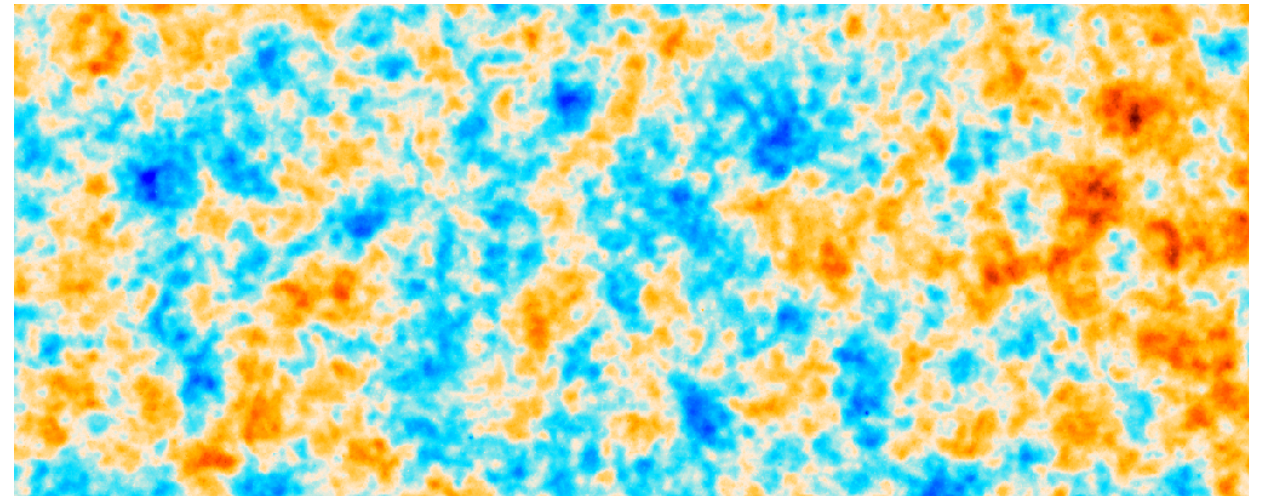
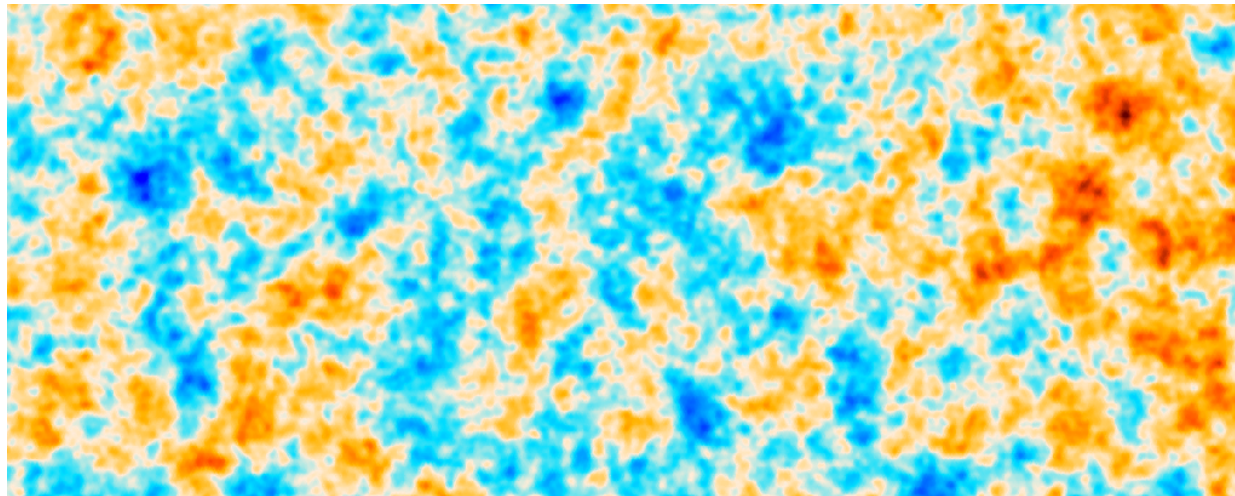


