STATISTICAL SUMMARIES FOR BAYESIAN ANALYSES IN EOR SCIENCE

TOM BINNIE – HANGZHUO 2024

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What we'll cover:

Methods

- Bayesian parameter estimation, Bayesian Model Selection, ABC
- 3 types of Summary statistic

- (Fourier) Power Spectrum likelihood + 3DCNN + Morlet PS likelihood (in Progress..)

Application

- FPS likelihood can be used reliably in a wide range of situations

- 3D-CNN likelihood-free inference can do model selection but with some flexibility caveats.

- MPS is still in development but looks very promising

Line of sight density structure modes contribute to cosmic variance

Intro to Bayesian Statistics

Likelihood — Prior

$$\frac{p(D|\mathcal{M},\theta)\ \ p(\theta|\mathcal{M})}{p(D|\mathcal{M})} = p(\vartheta|D,\mathcal{M})$$

Bayesian Evidence — Posterior

(with uniform priors) → $\mathcal{P} \propto \mathcal{L}$

- Parameter Estimation

we want $\mathcal{L}_{max}$

- Peak finding done by Emcee

(Foreman-Mackey et al. 2013)

1:

- can we retrieve fiducial parameters from mock data?

- Model Selection

we want $\mathcal{Z}_i = p(D|M_i)$

$$\mathcal{Z}_i = \int \mathcal{L}(\Theta)\Pi(\Theta)\mathrm{d}\Theta$$

- Integrated with MultiNest

(Feroz, Hobson et al. 2006)

$$\mathcal{B}_{12} = \frac{P(D|M_1)}{P(D|M_2)} = \frac{\mathcal{Z}_1}{\mathcal{Z}_2}$$

2:

- for a mock data set from each model can we rule out the *wrong* models?

Bayesian likelihoods vs Approximate Bayesian Computation

Both require simulating a forward model

Likelihood describes the distance to a data set

General likelihood:

$$ln\mathcal{L} = -\frac{1}{2}\left(\log 2\pi + \log|\mathcal{C}| + (\mathbf{x}-\mu)^T\mathcal{C}^{-1}(\mathbf{x}-\mu)\right)$$

(Typically assumes a Gaussian form around a data set)

Allows MCMC sampling
e.g. Nested Sampling (model selection)
Emcee (parameter estimation)

(AKA likelihood free inference or simulation based inference)

a likelihood is not tractable

Within a threshold, a distance metric selects the parameters that are close to the data.

$$x(D_{\text{true}}, D_{\text{sample}}) \leq \epsilon,$$

Parameters within criteria estimate the posterior.

Learning Posteriors with pyDelfi
(Alsing et al. 2018, 2019)

Both estimate the parameter posterior

Standard 21cm likelihood (recap)

Fourier Power Spectrum

Throughout, FPS refers to spherically averaged 21cm brightness temperature (Fourier) power spectrum

$$\Delta^2(\boldsymbol{k}) \equiv \frac{k^3}{2\pi^2 V} P(\boldsymbol{k})$$

$$\delta T_{\mathrm{b}} \approx 27 x_{\mathrm{HI}} (1+\delta) \left(\frac{H}{\frac{dv_{\mathrm{r}}}{dr} + H} \right) \left(1 - \frac{T_{\mathrm{CMB}}}{T_{\mathrm{s}}} \right) \times \left(\frac{1+z}{10} \frac{0.15}{\Omega_{\mathrm{M}} h^2} \right)^{\frac{1}{2}} \left(\frac{\Omega_{\mathrm{b}} h^2}{0.023} \right) \mathrm{mK},$$

Power Spectrum - the Fourier transform of the 2 point correlation function

$$P(\boldsymbol{k}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\boldsymbol{k}\boldsymbol{x}} \xi(\boldsymbol{x})\, d\boldsymbol{x}$$

Correlation function - the excess probability relative to a Poission distribution

$$P_{\mathrm{True}}(n|\boldsymbol{x}) = P_{\mathrm{poisson}}(n|\boldsymbol{x})[1 + \xi(\boldsymbol{x})]$$

FPS likelihood

$$ln\mathcal{L} = -\frac{1}{2}(\mathbf{x} - \mu)^T \mathcal{C}^{-1} (\mathbf{x} - \mu)$$

(Cross correlation terms ignored)

Simulation - 21CMMC (Greig & Mesinger 2015)

& 21cmFAST (Mesinger et al 2013 Murray et al. 2023)

- Semi-numerical simulation used for parameter estimation

1) Simple Model (FZH)

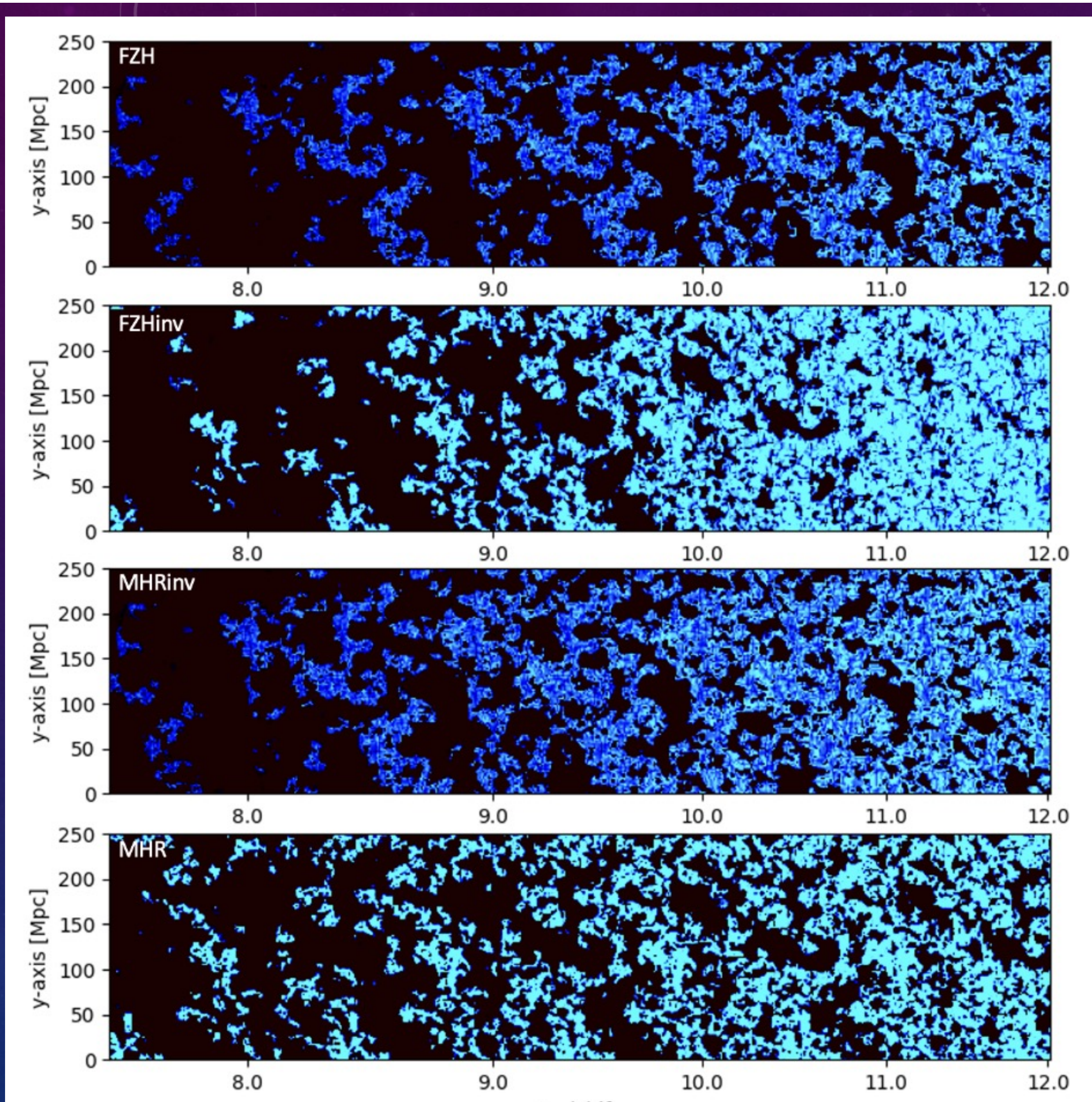
T_{vir} - the minimum virial temperature for galaxies.
ζ - UV ionising efficiency of galaxies.

- Each has a linear density field realization
- Ionization defined by comparing photons to the number of baryons in a given region.

2) Testing Morphologies
+ Ionization correlates with the density field directly - MHR
+ Mathematical Inverses (FZHinv, MHRinv)

3) Testing Astrophysics
+ Including Spin temperature,
+ Including a power law in halo mass for ζ
(with and without UV LF synergy.

