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Big Data and Quantum Computing

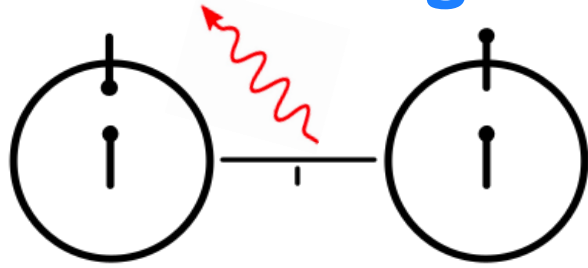
Optimal compression and Simulation-Based Inference of the cosmic 21-cm signal

David Prelogović, Andrei Mesinger

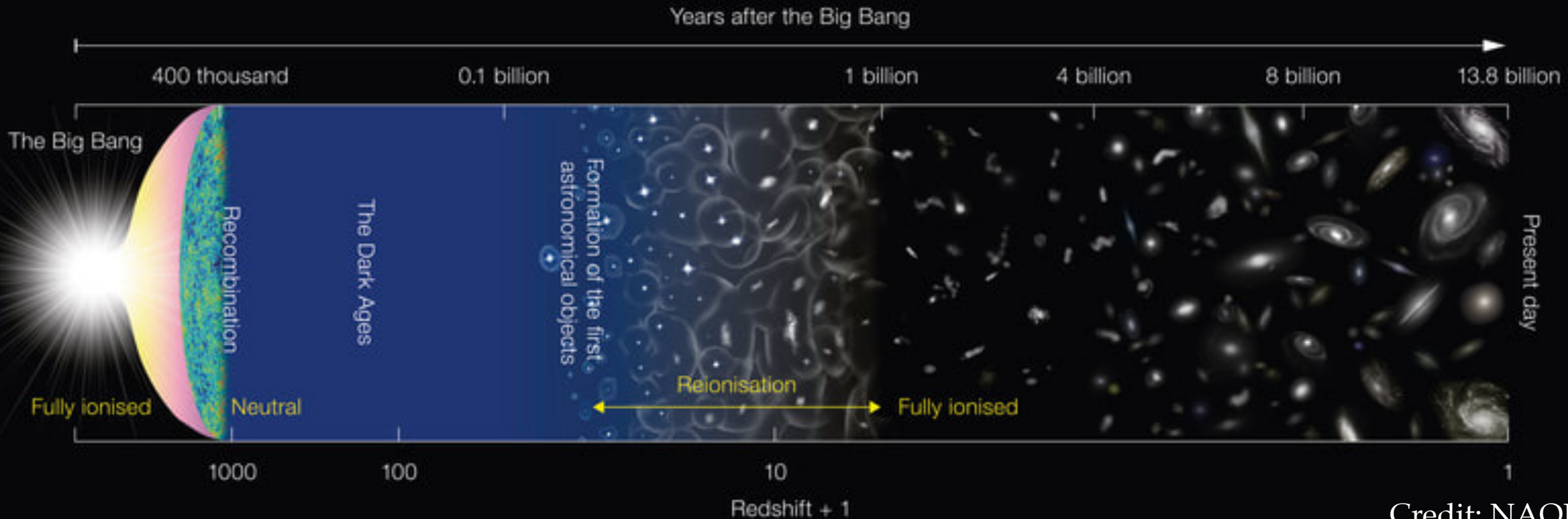
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Spoke 3 General Meeting, Elba 5-9 / 05, 2024

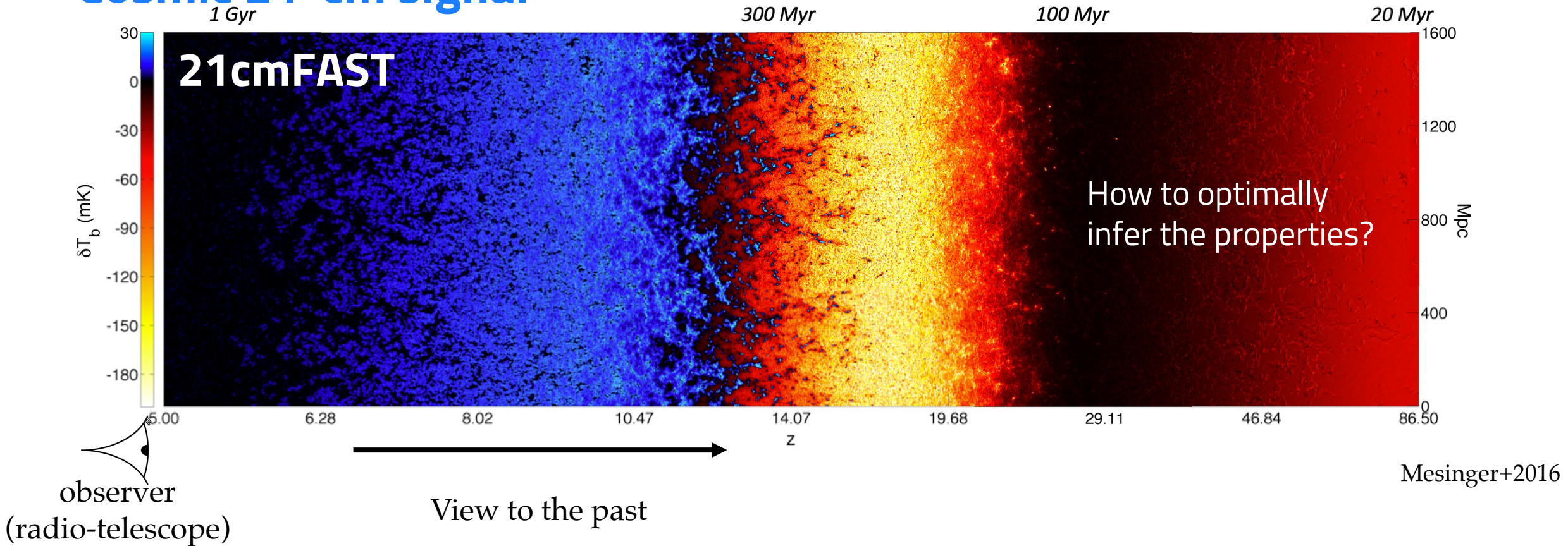
Cosmic 21-cm signal



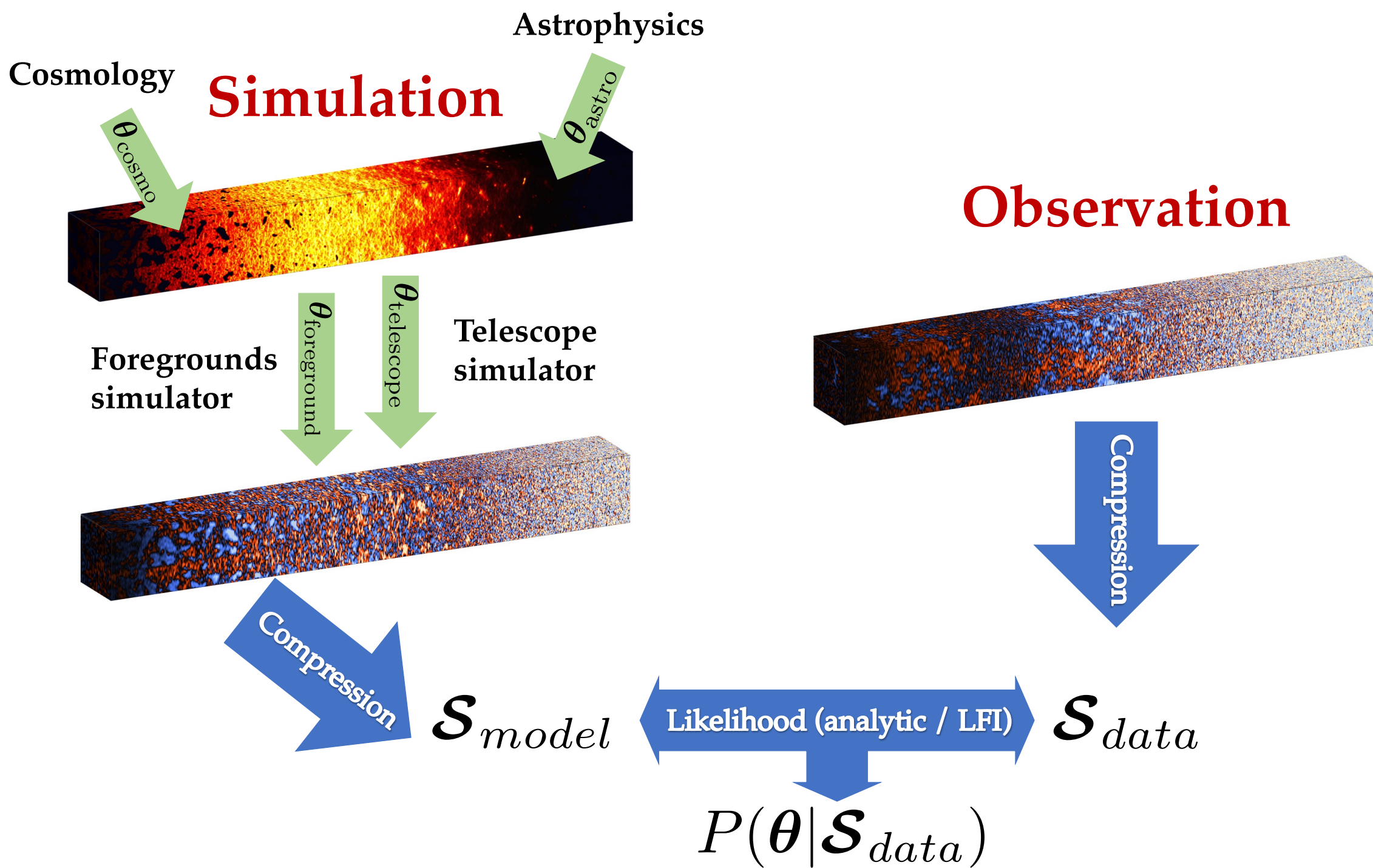
- Over 90% of the "normal" matter in the Universe is **hydrogen**



