

Toward a complete machine learning-based forward modelling pipeline

Daniela Breitman

Scuola Normale Superiore

Supervised by Andrei Mesinger

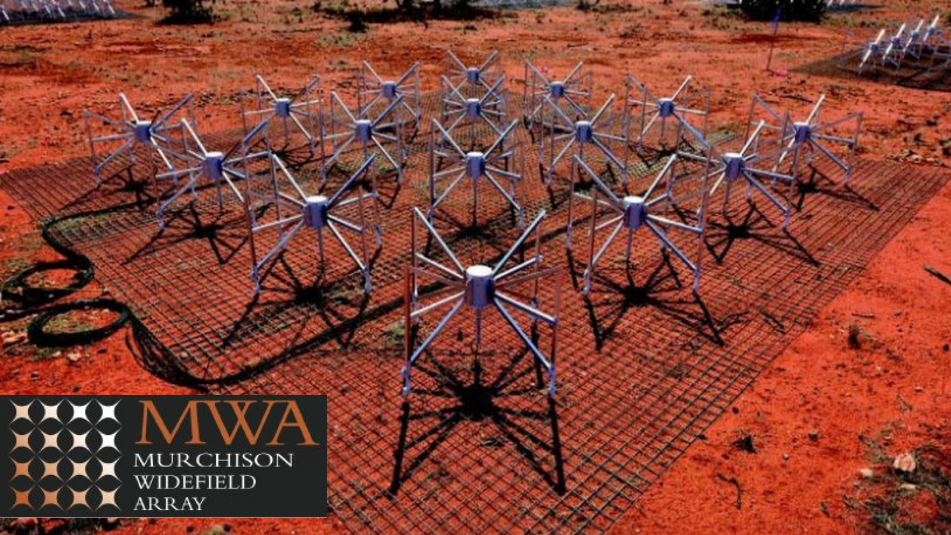
SKA CD/EoR ST Meeting, Tsinghua

July 18, 2024



SCUOLA
NORMALE
SUPERIORE

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How do we learn from this data?

BAYES' THEOREM

$$P(\theta|d) = \frac{P(d|\theta)P(\theta)}{P(d)}$$

Bayes' Theorem

- **What we want** $P(\theta|d)$ = updated knowledge on θ provided an observation d
- **Forward model** $P(d|\theta)$ = probability of reproducing observation d with model parameters θ
- $P(\theta)$ = prior on the model parameters θ

$$P(\theta|d) = \frac{P(d|\theta)P(\theta)}{P(d)}$$

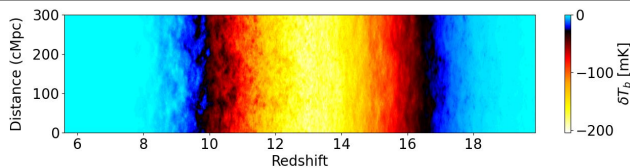
Sample params: $\theta_{\text{astro}} \sim P(\theta_{\text{astro}})$, θ_{cosmo} , ICs

Traditional Pipeline

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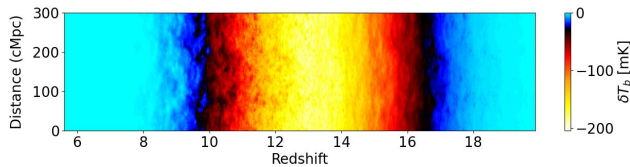
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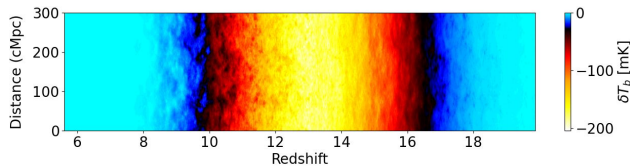


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Run 21cmFAST: Realisation $\Delta_i^2(k_{\perp}, k_{\parallel}, z)$

**$\gtrsim 300k$
CPU hrs**

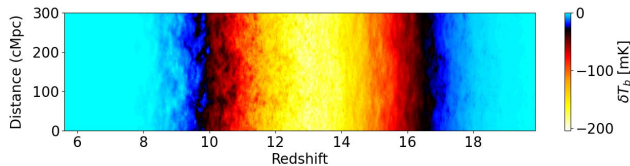


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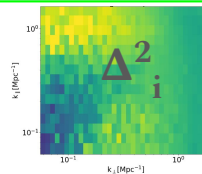
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This work

21cmEMU**v3**: Realisation $\Delta_i^2(k_{\perp}, k_{\parallel}, z)$

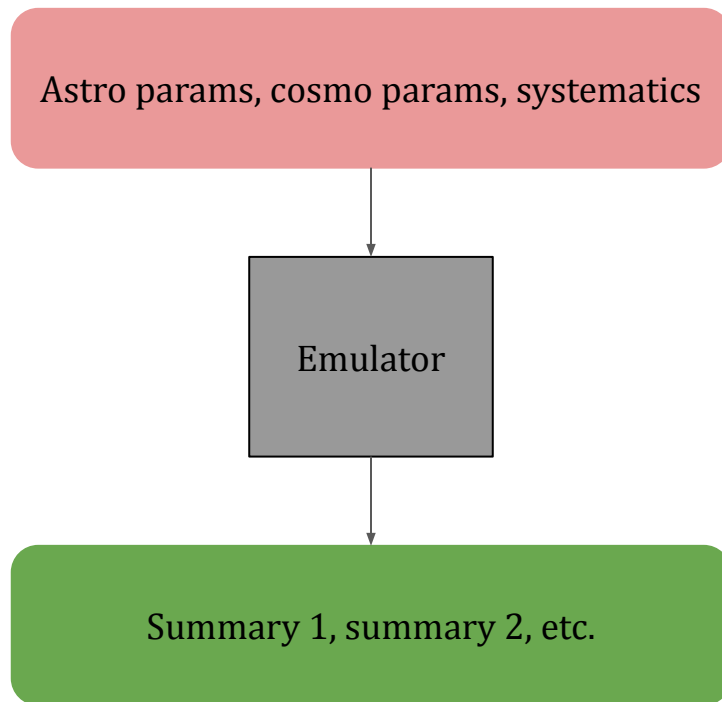
$\lesssim 1$ GPU day



, etc.

Breitman+in prep.