Mocking the Universe & Machine Learning Approaches to Large-Scale Structure

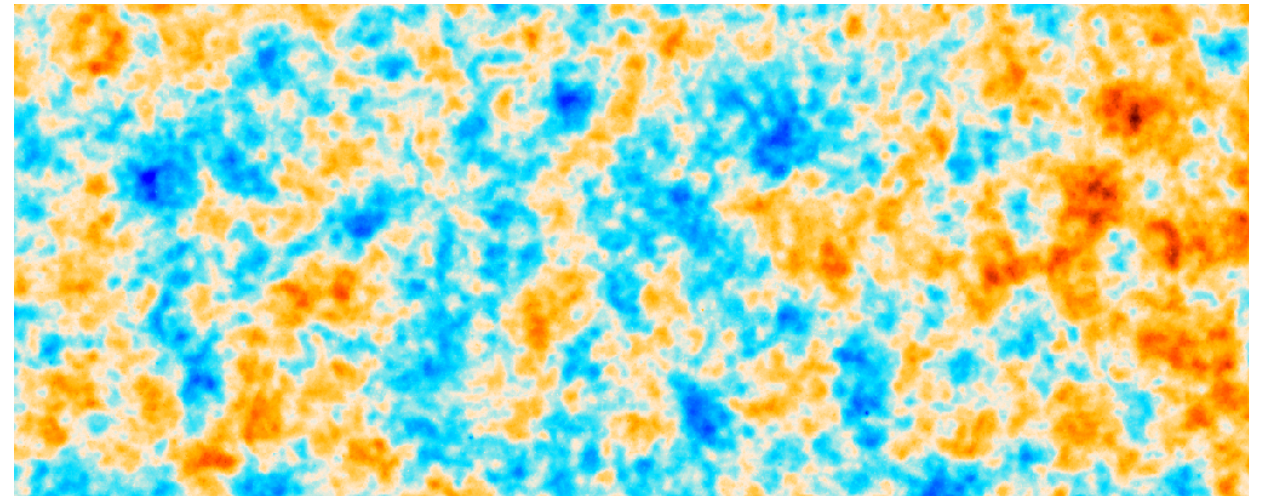
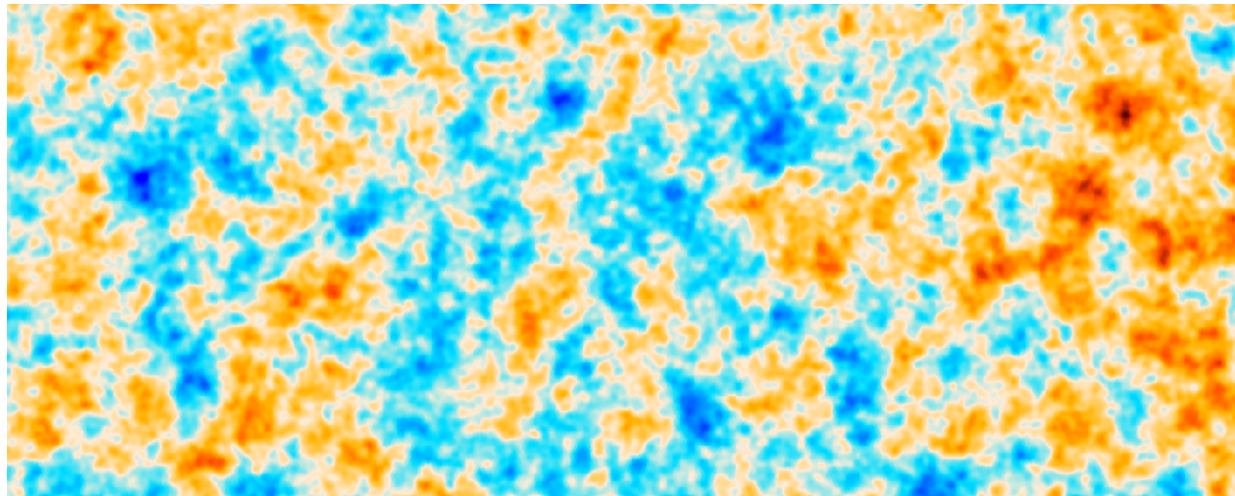
George Stein