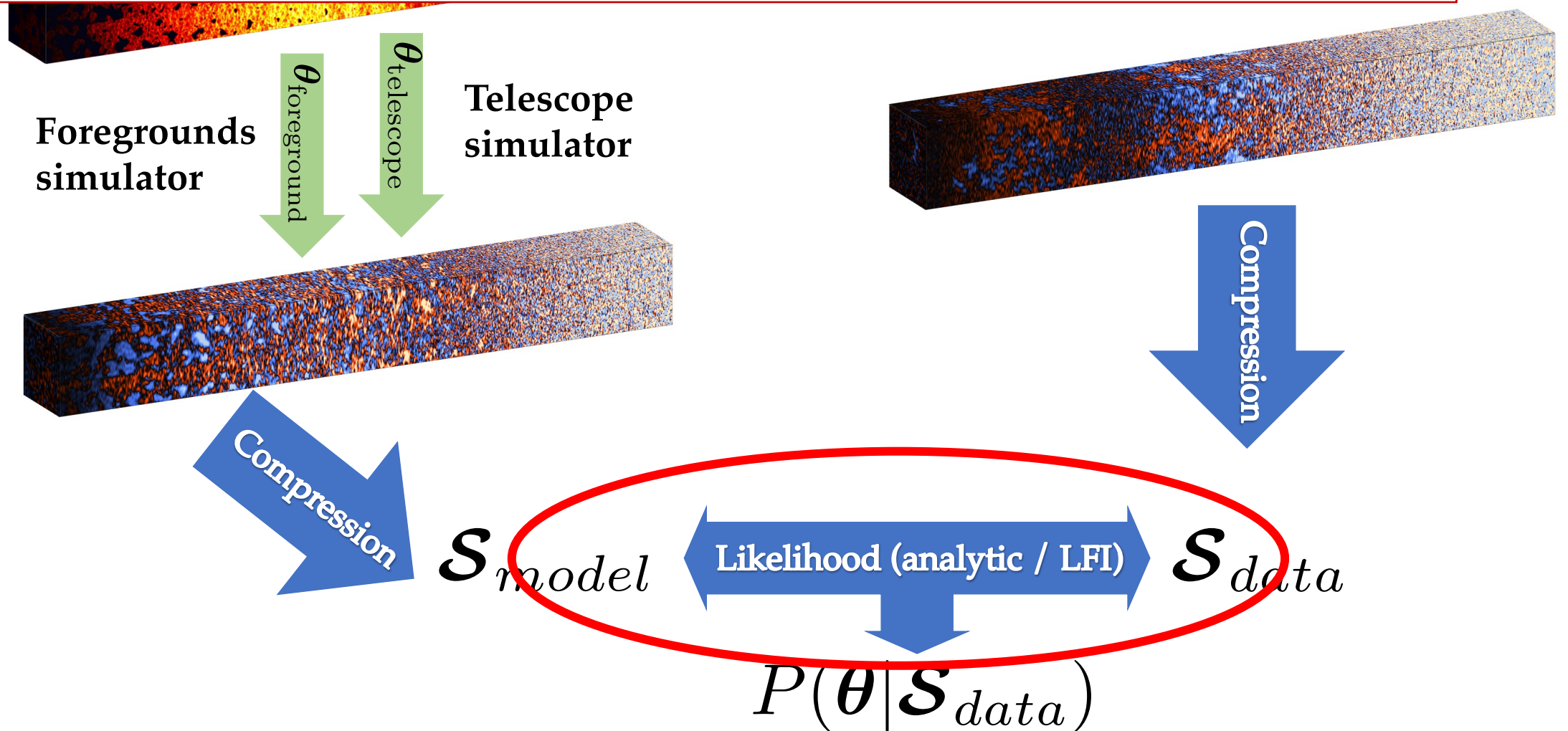
Cosmic 21-cm signal



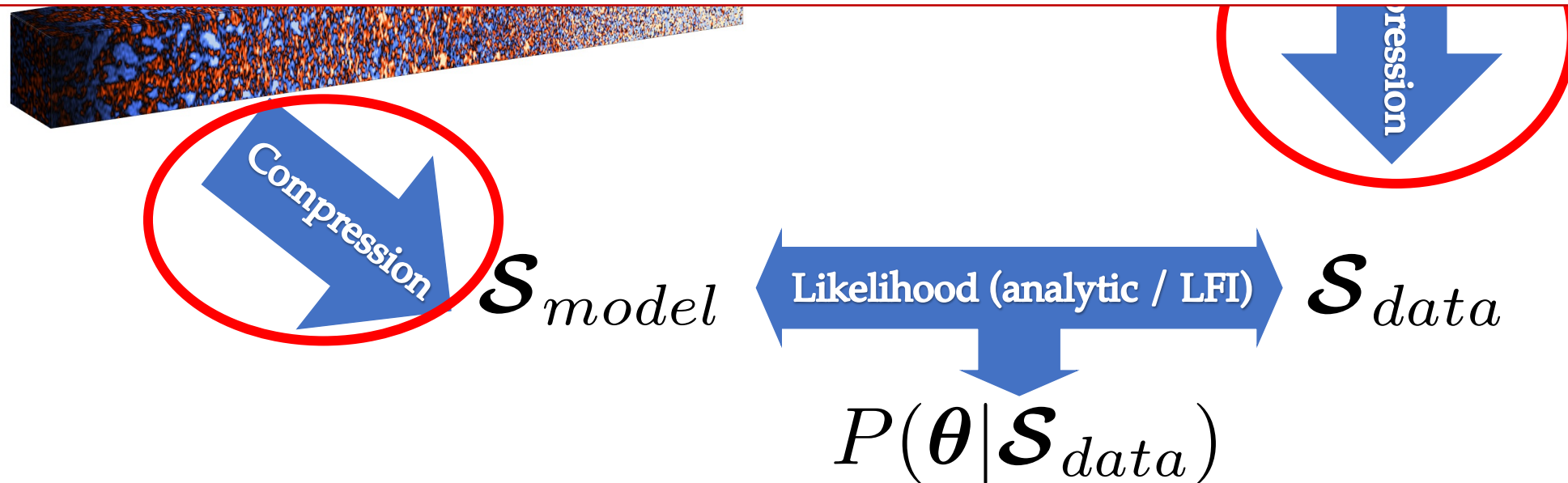
- The properties of the **unseen first galaxies** are encoded in the timings and patterns of this signal!



1) What is the correct form of the likelihood, for a given summary?



- 1) What is the correct form of the likelihood, for a given summary?
- 2) What summary extracts the most information from this non-Gaussian signal?



The background is a deep blue gradient. On the left side, there are numerous bright blue light trails and dots that appear to be moving towards the center, creating a sense of depth and motion. The trails are composed of many small, overlapping lines and points of light. The overall effect is reminiscent of a digital or data environment.

Simulation-Based Inference for the 21-cm PS

Is the PS likelihood Gaussian?

$$\ln \mathcal{L}(\Delta_{21 \text{ obs}}^2 | \boldsymbol{\theta}) \propto -\frac{1}{2} [\Delta_{21 \text{ obs}}^2 - \mu(\boldsymbol{\theta})]^T \Sigma^{-1} [\Delta_{21 \text{ obs}}^2 - \mu(\boldsymbol{\theta})]$$

Is the PS likelihood Gaussian?

model mean $\mu(\theta, k, z)$

(averaging over stochasticity: cosmic variance, noise)

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covariance $\Sigma(\theta, k_1, z_1, k_2, z_2)$

Is the PS likelihood Gaussian?

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variance (ignoring non-diagonal terms)

Is the PS likelihood Gaussian?

