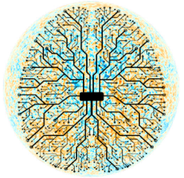
On the accuracy of posterior recovery with neural network emulators

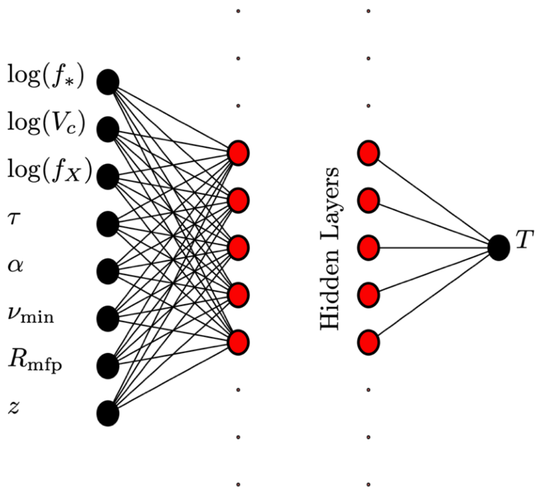
Harry Bevins
With Thomas Gessey-Jones and Will Handley


arXiv:2503.13263

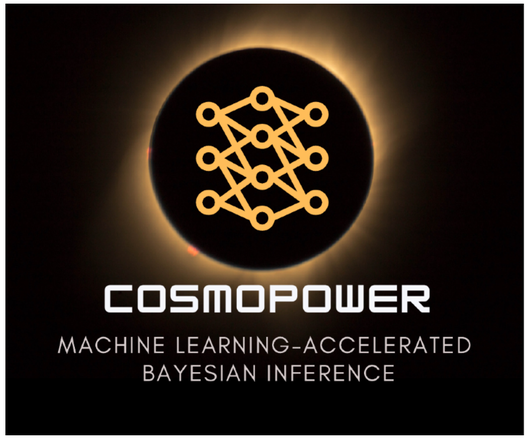
Emulators in Cosmology and Astrophysics

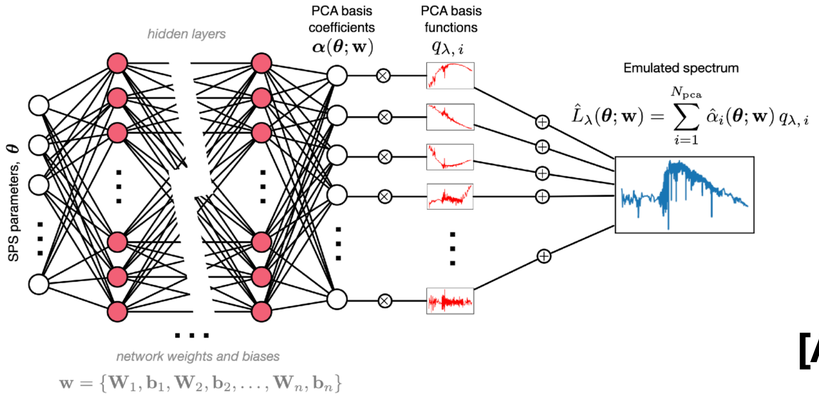
- Neural network emulators are really important in Cosmology and Astrophysics
- For fast inference on computationally expensive likelihoods
- Generating large training data sets for training simulation based inference algorithms



Cosmopower
[Spurio Mancini+2021]

globalemu [Bevins+21]
21cmLSTM [Dorigo Jones+2024]
21cmEMU [Breitman+ 2023]
21cmGEM [Cohen+2017]
And 21cmVAE [Bye+2022]





Speculator
[Alsing+2020]

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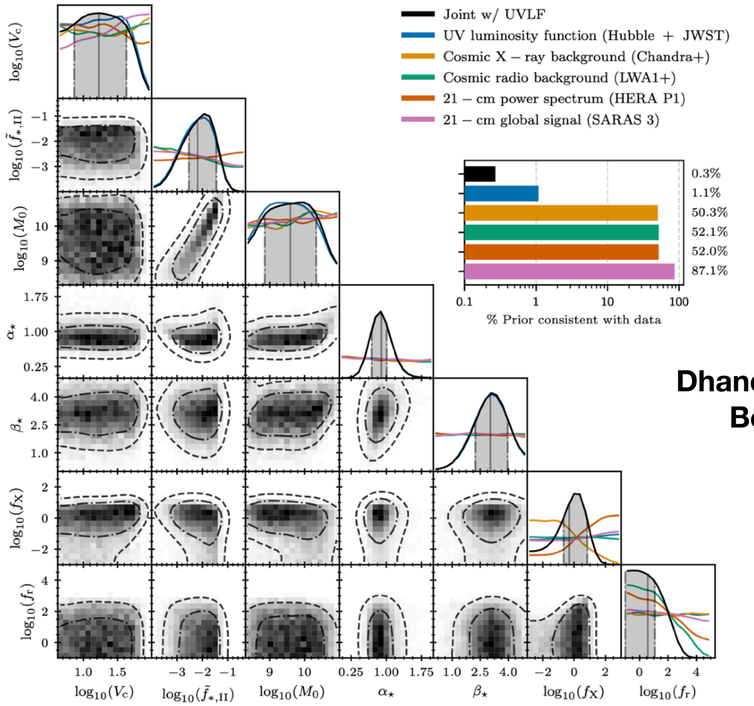
Emulators in Cosmology and Astrophysics

- In this work we are focused on likelihood based inference
- Semi-numerical simulations of cosmological signals are very computationally expensive
- Train emulators on example simulations and use these in the likelihood functions
- Established method for doing inference



Dhandha, Gessey-Jones, Bevins et al. 2025

(a) Cosmic shear with 37 (ΛCDM) and 39 (w_0w_aCDM) parameters, described in Sect. 4.

Method	$\log(z_{\Lambda\text{CDM}})$	$\log(z_{w_0w_a\text{CDM}})$	log BF	Total computation time
`CAMB` + nested sampling	-107.03 ± 0.27	-107.81 ± 0.74	0.78 ± 0.79	∼8 months (48 CPUs)
`CosmoPower-JAX` + NUTS + `harmonic`	40956.55 ± 0.06	40955.03 ± 0.04	1.53 ± 0.07	2 days (sampling, 12 GPUs) + 12 minutes (evidence, 1 GPU + 48 CPUs)
`CosmoPower-JAX` + NUTS + naïve flow estimator	400958 ± 5	40957 ± 4	1 ± 6	Similar to `harmonic`

Piras et al 2024

(b) 3x(3x2pt) with 157 (ΛCDM) and 159 (w_0w_aCDM) parameters, described in Sect. 5.

Method	$\log(z_{\Lambda\text{CDM}})$	$\log(z_{w_0w_a\text{CDM}})$	log BF	Total computation time
`CAMB` + nested sampling	Unfeasible	Unfeasible	Unfeasible	12 years (projected, 48 CPUs)
`CosmoPower-JAX` + NUTS + `harmonic`	$406689.6^{+0.5}_{-0.3}$	$406687.7^{+0.5}_{-0.3}$	$1.9^{+0.7}_{-0.5}$	8 days (sampling, 24 GPUs) + 17 minutes (evidence, 1 GPU + 48 CPUs)
`CosmoPower-JAX` + NUTS + naïve flow estimator	406703 ± 39	406701 ± 62	2 ± 73	Similar to `harmonic`

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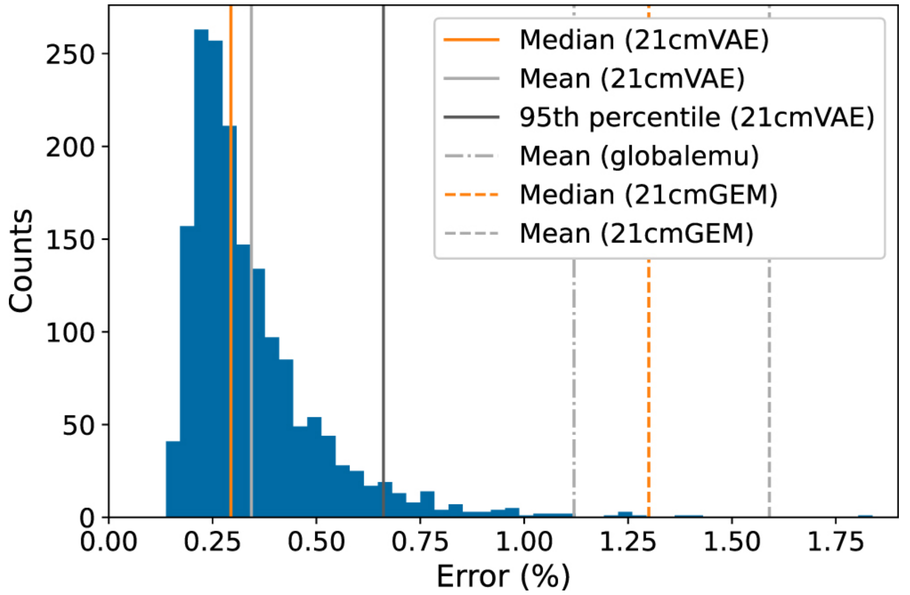
Defining required accuracy

- We measure accuracy by evaluating the networks on a test data set
- Typically we do this with something like RMSE

$$\epsilon = \sqrt{\frac{1}{N_\nu} \sum_i^{N_t} (S_{\rm true}(t) - S_{\rm pred}(t))^2}$$

- But what average value of ϵ over the test data is good enough?
- Generally we work with “rules of thumb”
- e.g. ***globalemu*** paper suggested $\bar{\epsilon} \approx 0.1\sigma$



