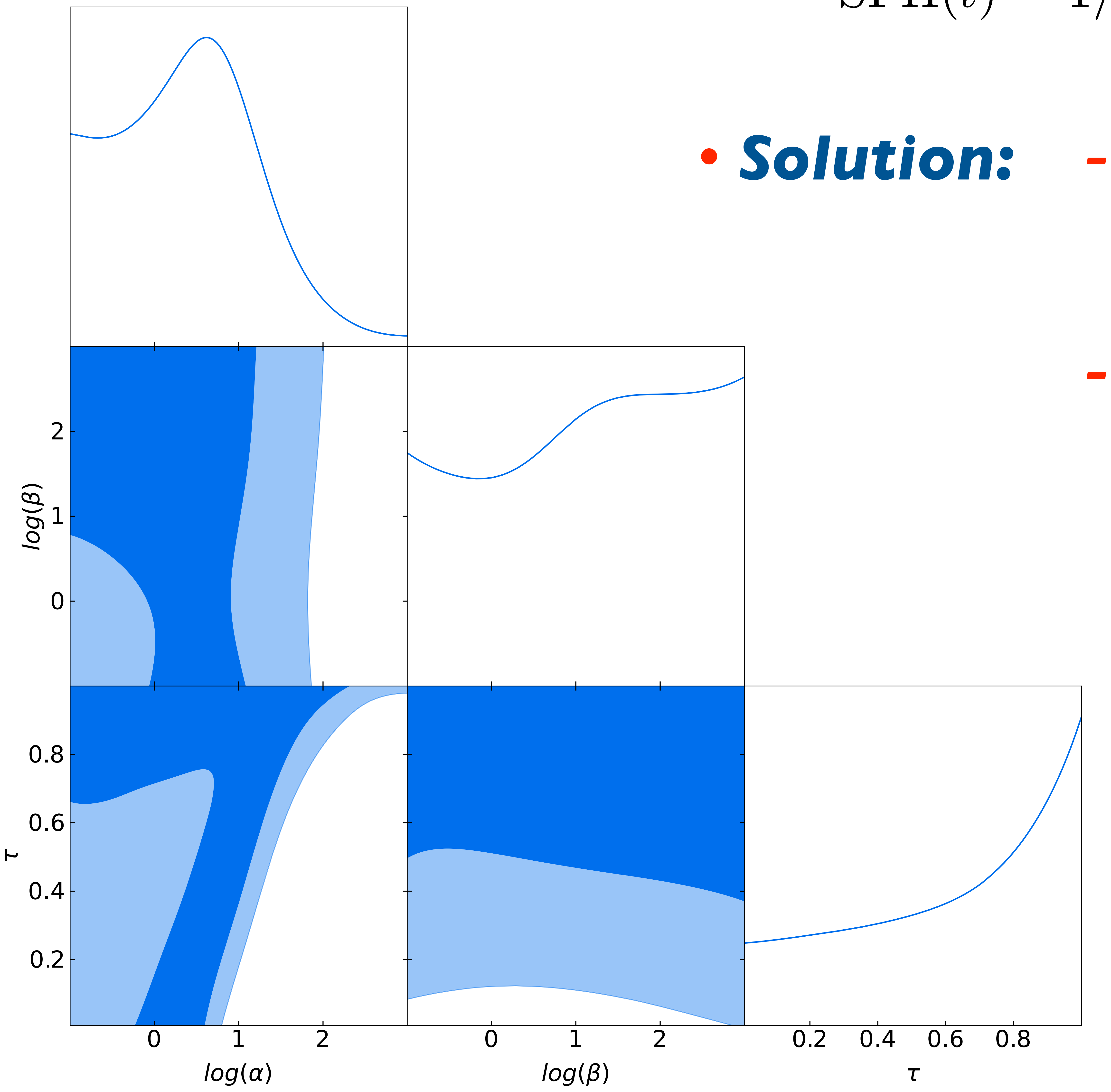
More realistic target prior encoding observations of (more "physical") derived SFH quantities

ALSING ET AL. (IN PREP); TARGET PRIOR FROM LEJA, SPEAGLE ET AL. (2021)

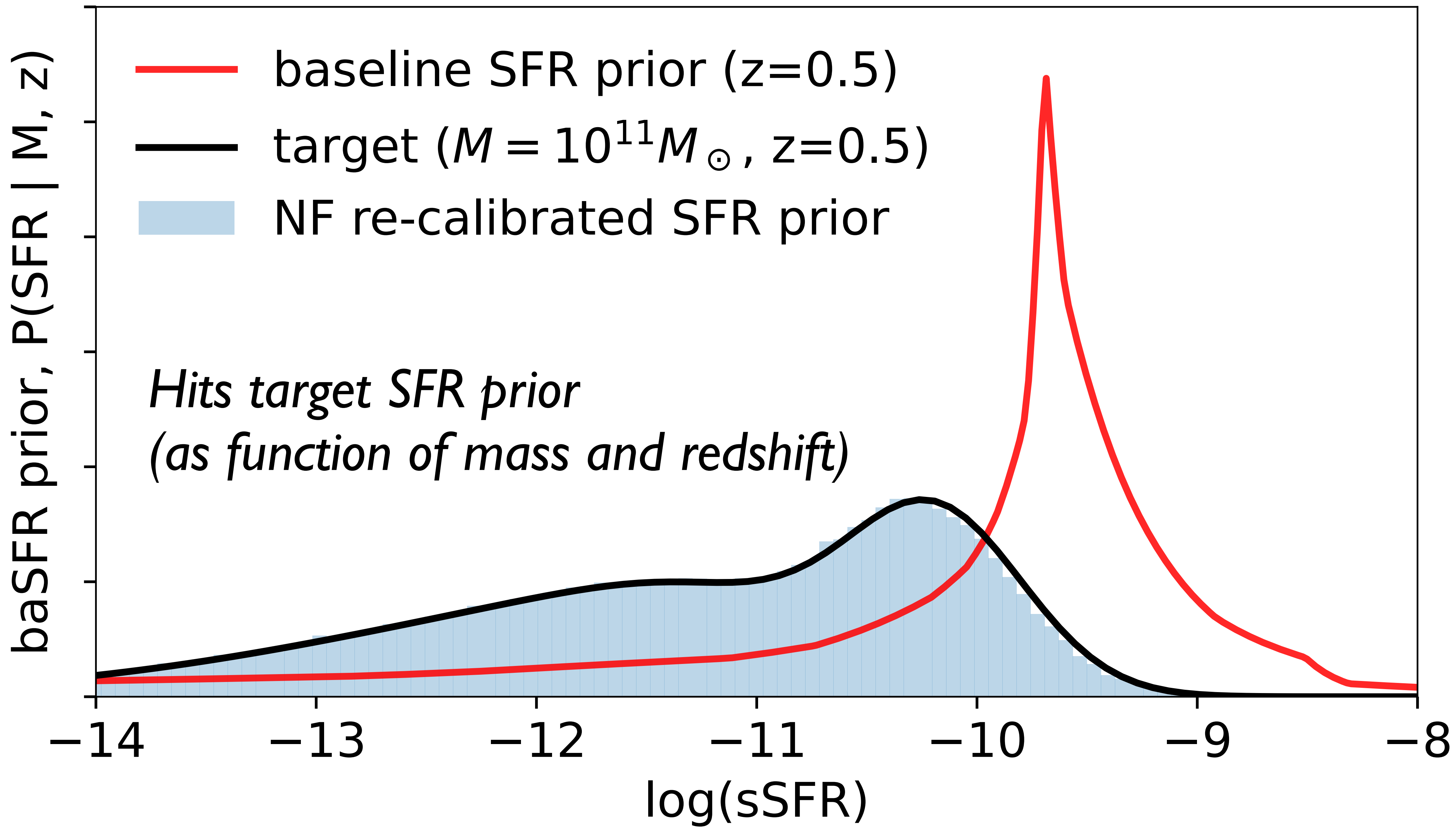
Normalising flows to the rescue

$$\mathrm{SFH}(t) \sim 1/\left[(t/\tau)^{\alpha} + (t/\tau)^{-\beta}\right]$$

- ***Solution:***
  - *Train normalising flow to learn implicit SFR prior P(SFR | z)*
  - *"Divide it out": re-weight prior measure to match target SFR prior P*(SFR | M, z)*