BERKELEY CENTER *for*
COSMOLOGICAL PHYSICS

Mocking the Universe & Machine Learning Approaches to Large-Scale Structure With

George Stein



(a small sampling of)
the Era of Large-Survey Precision Cosmology

Cosmic Microwave
Background (CMB)

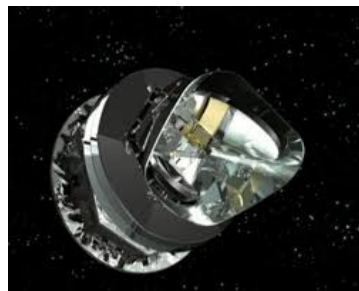
ACT



SPT

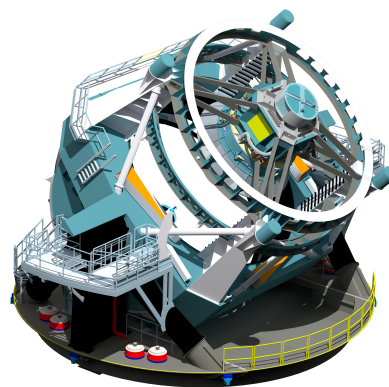


Planck

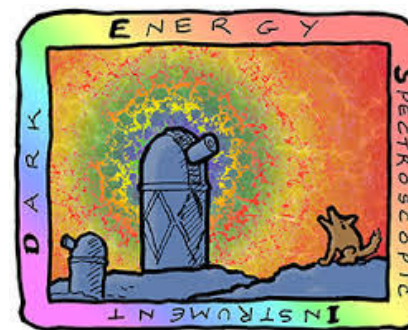


Large Scale
Structure (LSS)

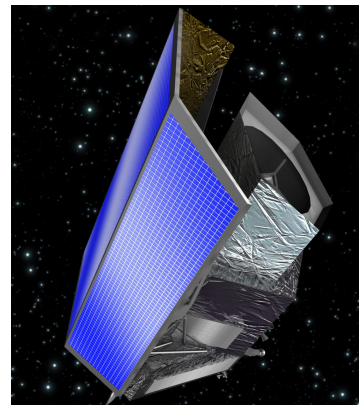
LSST



DESI



Euclid



Intensity Mapping
(IM)