Ideal Emulator



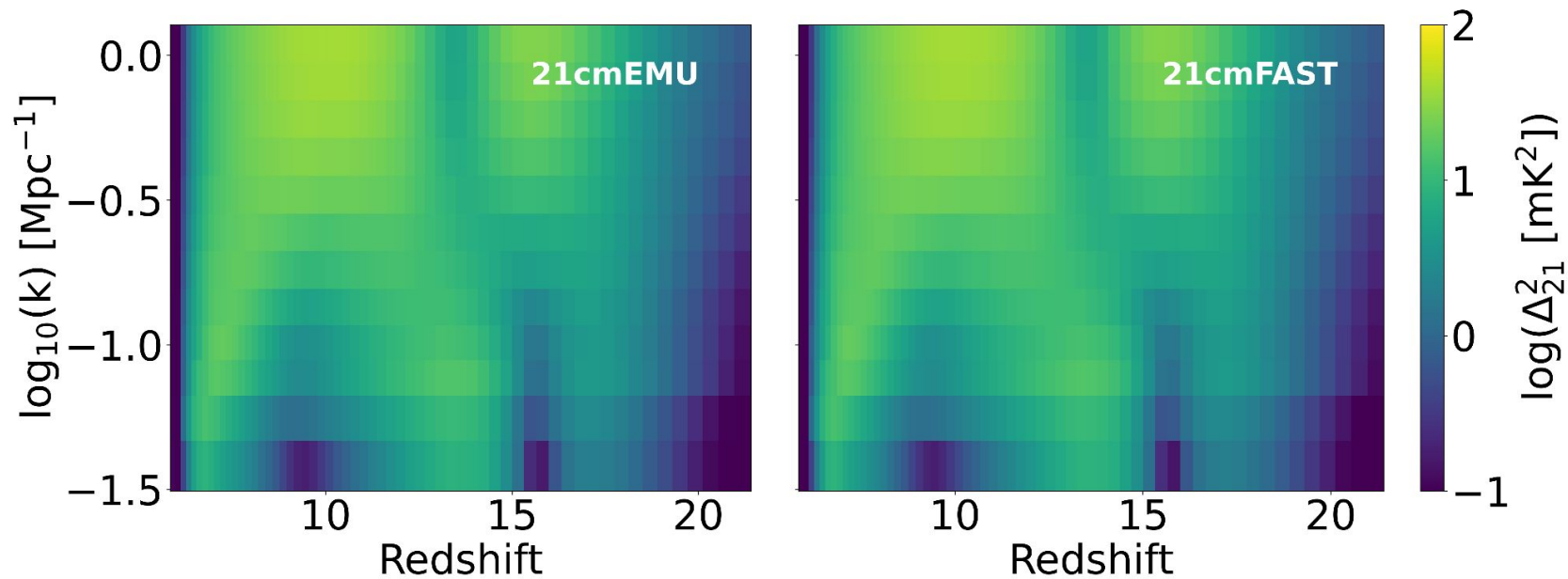
Summary Statistics

- $x_{\text{HI}}(\mathbf{z})$: Global fraction of neutral hydrogen
- $T_{\text{S}}(\mathbf{z})$: Global neutral IGM spin temperature $T_{\text{S}}^{-1} = \frac{T_{\gamma}^{-1} + x_{\alpha} T_{\alpha}^{-1} + x_{\text{c}} T_{\text{K}}^{-1}}{1 + x_{\alpha} + x_{\text{c}}}$
- $T_{\text{b}}(\mathbf{z})$: Global 21-cm brightness temperature [e.g. Bye+22, Bevins+21, Cohen+19]

$$\delta T_{\text{b}} \approx 27 x_{\text{HI}} (1 + \delta_{\text{b}}) \left(\frac{\Omega_{\text{b}} h^2}{0.023} \right) \left(\frac{0.15}{\Omega_{\text{m}} h^2} \frac{1+z}{10} \right)^{1/2} \times \left(\frac{T_{\text{S}} - T_{\text{R}}}{T_{\text{S}}} \right) \left[\frac{\partial_{\text{r}} v_{\text{r}}}{(1+z)H(z)} \right] \text{ mK}$$

- **21-cm power spectrum** ($\mathbf{k}, \mathbf{z}$): e.g. Kern+17, Schmit & Pritchard 18, Ghara+20, Mondal+21
- **UV luminosity function**: Source number density per magnitude vs z [Bouwens+15, 16]
- τ_{e} : Thomson scattering optical depth of CMB photons

Power Spectrum

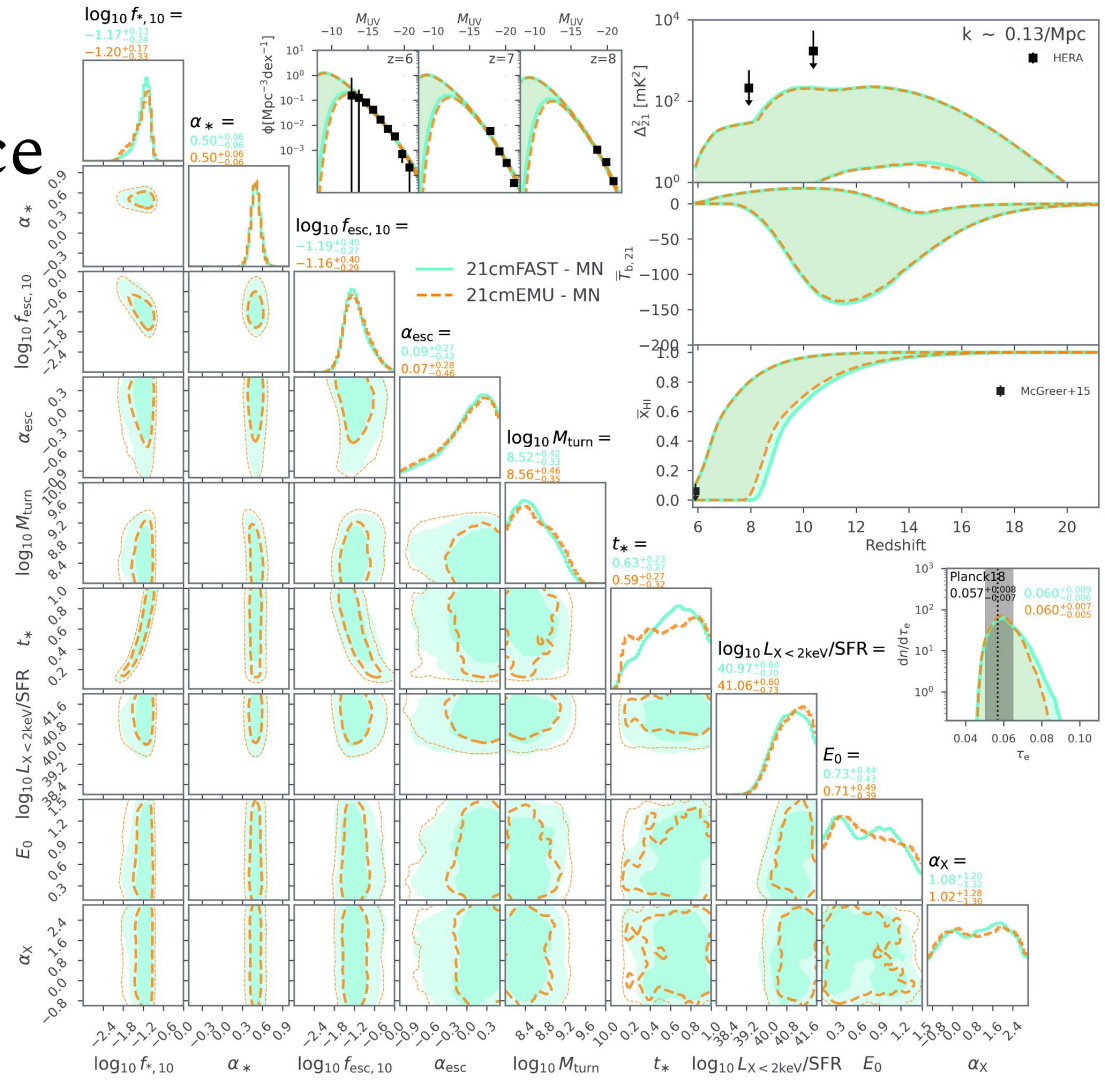


21cmEMU Performance

Summary	Median FE (%)	68% CL (%)
$\log \Delta_{21}^2$	0.55	2.4
$\overline{T}_b$	0.34	1.2
$\log \overline{T}_S$	0.032	0.13
$\overline{x}_{\text{HI}}$	0.0073	0.10
τ_e	0.11	0.26
$\log \phi$	0.50	2.1