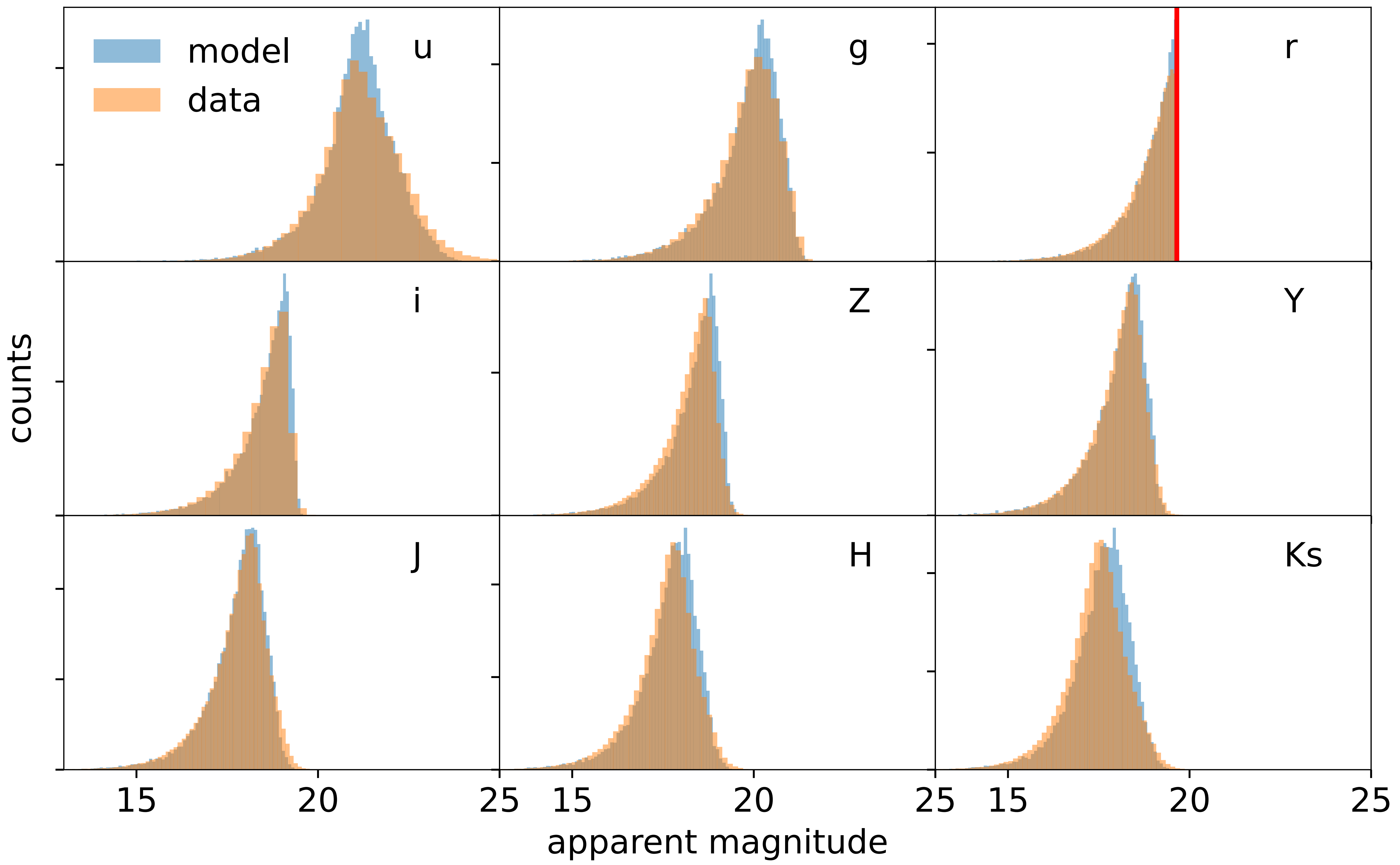
Normalizing flow recalibrated prior on SFH parameters (example at M = 10^{11}, z=0.5)



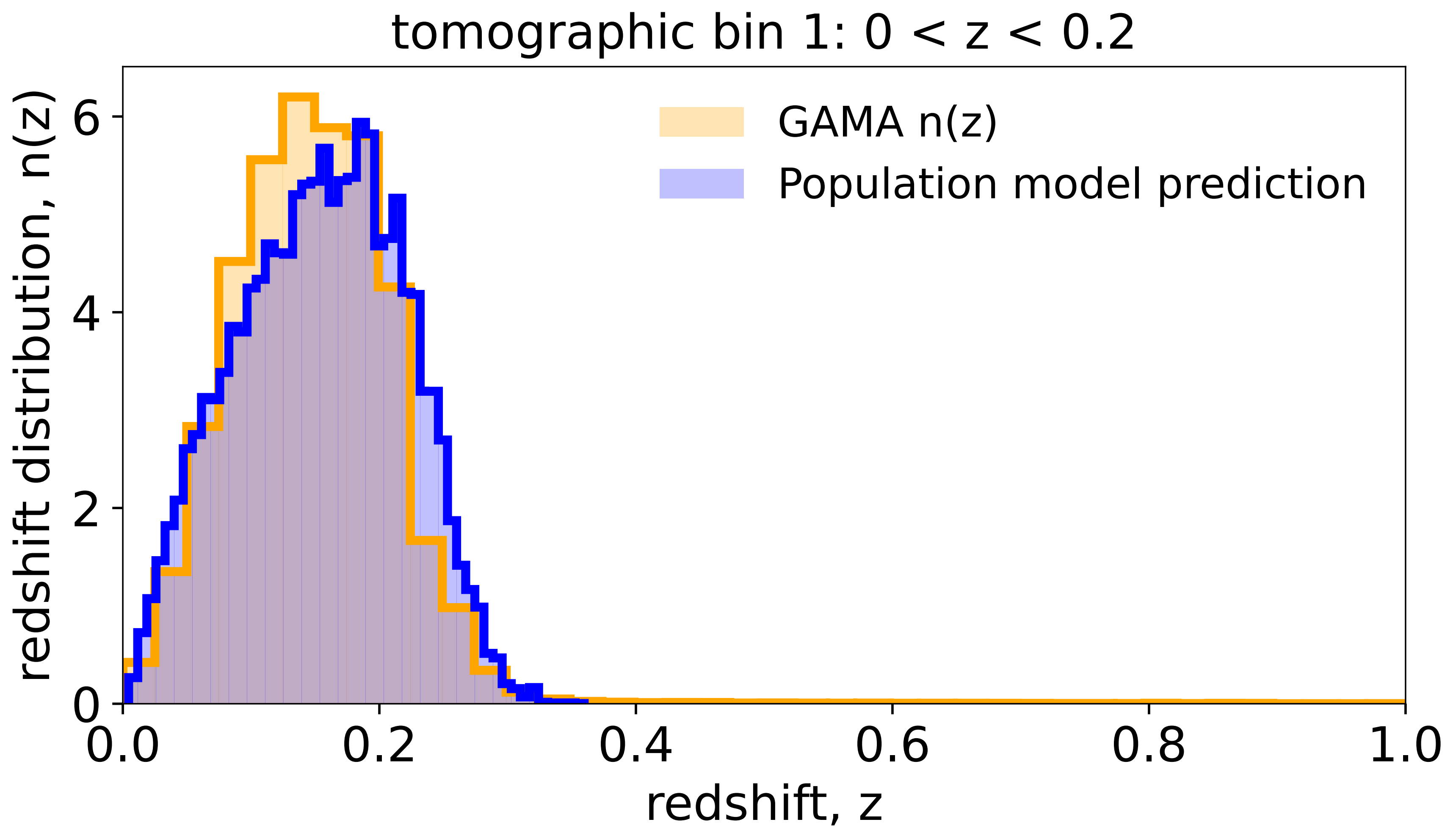
ALSING ET AL. (IN PREP); TARGET PRIOR FROM LEJA, SPEAGLE ET AL. (2021)

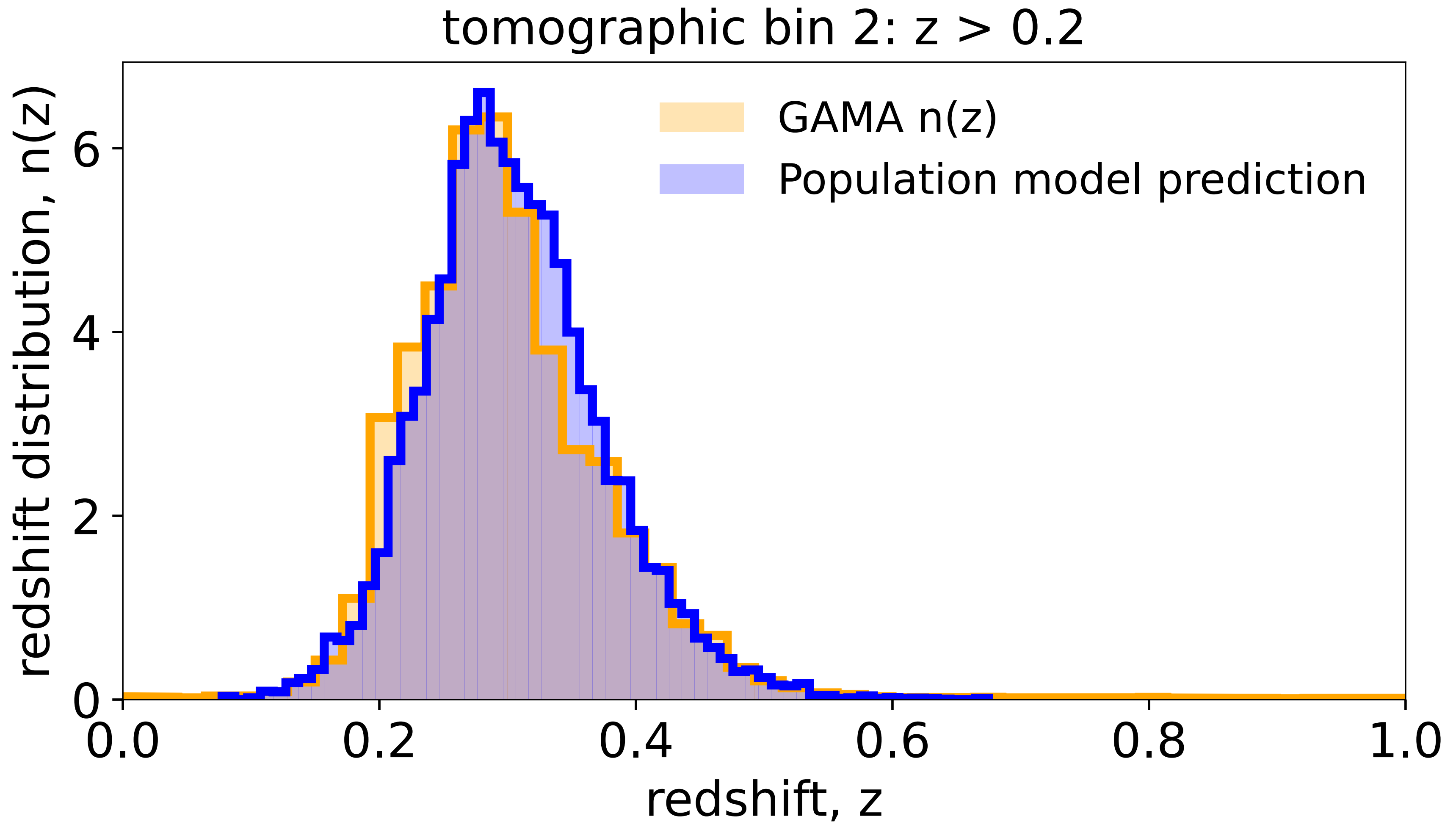
WiP: Population modelling for redshift distribution inference