CHIME



COMAP



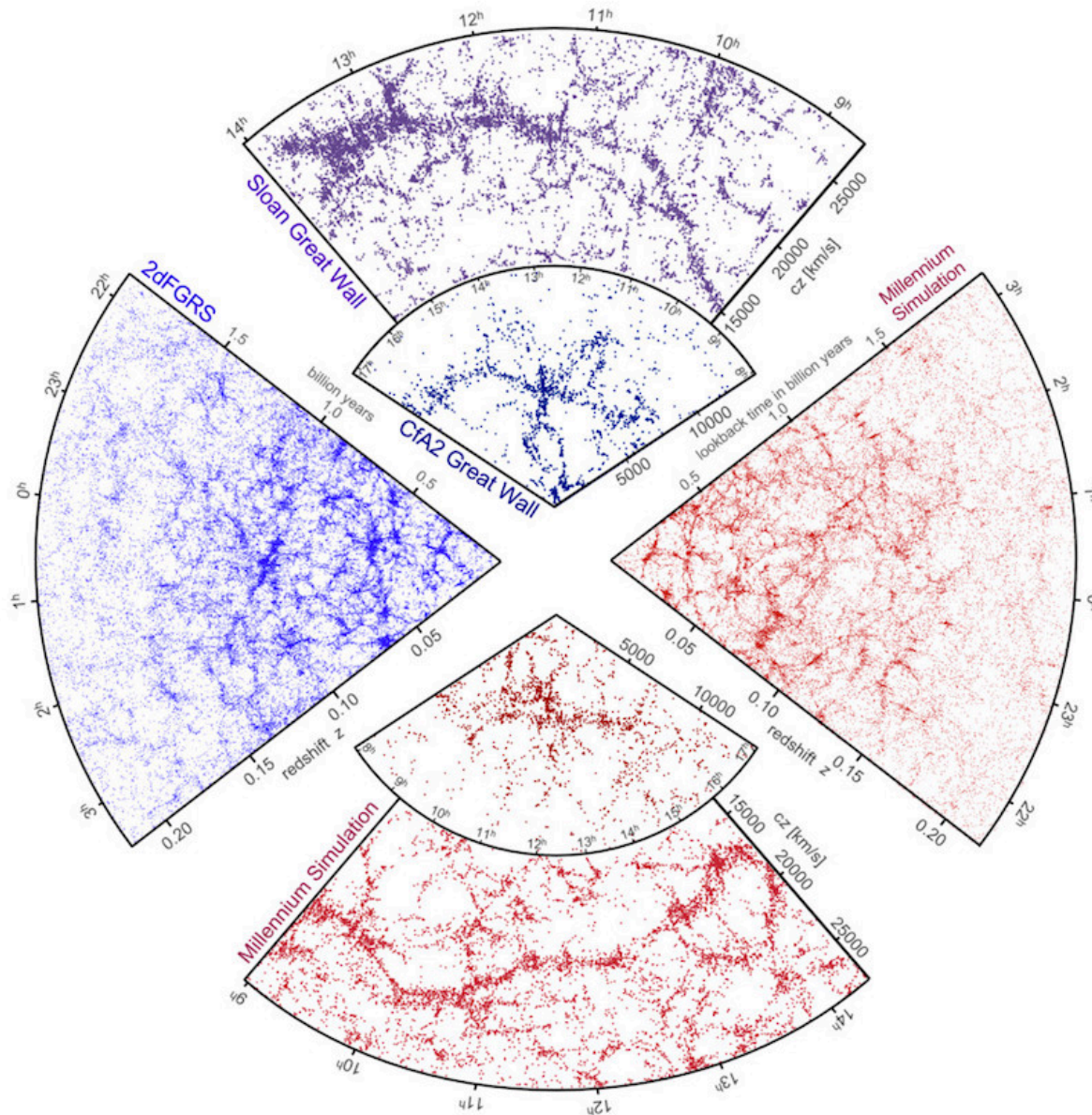
How do we interpret the data?



**Theory/
Initial Conditions**



Observables



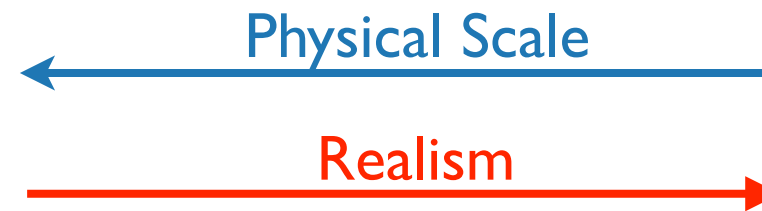
Cosmological simulations are required to:

- forecast the expected effects of cosmological scenarios
- analyze current and near-future cosmological datasets
- develop and test operational pipelines