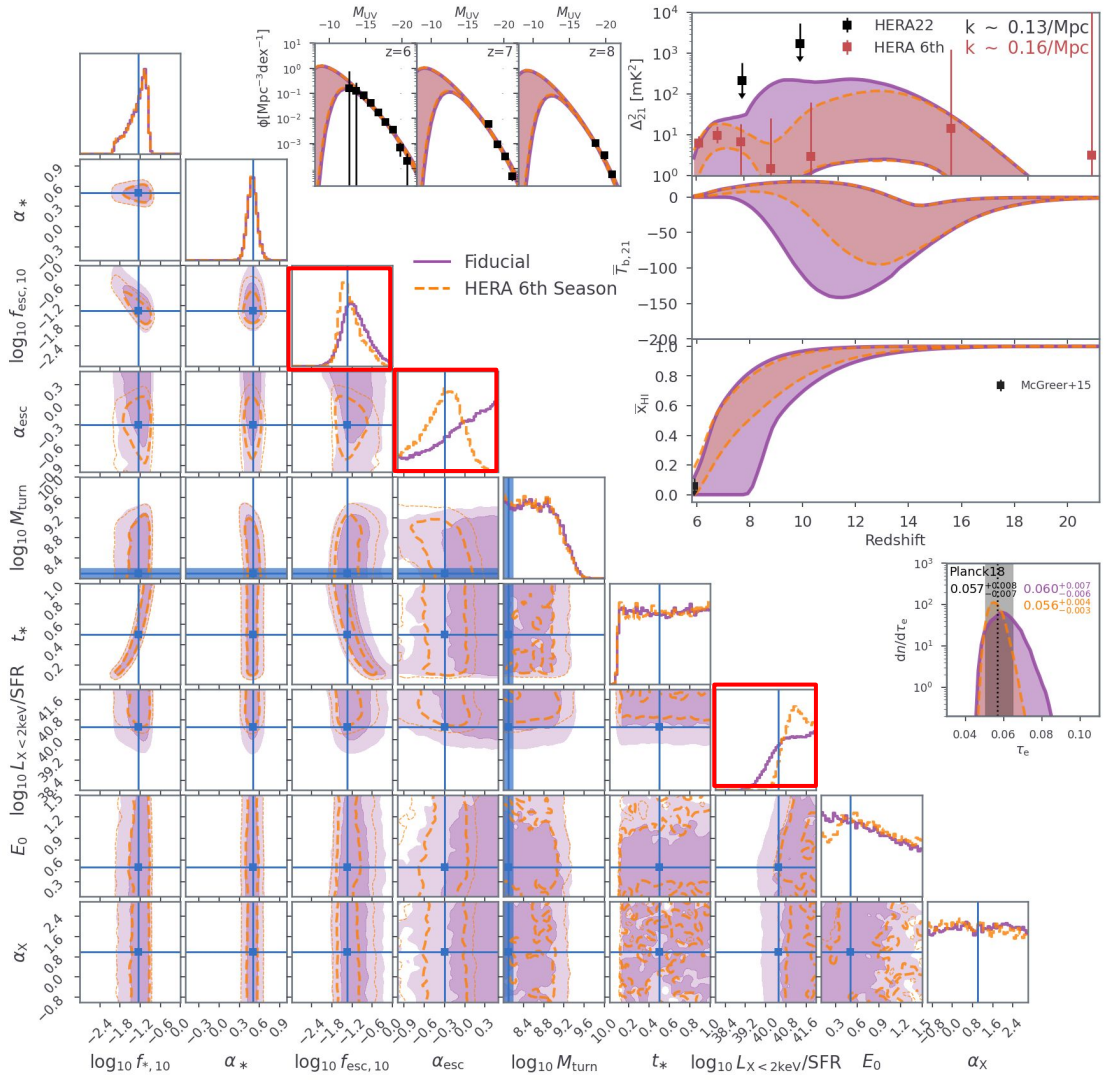
Small errors, but do they impact the inference?

21cmEMU can reproduce
21cmFAST results.



Forecast for HERA Phase II 6th-Season Observations

New HERA data + tighter prior on
systematics improve the
constraints for many astrophysical
parameters

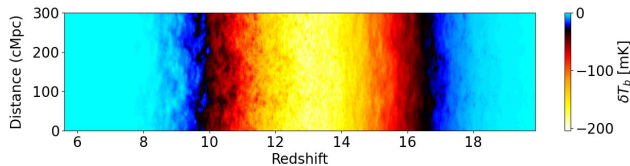


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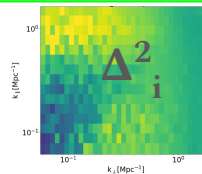
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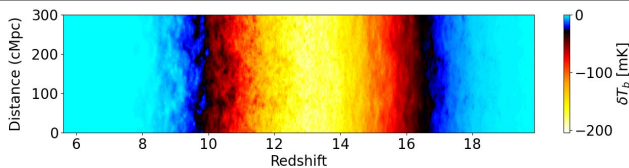
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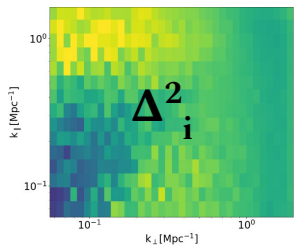
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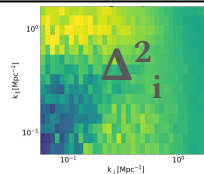
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21-cm Power Spectrum

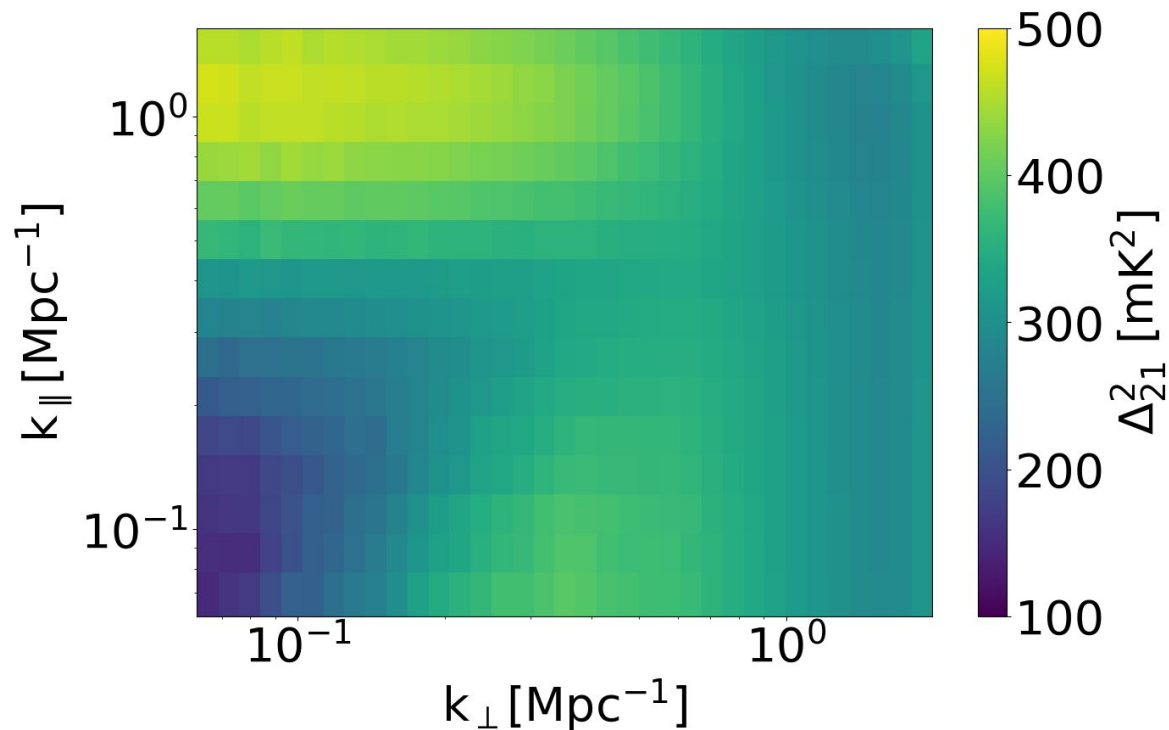
$$P(k) \propto \mathcal{F}(T_b) \mathcal{F}^*(T_b)$$