Does it work? *Simulated galaxy population (encoding galaxy evolution calibrated to observations), combined with data model and selection cuts, should be able to predict redshift distribution.*

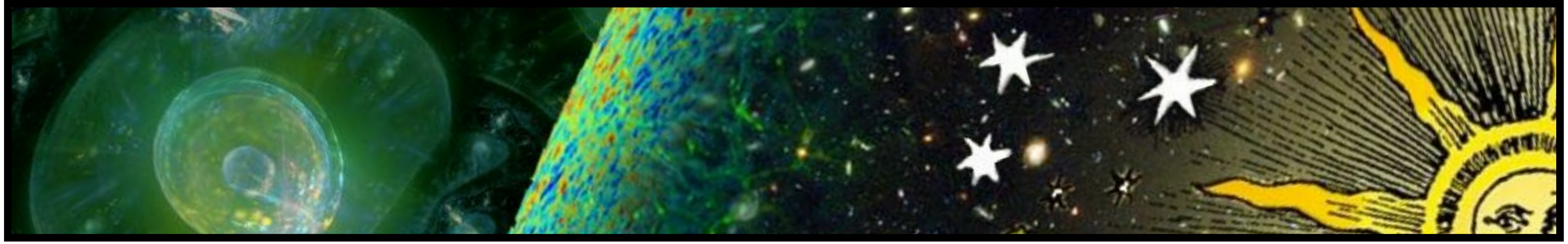


Tomographic selection (based on photo-z estimator) applied to GAMA survey (r-band flux cut, and additional colour cuts for star-galaxy separation)





Alsing et al. (In prep)



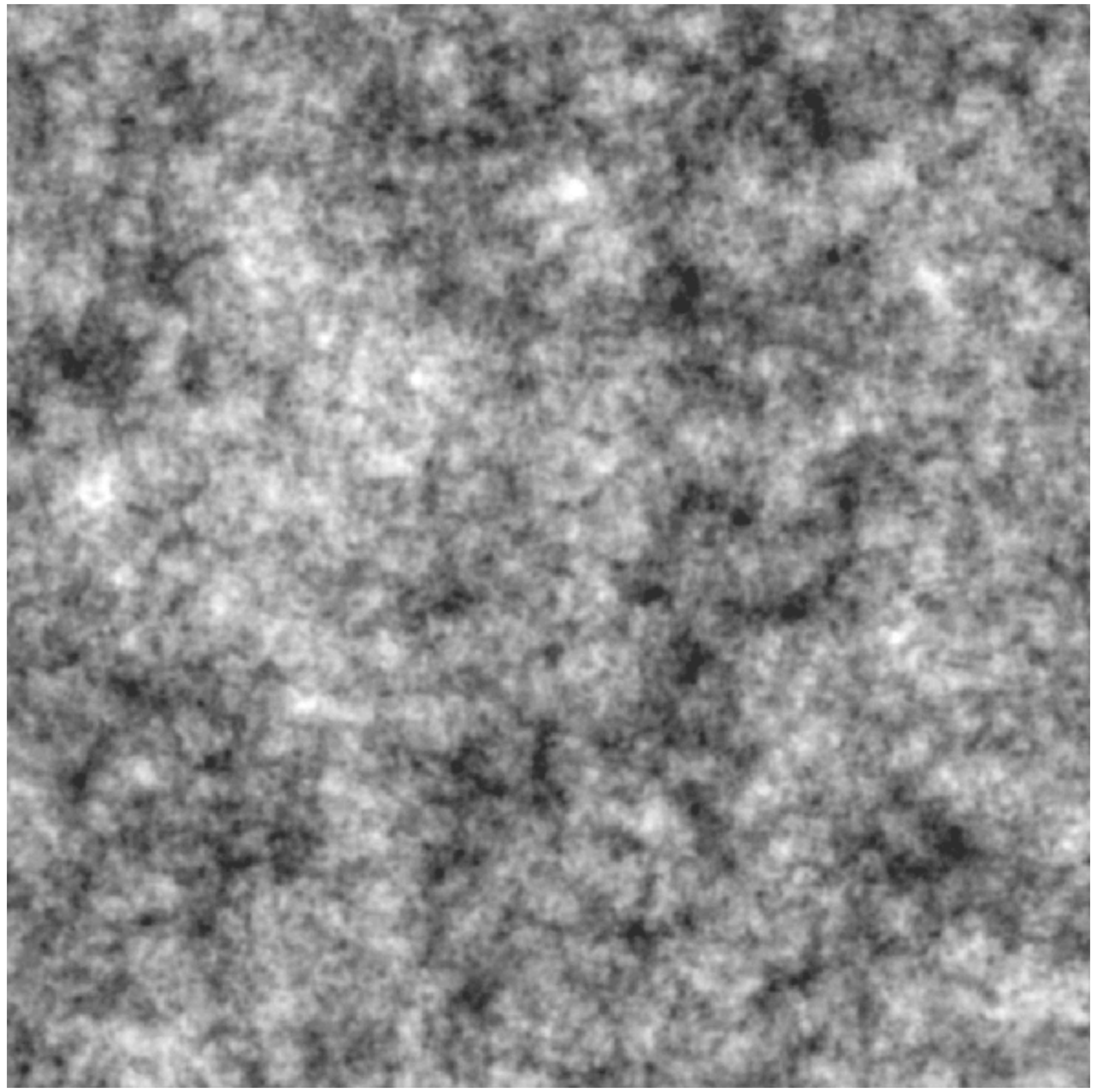
Knowledge extraction using deep learning

Luisa Lucie-Smith
(MPA/Garching)

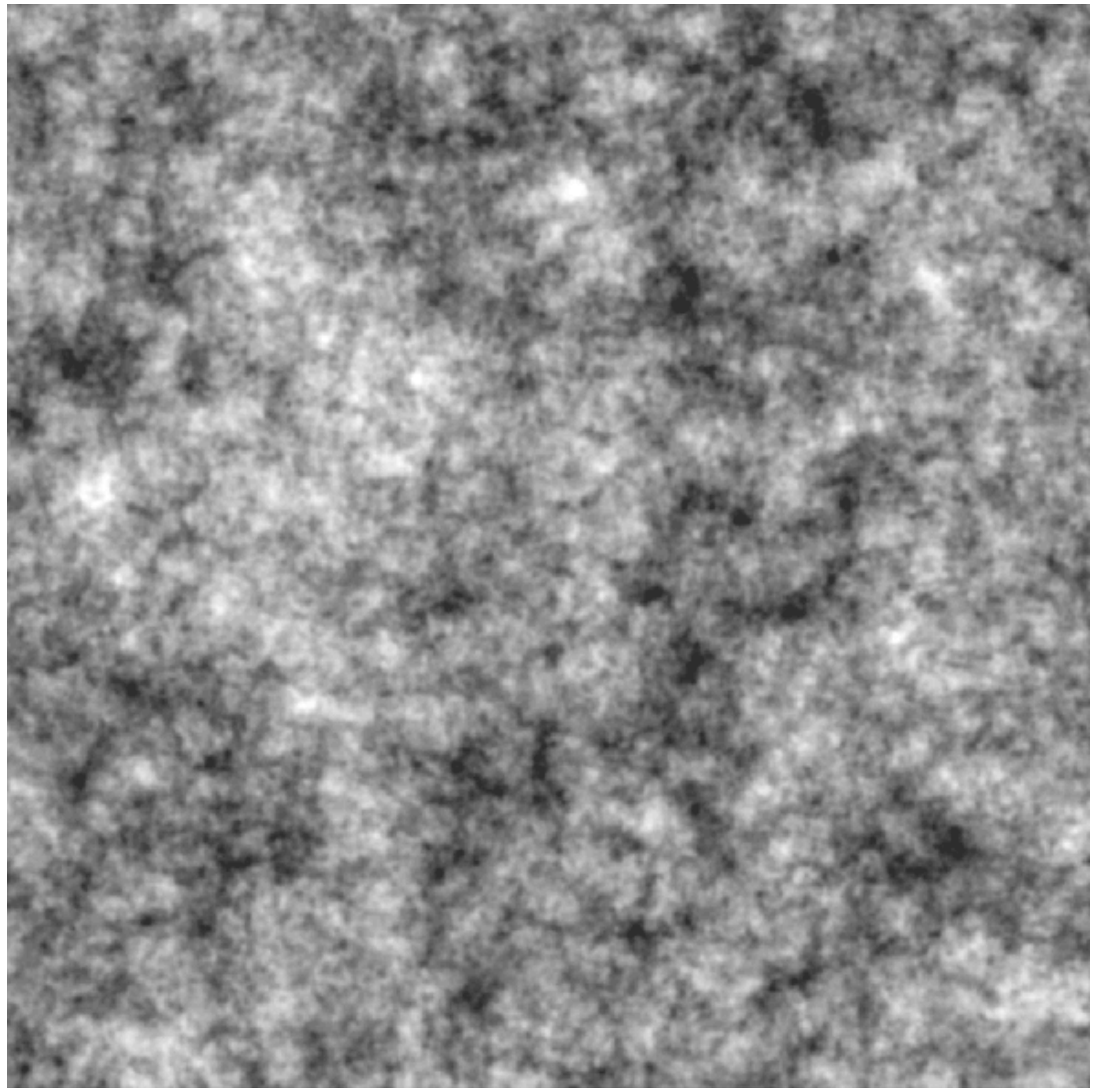
Andrew Pontzen
(UCL)