Morphological light-cones



(21cmFast)
Inside-Out

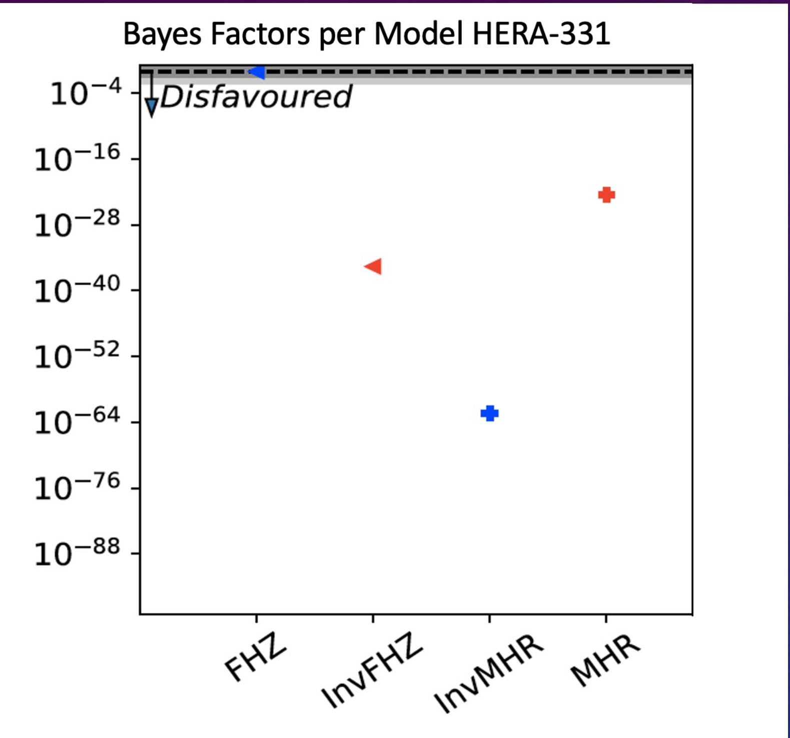
Outside-In

Inside-Out

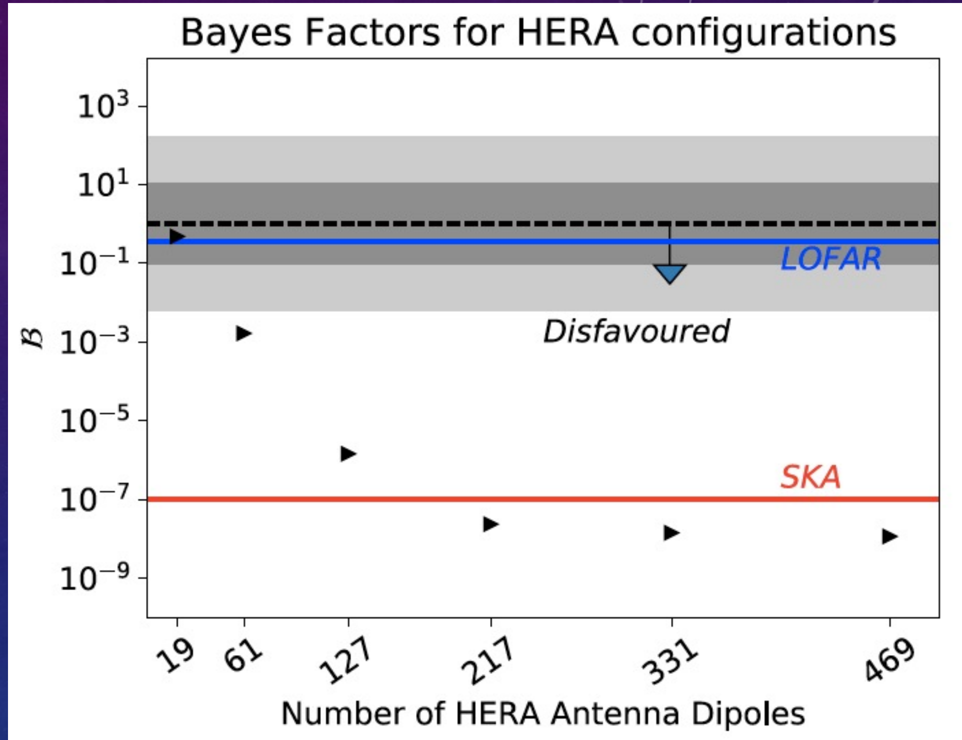
Outside-In

(Watkinson & Pritchard 2014)
(Binnie & Pritchard 2019)
(Furlanetto, Zaldarriaga & Hernquist 2004)
(Miralda-Escudé, Haenelt, Rees 2000)
(Binnie et al in prep.)

FPS results example



BMS can answer interesting questions:



(Most competitive model)

< = Global
+ = Local

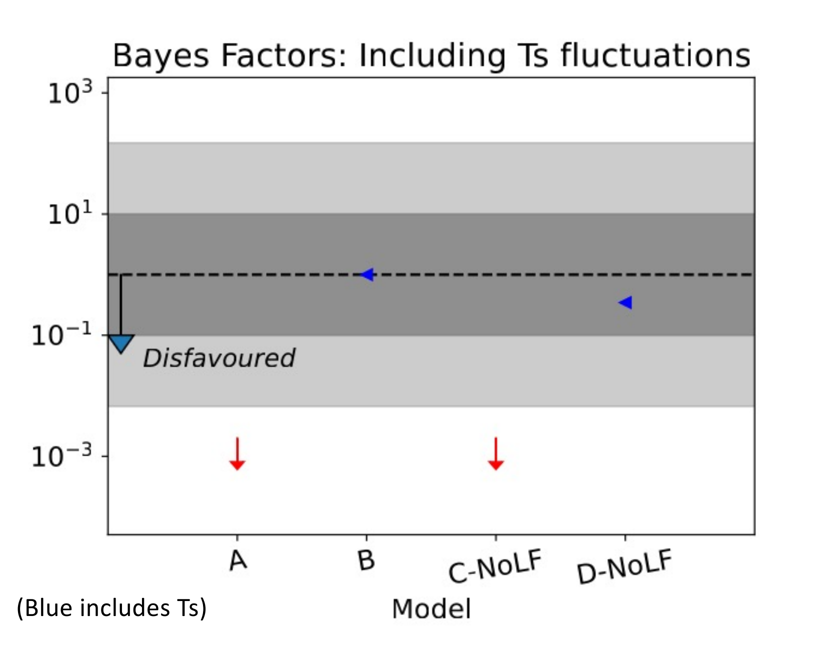
red = outside-in
blue = inside-out

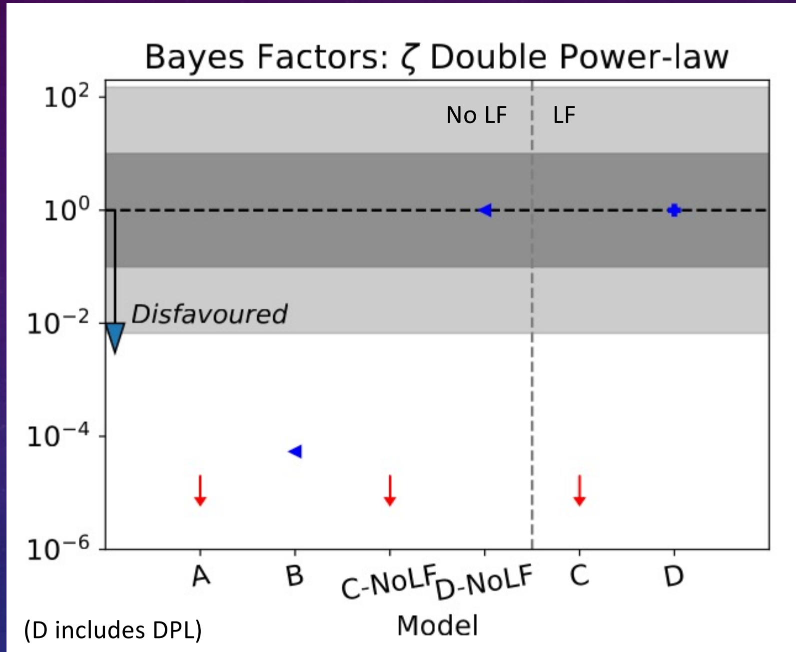
Telescope Simulations with 21cmSense Pober (2016)

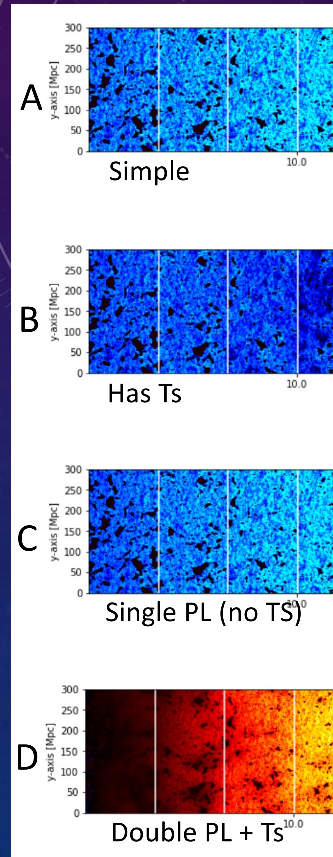
1080hr

For full results see https://arxiv.org/pdf/1903.09064

FPS results with Astrophysical models





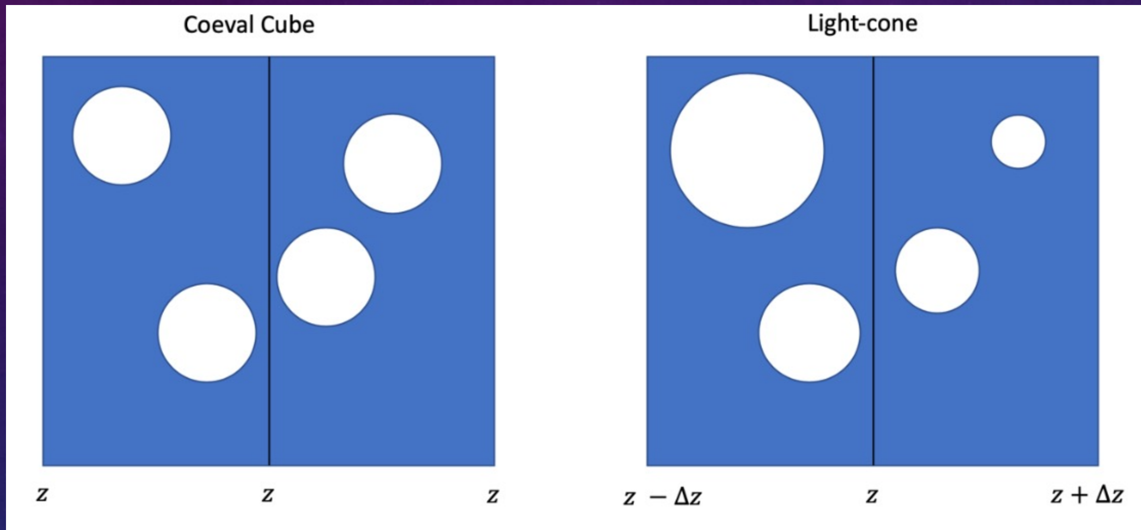


We can decisively distinguish between Astrophysical models.

– If the heating realization is significant.

BUT…

- Light-cone signal evolves along line of sight
- FPS is not ergodic of light-cone
- With the FPS must take chunks to approximate ergodicity



(Datta et al 2012, 2014)

The 3D-CNN and Morlet Power Spectrum both try to interpret the entire light-cone

What is the 3D-CNN?

Before, we summarised the 21cm light-cone with the power spectrum

$$\Delta^2_{21}(k,z) \equiv \frac{k^3 \bar{T}_b^{\,2}(z)}{2\pi^2 V} \langle |\tilde{\delta}_{21}(\mathbf{k},z)|^2 \rangle_k$$

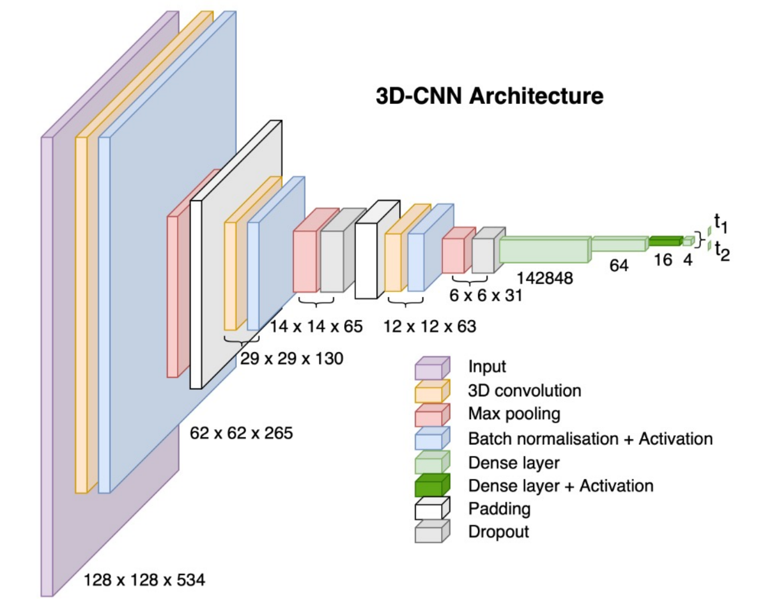
$$\delta_{21} = \frac{T_b(\mathbf{x},z)}{\bar{T}_b(z)} - 1$$

Now, 21cm brightness temperature light-cones are compressed by the 3D-CNN into Summaries (t).