$$\Delta_{21}^2 = P(k) k^3 / (2 \pi^2) [\text{mK}^2]$$

This is a 3D quantity

1D PS = spherical average

2D PS = cylindrical average



21-cm Power Spectrum

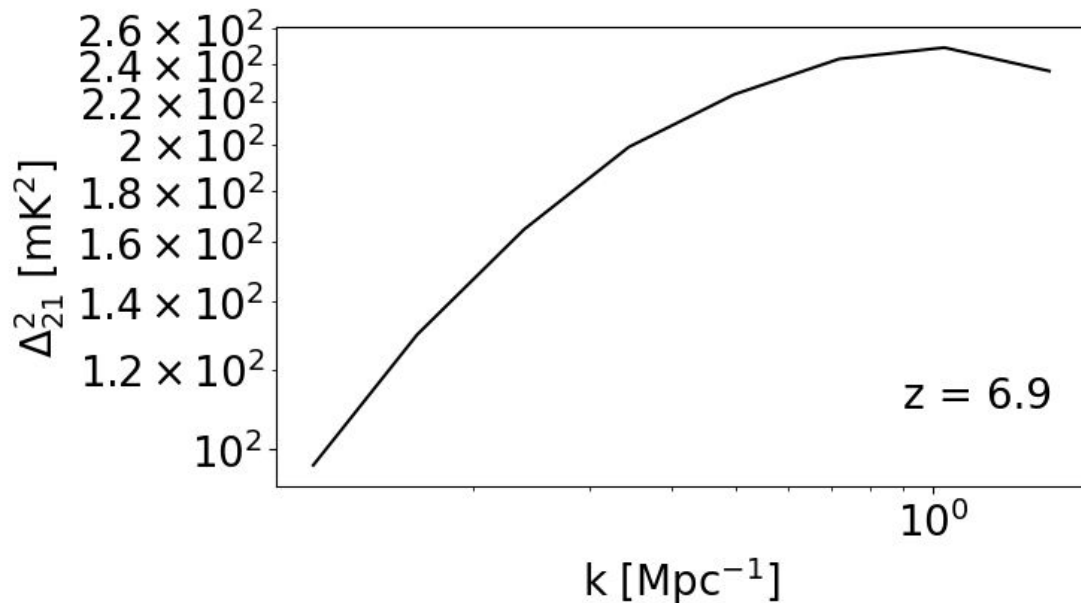
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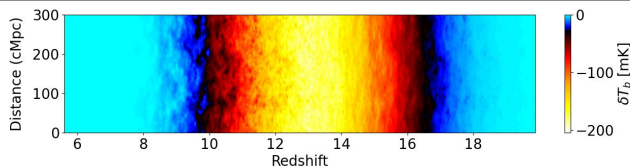


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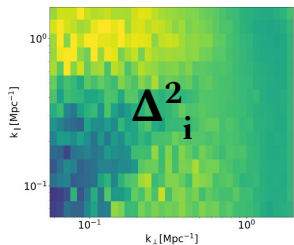
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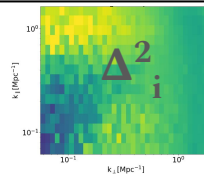
Spherical
averaging



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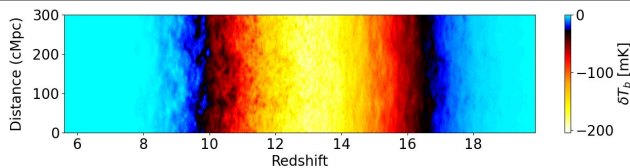
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Run 21cmFAST: Realisation $\Delta^2_i(k_{\perp}, k_{\parallel}, z)$

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CPU hrs



$\mu(\theta) \approx \Delta^2_i$
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Spherical
averaging

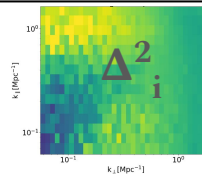
Gaussian likelihood: $P(d|\theta)$

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

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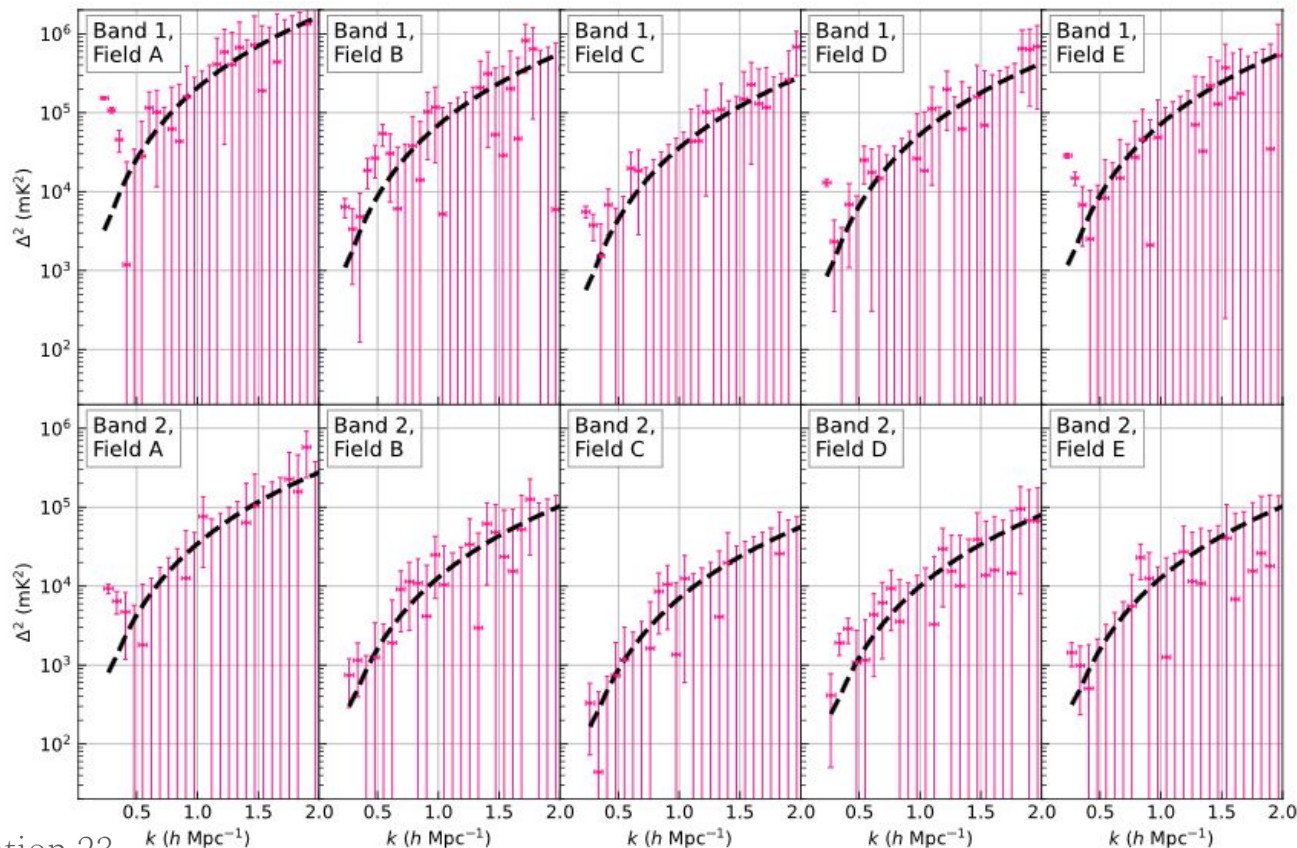


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21-cm Power Spectrum

Δ_{21}^2
obs



But are we actually comparing like to like in the forward modelling process?

A few caveats...