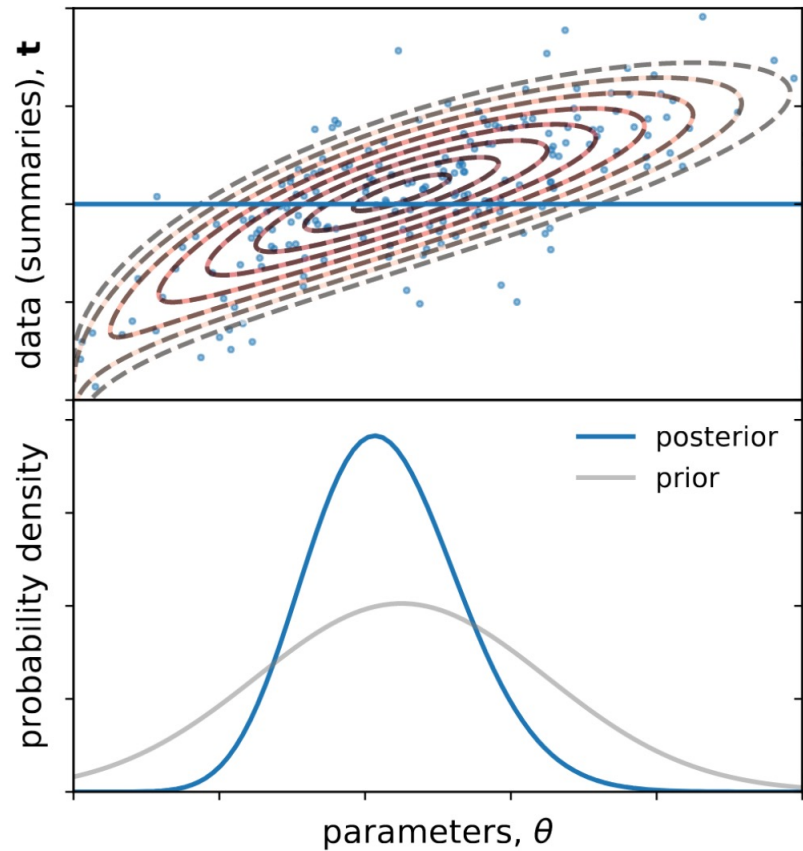
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Common assumptions:

- *Is the likelihood Gaussian?*
- *Can we ignore non-diagonal terms in the covariance btw k and z ?*
- *Can we estimate the mean from a single realization?*
- *Can we estimate (co)variance at a single, “fiducial” parameter value*

We can actually map the ***TRUE*** likelihood with
Simulation Based Inference

Simulation-Based Inference (SBI)

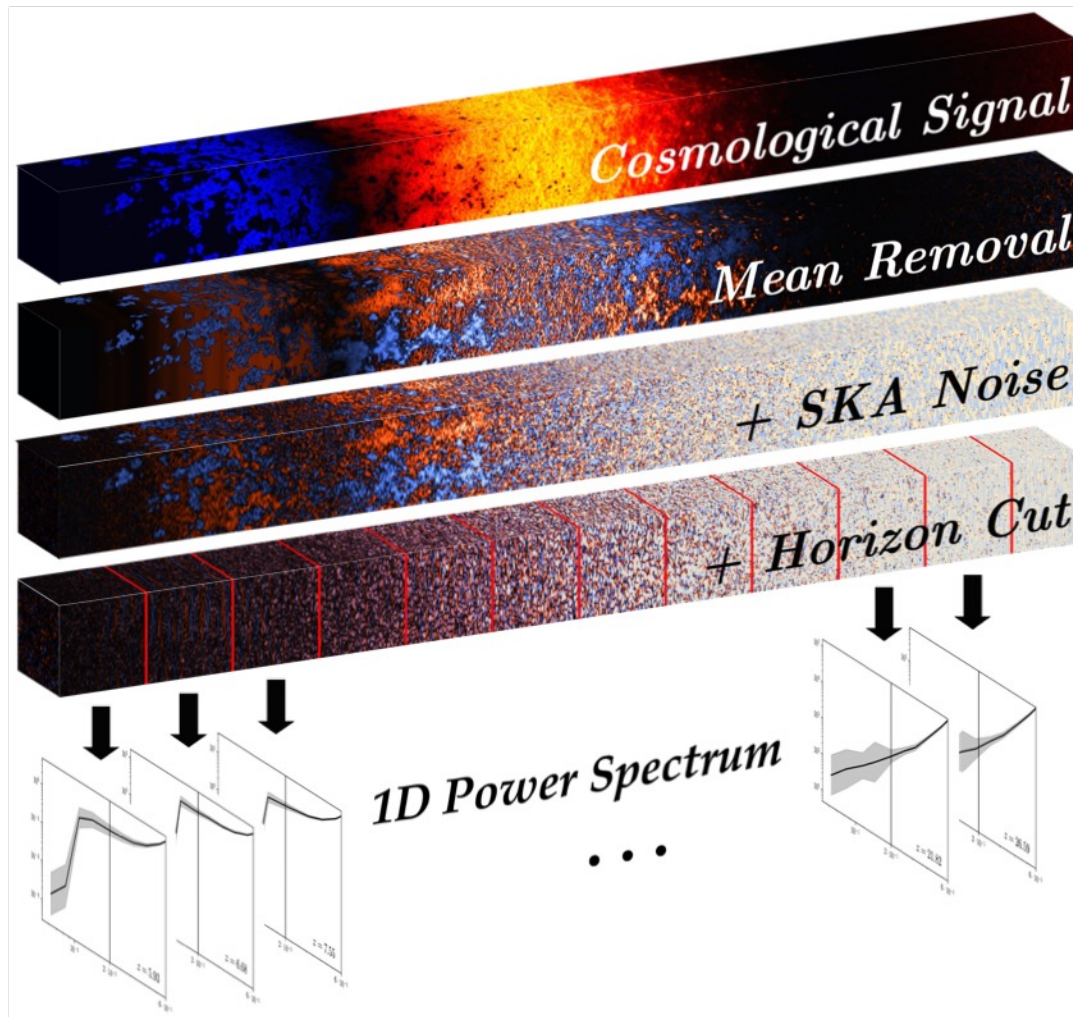


- Pull from the prior $\tilde{\theta} \sim p(\theta)$
- Pull from the likelihood $\tilde{t} \sim p(t|\tilde{\theta})$
 - Use simulator to simulate the data
$$\tilde{d} = \text{simulator}(\tilde{\theta})$$
 - Optionally compress the data to summary
$$\tilde{t} = \text{compressor}(\tilde{d})$$
- Repeat many times to construct a set
$$\{(\tilde{t}_1, \tilde{\theta}_1), (\tilde{t}_2, \tilde{\theta}_2), \dots, (\tilde{t}_N, \tilde{\theta}_N)\}$$
- It is assumed the simulator is perfect, i.e. it pulls from the actual likelihood

$$p(d|\tilde{\theta})$$

Simulation Based Inference (SBI)

Precompute database of forward models (varying cosmic ICs, noise, etc.) and train density estimators to fit the likelihood.