<https://wwwmpa.mpa-garching.mpg.de/millennium/>



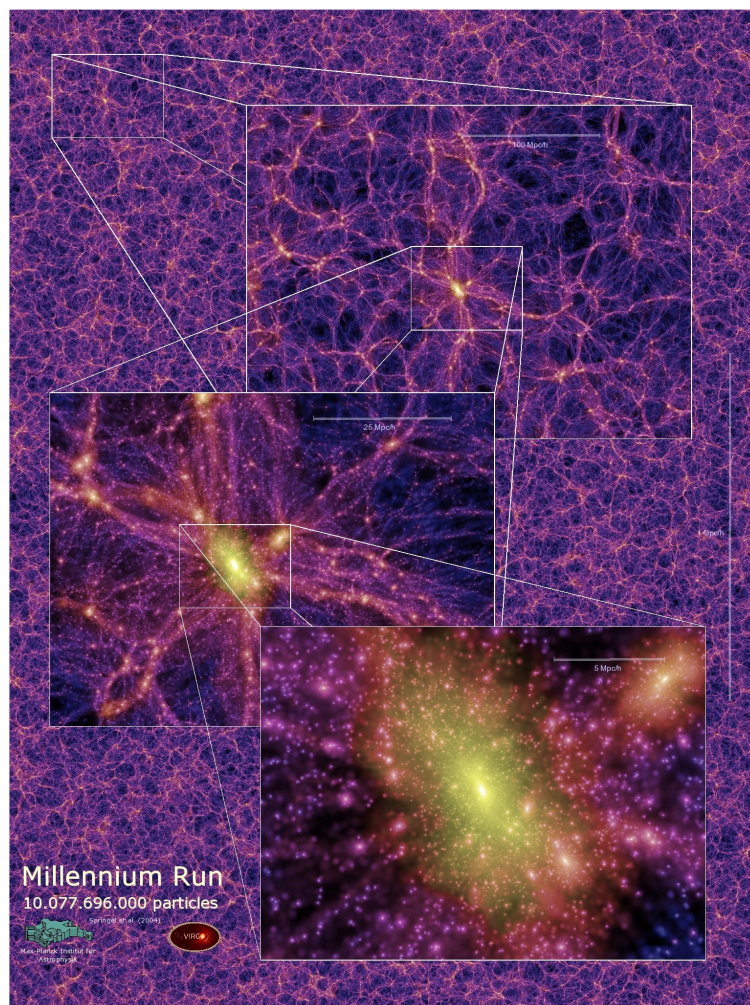
Modern Cosmological Simulations



Modern Cosmological Simulations



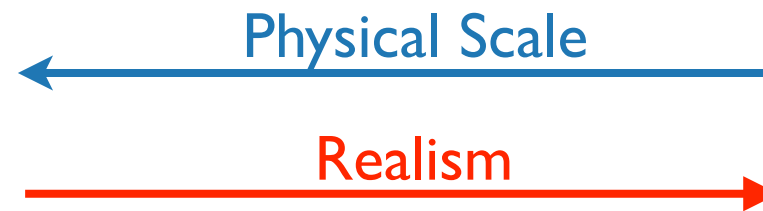
ultra large box, gravity only
Cosmic Web



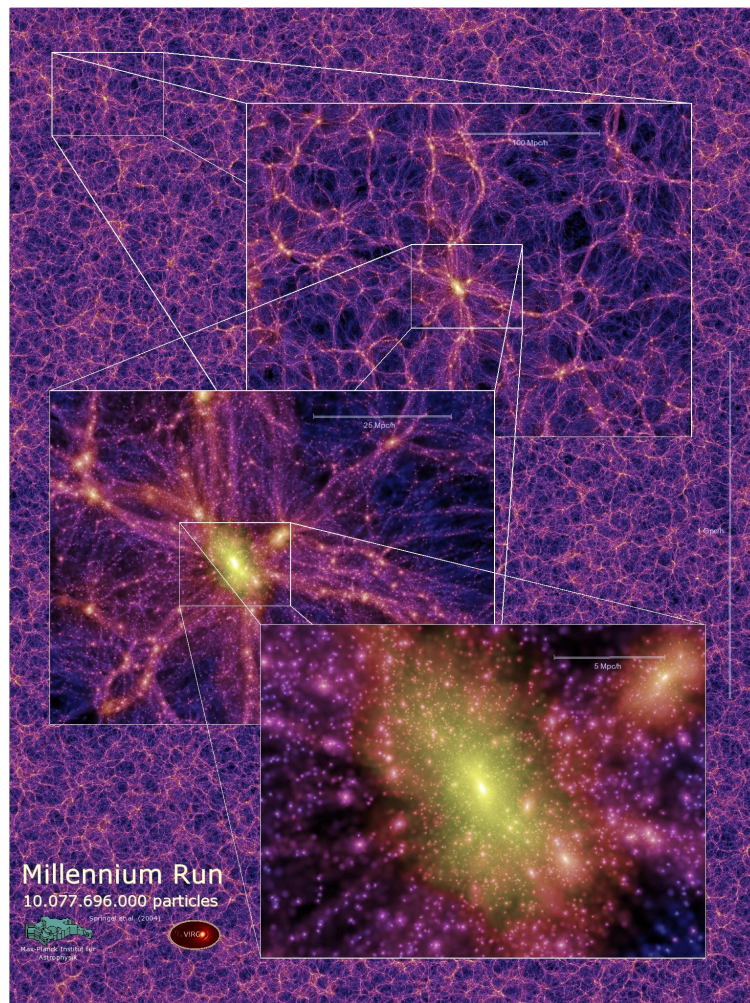
N-body or 'approximate methods'