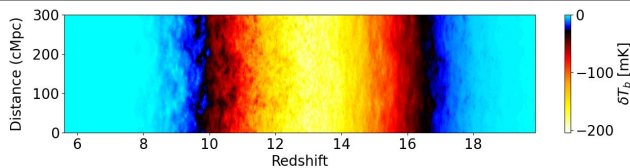
- Forward model volume $\ll$ survey volume

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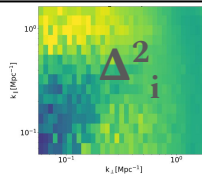
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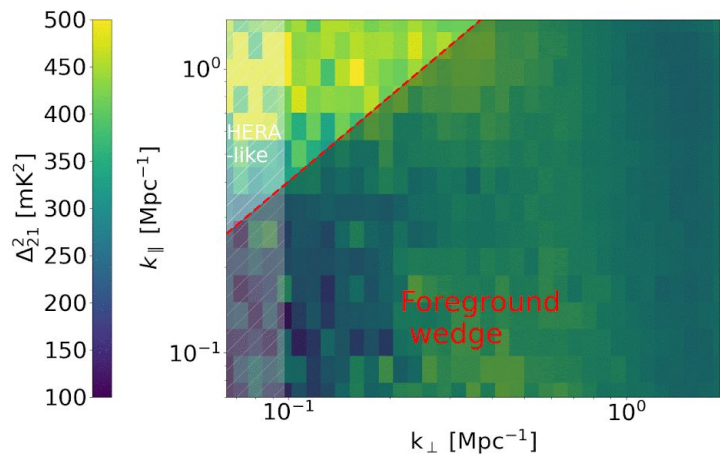
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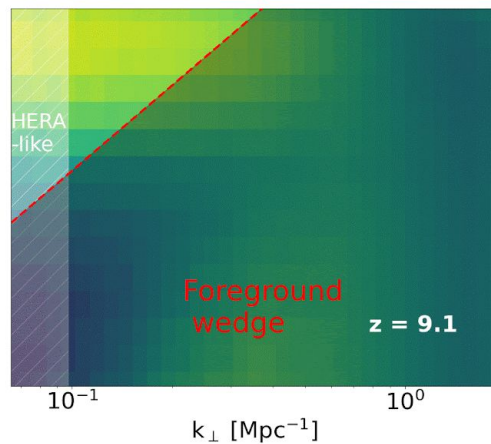
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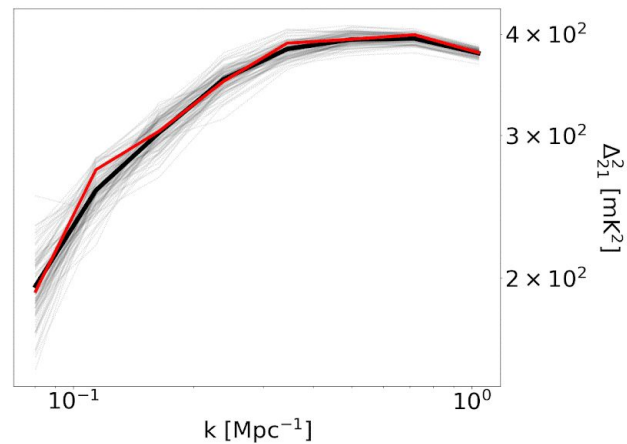
Sample Variance



One sample



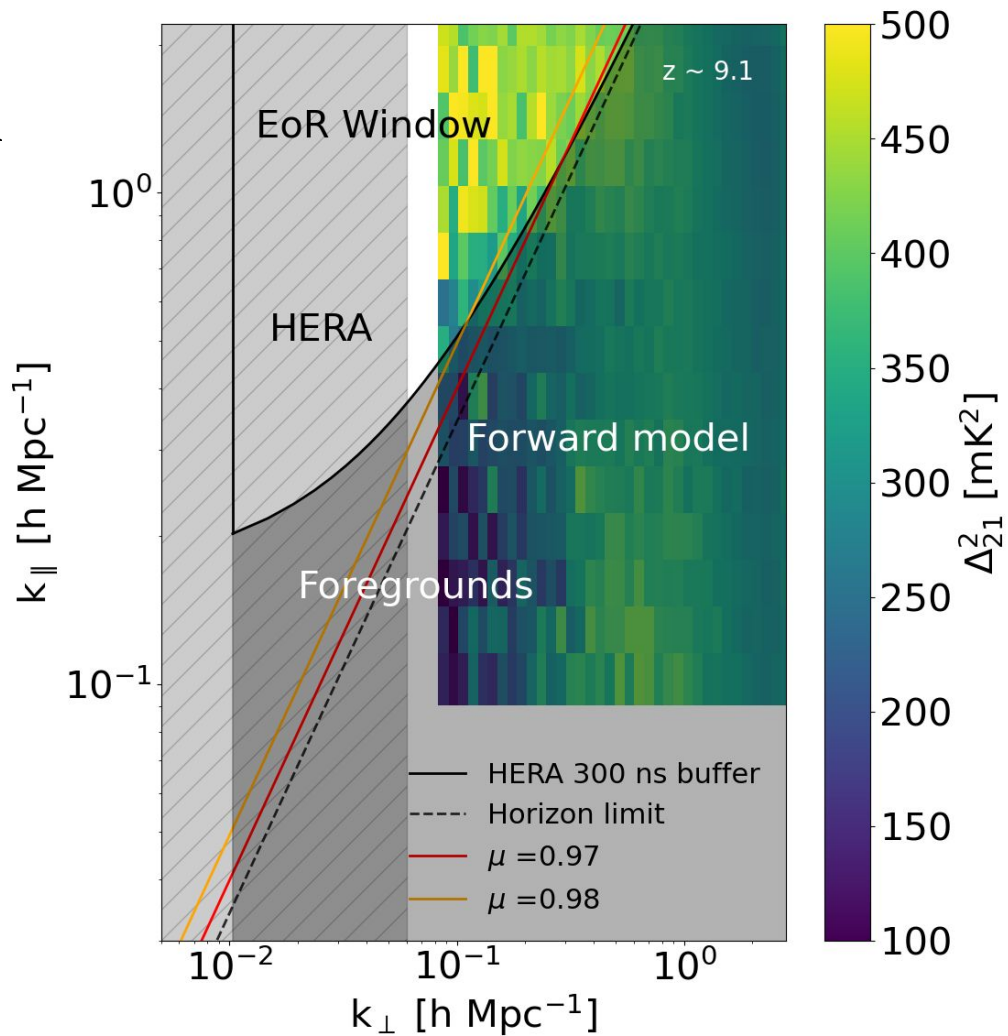
Mean of ~ 200 samples



Why not increase the model volume?

A typical inference requires $\gg 100k$ forward models.

Even with state-of-the-art simulators, it is not practical to forward-model volumes as large as a typical survey in an inference context.

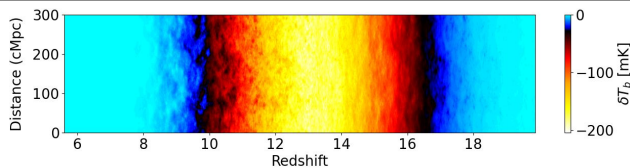


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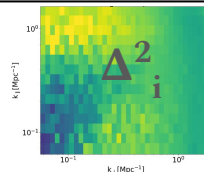
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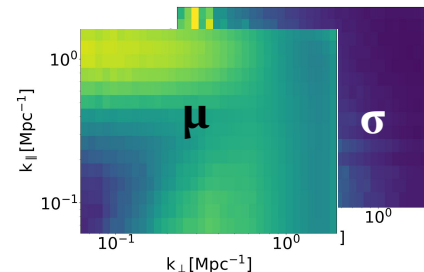
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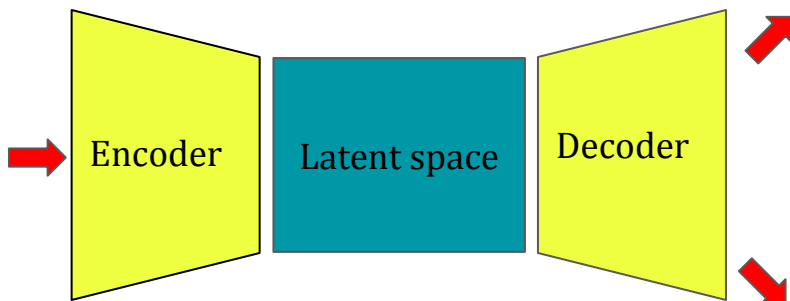
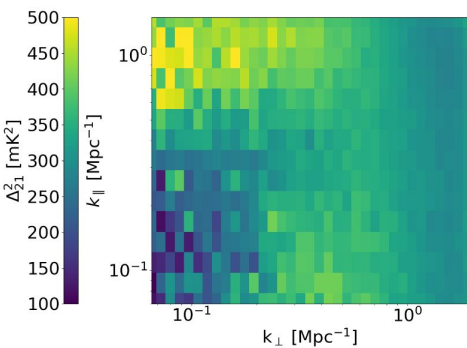
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Breitman+in prep.