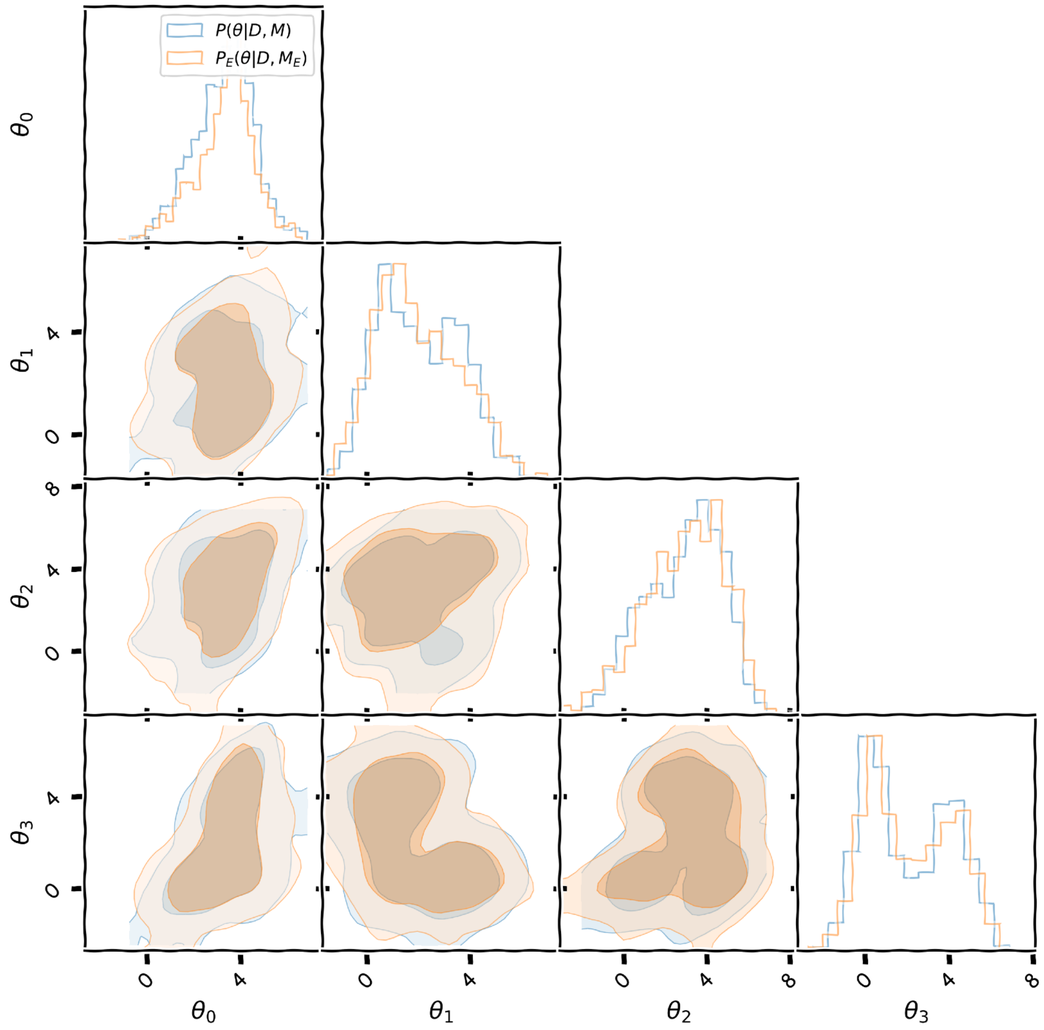
Impact on posterior recovery?

- Really interested in is how well can we recover the posteriors if we use an emulator rather than the full simulation?

$$\log L \to \log L + \delta \log L$$

$$P(\theta \,|\, D, M) = \frac{L\pi}{\int L\pi d\theta} \to P_E(\theta \,|\, D, M_E) = \frac{L\pi e^{\delta \log L}}{\int L\pi e^{\delta \log L} d\theta}$$

- Is $\bar{\epsilon} \approx 0.1\sigma$ good enough?



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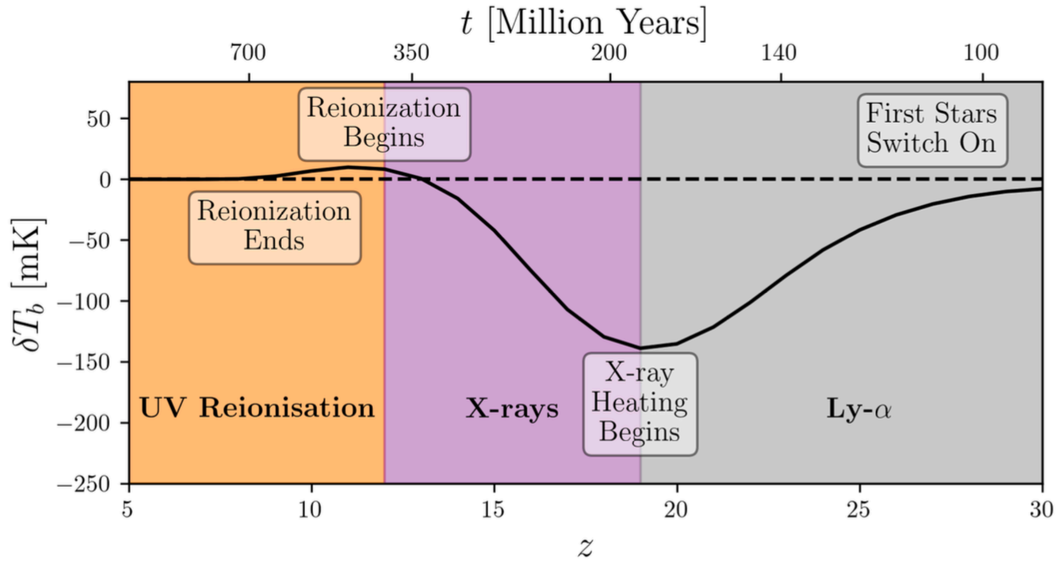
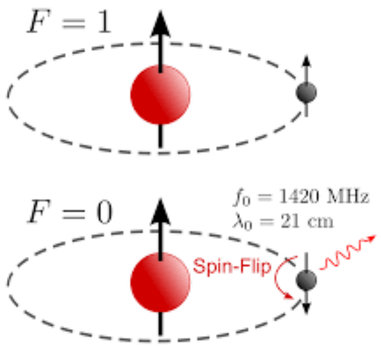
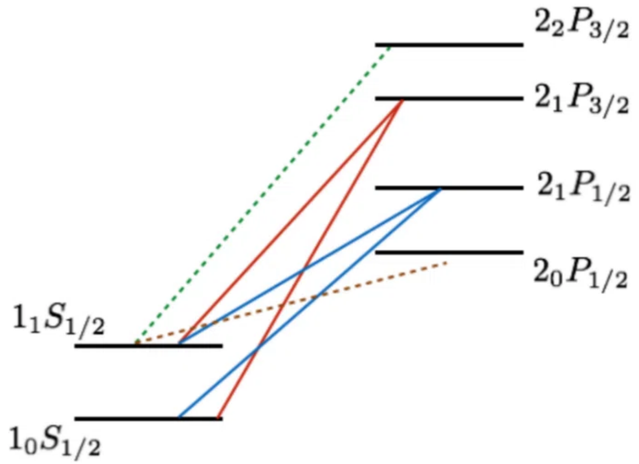
21cm Cosmology

- Looking at relative brightness of 21cm signal from neutral hydrogen and the background CMB
- 21cm signal brightness measured by a statistical temperature
- Relative number of atoms with aligned and anti-aligned proton and electron spins driven by many different processes
  - Cosmology ($z < 30$)
  - Star formation ($30 < z < 15$)
  - X-ray heating ($15 < z < 8$)
  - Ionisation ($8 < z < 5$)
  - With some overlap
  - And many other processes







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Dorigo Jones+23

- Dorigo Jones+23 tried to answer questions of emulator accuracy
- Ran inference with ARES and compared recovered posteriors to posteriors recovered with an emulator of ARES
- ARES is a 1D radiative transfer code which evaluates in about 1s
- Want to do inference with semi-numerical or hydro simulations which take hours to days to run per parameters set

OPEN ACCESS

Validating Posteriors Obtained by an Emulator When Jointly Fitting Mock Data of the Global 21 cm Signal and High-*z* Galaxy UV Luminosity Function

J. Dorigo Jones[1], D. Rapetti[1,2,3], J. Mirocha[4,5], J. J. Hibbard[1], J. O. Burns[1], and N. Bassett[1]

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Citation J. Dorigo Jones *et al* 2023 *ApJ* **959** 49