Modern Cosmological Simulations

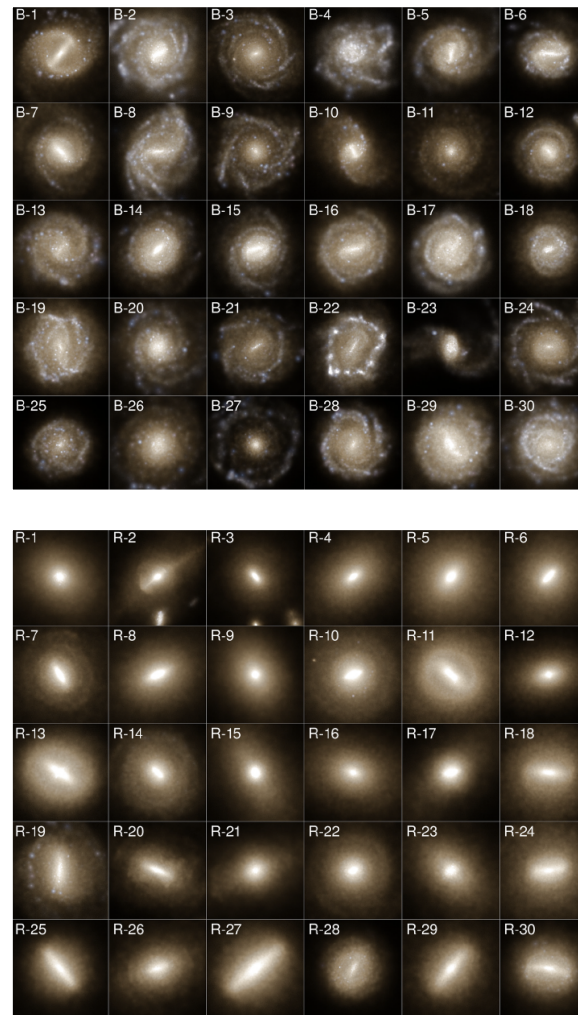


ultra large box, gravity only
Cosmic Web



N-body or 'approximate methods'

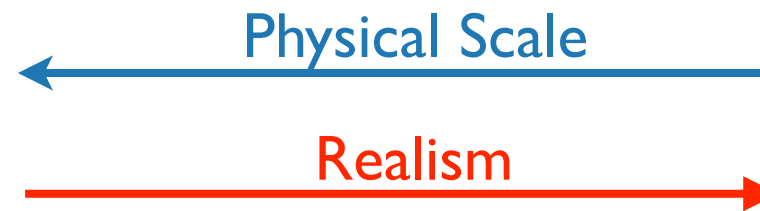
full physics, medium sized box
The properties of dark matter halos