With: Brian Nord, Jeyan Thiyagalingam, Davide Piras, Lillian Guo

Understanding cosmological structure formation



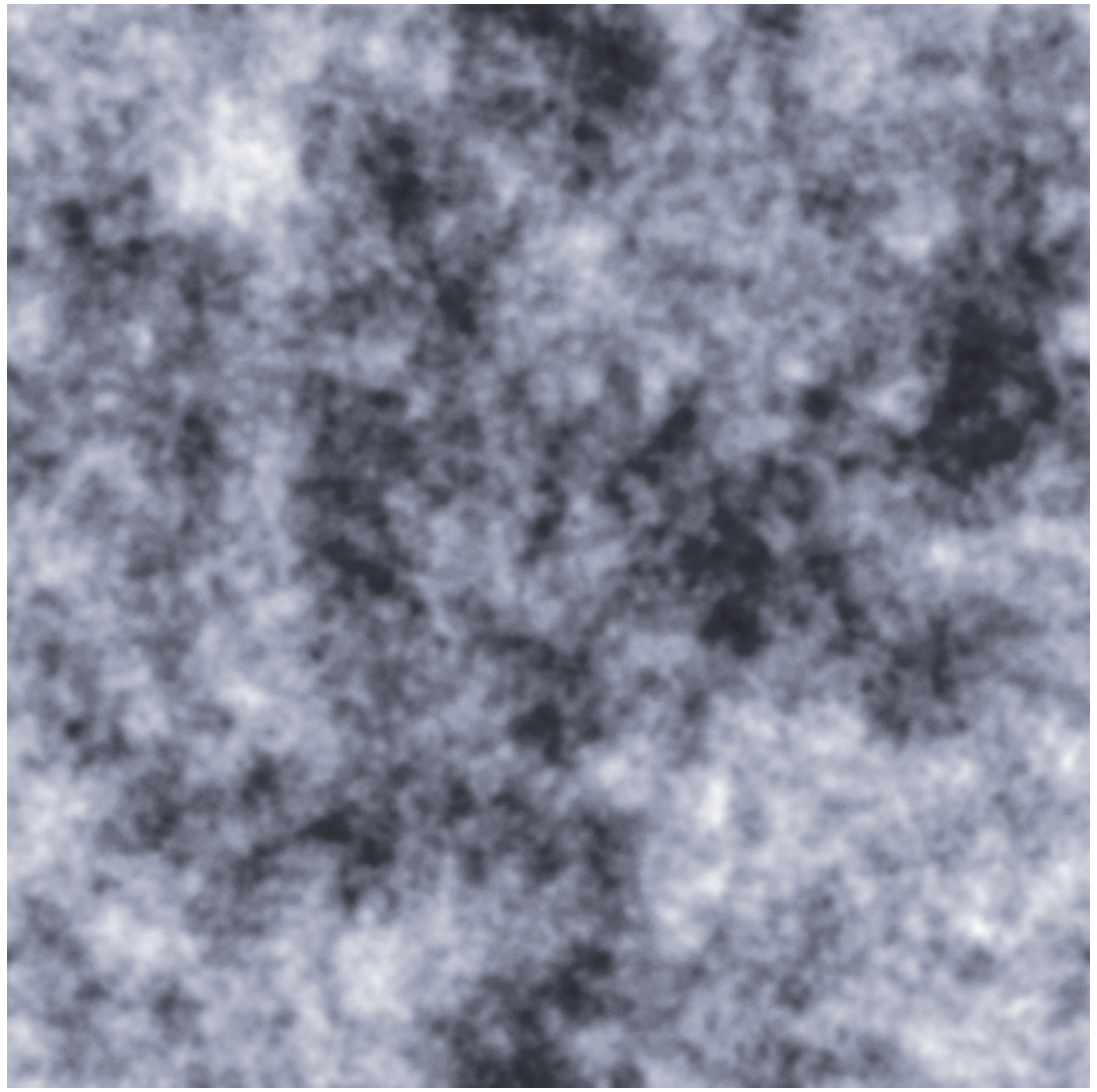
Perturbations in matter density at early times

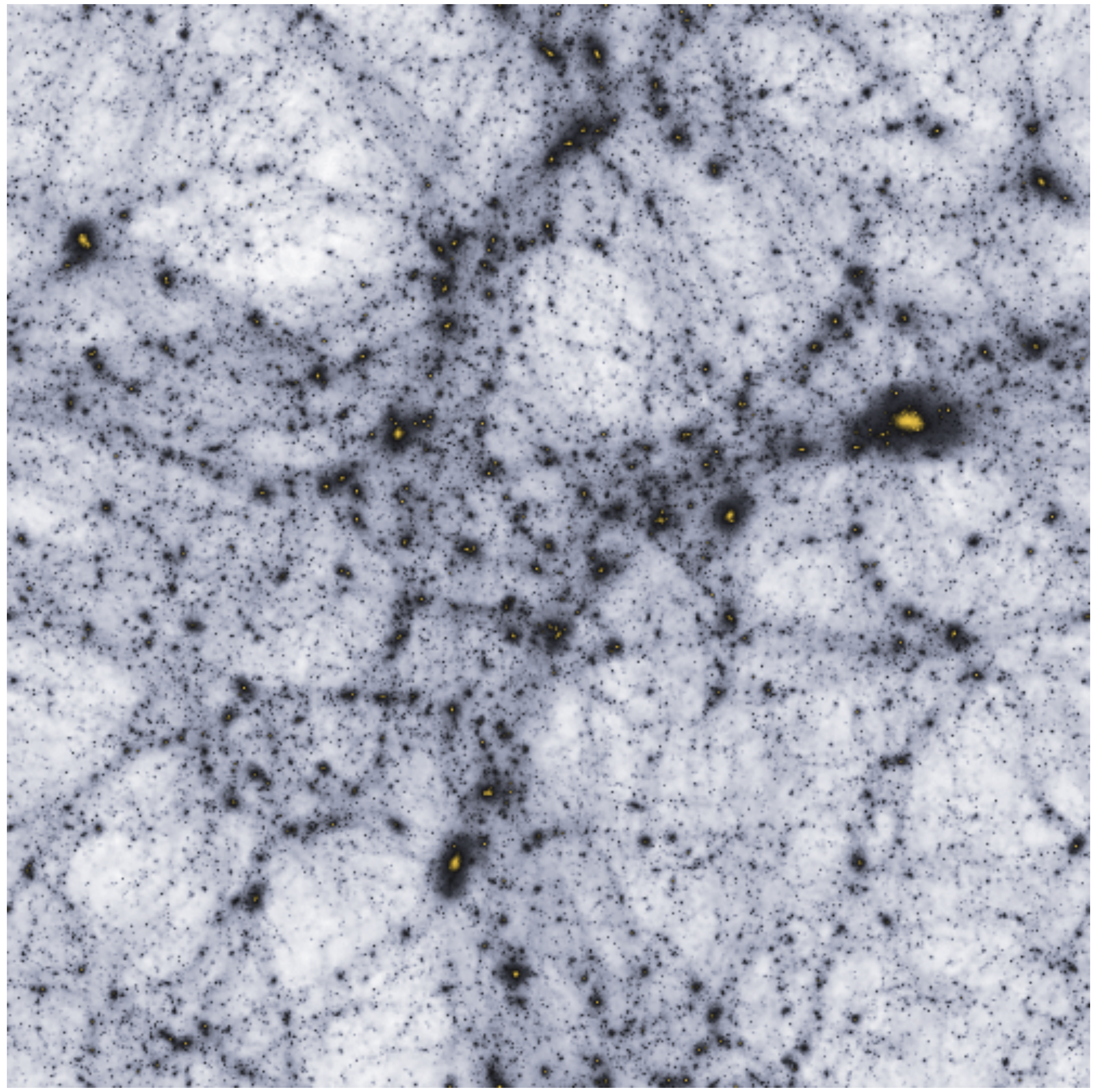


Large-scale structure at late times

Movie: Pontzen et al. (2016)

Understanding cosmological structure formation





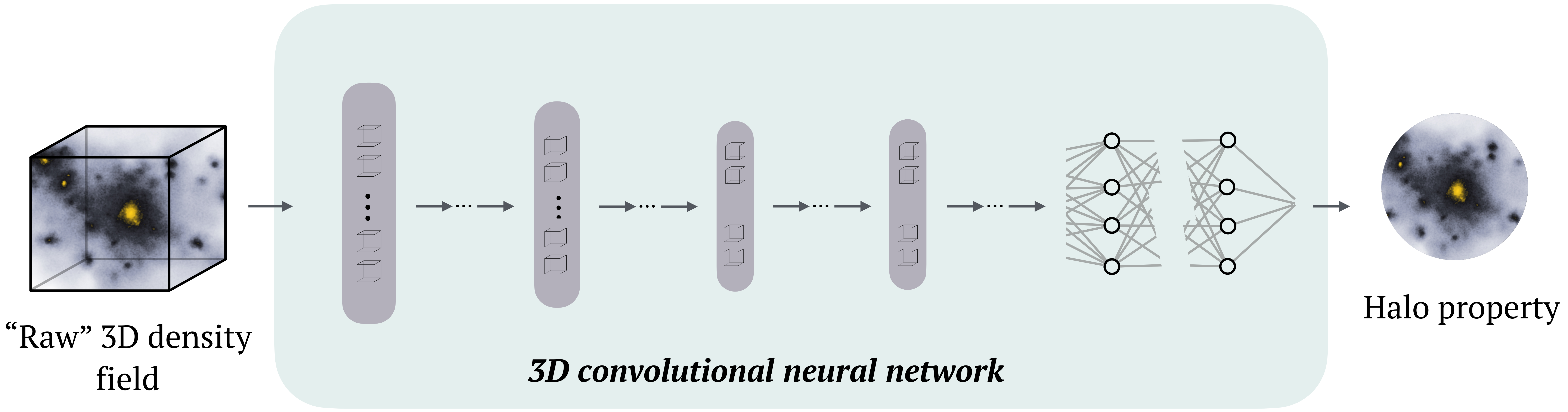
Law of gravity determines mapping
But does not give an *explanation* of mapping
(cf biochemistry vs biology)

“More is different”: emergent phenomena in cosmology

- Can we reliably access rich information in **cosmic web**?
- Can we understand **“mesoscale” phenomena** in structure formation?
- How do “universal” properties emerge?
- Can machine learning play a role in building accurate mesoscale models of complex phenomena?