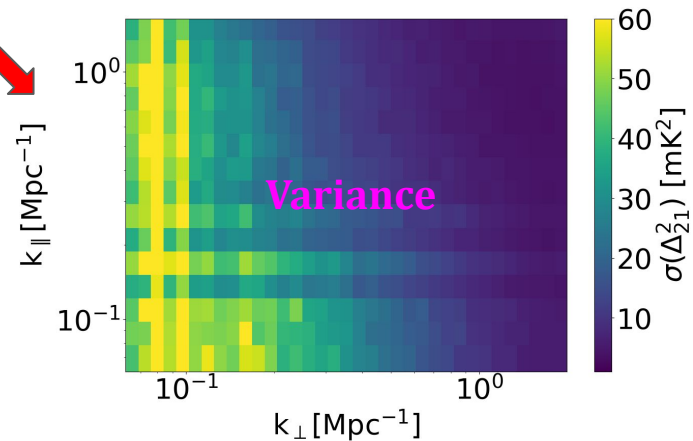
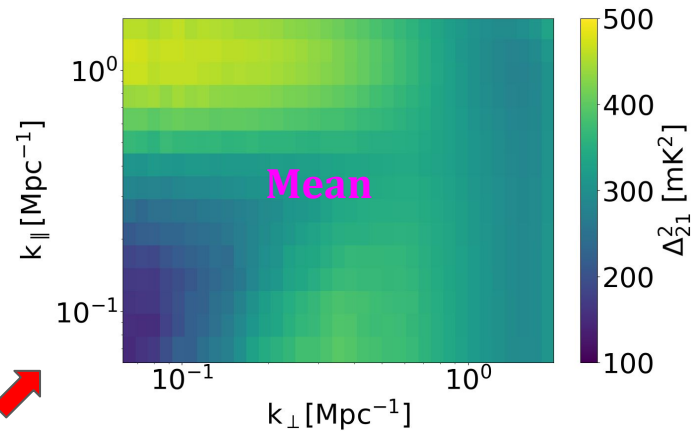
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Sample Variance Denoiser Network



Vary θ_{astro} and ICs

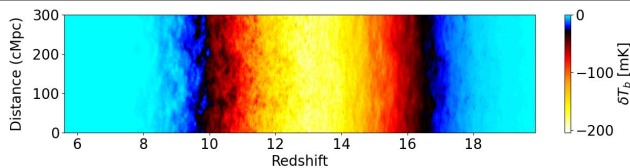


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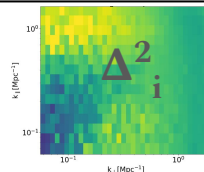
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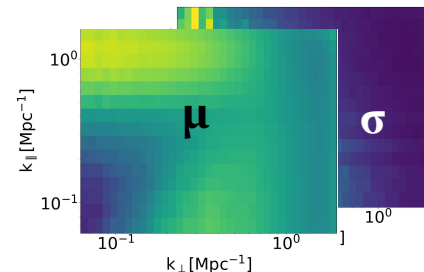
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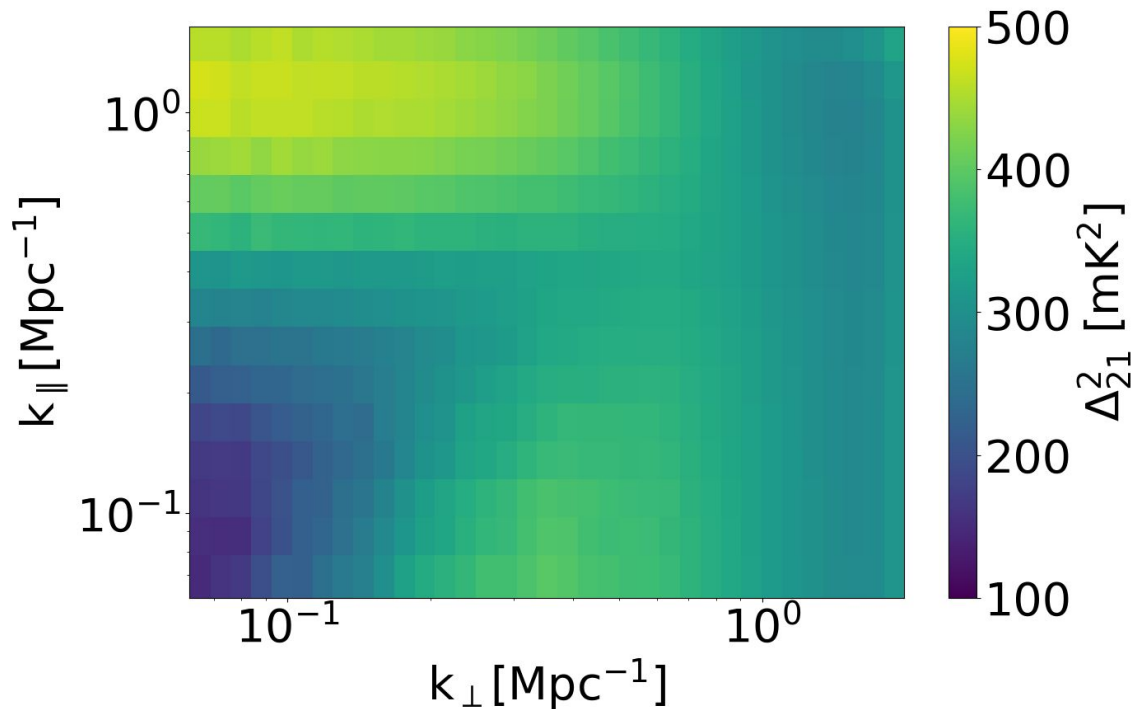
- Forward model volume $\ll$ survey volume
- Spherically-averaging the (non-isotropic) PS is the same for the forward model and the data

The 21-cm PS is not isotropic

Two main causes:

- Redshift space distortions (RSDs)
- Lightcone evolution along the line of sight

Both contribute to increasing the power along the line of sight.