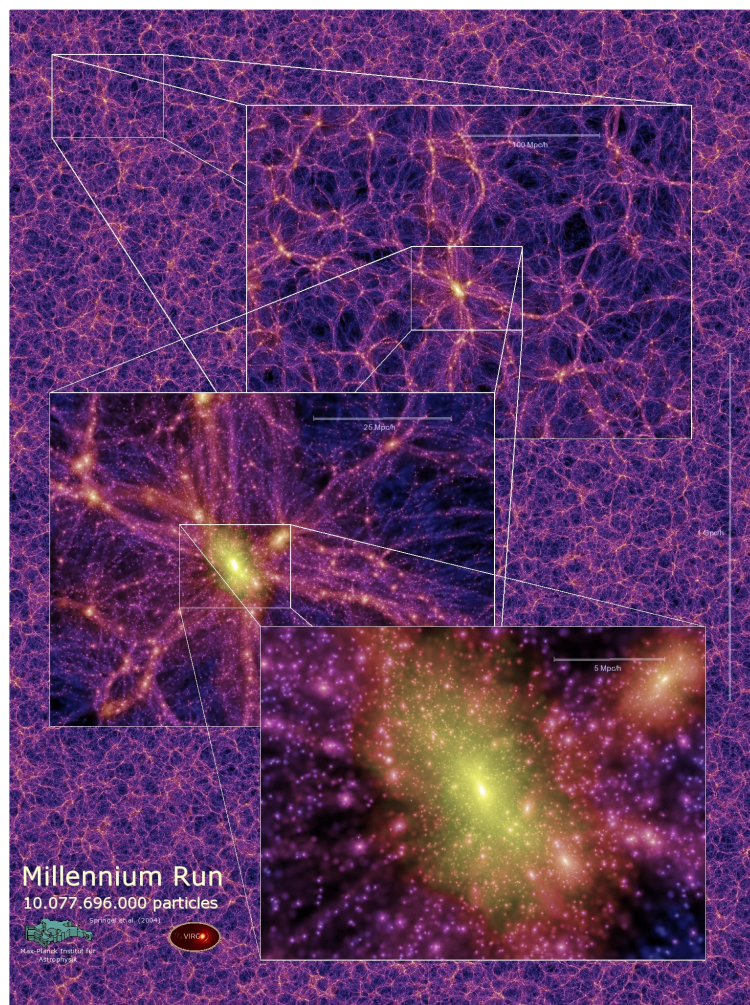
e.g. Illustris



Modern Cosmological Simulations

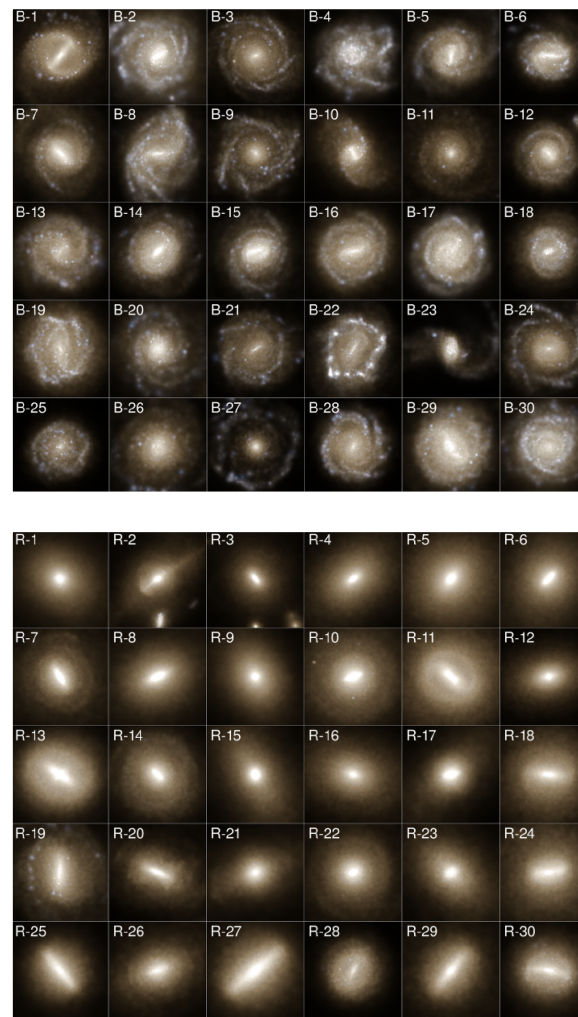


ultra large box, gravity only
Cosmic Web



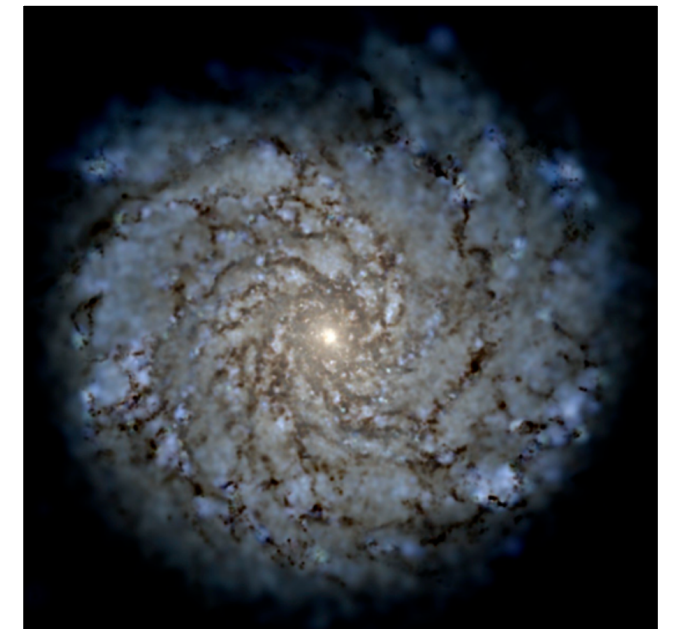
N-body or 'approximate methods'

full physics, medium sized box
The properties of dark matter halos



e.g. Illustris

full physics, small sized box
Detailed substructures of halos & galaxies



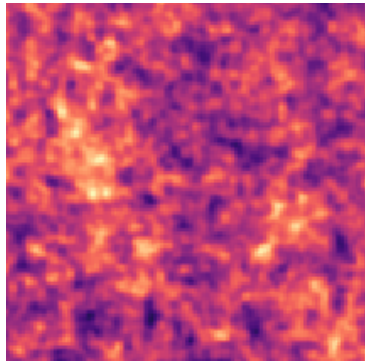
e.g. FIRE



Approximate Cosmological simulations

*map from initial conditions to final observable as fast as possible,
with an appropriate accuracy

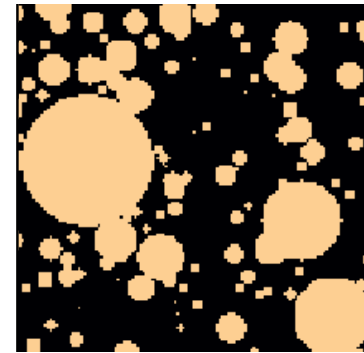
Initial Conditions



Physical Approximation



Final Matter Density/Halo Catalogue



Approximate Cosmological simulations

*map from initial conditions to final observable as fast as possible,
with an appropriate accuracy

I.) stochastic methods

1. **EZmocks (2014)** - Chuang et al.
 - Zeldovich + PDF mapping
2. **HALOGEN (2014)** - Avila et al.
 - LPT + stochastic halo biasing
3. **Log-normal (1991)** - Coles, Jones
 - +many others since
4. **PATCHY (2013)** - Kitaura, Yepes, Prada
 - APT + nonlinear stochastic biasing
5. **PThalos (2001)** - Scoccimarro, Sheth
 - 2LPT + $n(m, \delta | z)$ assignment using merger tree + NFW particle placement
 - ★ Manera et al. (2012)
 - 2LPT + fof (linking length = 0.38) + HMF
6. **QPM (2013)** - White, Tinker, McBride