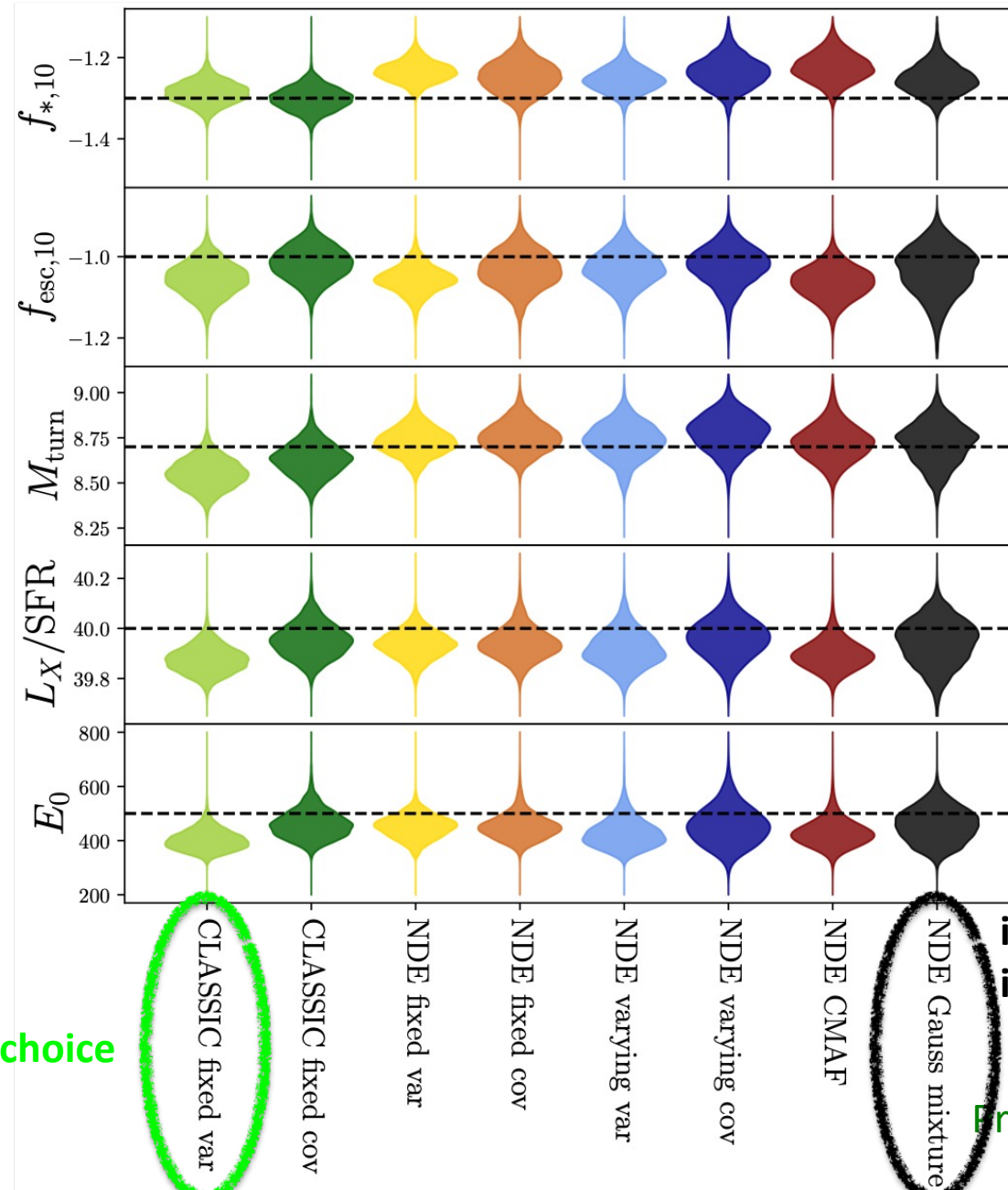


Rapidly becoming popular in 21cm:
Zhao+2022ab, Saxena+2023

Use different functional forms to test the assumptions

	non-Gaussian	non-diagonal covariance	(co)variance is a function of θ	mean by averaging over realizations
CLASSIC fixed var	✗	✗	✗	✗ (single, well-chosen seed)
CLASSIC fixed cov	✗	✓	✗	✗ (single, well-chosen seed)
NDE fixed var	✗	✗	✗	✓
NDE fixed cov	✗	✓	✗	✓
NDE varying var	✗	✗	✓	✓
NDE varying cov	✗	✓	✓	✓
NDE CMAF	✓	N/A	N/A	N/A
NDE Gauss mixture	✓	N/A	N/A	N/A

Use different functional forms to test the assumptions



~ most common choice

CLASSIC fixed var

CLASSIC fixed cov

NDE fixed var

NDE fixed cov

NDE varying var

NDE varying cov

NDE CMAF

NDE Gauss mixture

implicit likelihood SBI is most accurate

Prelogovic & AM (2023)

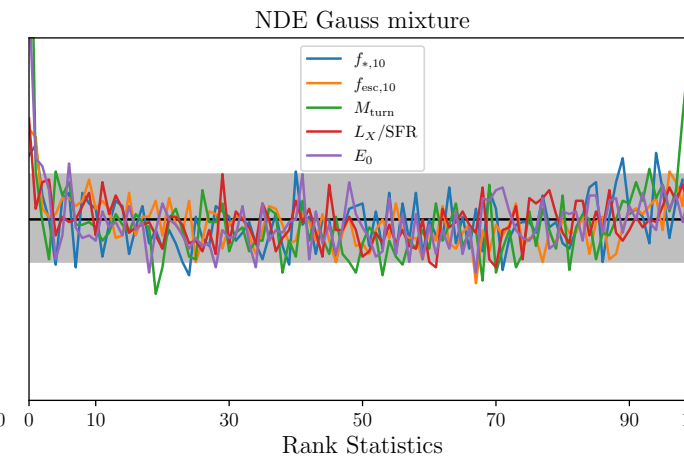
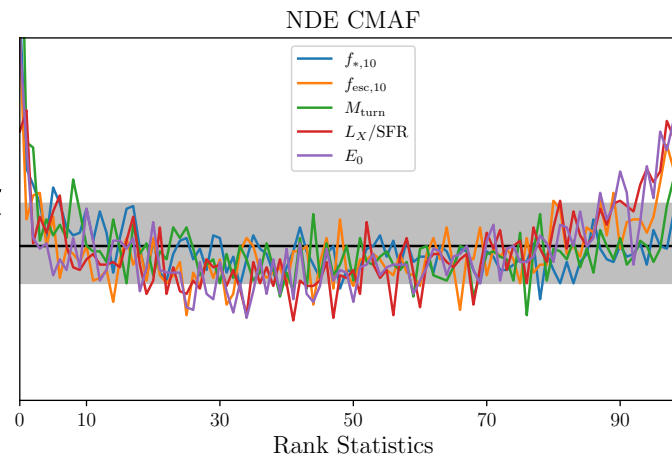
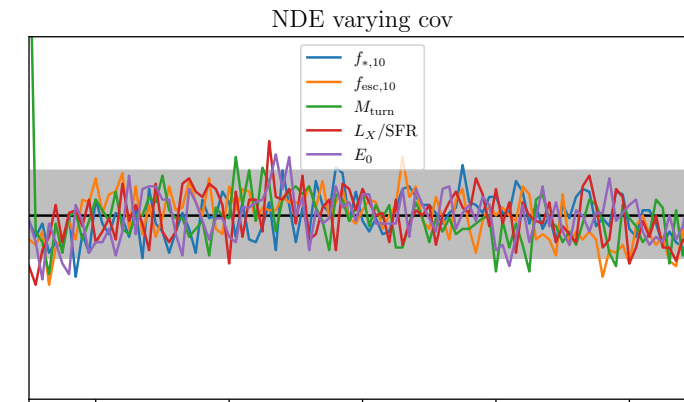
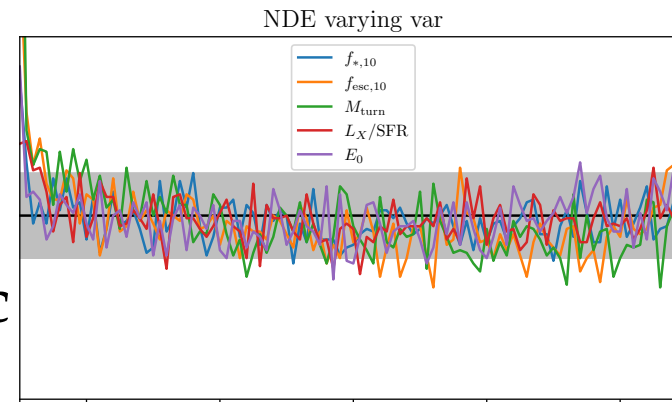
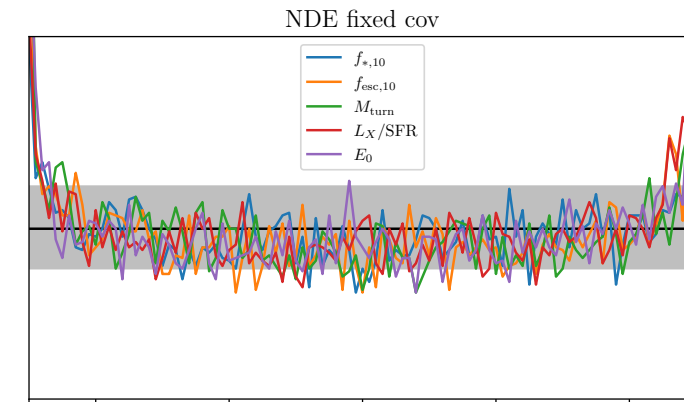
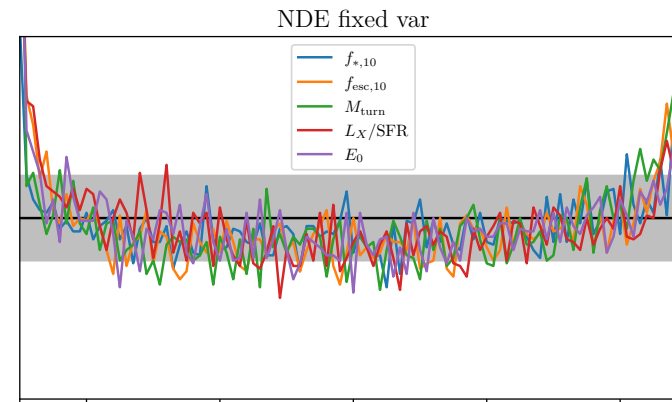
Simulation Based Calibration (SBC)

• “prior” = “data averaged posterior” $P(\boldsymbol{\theta}) = \int P(\boldsymbol{\theta}|\tilde{\mathbf{y}}) P(\tilde{\mathbf{y}}|\tilde{\boldsymbol{\theta}}) P(\tilde{\boldsymbol{\theta}}) d\tilde{\mathbf{y}} d\tilde{\boldsymbol{\theta}}$