3D-CNN uses parameters to obtain summary values instead of simulating

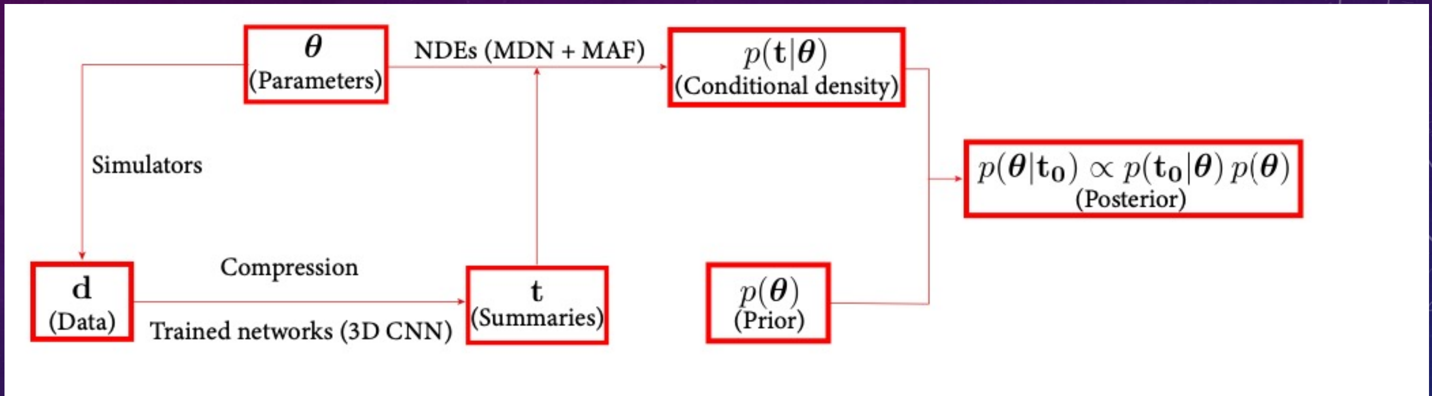
A different 3D-CNN is trained on each of the 4 EoR models with 10000 light-cones.

Mock data summaries are produced by summarizing a fiducial parameter simulation with the trained network.



What is Pydelfi?

Pydelfi uses these summaries to asymptotically estimate the true posterior



Credit: Zhao et al. 2022

- Neural Density Estimators (NDE) - a combination of Mixture Density Networds and Masked Auto-regressive Flows
- Delfi uses 5 MDN & 1 MAF (Bishop 1994, Papamakarious et al. 2017)

- Training is achieved by minimizing the cross-entropy

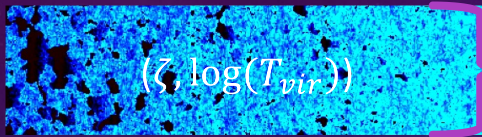
(information content is related to the log probability Q ∝ lnP)

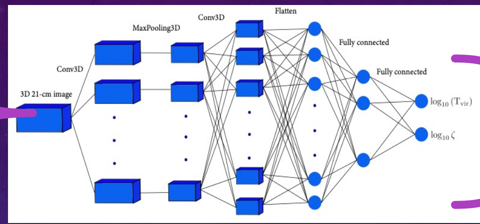
Pydelfi + 3DCNN

Process iterates

We can then learn $\mathcal{P}$ and find the MAP θ.

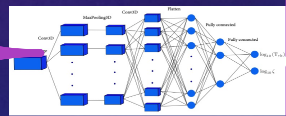
Sampler suggests parameters





(t1, t2)

Pydelfi compares the entropy of sampled data summary to the mock data summary.



$(t1_{Mock}, t2_{Mock})$

Can we recover the mock data's model?

$$\int \mathcal{P}\, d\theta = \mathcal{Z}\,,$$

$$\rightarrow \quad \mathcal{B} = \frac{\mathcal{Z}_{test}}{\mathcal{Z}_{mock}} \leq 1$$

Can we recover the parameters that model used to produce the mock data?

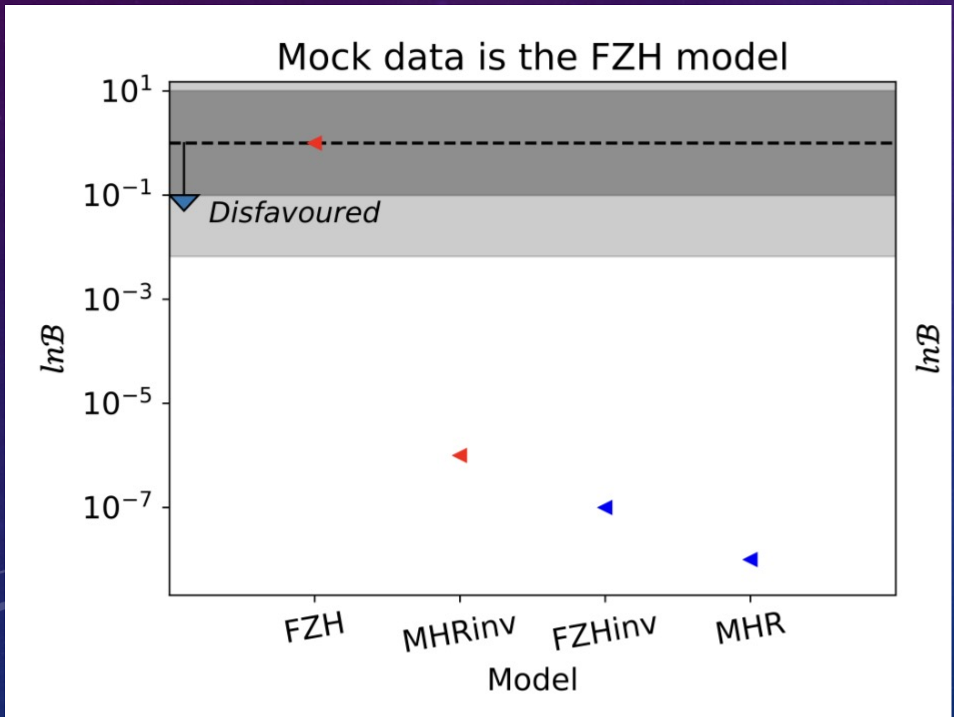
Is $\mathcal{P}_{max} = \mathcal{P}(\theta_{mock})$?

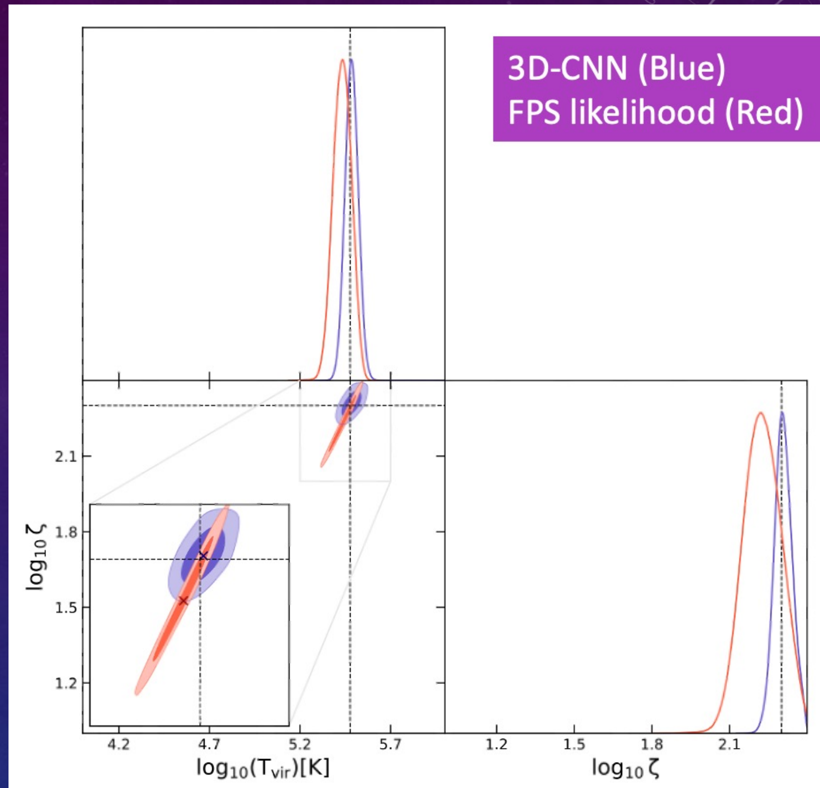
$$P(D|M) \propto^{?} \int d\Theta \sum_{i}^{NDE} W_i\, P_i(t|\Theta, \omega)$$

- Can the learnt-Posterior be used for Bayesian inference?

3D-CNN Results

Posterior Precision and accuracy improves with the Delfi-3DCNN compared to the FPS for the FZH (inside-out) model

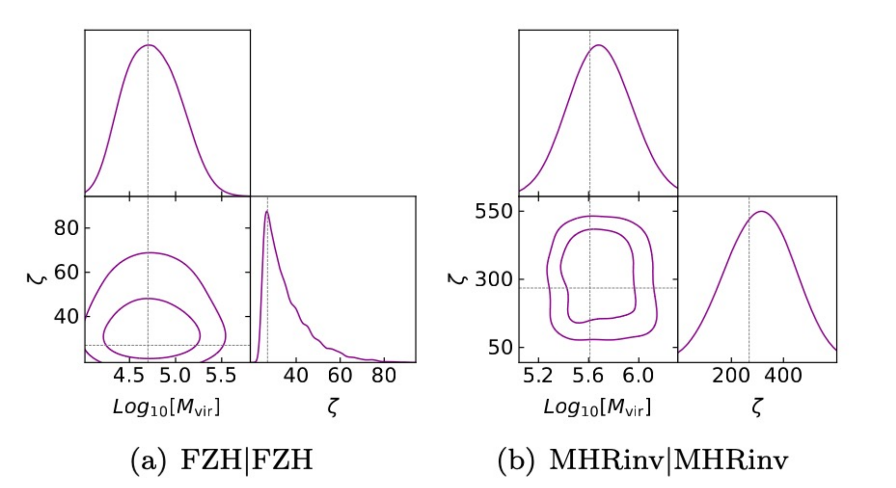




Credit: Zhao et al. 2022

Models can also be decisively distinguished by the 3D-CNN + pyDelfi for all 4 of our morphological models