CREDIT: UCL / PONTZEN

Why convolutional neural networks?



Advantages:

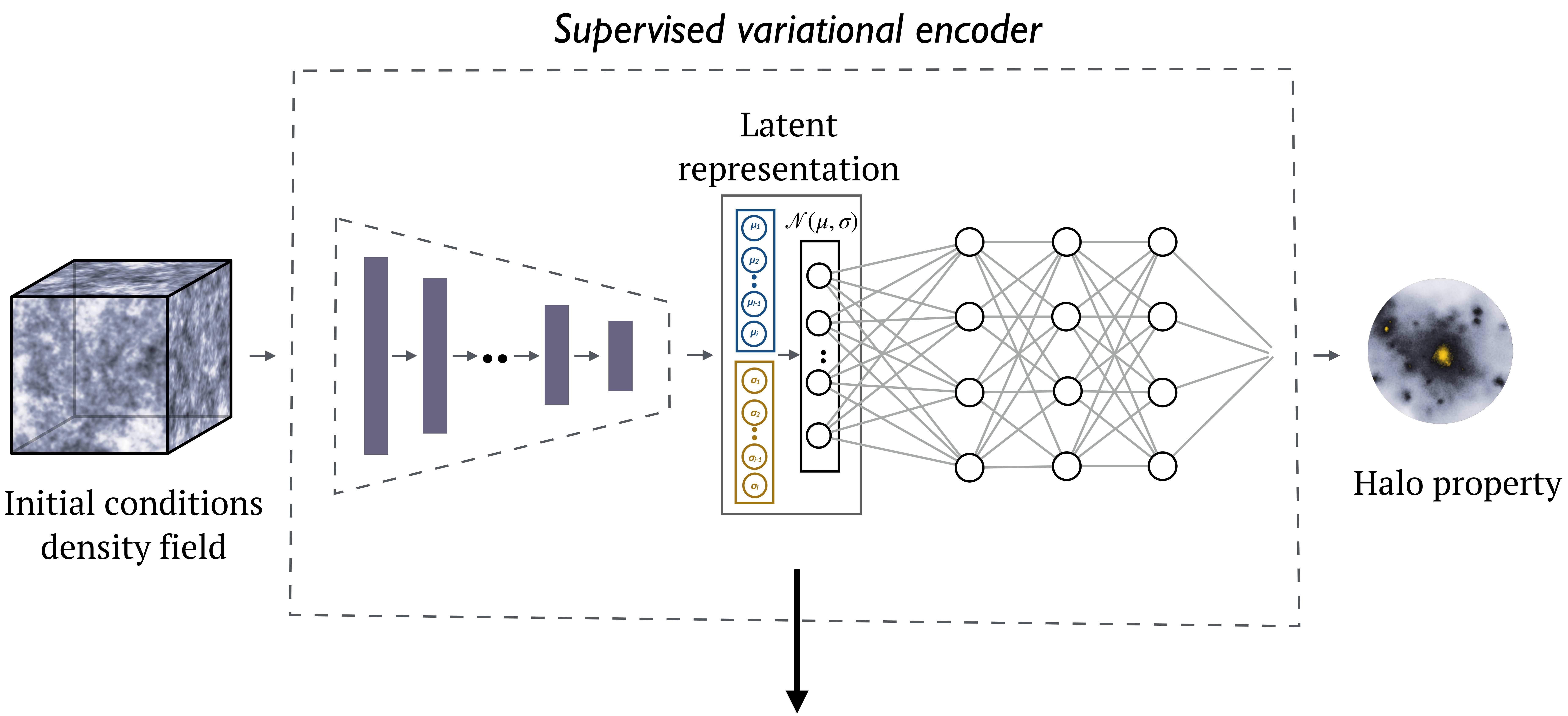
- no *featurization:* CNN learns directly from "raw data"
- CNN learns which features of the raw data are relevant for halo property
- CNNs are able to effectively learn complicated highly non-linear mappings

Disadvantages:

- DL algorithms are "black-box" algorithms, encoding features in very high-dimensional models.

How do we extract physical knowledge from a DL algorithm?