1. Pull from prior $\tilde{\boldsymbol{\theta}} \sim P(\boldsymbol{\theta})$
2. Pull the data from the likelihood $\tilde{\mathbf{y}} \sim P(\mathbf{y}|\tilde{\boldsymbol{\theta}}) \Leftrightarrow \tilde{\mathbf{y}} = \text{simulator}(\tilde{\boldsymbol{\theta}})$
3. Calculate the posterior the sample $P(\boldsymbol{\theta}|\tilde{\mathbf{y}})$
4. Repeat and average posteriors $P(\boldsymbol{\theta}) \approx \frac{1}{N} \sum_{i=1}^N P_i(\boldsymbol{\theta}|\tilde{\mathbf{y}}_i)$

SBC for 21-cm PS

- *Expensive to compute!*
 - *10 000 posteriors*
- However, once likelihood is trained, no new simulations are needed
 - “amortized inference”
- Procedure would be useful for classic inference too, but is impossible to compute
- NDE fixed var & cov – overconfident
- NDE varying var & cov – good
- NDE CMAF – overconfident
- NDE Gauss mixture – the best

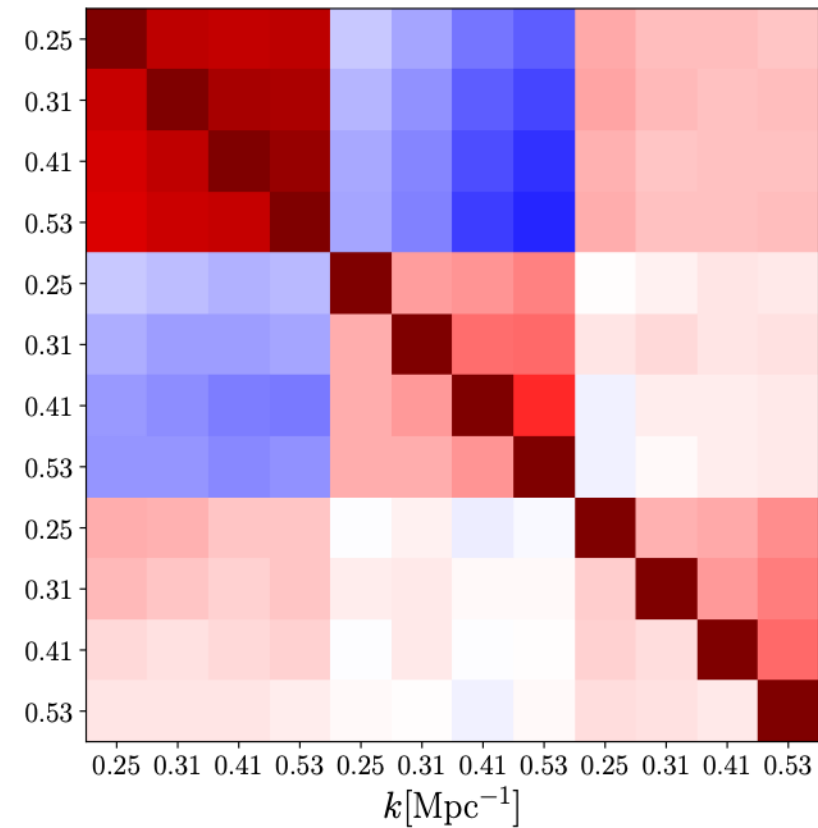
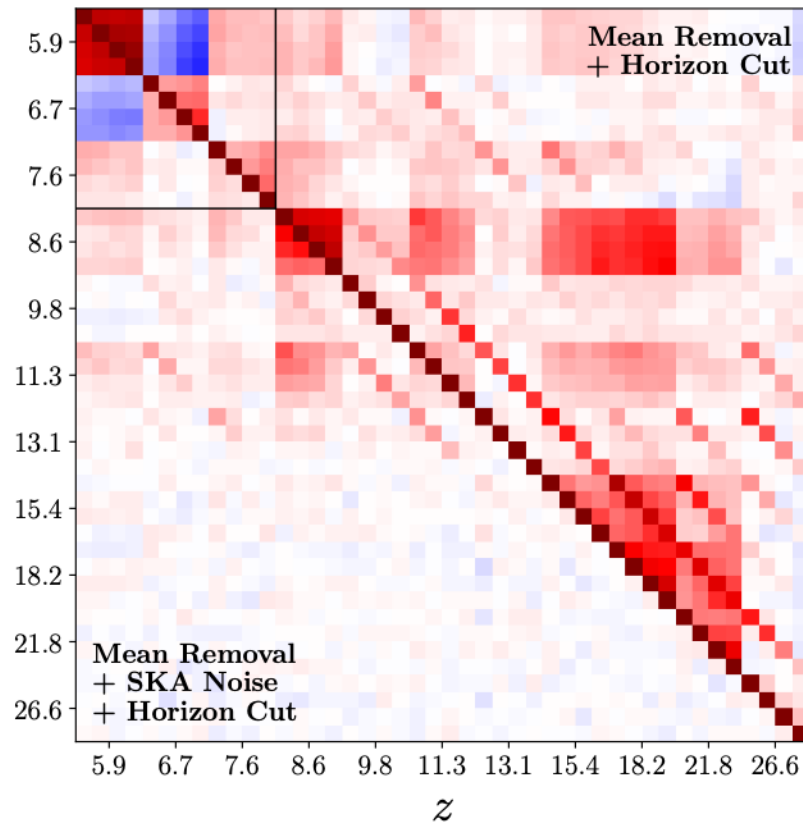


So... Is the PS likelihood Gaussian?

- Is the likelihood close to Gaussian? —> *close enough (assuming wedge excision)*

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- Is the likelihood close to Gaussian? —> **close enough**
- Can we ignore 2pt covariance btw k and z ? —> **No**
- Can we estimate the mean from a single realization? —> **Only if you choose well**
- Can we estimate (co)variance at a single, “fiducial” parameter value —> **No**

But we don't have to worry about it because:

SBI gives more accurate posteriors using an order of magnitude fewer simulations than MCMC/Nested sampling

- *no “emulation error” that is difficult to characterize over parameter space -> NDE error easier to mitigate*
- *once likelihood is learned, new inference from updated data can be done ~ instantaneously (“amortized” cost)*

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Optimal Compression of the 21-cm lightcones

Ad-hoc compressions

- Without good a-priori physical motivation, we cannot know what is THE optimal compression/summary, i.e. providing tightest recovery of astrophysics and cosmology

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Solution:

Let the machines figure it out for us!

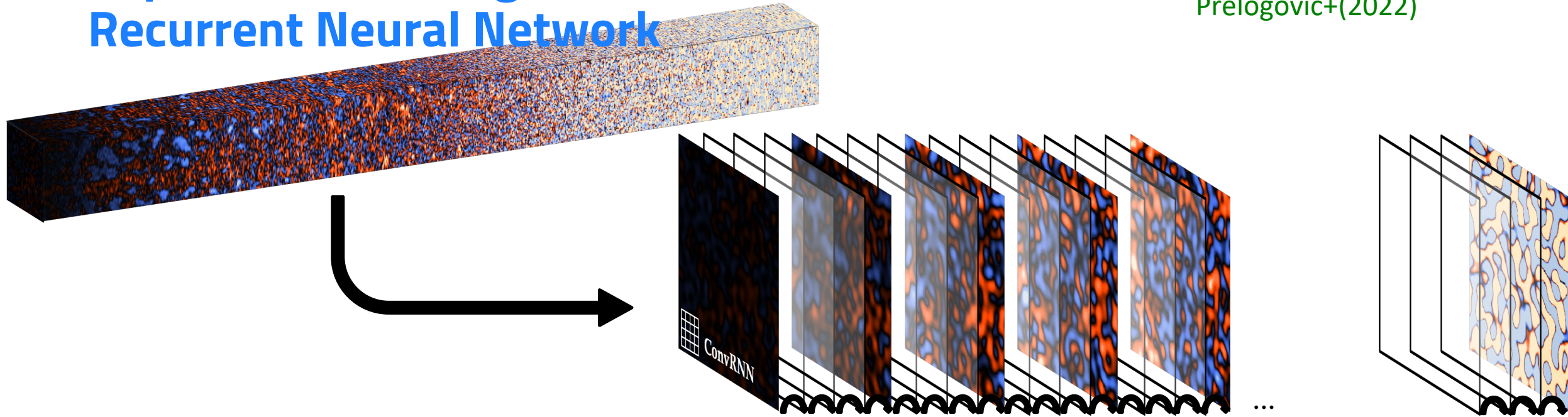
(Neural Network)

- Gillet+2018
- La Plante & Ntampaka 2019
- Makinen+2020
- Mangena+2020
- Hortúa+2020
- Prelogović+2021
- +++



Supervised learning: Recurrent Neural Network

Prelogovic+(2022)