3D-CNN Results

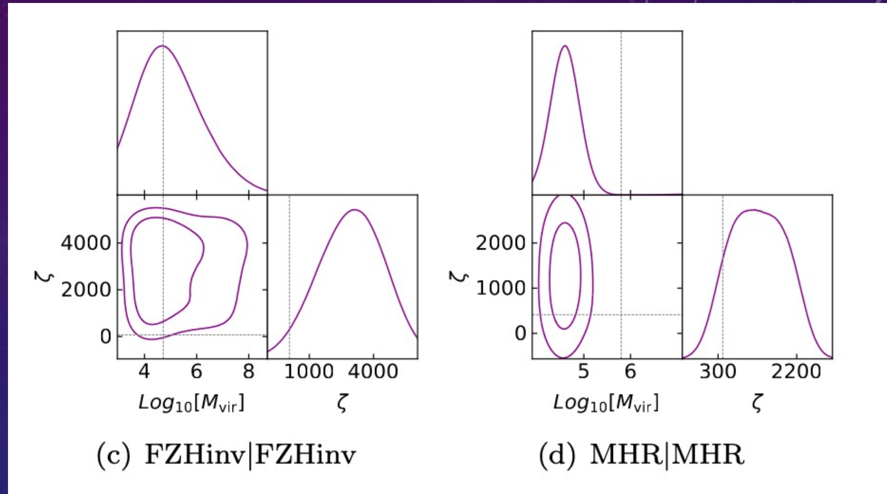


(a) FZH|FZH (b) MHRinv|MHRinv

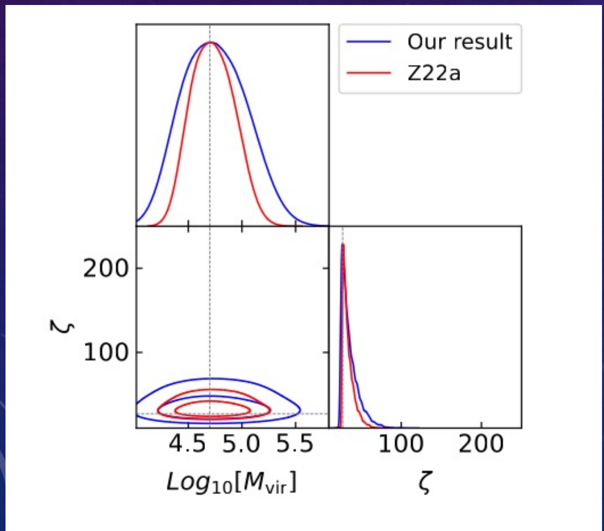
Inside-out models work well

BUT...

3D-CNN does not predicts accurate posteriors for outside-in morphology !



(c) FZHinv|FZHinv (d) MHR|MHR



Increasing the simulation resolution worsened parameter precision!

The Morlet Power Spectrum

$$P(\boldsymbol{k}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\boldsymbol{k}\boldsymbol{x}} \xi(\boldsymbol{x})\, d\boldsymbol{x}.$$

- Each Morlet Bases Υ, wrapped with Gaussian Envelopes

$$\Upsilon(\nu_i|\eta, \nu_c) = e^{-\eta^2(\nu_i - \nu_c)^2} e^{2\pi i \eta(\nu_i - \nu_c)}$$

$k_{\parallel} \sim \eta(z)$

$\nu_c =$ Line of sight position [Hz]

- Envelopes adapts to evolution of the light-cone (based on Nyquist frequency)
- Ergodic statistics

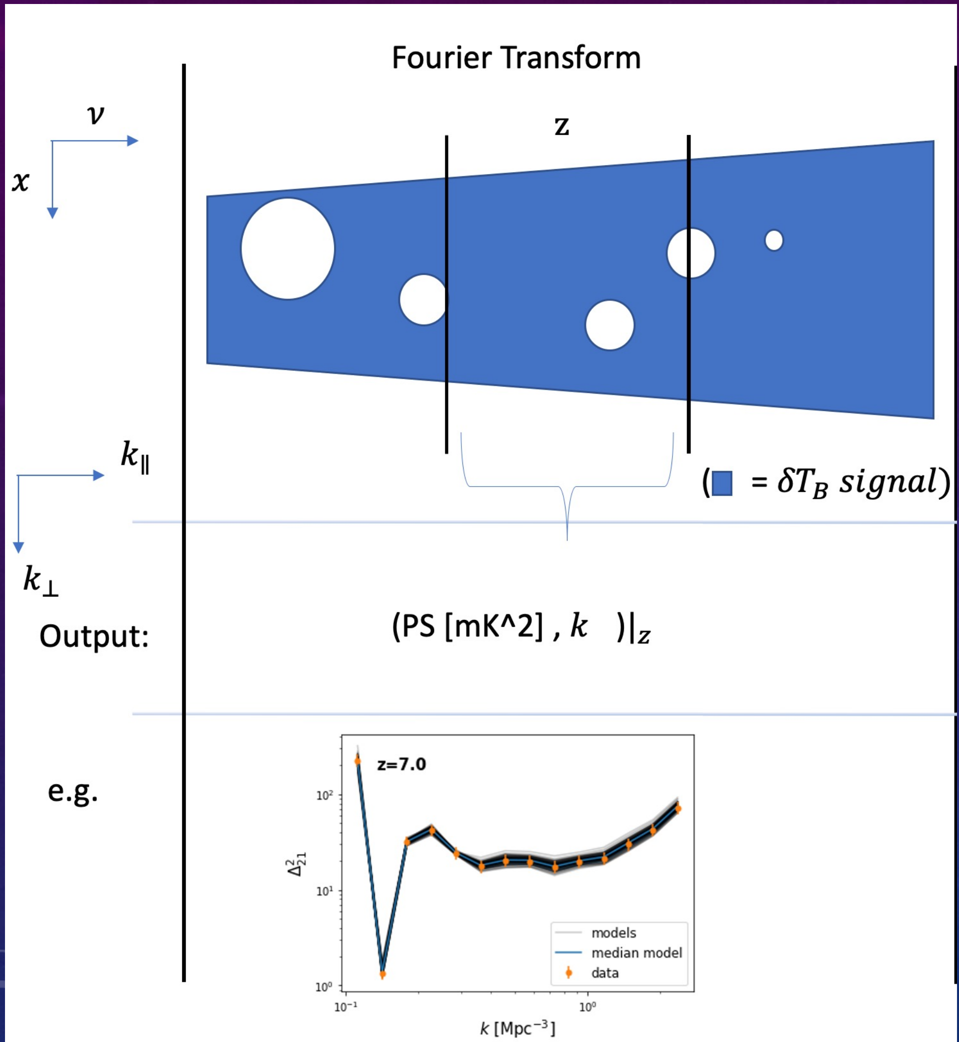
$$P_{\mathrm{MPS}}(z, k_{\parallel}|k_{\perp}) = \frac{1}{V(k_{\parallel}, z)} |\Upsilon|^2 \ \mathrm{mK}^2 h^{-3} \mathrm{Mpc}^3$$

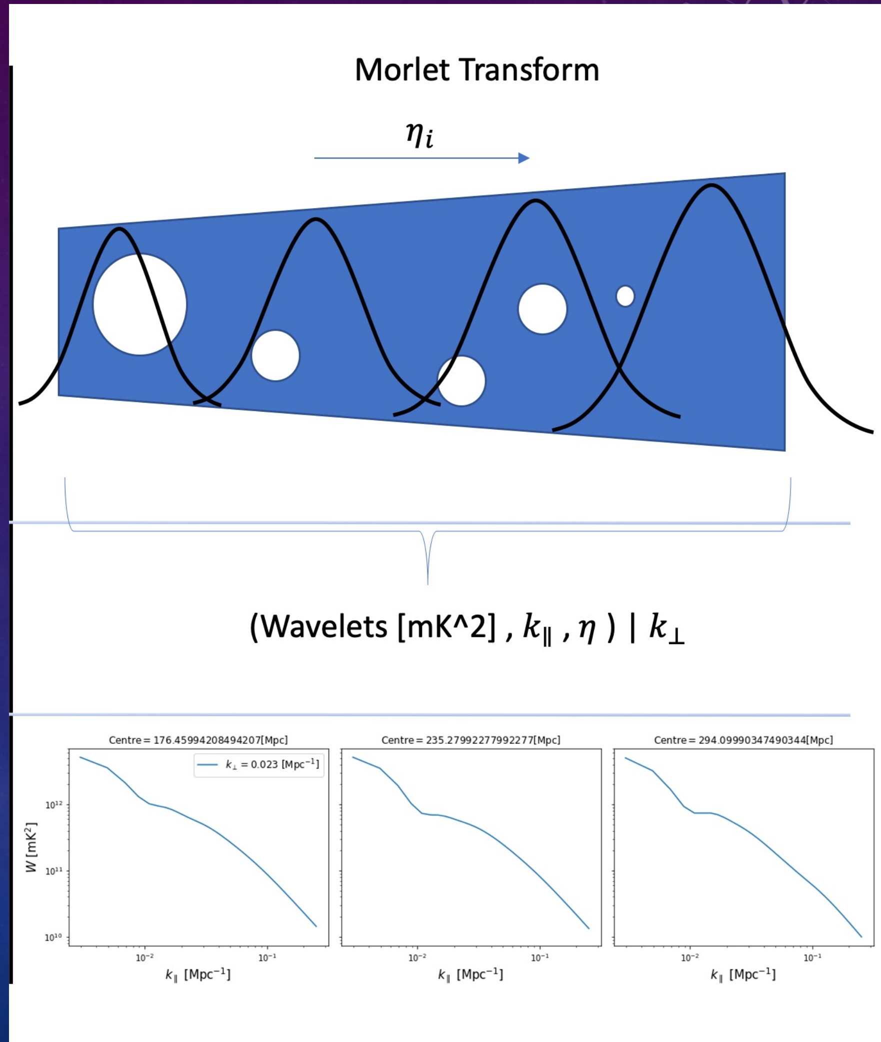
- See Trott (2016) for more info

$$ln\mathcal{L} = -\frac{1}{2}\left(\log 2\pi + \log|\mathcal{C}| + (\mathbf{x} - \mu)^T \mathcal{C}^{-1} (\mathbf{x} - \mu)\right)$$