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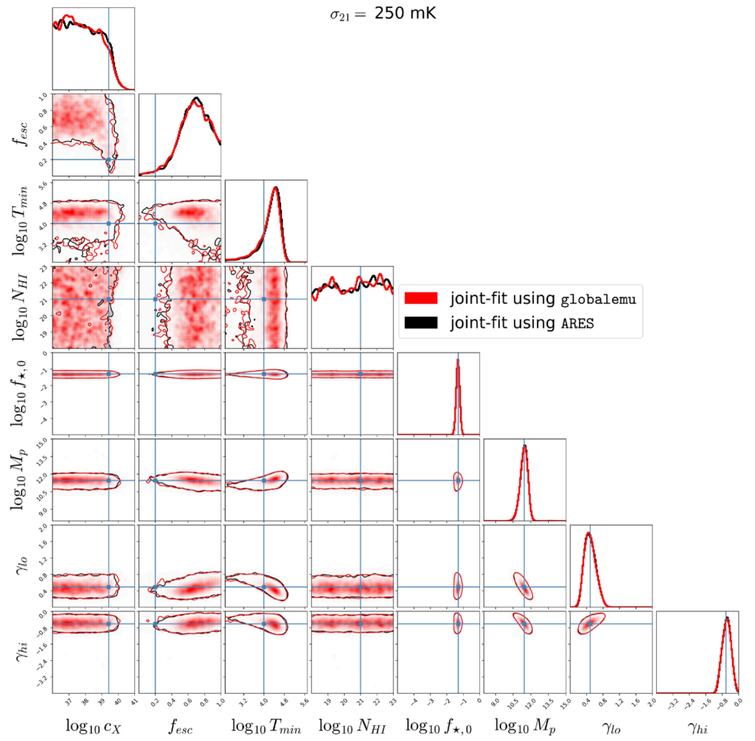


arXiv:2503.13263

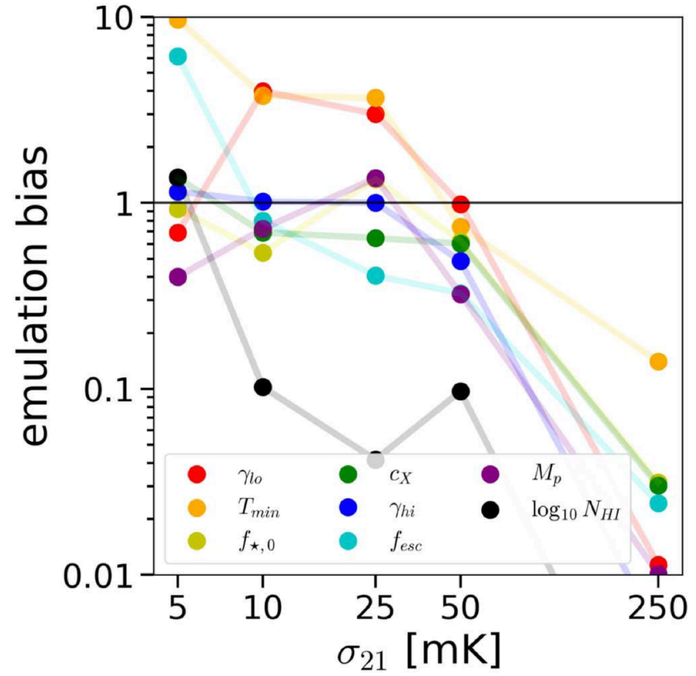
Dorigo Jones+23

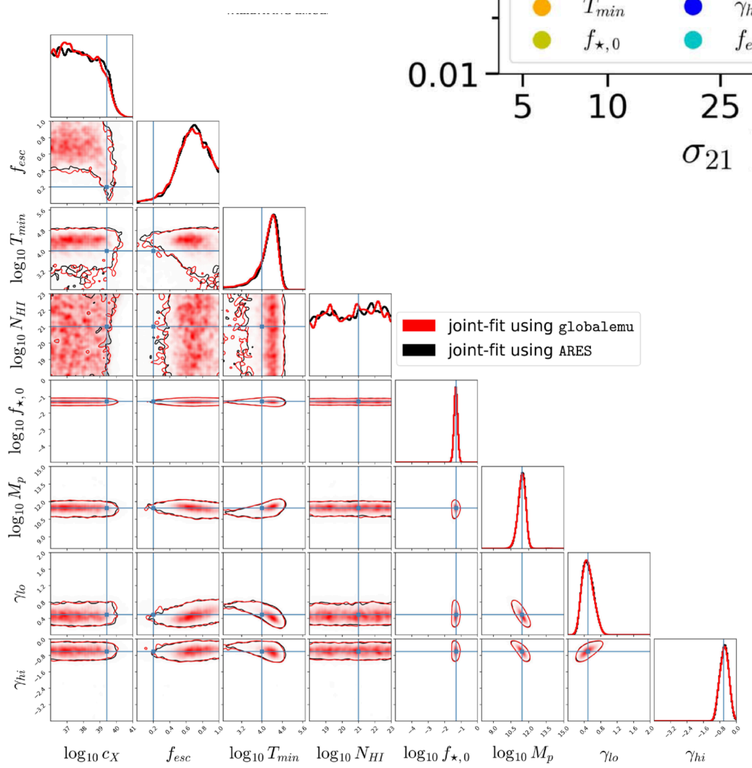
- Measured posterior accuracy with two metrics

$$\text{emulator bias} = \frac{|\mu_{\text{globalemu}} - \mu_{\text{ARES}}|}{\sigma_{\text{ARES}}}$$

$$\text{true bias} = \frac{|\mu_{\text{ARES}} - \theta_0|}{\sigma_{\text{ARES}}}$$

- They concluded that even for $\bar{\epsilon} \approx 0.05\sigma$ they can't accurately recover the posteriors with ***globalemu***





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Why this is concerning?

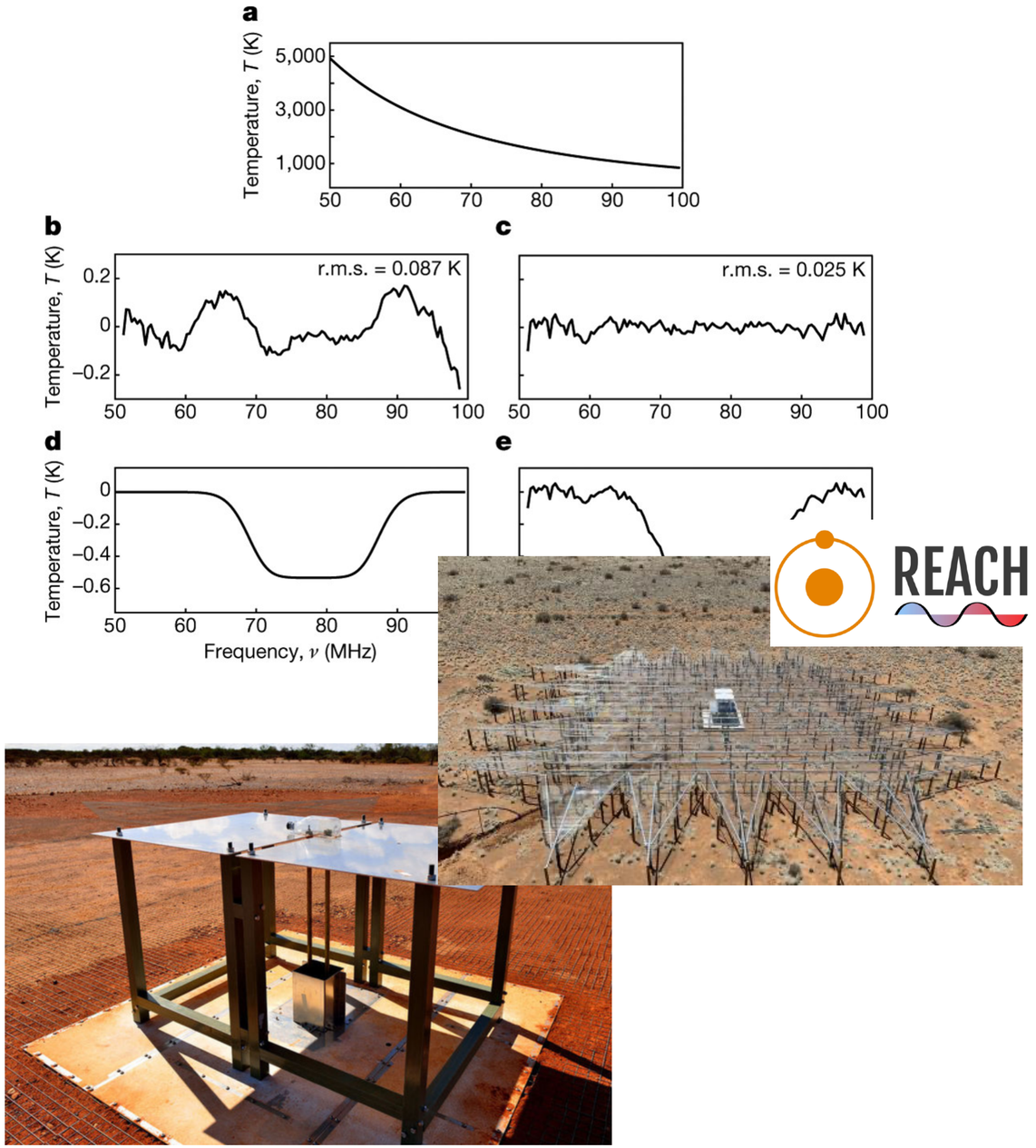
- Most experimentalists agree that we need to go down to around 25 mK noise to confidently detect the 21cm signal

- Most emulators have $\bar{\epsilon} \approx 1\ \mathrm{mK} \approx 0.05 \times 25\mathrm{mK}$ and it seems challenging to go beyond this