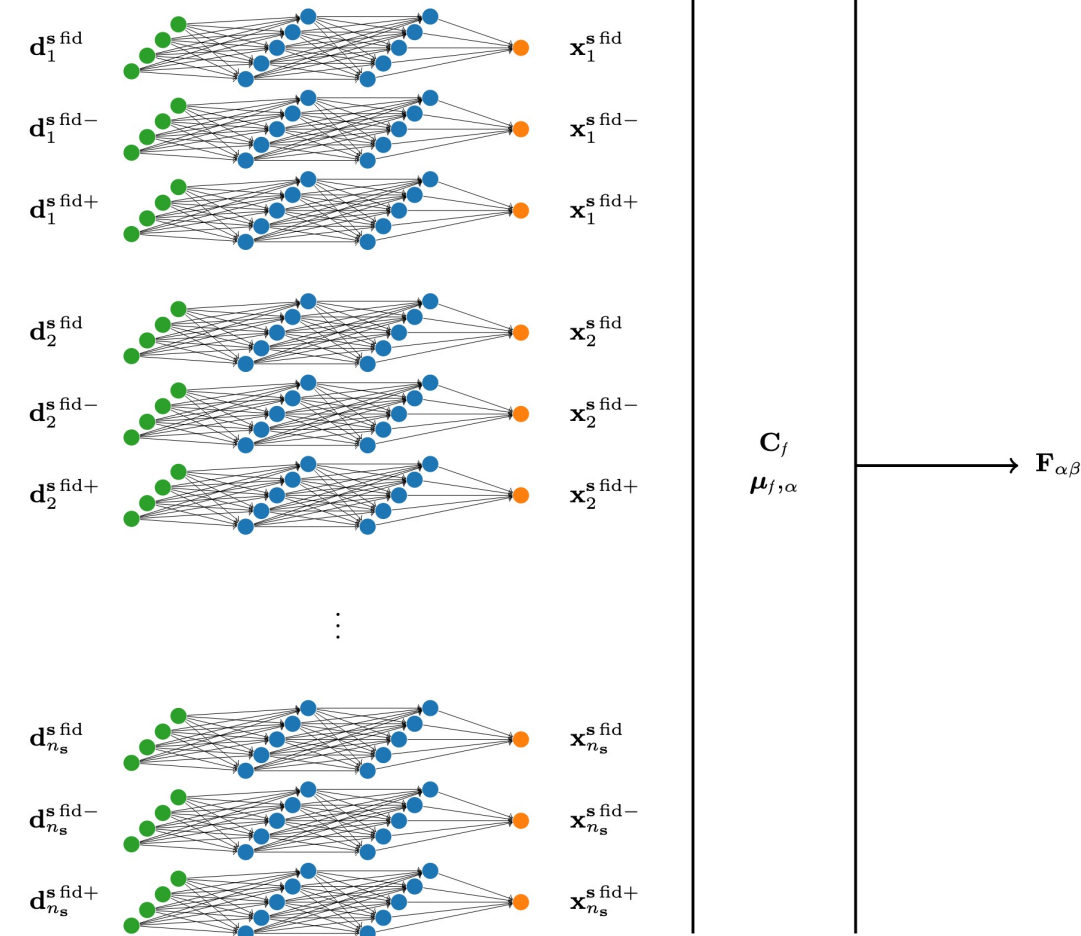


- RNN – encoding correlations across all frequency bins at once
- 2D Convolutional NN– local correlations in sky-plane

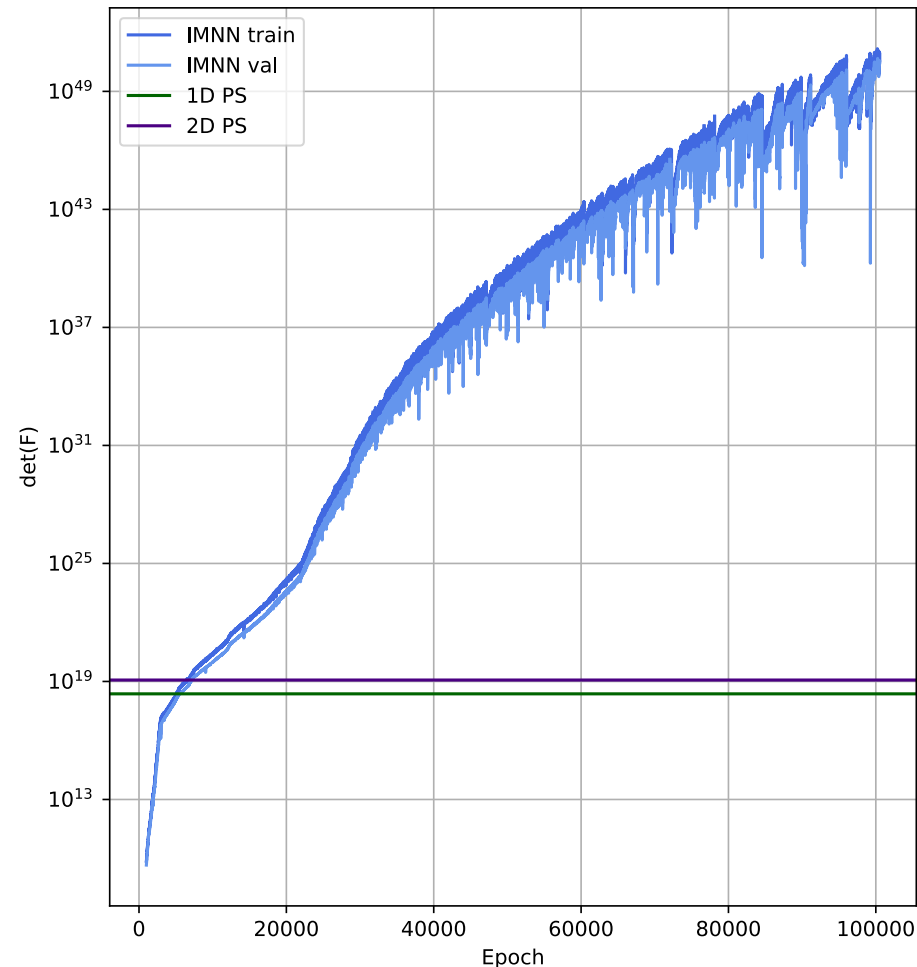
Unsupervised learning: Information Maximizing Neural Network

- Simulate the data at a fiducial parameter set: $\mathbf{d}(\boldsymbol{\theta}_{\text{fid}})$
- Simulate around the fiducial parameters: $\mathbf{d}(\boldsymbol{\theta}_{\text{fid}}^+)$, $\mathbf{d}(\boldsymbol{\theta}_{\text{fid}}^-)$
- Calculate compressed summary:
$$\mathbf{s}(\boldsymbol{\theta}) = \text{NN}(\mathbf{d}(\boldsymbol{\theta}))$$

- Maximize Fisher information:
$$L = -\ln |F|$$



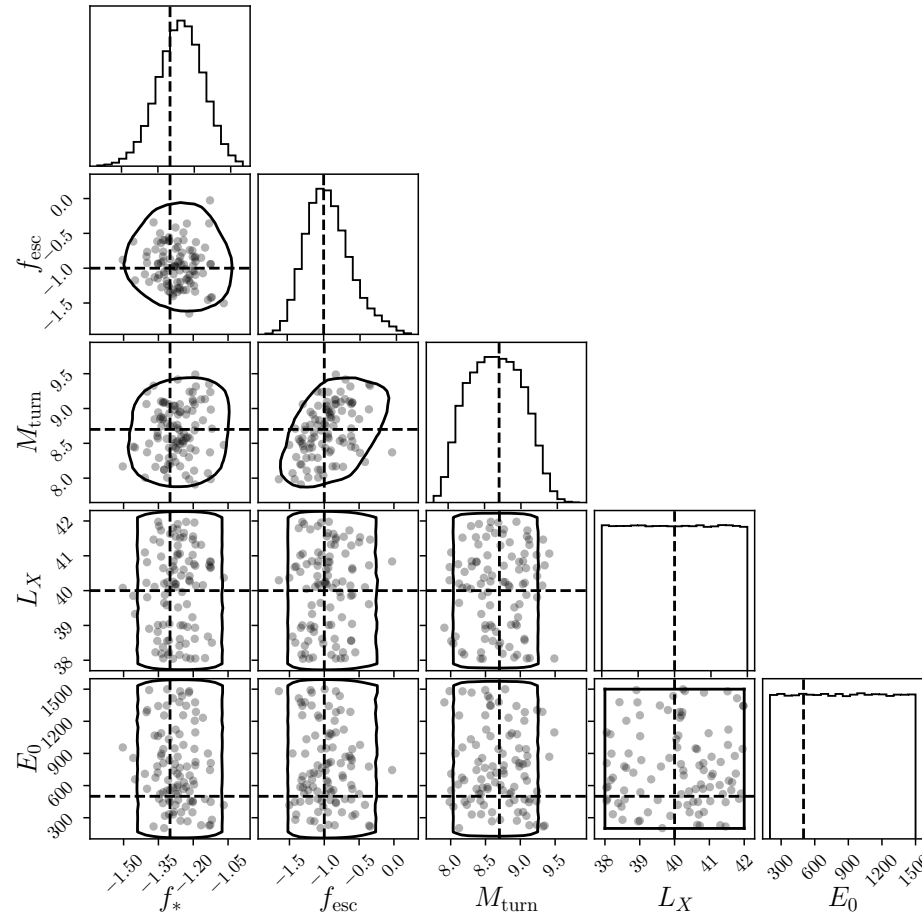
IMNN Fisher information at fiducial



Prelogović & Mesinger (2024)