New framework for knowledge extraction using AI

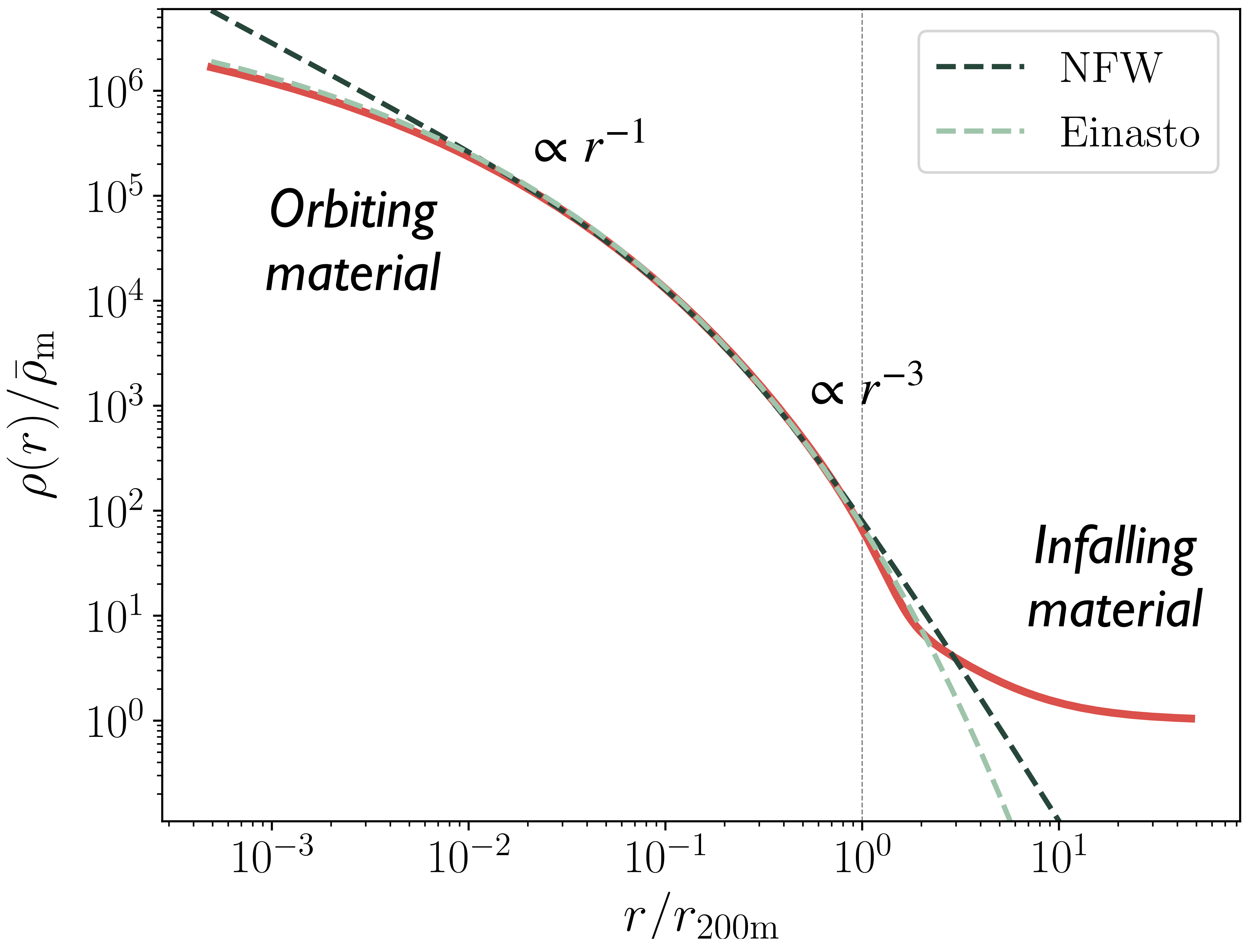


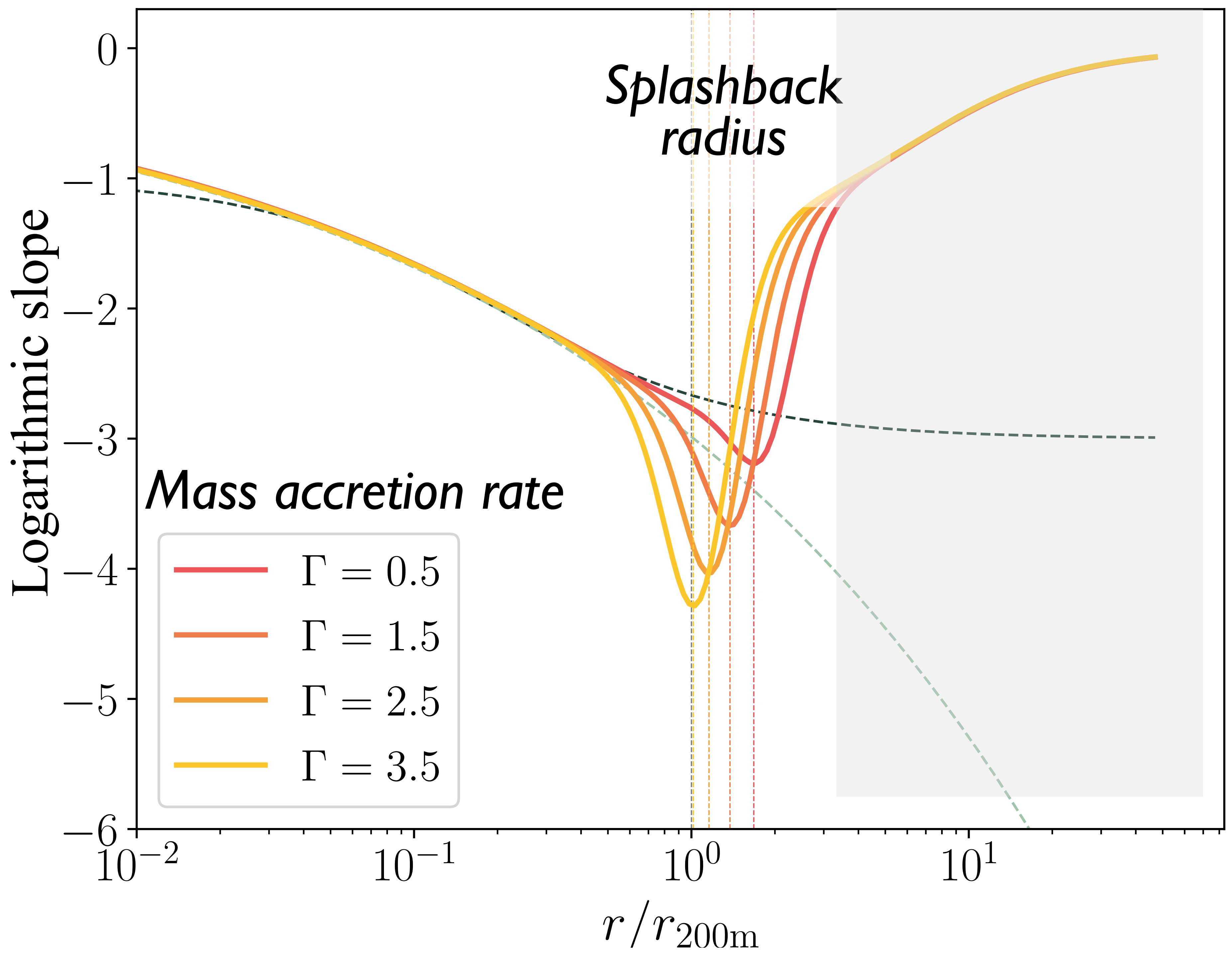
Latent variables encode most relevant aspects of initial conditions about final halo property

Model compression to enable "explainable" AI

ITEN ET AL (PHYS. REV. LETT. 2020), LUCIE-SMITH, PEIRIS, PONTZEN, NORD,, PIRAS (ARXIV:2203.08827)

Case study: can neural networks discover the building blocks of dark matter halo profiles?

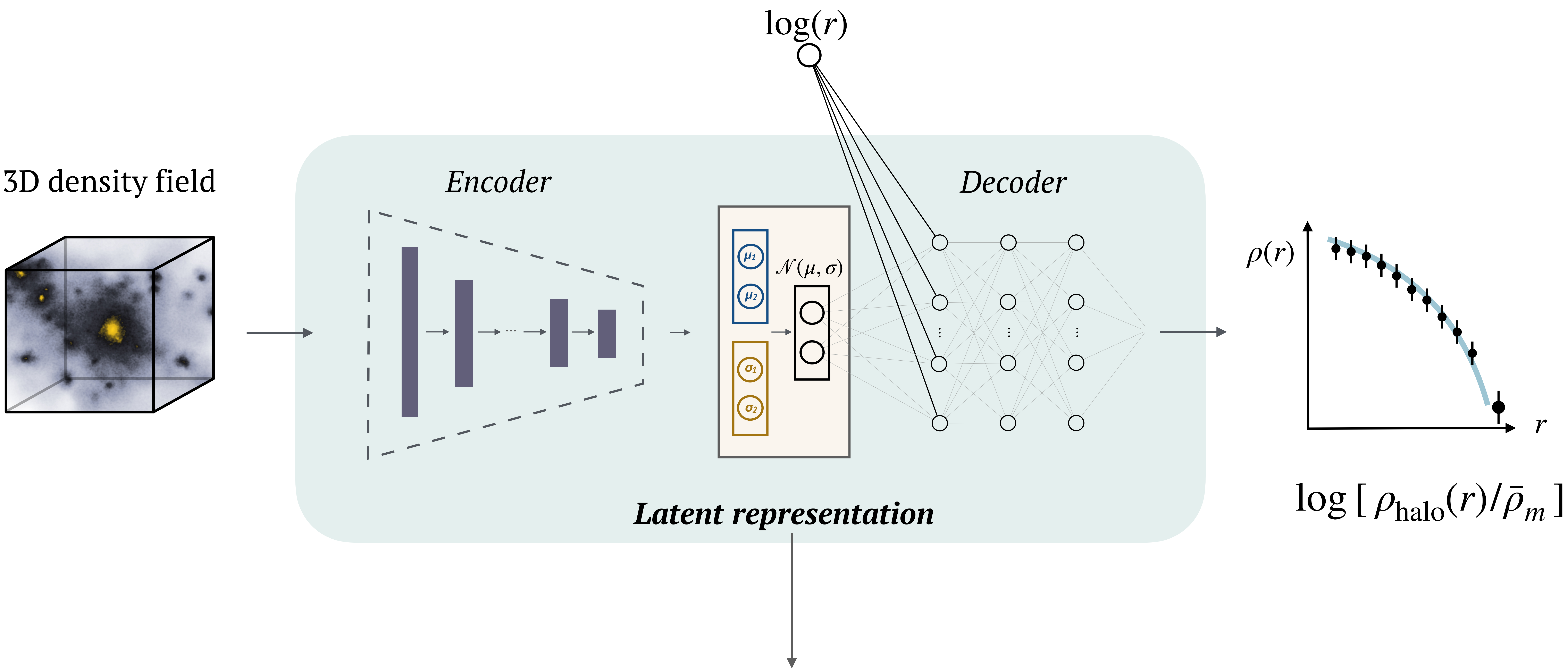




*Existing physical models, based on empirical fitting functions, lack **explainability***

Navarro, Frenk, White (1996, 1997); Einasto (1965); Diemer & Kravstov (2014); Adhikari et al. (2014); More et al. (2015)

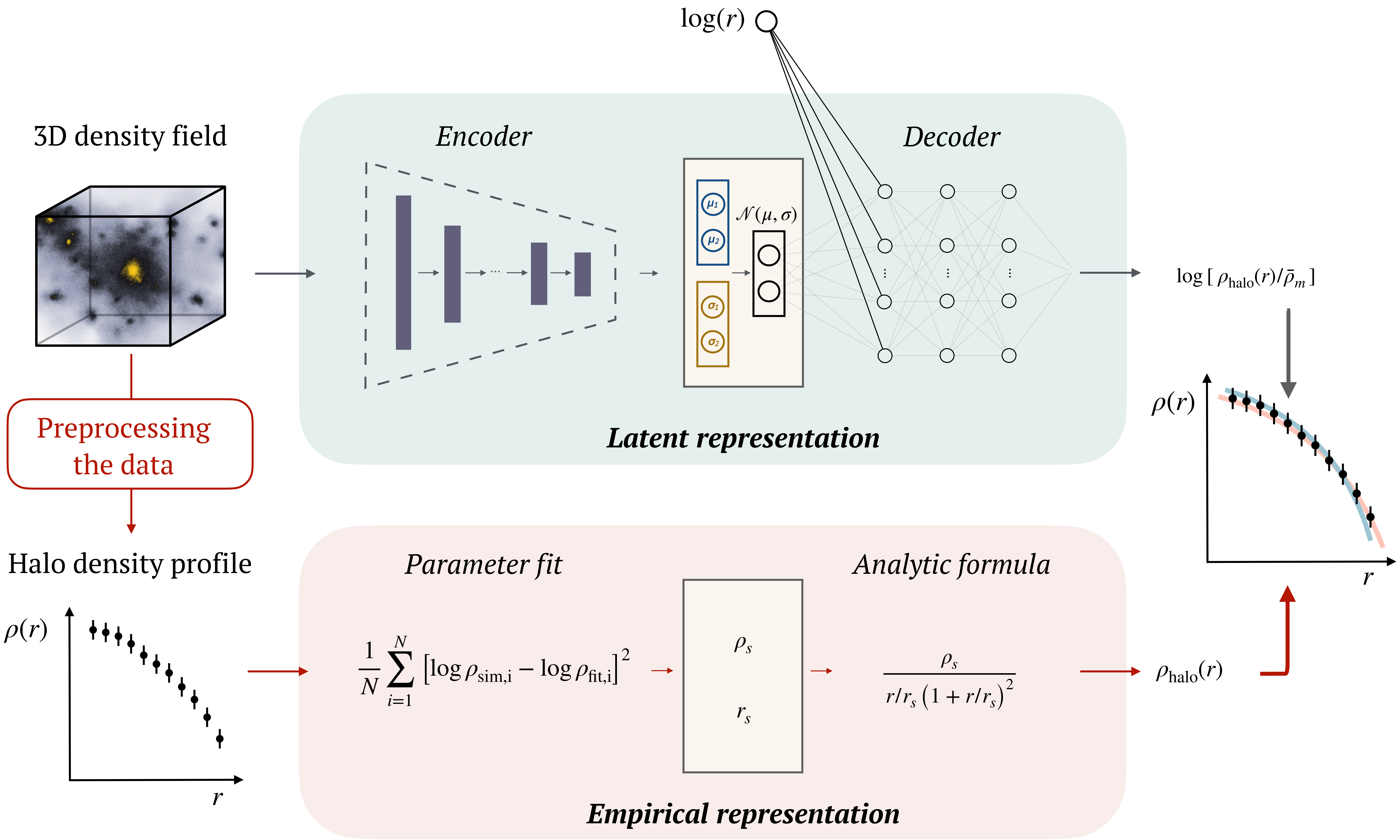
Designing an interpretable variational encoder for knowledge extraction



Latent representation retains all the information used by model to predict density profiles