- Assuming a Gaussian likelihood and

$$\sigma^2 = \sigma^2_{\mathrm{instrument}} + \bar{\epsilon}^2$$

we would expect the uncertainty from the instrument to dominate the posteriors



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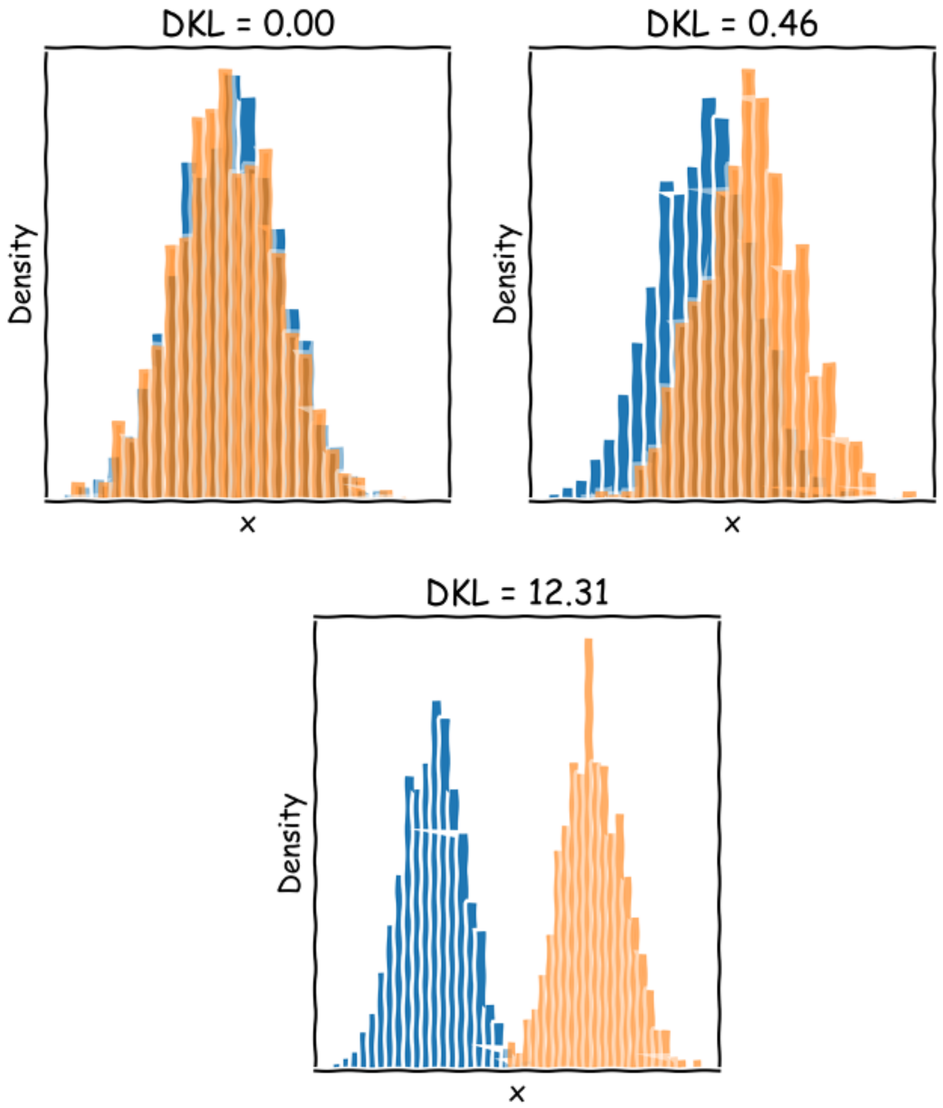
Measuring the impact of the emulator

- The emulator bias defined in Dorigo Jones+23 is fine but its only really considers the difference in 1D

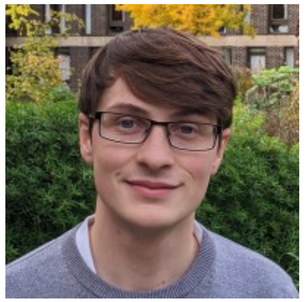
- A more comprehensive measure of the difference between the true and emulated posteriors is the Kullback-Leibler Divergence

$$D_{\mathrm{KL}} = \int P \log\left(\frac{P}{P_\epsilon}\right) d\theta$$

- The issue is that we typically do not have access to P else we wouldn't be interested in emulators



Measuring the impact of the emulator

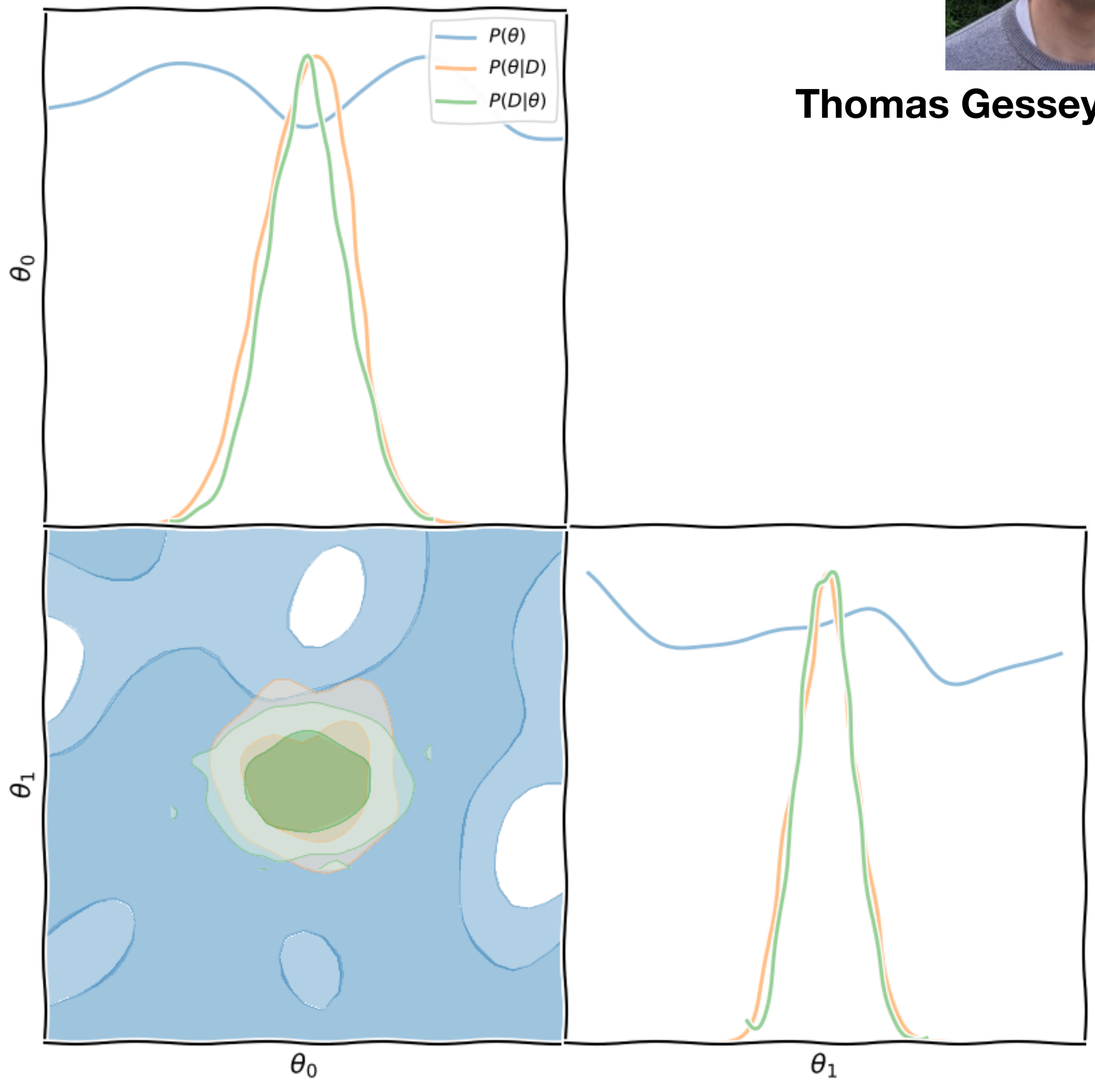


Thomas Gessey-Jones

- Can make progress if we make some assumptions
- Firstly we assume that the likelihood function is Gaussian

$$L \propto \exp\left(-\frac{1}{2}(D - \mathscr{M})^T \Sigma^{-1} (D - \mathscr{M}) \right)$$

And our prior is uniform such that the posterior is also Gaussian



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Measuring the impact of the emulator

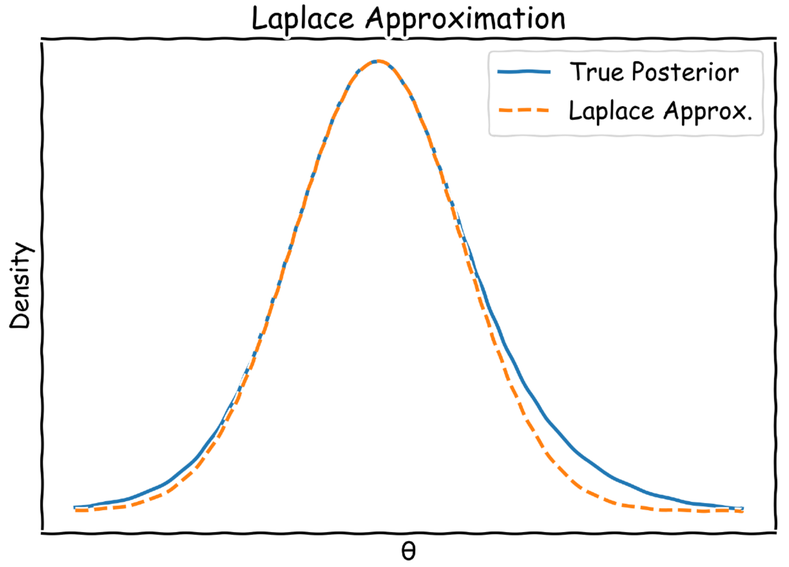
- Assume a linear model and linear emulator error