→ Simulated and Analytical covariances agree

The Morlet Power Spectrum

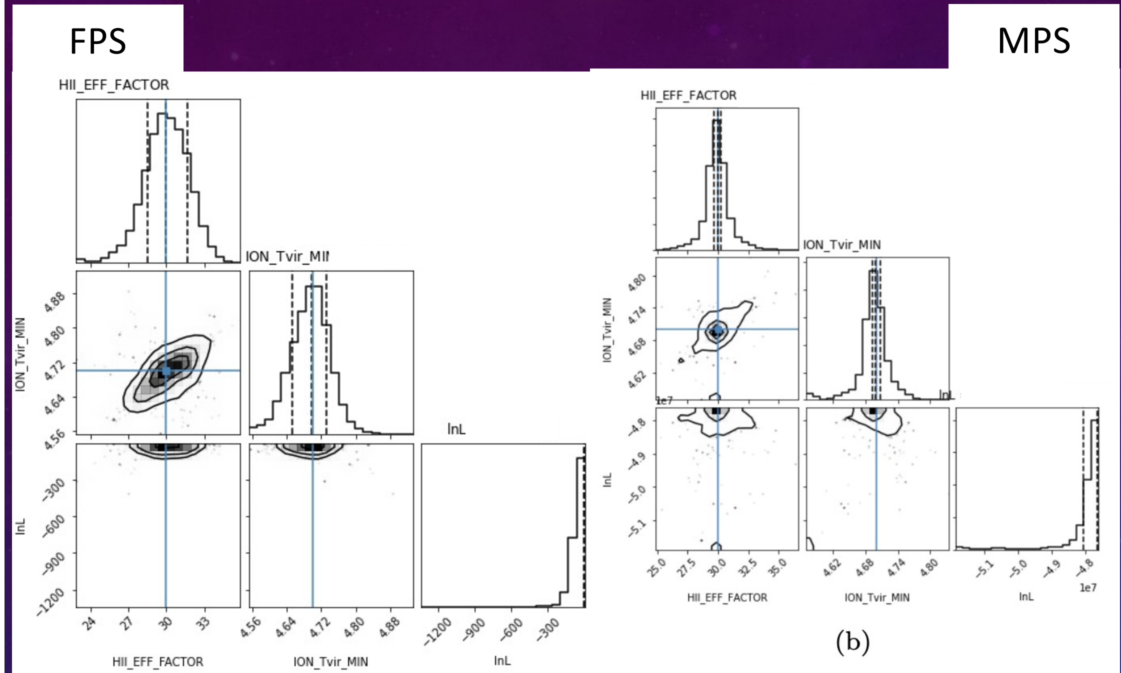




Interpretation is analogous to the 1D FPS

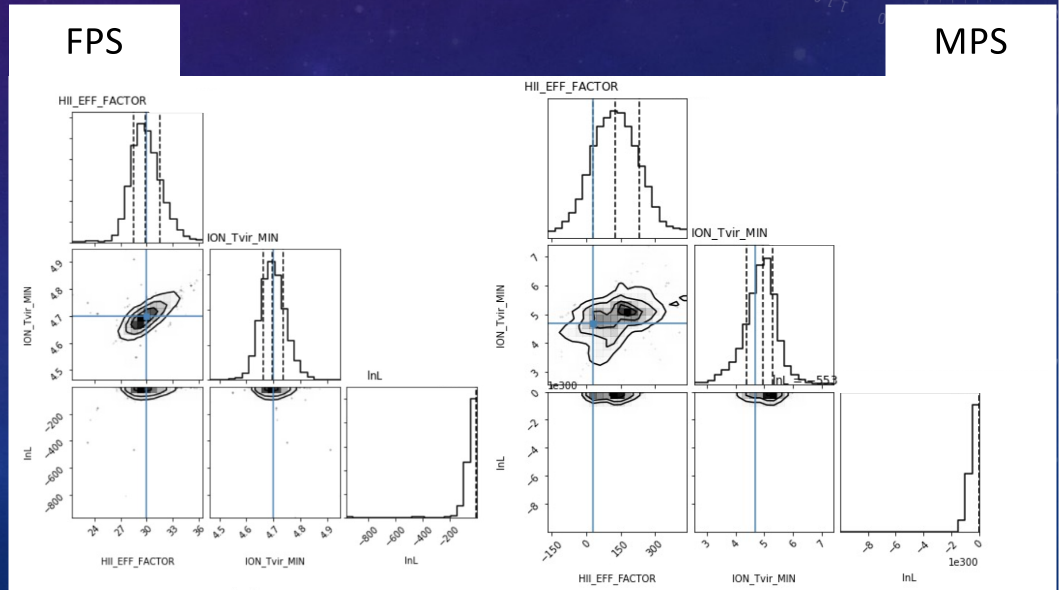
MPS Comparison with FPS

MCMC $\sim 10^4$ points, 2 parameter FZH,
250Mpc box light-cone (redshifts 8-10) sliced into:



← 1 chunk

3 chunks ↓

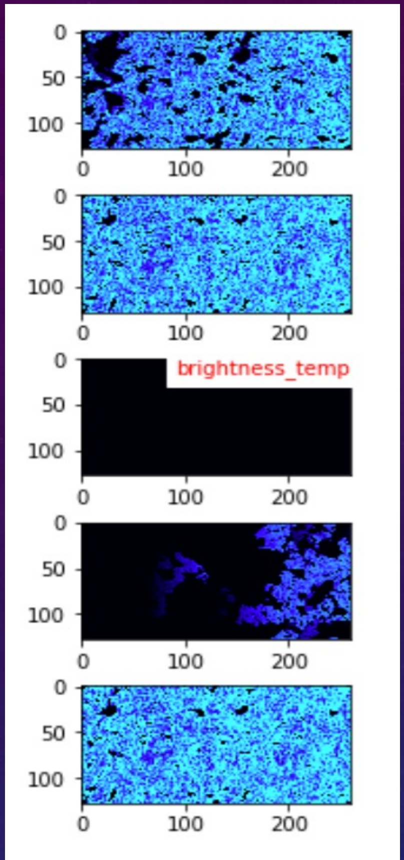


- 3 chunk MPS receives no largescale modes (the wavelet just filters the data for no reason)

- 1 chunk FPS suffers badly from the LC effect

No telescope noise yet.

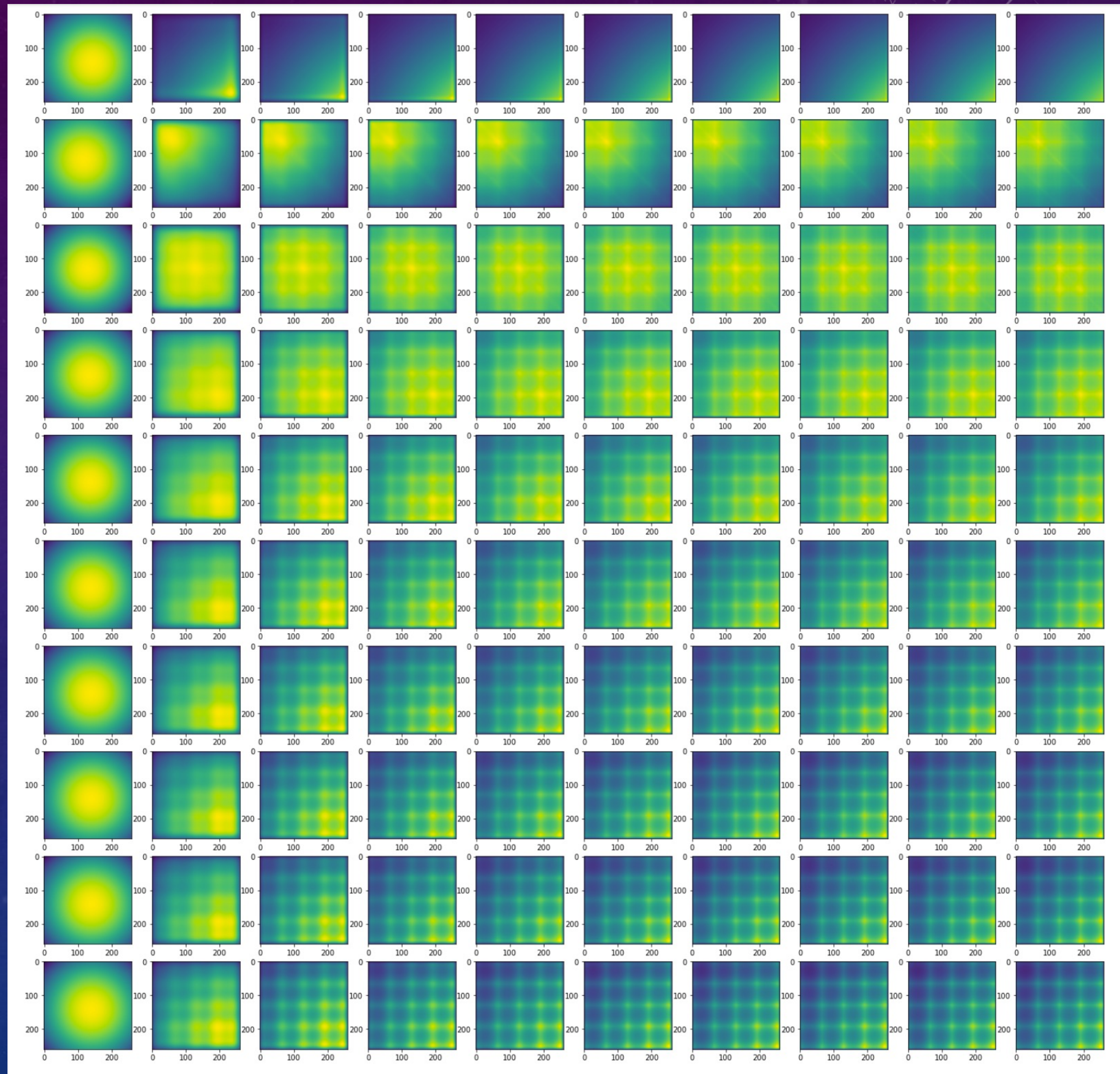
MPS Covariance interpretation is hard



$$ln\mathcal{L} = -\frac{1}{2}\left(\log 2\pi + \log|\mathcal{C}| + (\mathbf{x}-\mu)^T\mathcal{C}^{-1}(\mathbf{x}-\mu)\right)$$

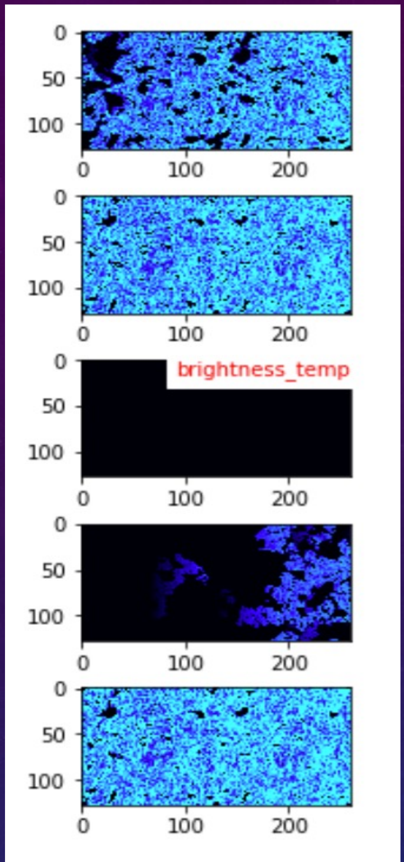
Box coordinates^2 plot per $k_{\parallel}$ (given $|k_{\perp}|$)