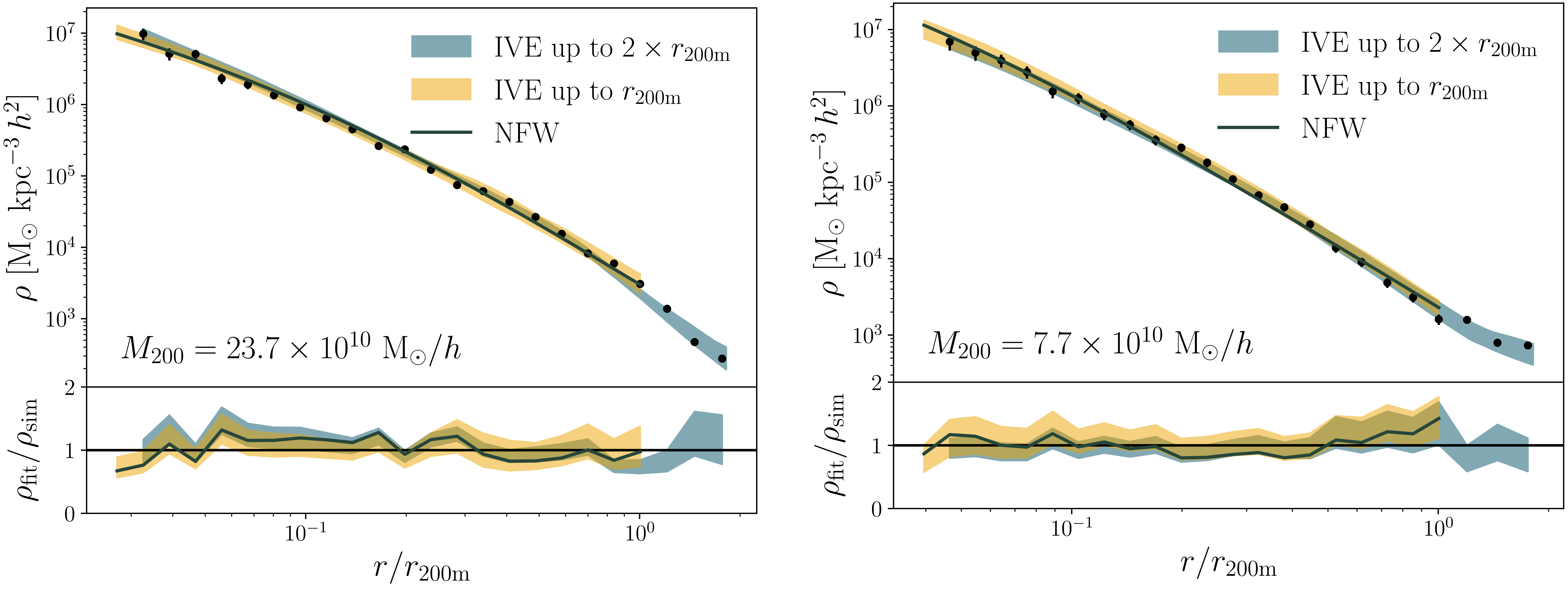
Lucie-Smith, Peiris, Pontzen, Nord + (2022)

Case study: can neural networks discover the building blocks of dark matter halo profiles?



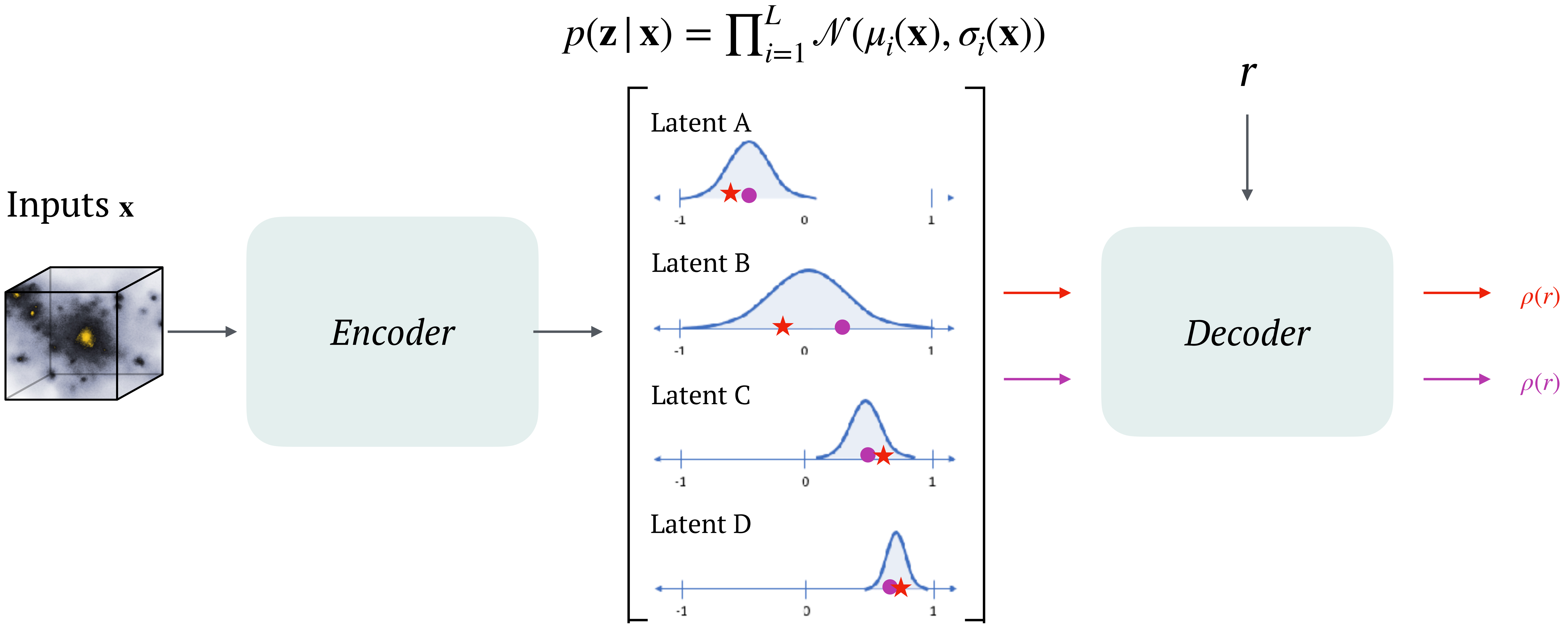
LUCIE-SMITH, PEIRIS, PONTZEN, NORD + (2022)

Examples of fits created by interpretable variational encoder



LUCIE-SMITH, PEIRIS, PONTZEN, NORD + (2022)

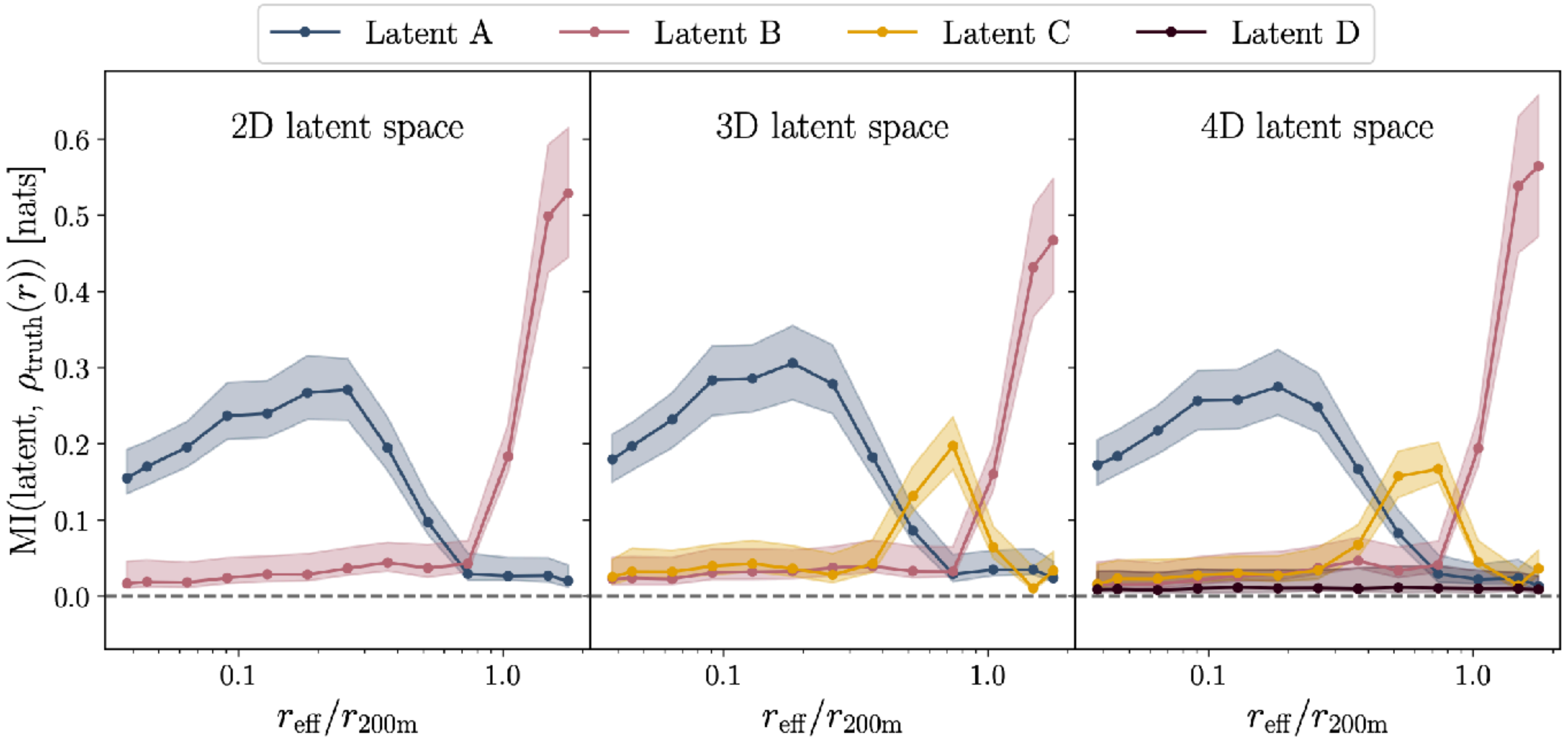
Desired latent representation properties for interpretability