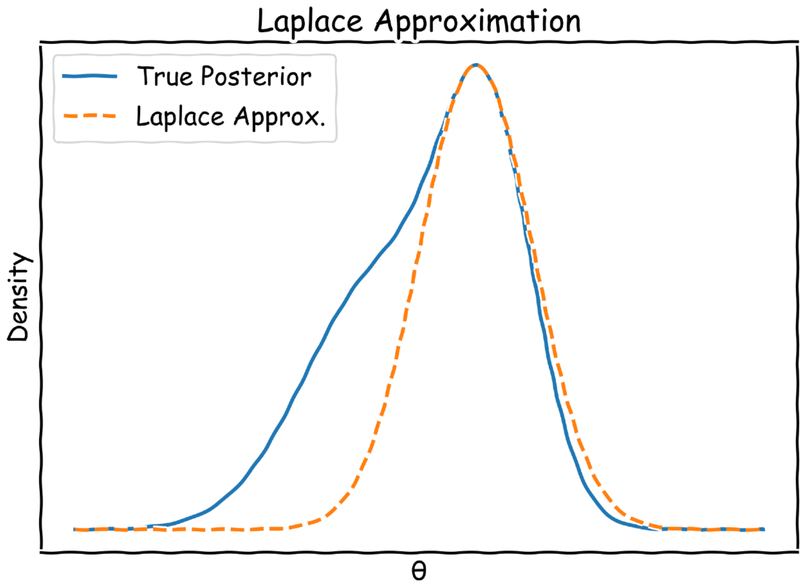
$$\mathscr{M}(\theta) \approx M\theta + m \text{ and } E(\theta) \approx E\theta + \epsilon$$

Such that $M_\epsilon(\theta) = (M + E)\theta + (m + \epsilon)$

- Comes from Taylor expansion of model around the MAP and the assumption that the posterior is sharply peaked so we can ignore higher order terms

$$M = \mathscr{J}(\theta_0)$$
$$m = M(\theta_0) - \mathscr{J}(\theta_0)\theta_0$$





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Measuring the impact of the emulator

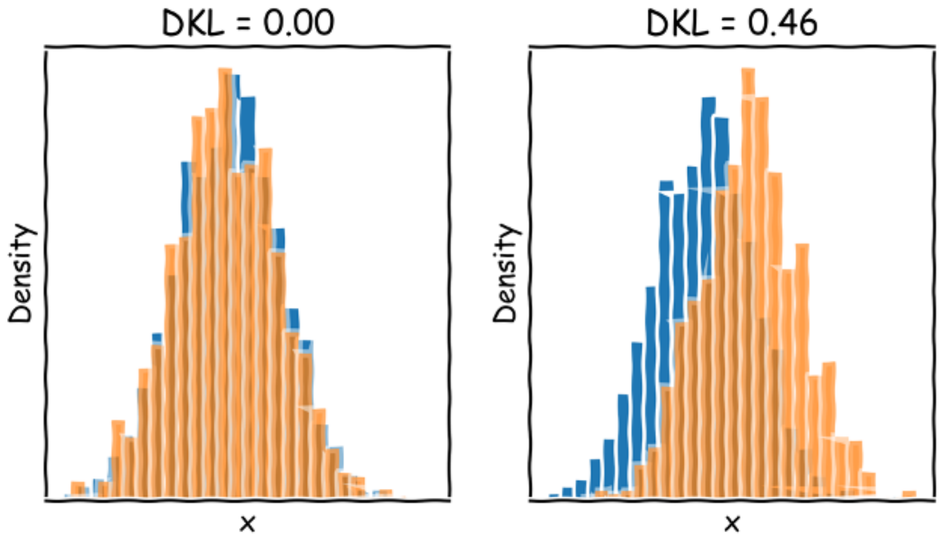
- KL divergence between two Gaussians is given by

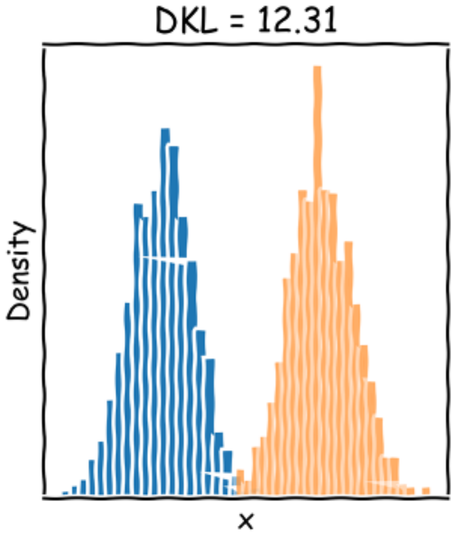
$$D_{KL} = \frac{1}{2}\left[\log\left(\frac{|C_E|}{|C|}\right) - N_\theta + \mathrm{tr}(C_E^{-1}C) + (\mu_E - \mu)^T C^{-1}(\mu_E - \mu)\right]$$

- Can show that

$$C = (M^T\Sigma^{-1}M)^{-1}$$
$$\mu = CM^T\Sigma^{-1}(D - m)$$
$$C_E = ((M + E)^T\Sigma^{-1}(M + E))^{-1}$$
$$\mu_E = C_E(M + E)^T\Sigma^{-1}(D - m - \epsilon)$$

- Make assumptions about $E \ll M$ and $\Sigma = \frac{1}{\sigma^2}\mathbf{1}_{N_d}$





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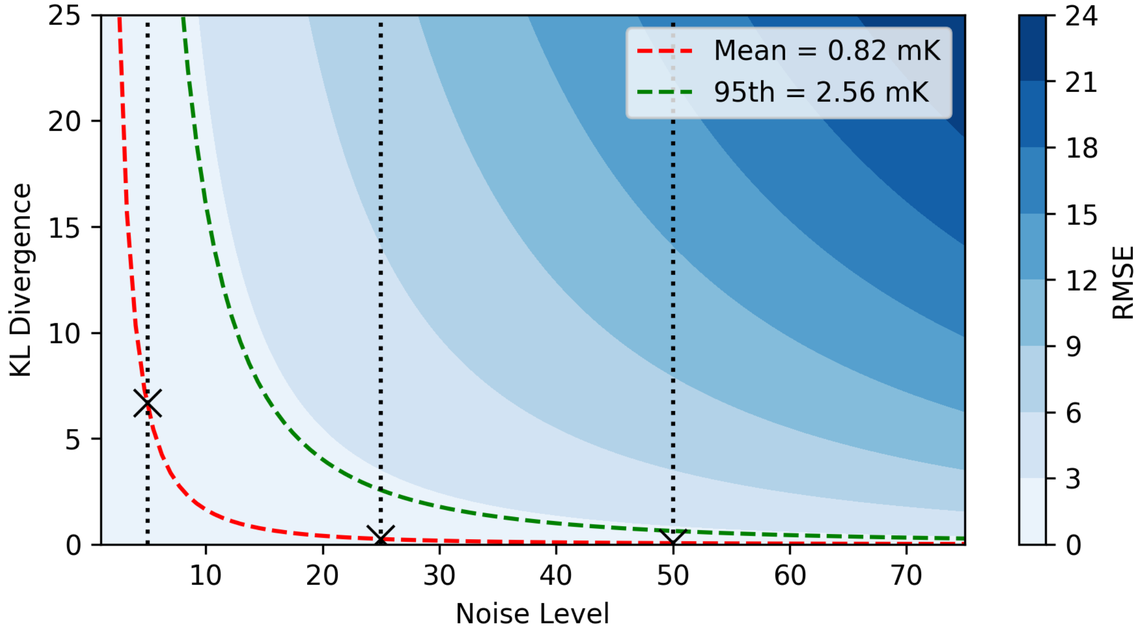
Measuring the impact of the emulator

$$D_{\mathrm{KL}}(P\,||\,P_E) \leq \frac{1}{2}\frac{1}{\sigma^2}||\epsilon||^2$$

$$D_{\mathrm{KL}}(P\,||\,P_\epsilon) \leq \frac{N_d}{2}\left(\frac{\mathrm{RMSE}}{\sigma}\right)^2$$

- An approximate upper bound on the KL divergence between P and P_ϵ given an emulator error RMSE, the noise in the data σ and the number of data points N_d
- Predictive function that can be used both to justify but also predict the required accuracy of an emulator