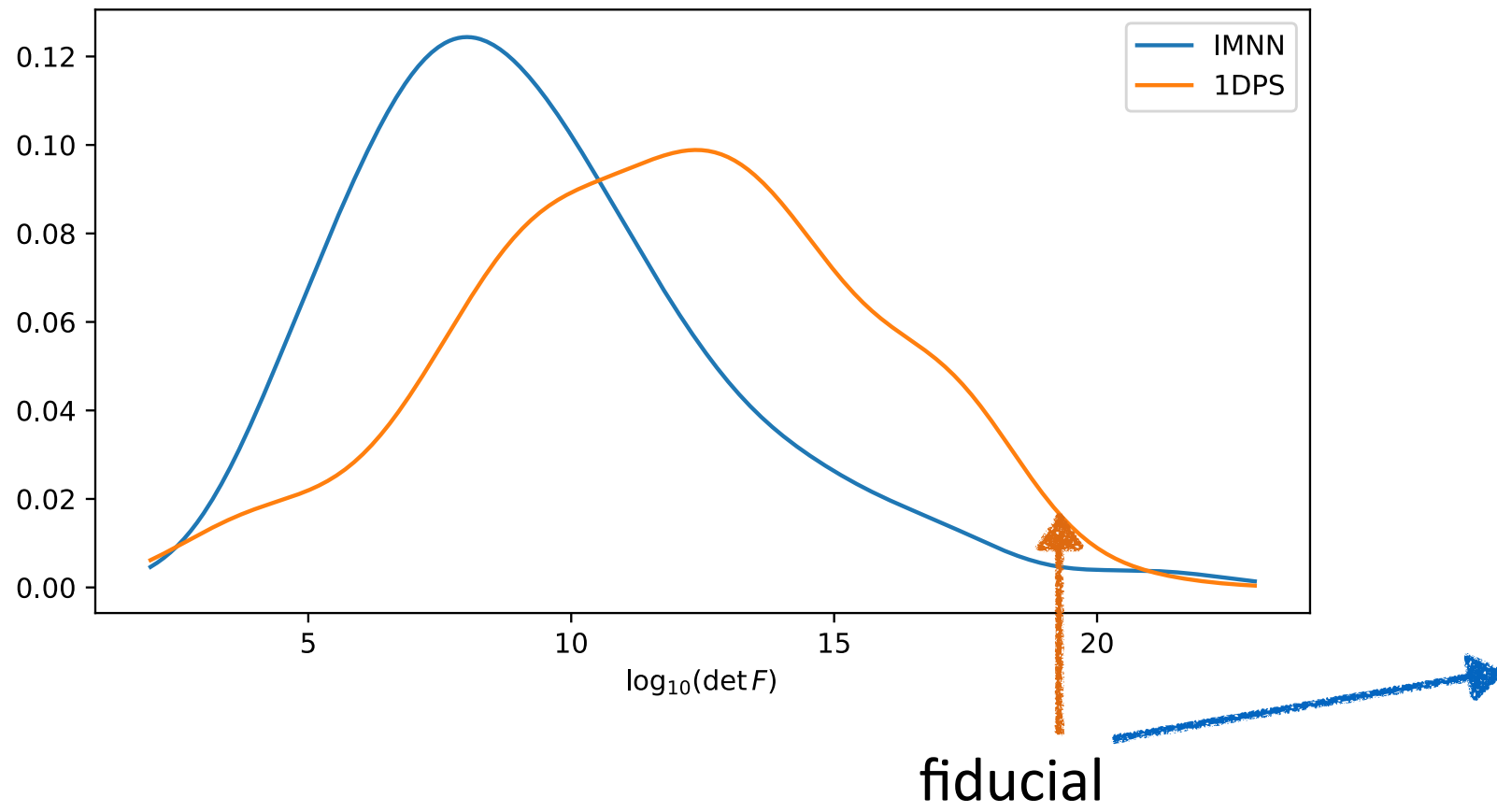
over 40 orders of magnitude improvement in Fisher information wrt power spectrum! $\sim 10^8$ times lower variance in parameter recovery!

How optimal is the compression for different fiducial parameter choices?

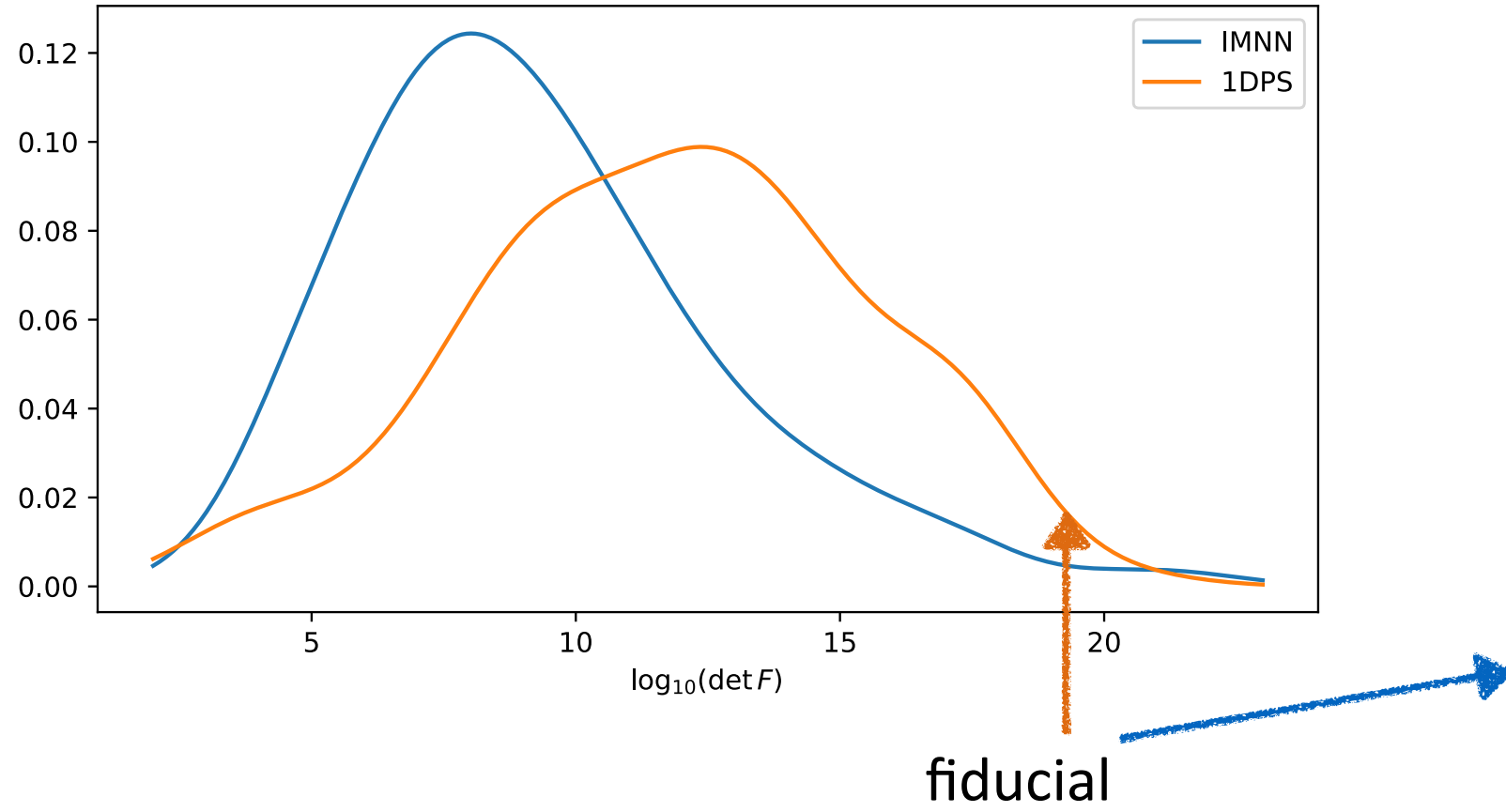


sample your prior volume and evaluate Fisher information throughout -> *prior weighted Fisher information*