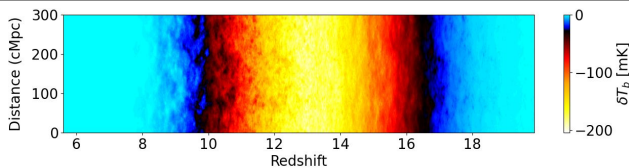


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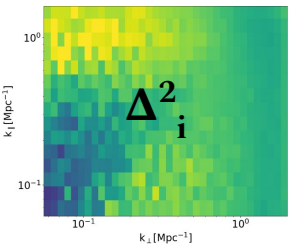
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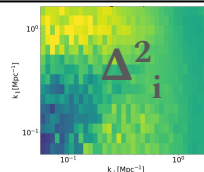
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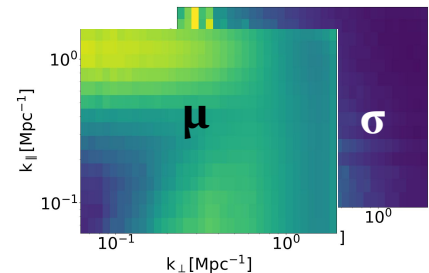
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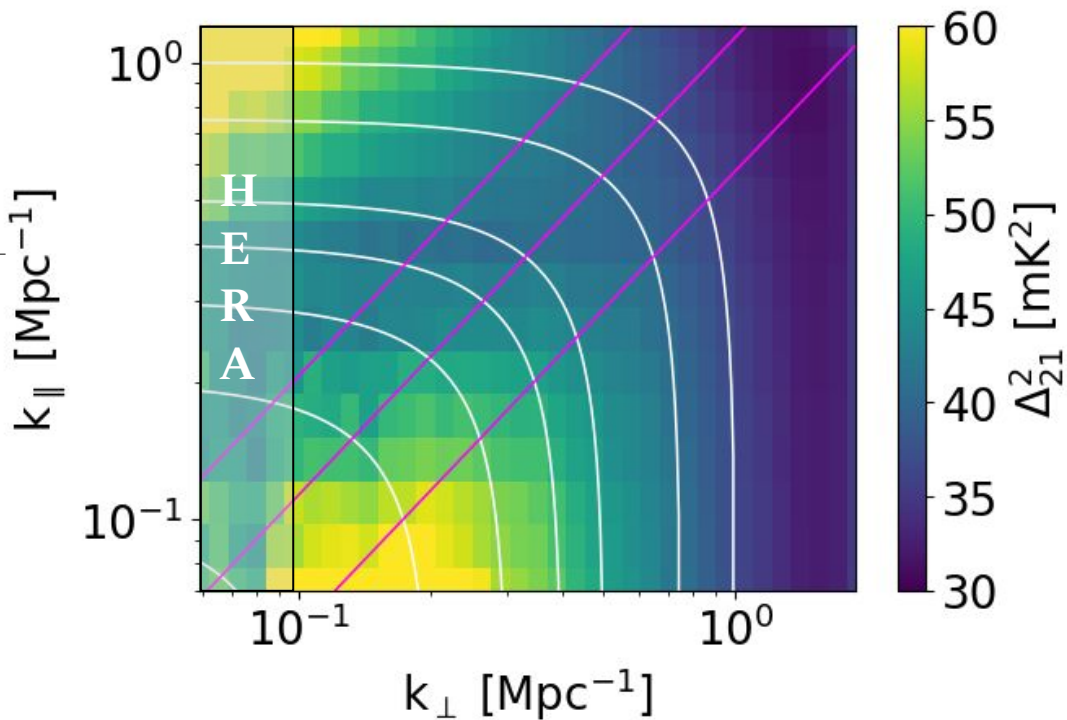
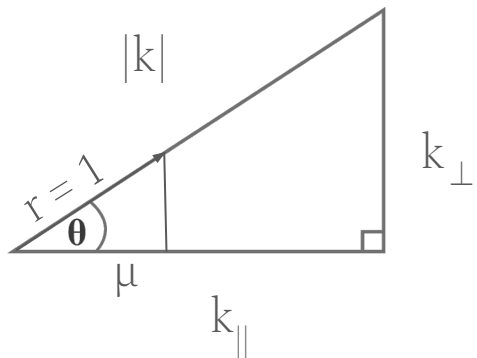
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Anisotropy of the 21-cm Cylindrical Power Spectrum

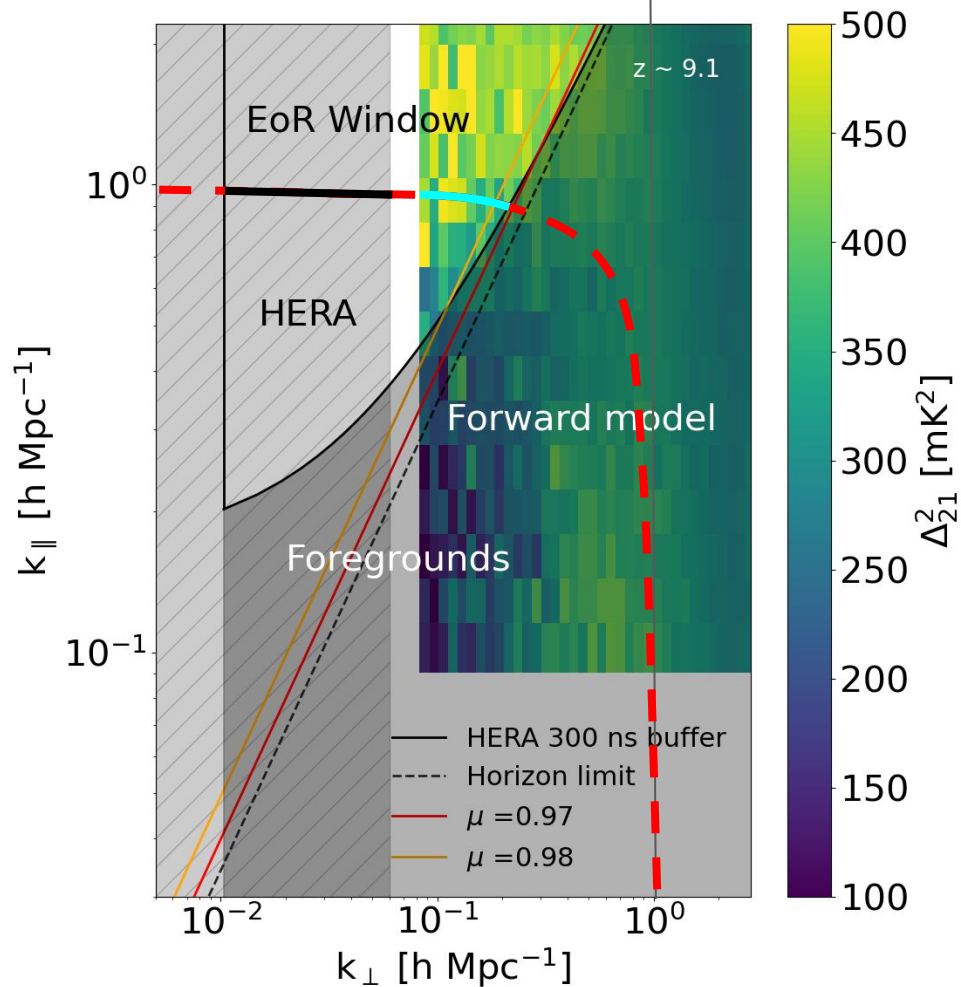
- White: Constant $|k|$ contours
- Magenta: Constant $\mu = \cos(\theta)$
 - θ = angle between $k_{\parallel}$ and $k_{\perp}$



Forward Model

Anisotropy $\Rightarrow$ spherically averaging over the entire power spectrum introduces a bias in the forward model.

Solution: Put a cut $\mu_{\min} = 0.97$ on the forward-modelled data to reduce the bias in the spherically-averaged 21-cm PS.

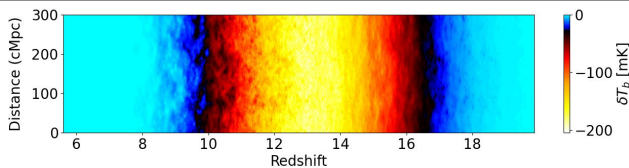


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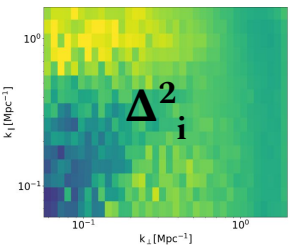
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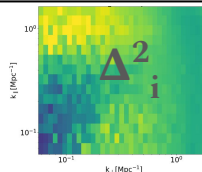
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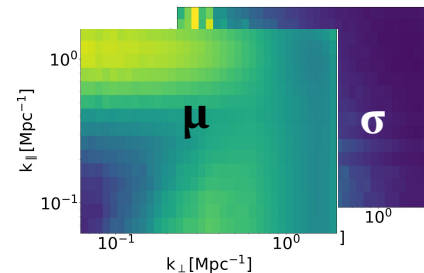
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$\mu(\theta) \approx \text{NN}(\Delta_i^2)$
 $\Sigma(\theta) \approx \text{NN}(\Delta_i^2)$

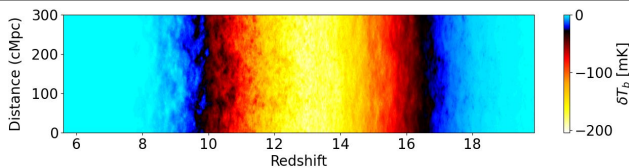


Sample params: $\theta_{\text{astro}} \sim P(\theta_{\text{astro}})$, θ_{cosmo} , ICs