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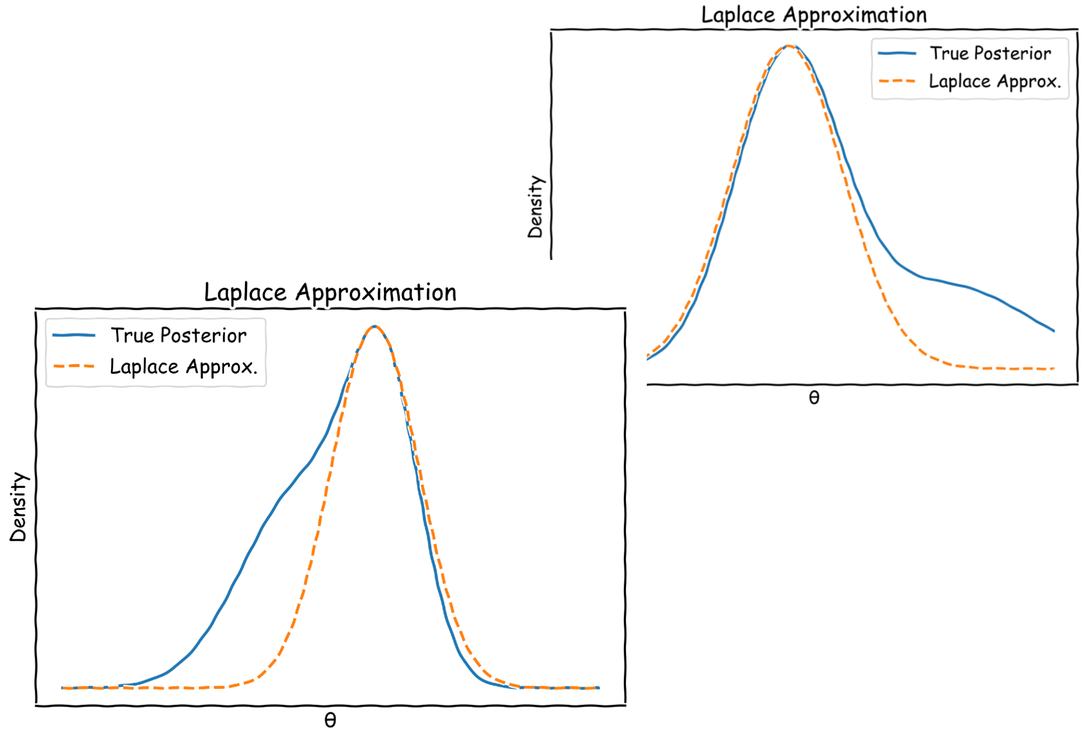
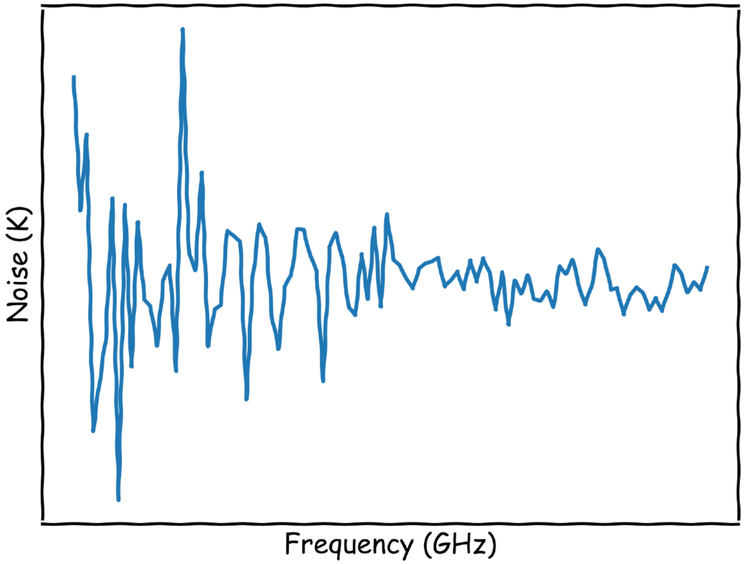
Limitations of the approximation

- The approximation assumes linearity around the peak of the posterior which might not hold in higher dimensions
- Posteriors become curved or multi modal
- Assuming a Gaussian likelihood and posterior
- Assumes uncorrelated noise in the data
- Assumes noise is constant across the data





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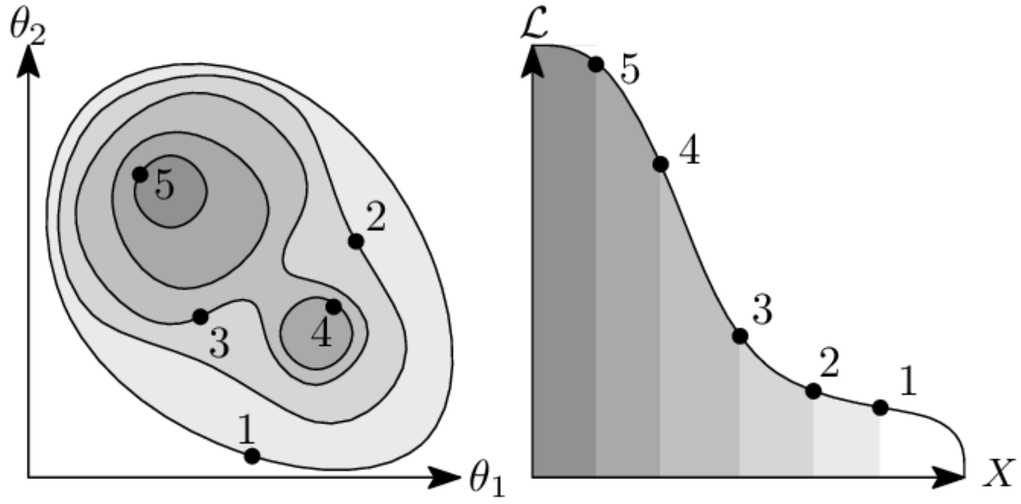
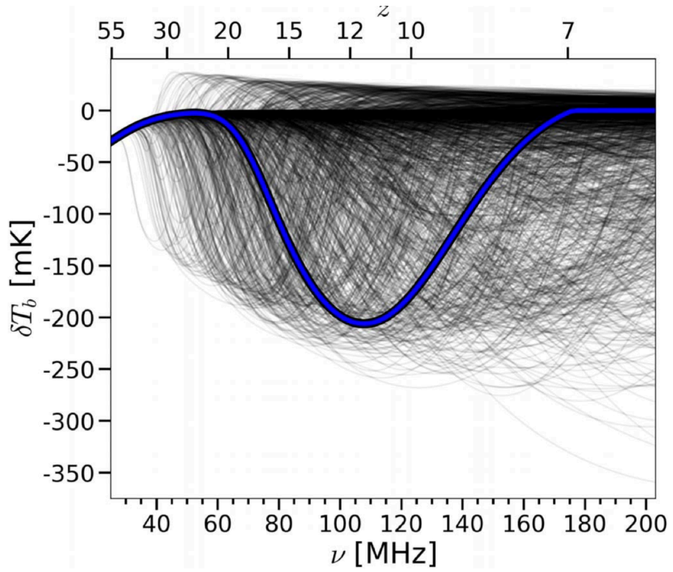
Testing on a 21cm Cosmology problem

- Assuming the data comprises of signal plus noise
- Same fiducial signal as in Dorigo Jones+23
- Same prior range and same sampler
- Assuming as Gaussian likelihood as was done in their paper
- Assuming absolute knowledge of the level of noise in the data
- Running for 5, 25, 50 and 250 mK





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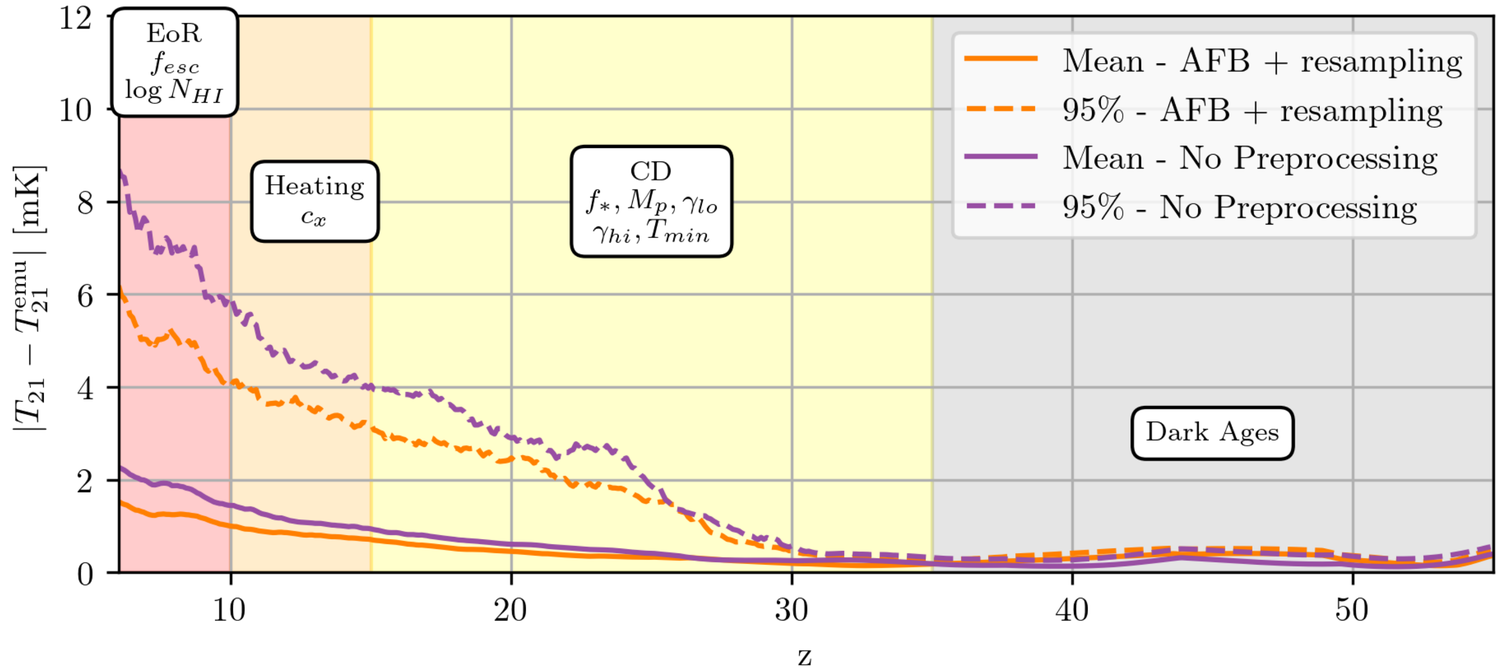
globalemu performance and ARES modelling