Implementing the Morlet Transform

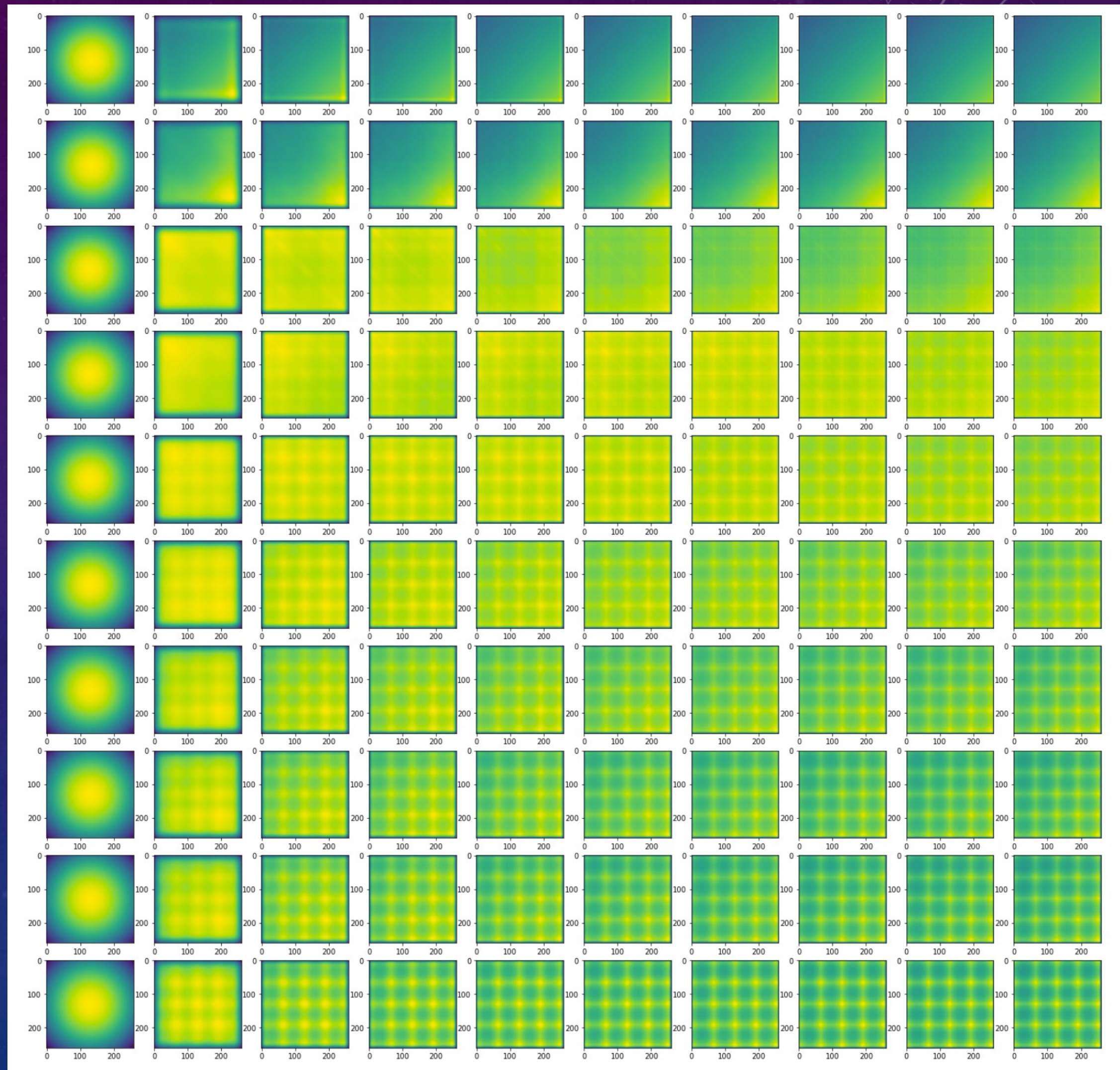


BUT... Cross hairs line up with Simulation artifacts.

MPS Covariance interpretation is hard



Implementing the Morlet Transform



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Box coordinates^2 plot per $k_{\parallel}$ (given $|k_{\perp}|$)

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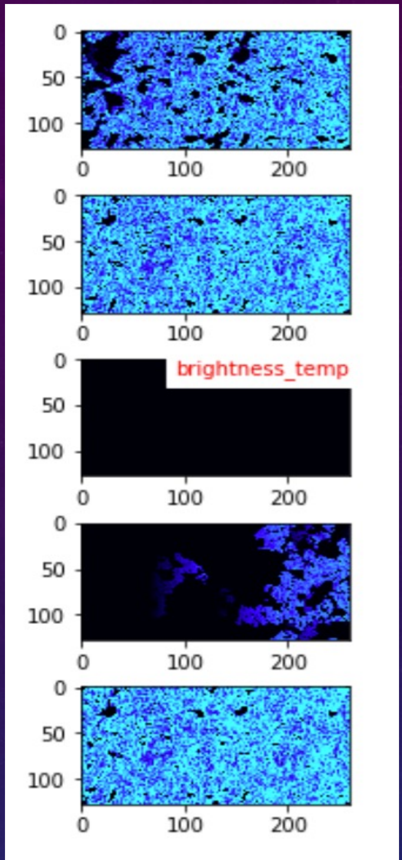

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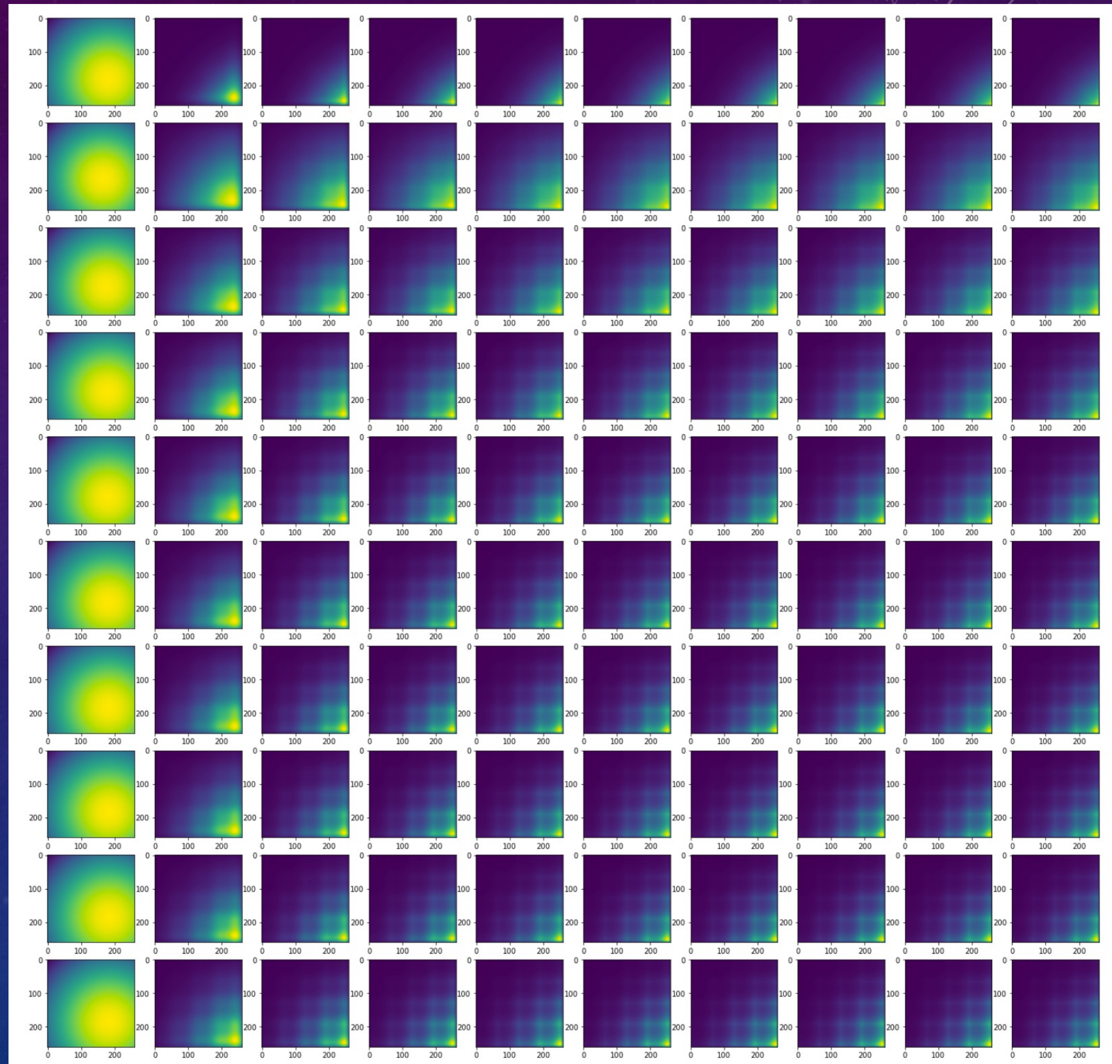

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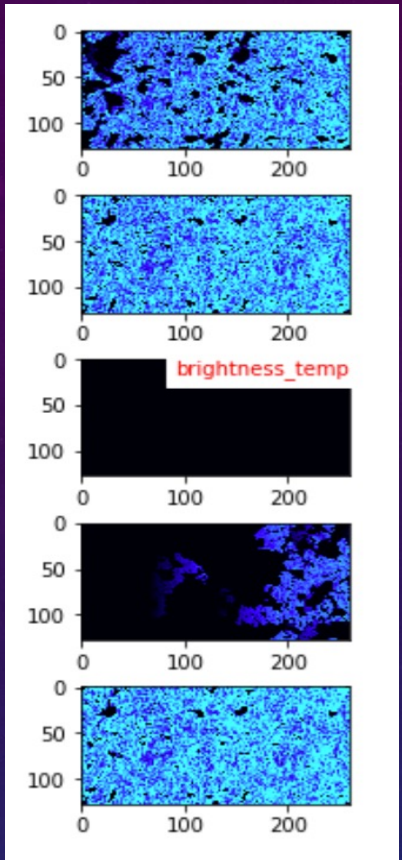