- ***Interpretability*** *can be achieved if latent space is* ***disentangled****:* *independent factors of variation in profiles captured by different latents*
- *Disentanglement encouraged via loss function optimised during training*
- *Degree of disentanglement measured using* ***mutual information*** *between latents*

Lucie-Smith, Peiris, Pontzen, Nord + (2022)

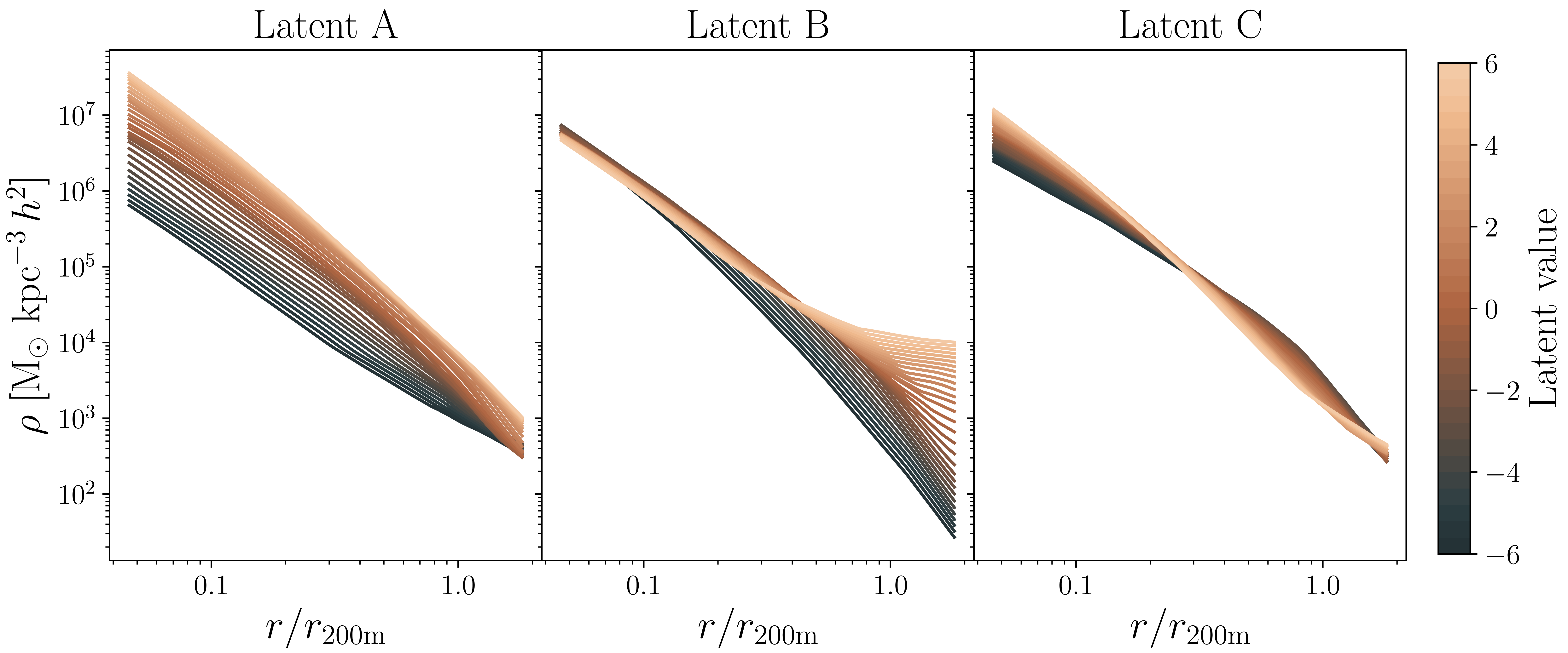
Interpreting the latent space using mutual information



Explainability *achieved by evaluating mutual information between latents and ground truth density profile*

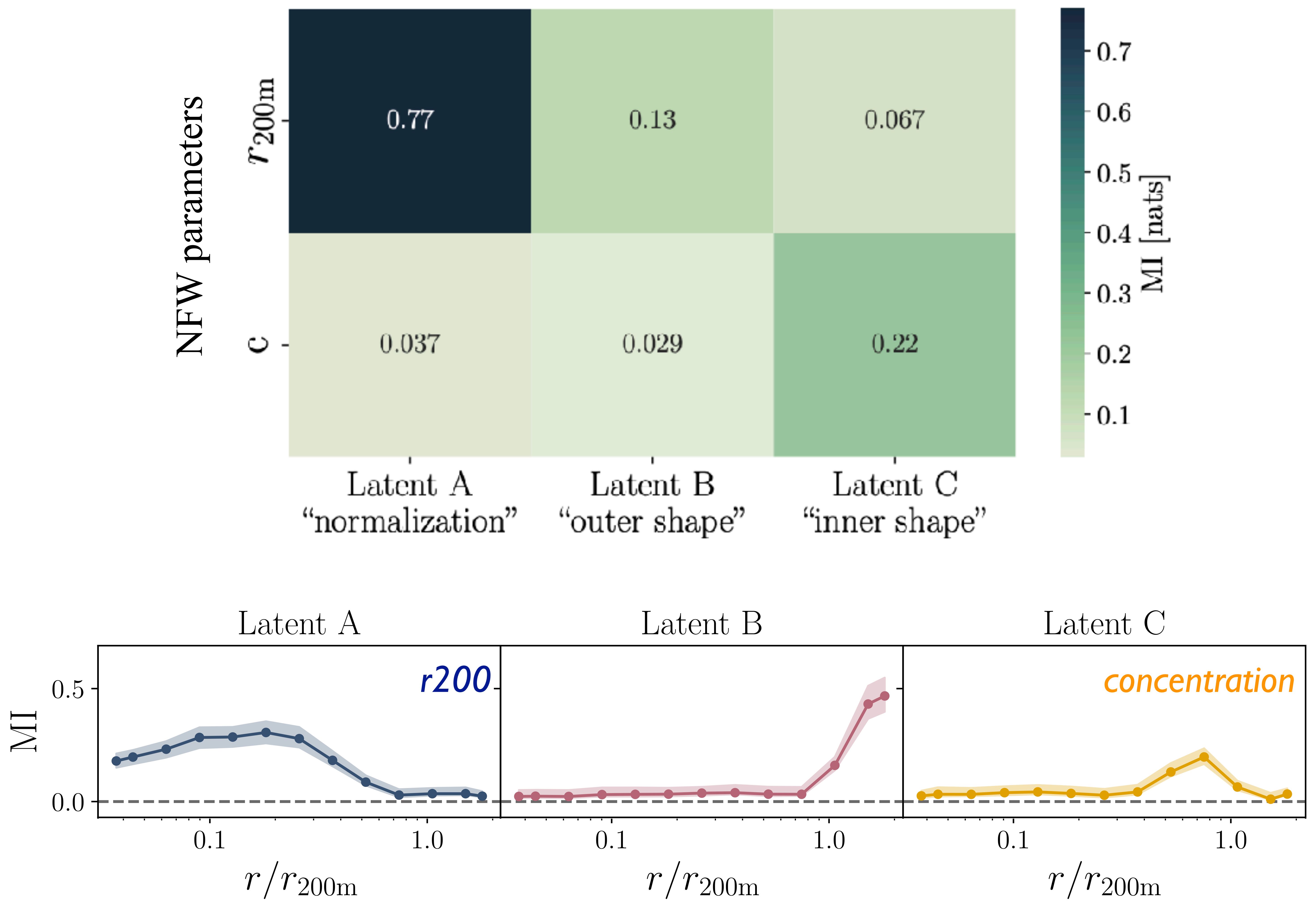
LUCIE-SMITH, PEIRIS, PONTZEN, NORD + (2022)

What has the machine learnt?



normalisation of profile *shape of outer component* *steepness of profile*

IVE re-discovers NFW parameters + additional "splashback" feature

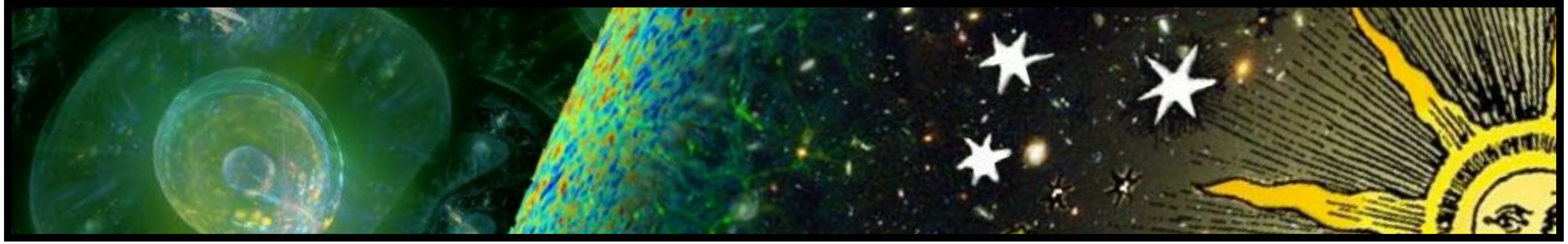


IVE for model compression + mutual information for interpretability enabled ML-driven discoveries

European Research Council
Established by the European Commission

CosmicExplorer: Exploring the Cosmos with the Vera Rubin Observatory

Aims: (i) AI-boosted modelling for cosmological analysis (ii) new cross-validation methods for diagnosis of systematics (iii) explainable AI to develop cosmic web as robust cosmological probe.



Powerful methods available now to enable cosmology with complex, costly models.

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Cosmoparticle, www.peneloperosecowley.com