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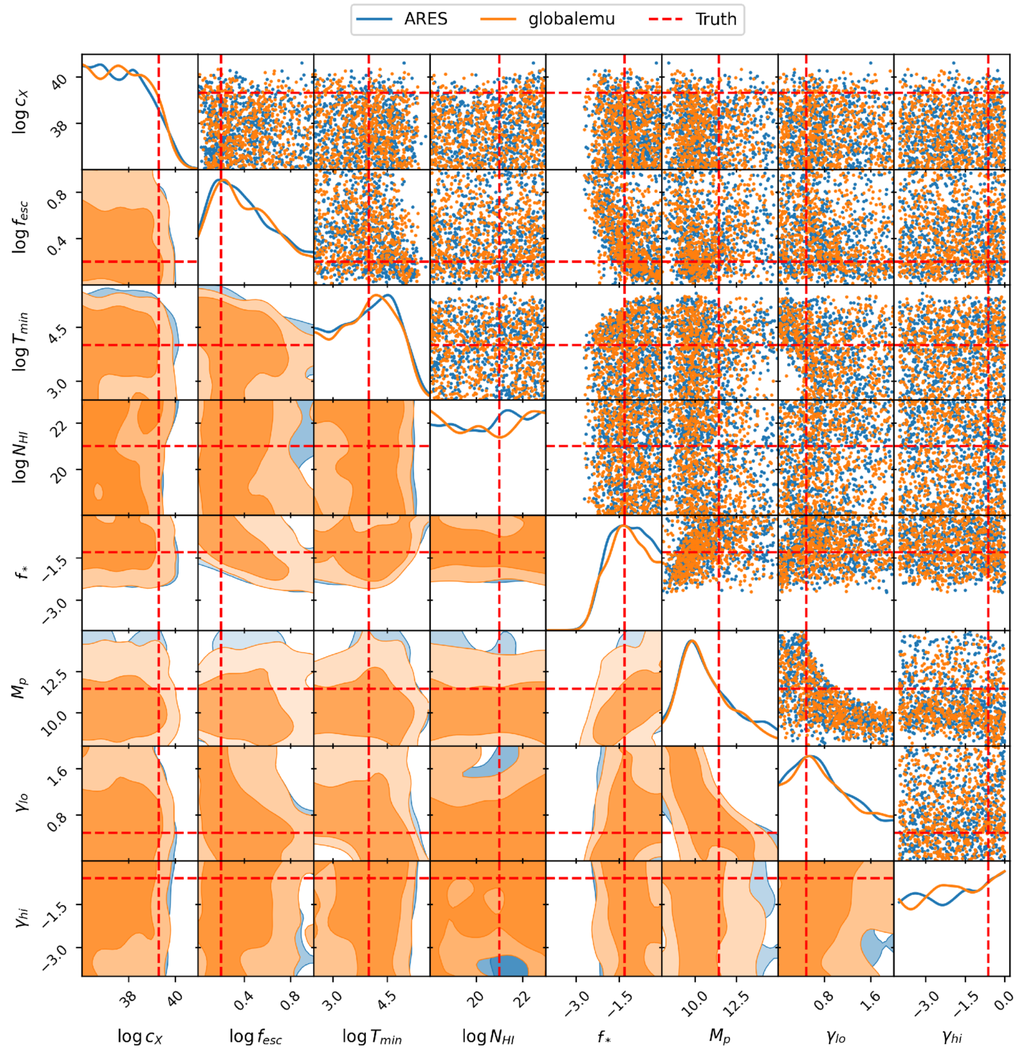
Running the analysis - 250 mK



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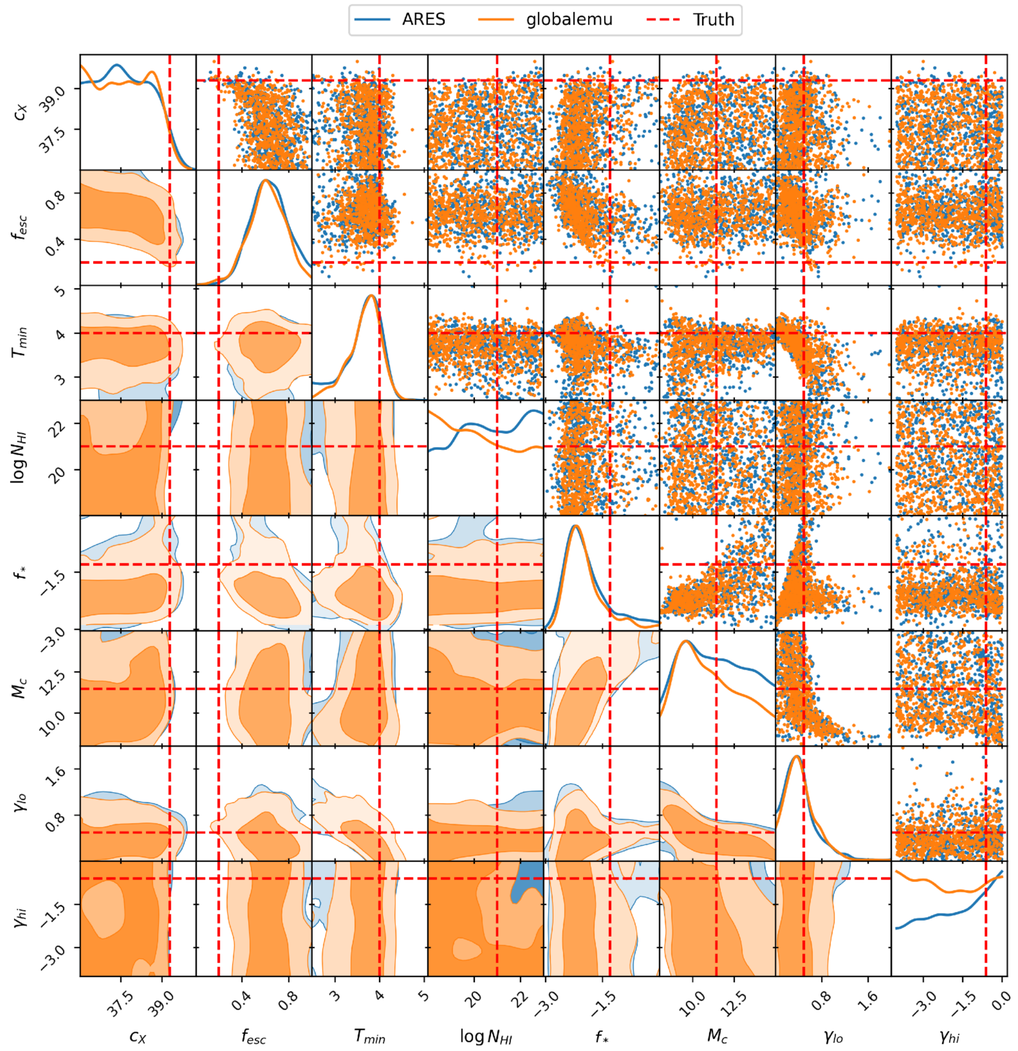
Running the analysis - 50 mK



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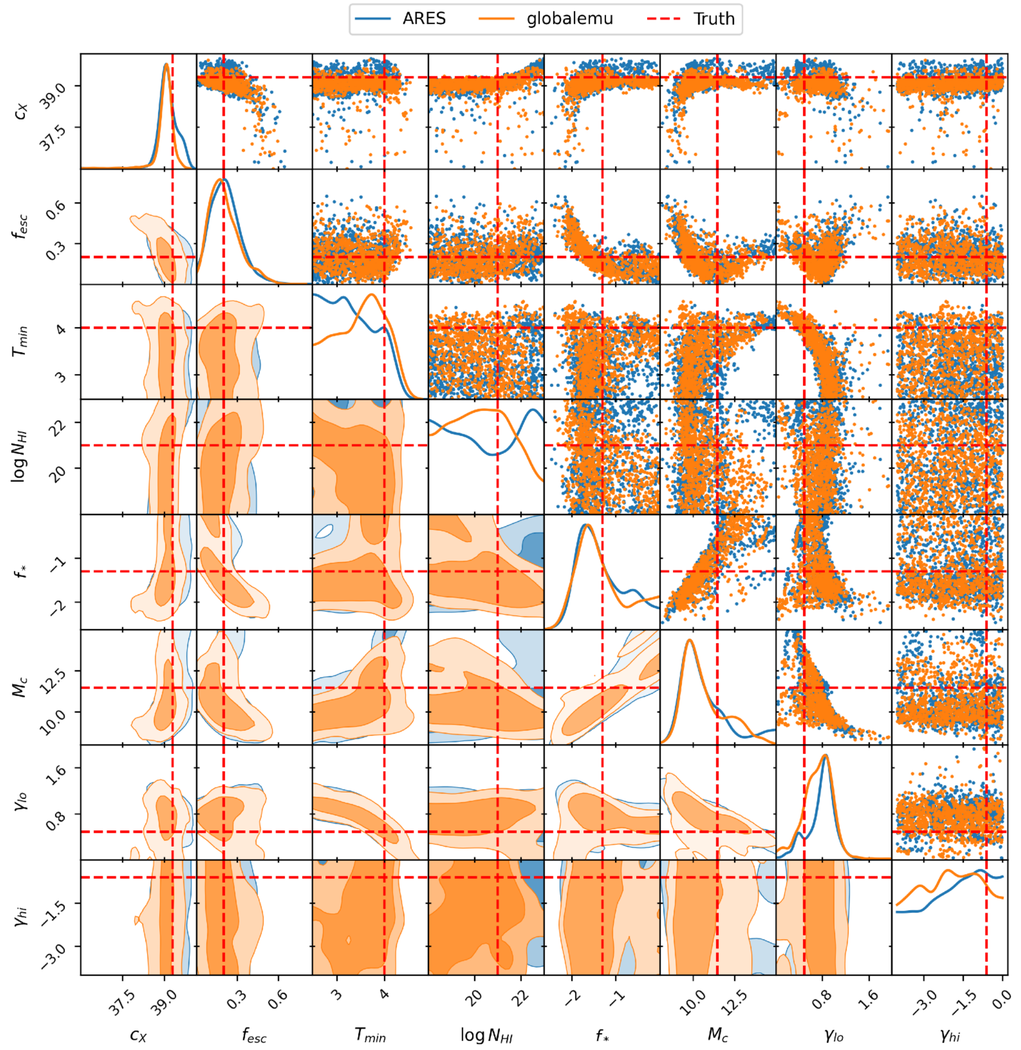
Running the analysis - 25 mK