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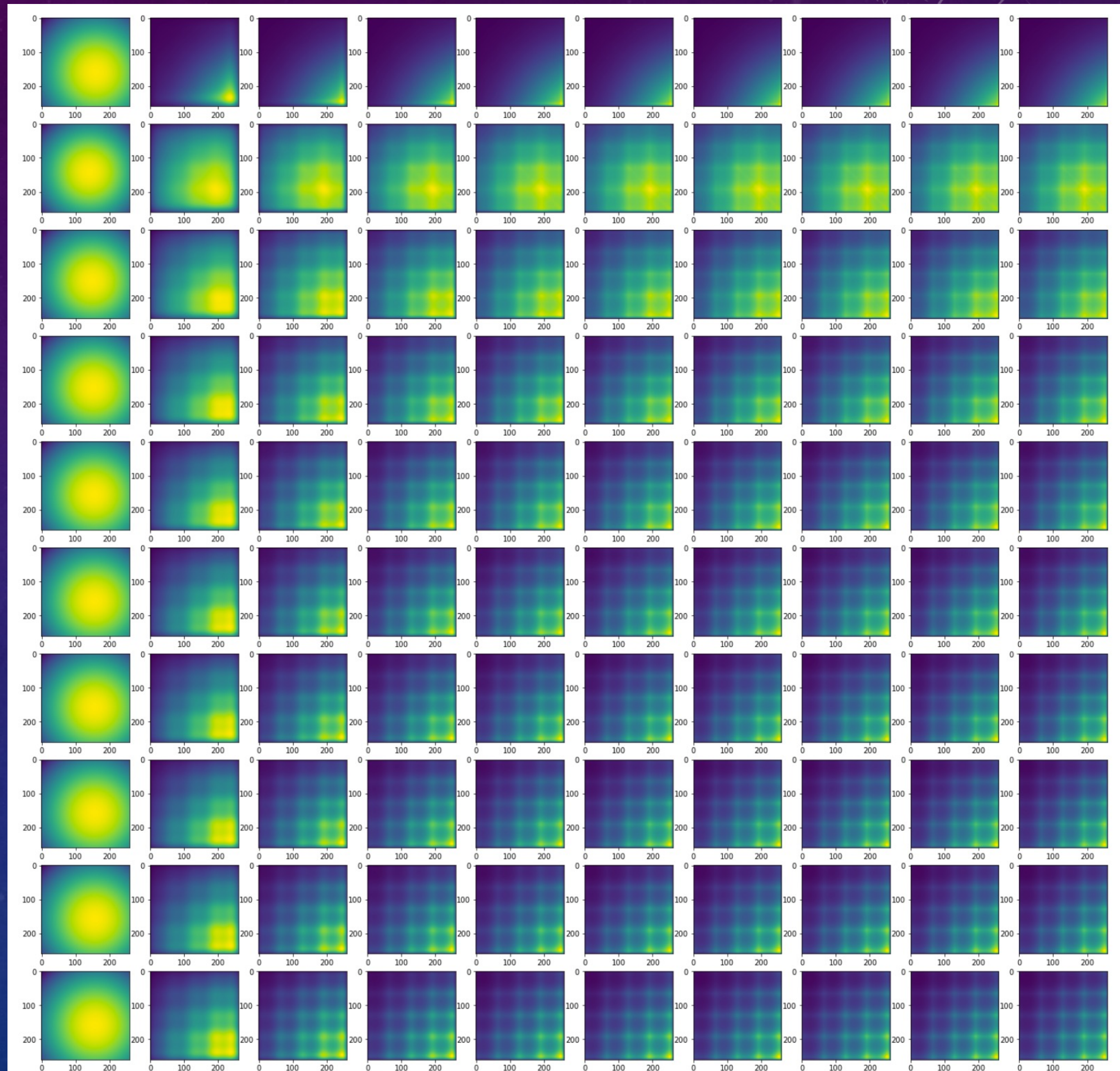

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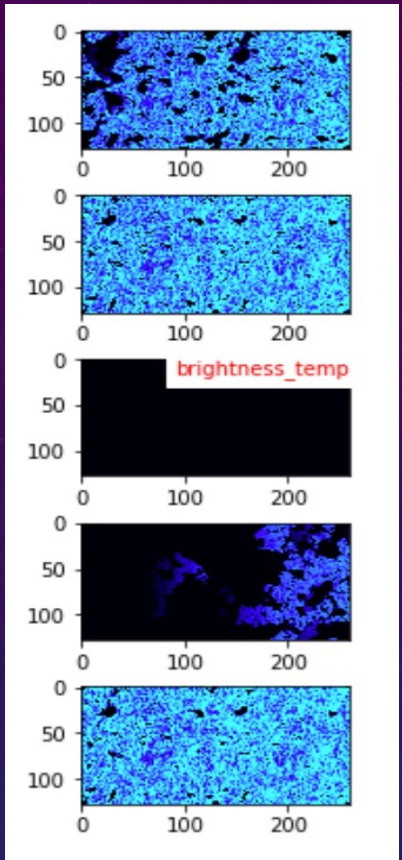

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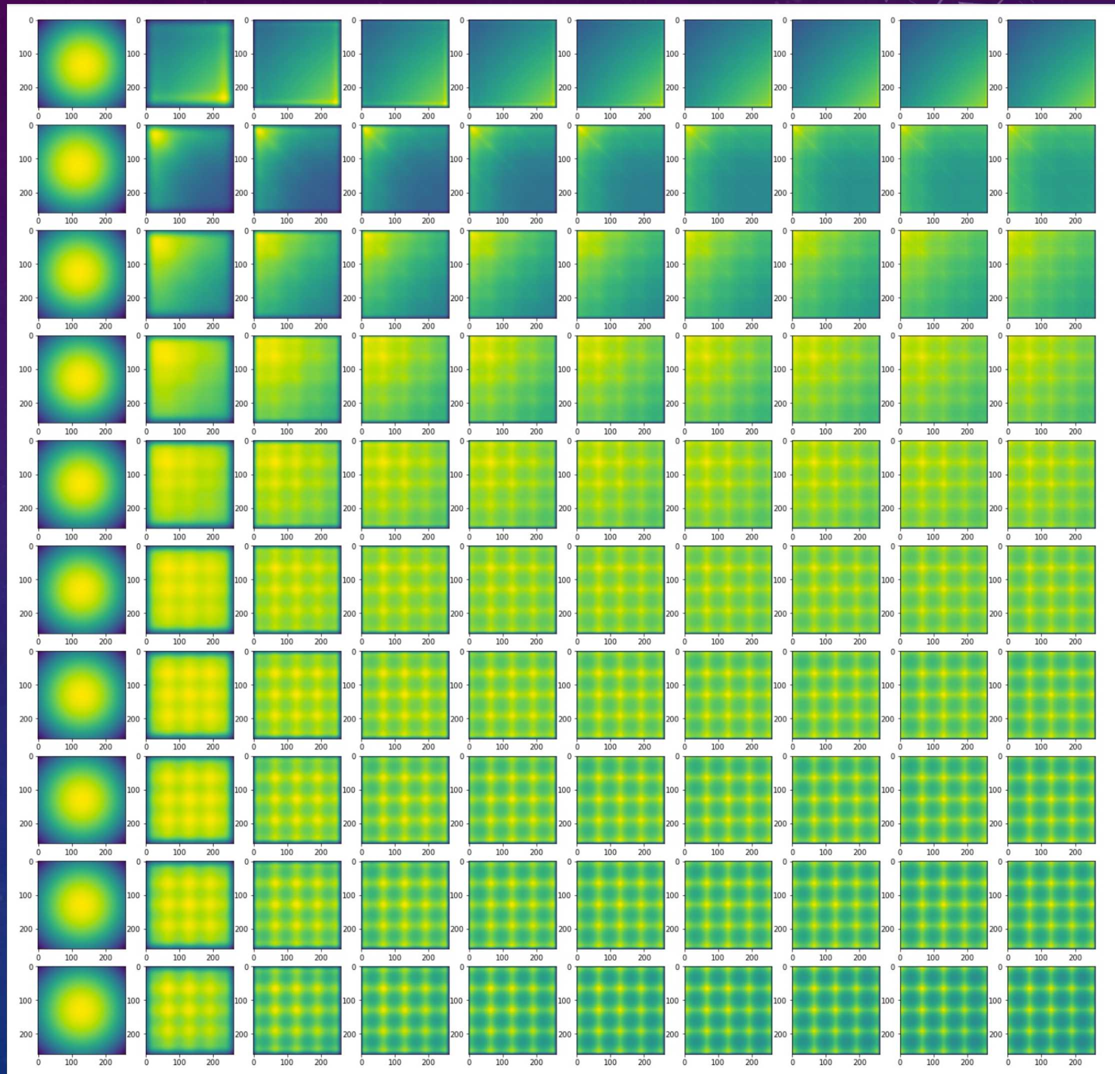
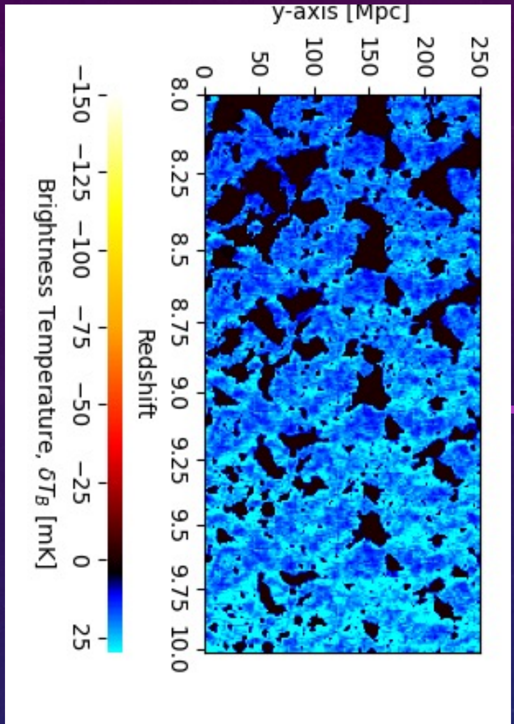


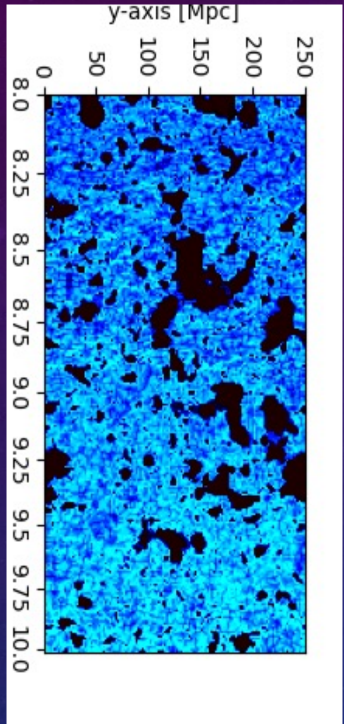
BUT... Cross hairs line up with Simulation artifacts.