Traditional Pipeline

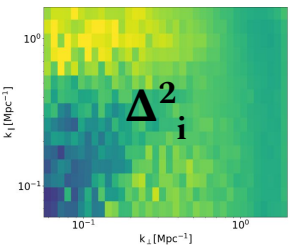
Run 21cmFAST: Realisation $\Delta_i^2(k_{\perp}, k_{\parallel}, z)$

$\gtrsim 300k$
CPU hrs



$\mu(\theta) \approx \Delta_i^2$
 $\Sigma(\theta) \approx \Sigma(\theta_{\text{fid}})$ Fixed

Spherical
averaging



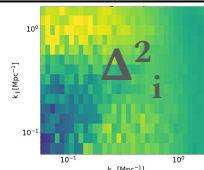
Gaussian likelihood: $P(d|\theta)$

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

This work

21cmEMU**v3**: Realisation $\Delta_i^2(k_{\perp}, k_{\parallel}, z)$

$\lesssim 1$ GPU day

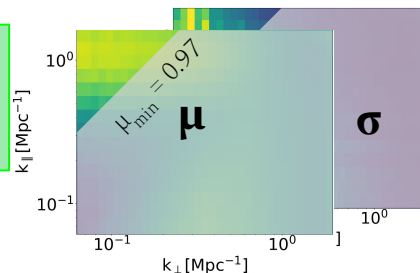


, etc.

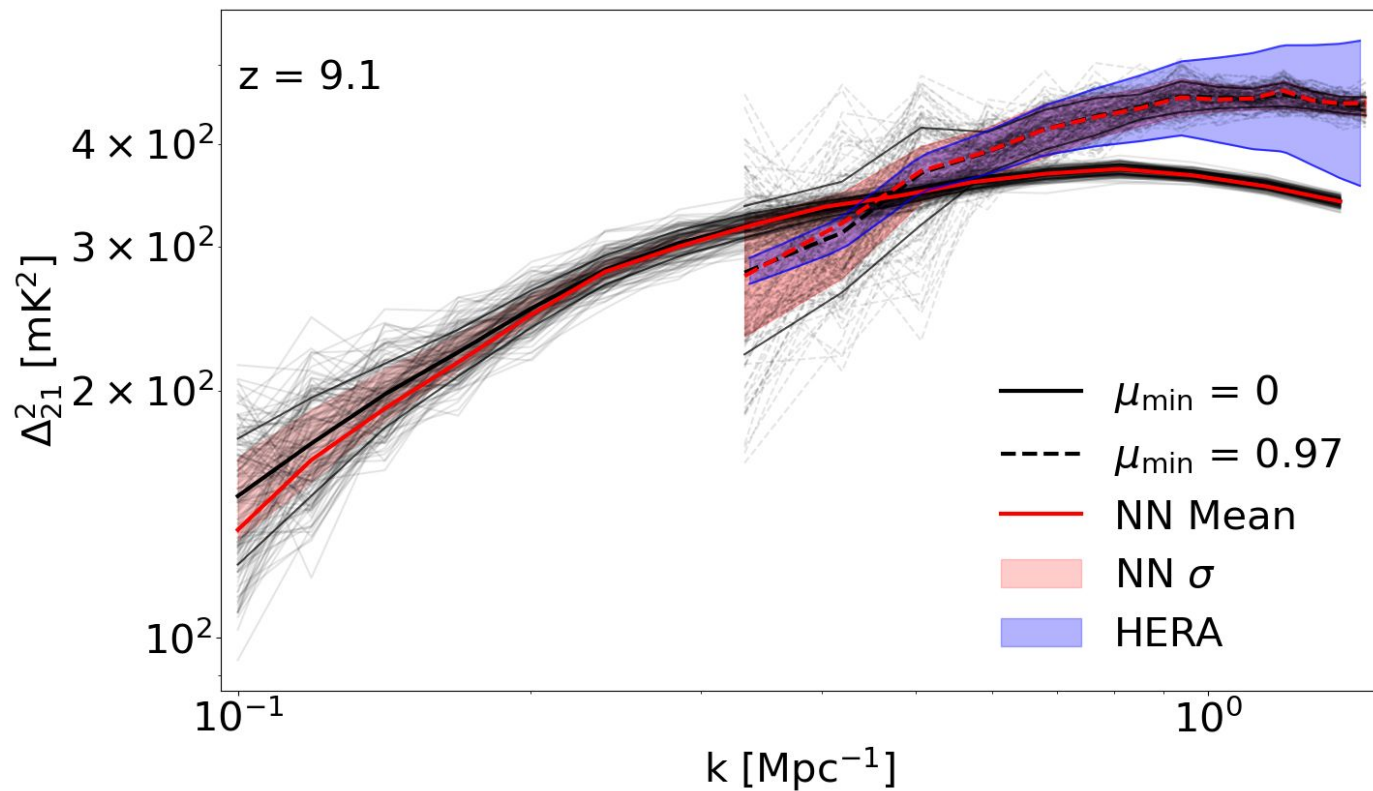
Breitman+in prep.

$\mu(\theta) \approx \text{NN}(\Delta_i^2)$
 $\Sigma(\theta) \approx \text{NN}(\Delta_i^2)$

Exclude PS under
 $\mu_{\text{min}} = 0.97$



Performance on a single θ_{astro} from the test set



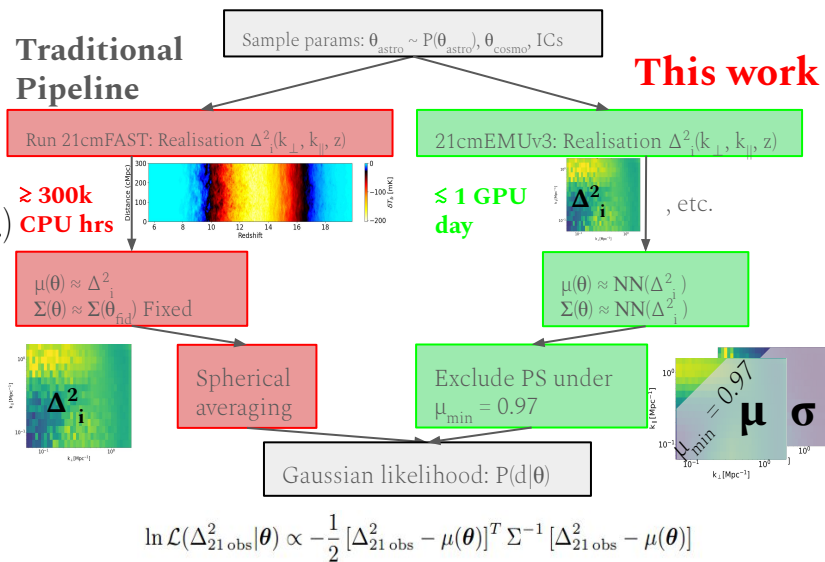
Conclusions

Problems:

- **21cmFAST simulator:** Too slow to perform inferences as new data comes out.
- **Sample variance:** We cannot perform Bayesian inference while forward modelling boxes large enough to cover the survey volume.
- **Anisotropy of the 21-cm PS:** RSDs and lightcone evolution make the 21-cm PS anisotropic. As a consequence, averaging over different regions of PS space than the observation leads to a bias in the model used in the inference $\Rightarrow$ biased posterior.

Solutions:

- **21cmEMUv3:** Emulate 21-cm summaries (2D PS, etc.)
- Neural network to correct for sample variance:
 - **Provides $\text{var}(\theta)$ estimate**
 - **$> 10^5$ times faster than traditional methods**
- Exclude signal above $\mu_{\min} = 0.97$, just like the observation, to **reduce the bias due to the anisotropy**.



Now available!!

pip install py21cmemu

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

Breitman+23