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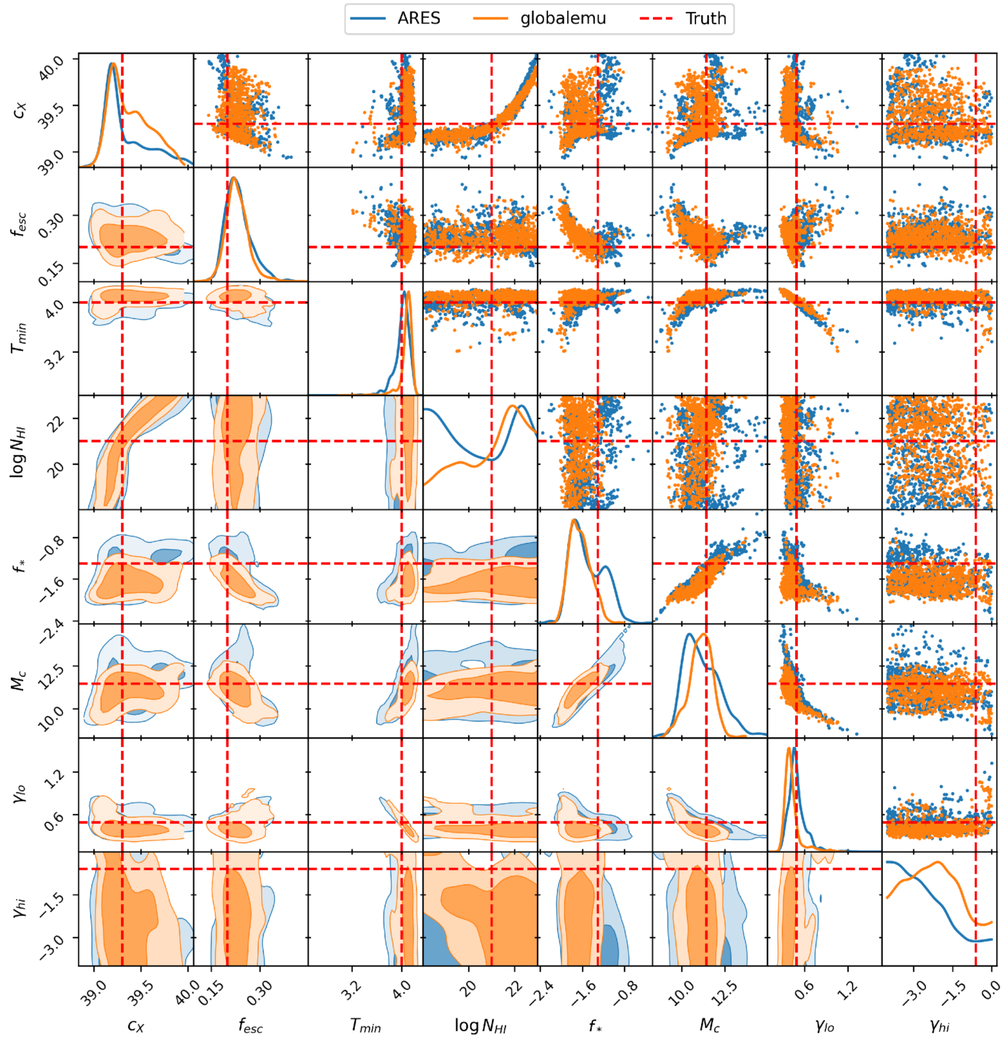
Running the analysis - 5 mK



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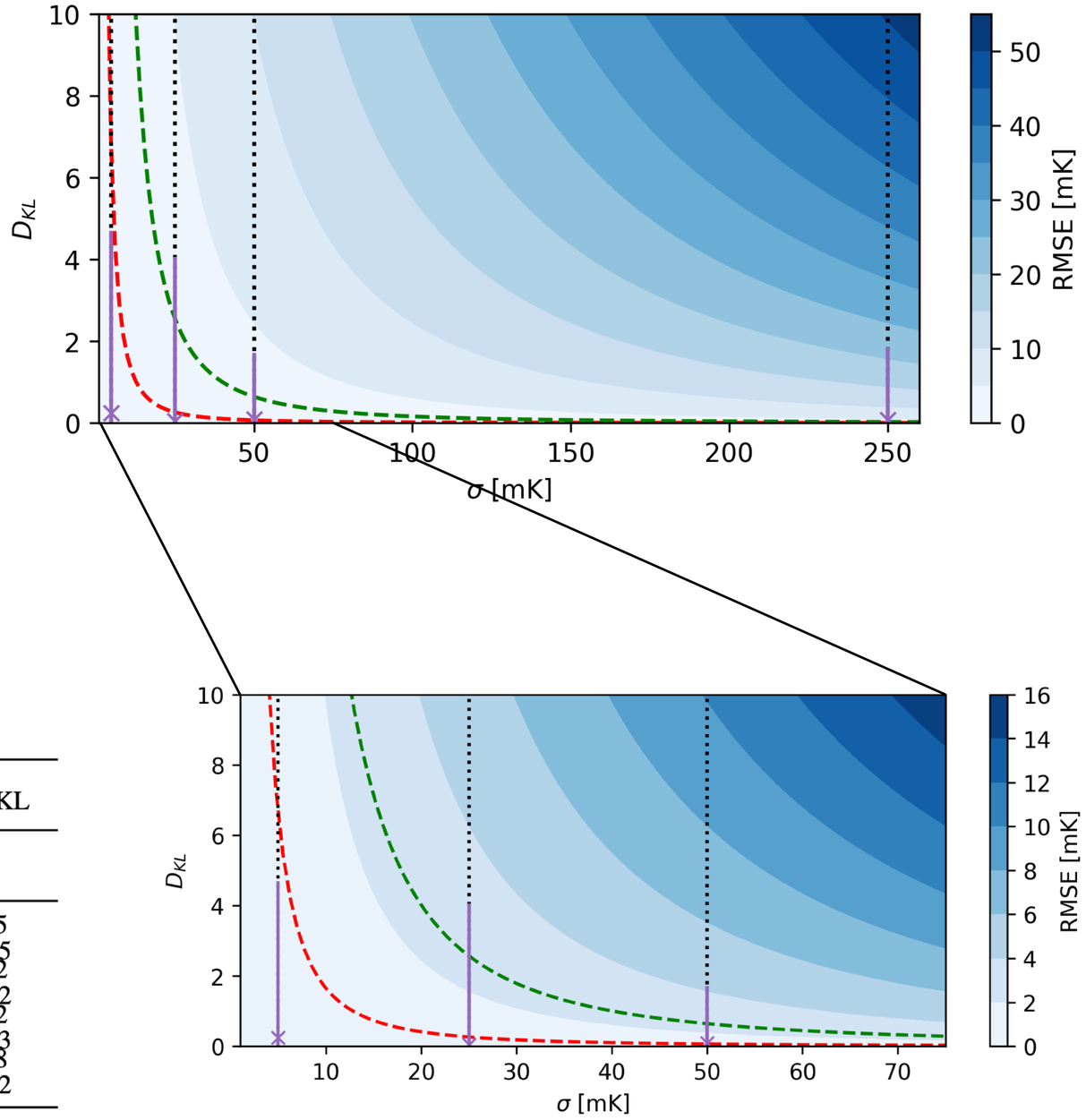
How about the D_{KL}?

- Need to be able to evaluate the log-probability for sets of samples on both distributions to get D_{KL}
- Use normalising flows implemented with ***margarine*** [see Bevins et al 2022, 2023, arXiv:2207.11457, arXiv:2205.12841]
- Compare calculated D_{KL} with predicted upper limits

Noise Level [mK]	Estimated $\mathcal{D}_{\mathrm{KL}} \leq$		Actual $\mathcal{D}_{\mathrm{KL}}$
	Mean RMSE	95th Percentile	
5	9.60	96.62	$0.25^{+4.45}_{-0.25}$
25	0.38	3.86	$0.05^{+4.02}_{-0.52}$
50	0.10	0.97	$0.09^{+1.62}_{-0.03}$
250	0.004	0.039	$0.08^{+1.78}_{-0.02}$



Conclusions

- We are presenting a useful upper bound on the incurred information loss from using emulators in inference
- Broadly applicable beyond 21cm
- We demonstrated that we can accurately recover posteriors even with $\bar{\epsilon} \approx 0.2\sigma$
- arXiv:2503.13263
- https://github.com/htjb/validating_posteriors