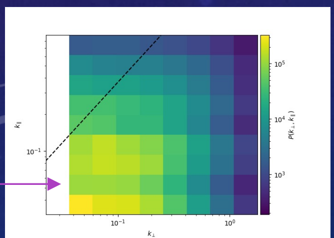
Long-mode lightcones

Original 21cmFast
- init box wraps
(below is exaggerated)

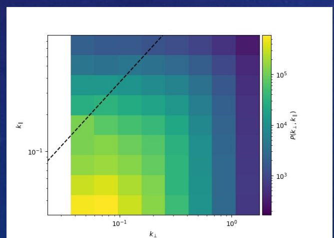


Cuboidal init box
Credit: Steven Murray
& Brad Greig





x8 dip in power
at $k_{\parallel}$ bin
For $\sim 250 Mpc$



BUT…

Longer line of sight density modes
produce cosmic variance

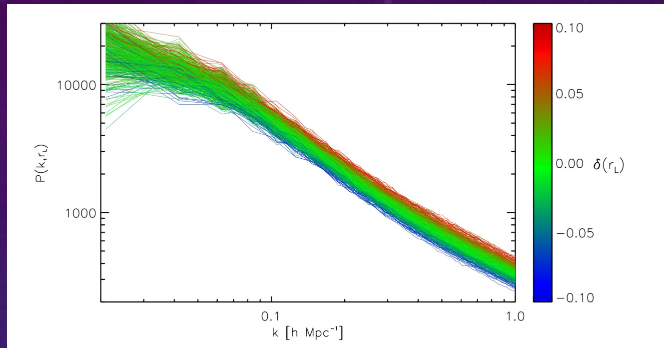
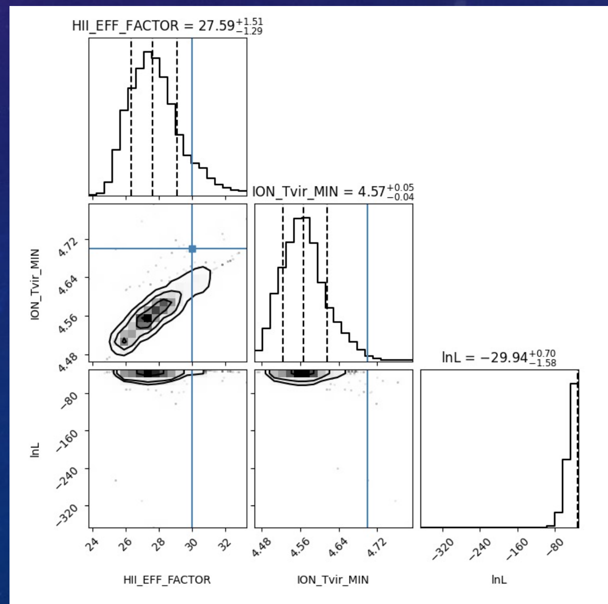


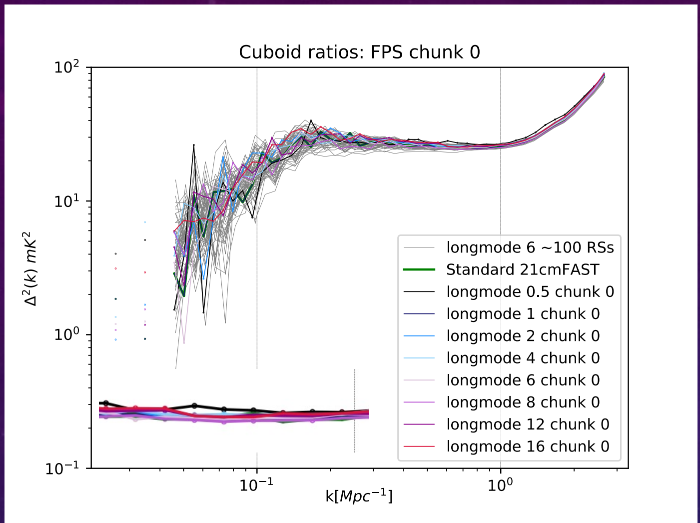
Figure 1: Position-dependent power spectra measured from 512 subvolumes with $L = 300\ h^{-1}$ Mpc in one realization. The color represents $\bar{\delta}(\mathbf{r}_L)$ of each subvolume.

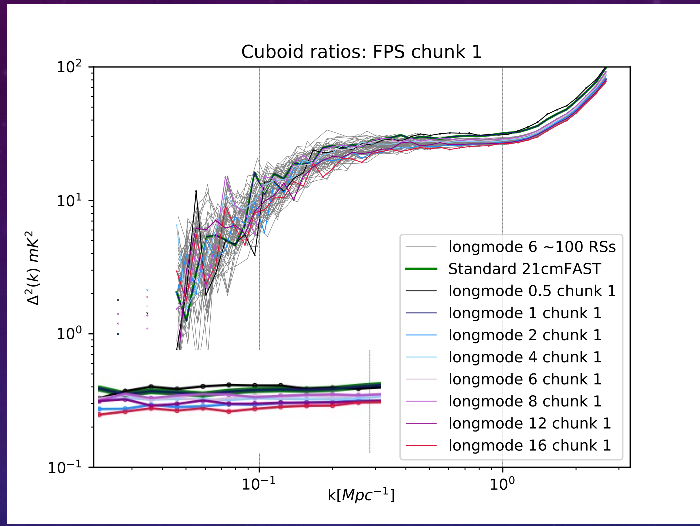
Chiang et al. 2014
'position dependent power spectrum'
is used to measure the Bispectrum
(Giri et al. 2020)

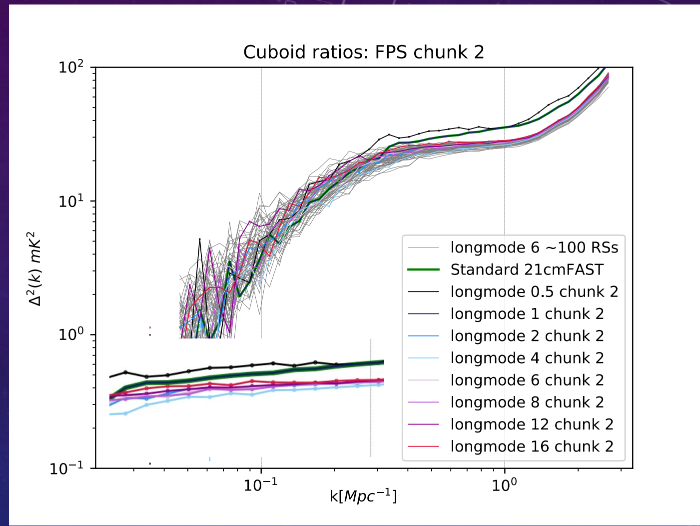
if longer modes are
in the Data set
FPS posteriors
can be biased $>2\sigma$



LoS Cosmic Variance with the FPS







(Colours) Different length init cuboids cause different FPS.

– Including modes longer than the light-cone seem to converge.

(Grey) Different random seeds for a light-cone-length init field also converge

– Cosmic Variance

– These agree with each other BUT don't average to the wrapped box method

(In progress: simulated ~100/1000 LCs + try with longer lightcones + will this also bias the MPS?

SUMMARY

- Bayesian model selection works in a wide variety of situations
- Decisive disfavouring of EoR morphologies & astrophysics with with HERA and The SKA soon!
- Statistical inference with CNNs is not flexible enough for use in EoR science.

(But L-free remains promising! Literature contains lots of alternatives… IMNN, Recurrent Neural Networks, Scattering transform etc.)

- The Morlet Power Spectrum is very promising but needs work.

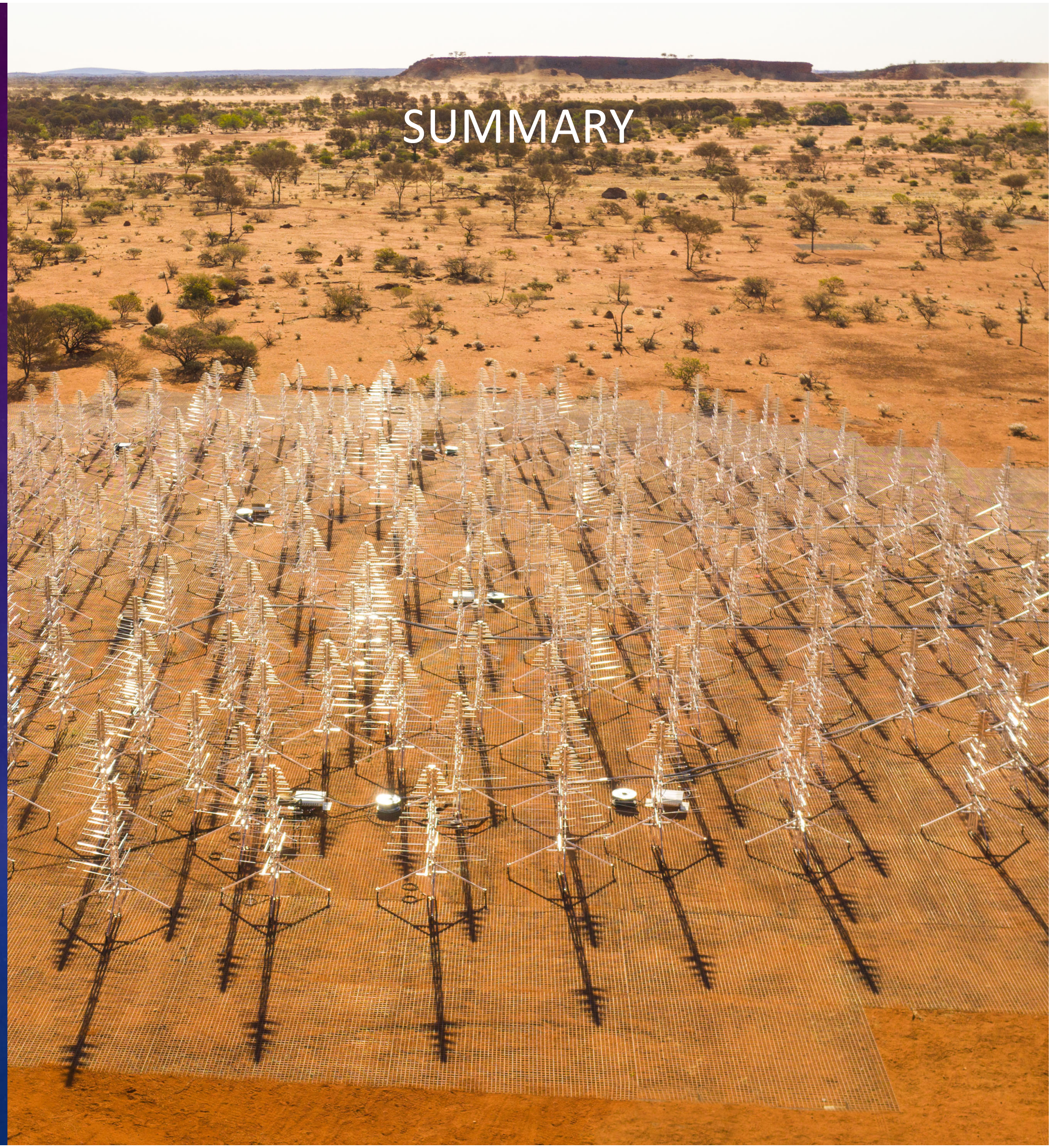
In progress…
- Adding Telescope noise
- Addressing LoS cosmic variance

Simple 21cmFast Posterior variance [ζ, Log[T_{vir}]]

FPS – [± 2.0, ± 0.09],

3D-CNN - [± 1.6, ± 0.04],

MPS – [±0.03, ±0.01],



Thanks for Listening!

Questions?

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