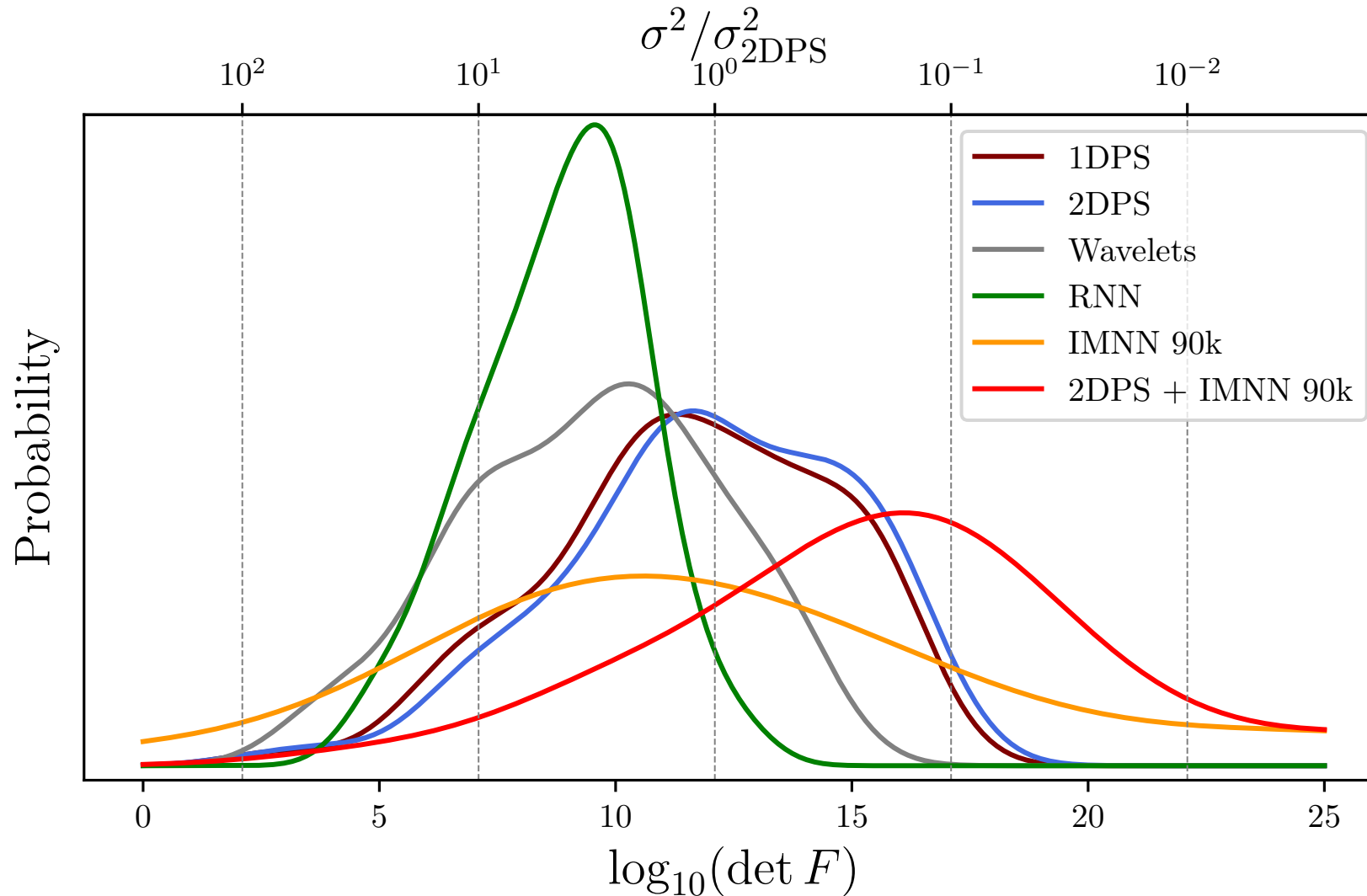
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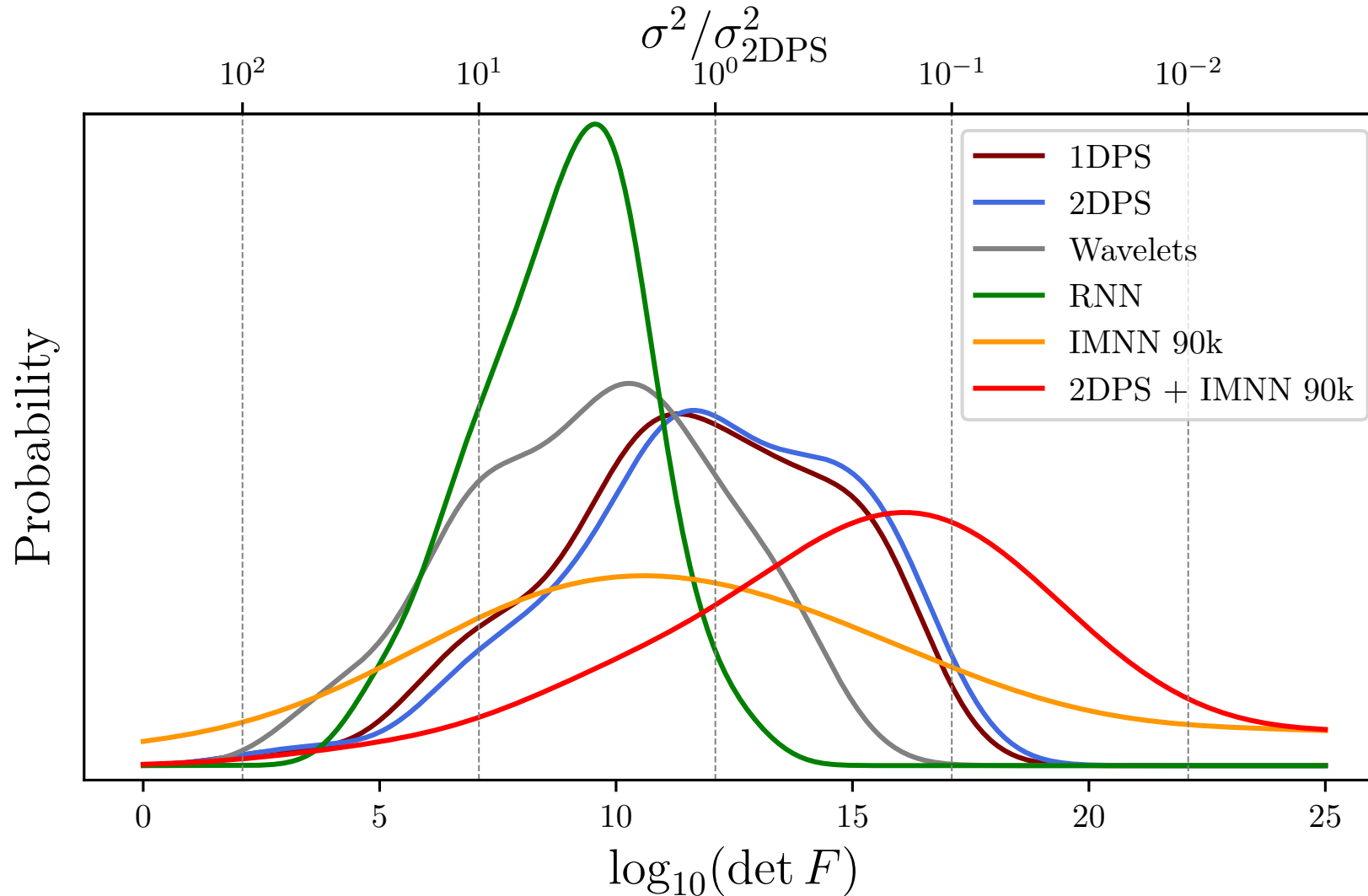
IMNN overspecializes to the Fisher of the *fiducial*... The mean Fisher over the prior is actually lower than the PS



Comparing various 21cm summaries using the prior-weighted Fisher information



Combining 2D PS & IMNN gives a constraining summary throughout the prior volume



The background is a deep blue gradient. On the left side, there are numerous light trails and dots in shades of cyan and white, creating a sense of depth and movement, similar to a data visualization or a futuristic tunnel. The word "Summary" is centered in the middle of the image.

Summary

Milestones and KPIs

Construction of databases:

- SBI database ~100 000 **21cmFAST** simulations
- IMNN database ~ 20 000
- Fisher database ~ 50 000

NN trainings:

- IMNN – 5 000 GPU h per model
- RNN – 1 000 GPU h per model
- SBI NDEs – relatively cheap (~few GPUh per model)

Bottlenecks:



Milestones and KPIs

Code release:

<https://github.com/dprelogo/21cmLikelihoods>

https://github.com/dprelogo/conditional_kde

<https://github.com/21cmfast/21cmEMU>

<https://github.com/dprelogo/21cmIMNN>

Publications:

Exploring the likelihood of the 21-cm power spectrum with simulation-based inference
[arXiv:2305.03074](https://arxiv.org/abs/2305.03074) (Prelogovic & Mesinger; MNRAS 524, 2023)

21CMEMU: an emulator of 21CMFAST summary observables
[arXiv:2309.05697](https://arxiv.org/abs/2309.05697) (Breitman, AM+; MNRAS 527, 2024)

How informative are summaries of the cosmic 21cm signal?
[arXiv:2401.12277](https://arxiv.org/abs/2401.12277) (Prelogovic & Mesinger; A&A submitted)