 - low-res PM, halos sampled from particles based on local densities



Approximate Cosmological simulations

*map from initial conditions to final observable as fast as possible,
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1.) stochastic methods

2.) abridged particle mesh methods

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1. **COLA (2013)** - Tassev, Zaldarriaga, Eisenstein
 - Nobody in frame comoving with 2LPT observers
2. **FastPM (2016)** - Feng, Chu, Seljak
 - PM + broadband correction at each timestep to enforce correct linear evolution



Approximate Cosmological simulations

*map from initial conditions to final observable as fast as possible,
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1.) stochastic methods

2.) abridged particle mesh methods

3.) predictive methods

1. **EZmocks (2014)** - Chuang et al.
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2. **HALOGEN (2014)** - Avila et al.
 - LPT + stochastic halo biasing
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 - PM + broadband correction at each timestep to enforce correct linear evolution

Physics Based

1. **Peak Patch (1993)** - Bond, Myers
 - Homogeneous ellipsoid collapse + LPT
 - ★ Stein, Alvarez, Bond (2018)
 - parallel HPC version
2. **PINOCCHIO (2002)** - Monaco et al.
 - LPT + Inverse collapse time for particles + fragmentation criteria to create distinct halos

Machine Learned

1. **D3M (2018)** - He et al.
 - CNN to find correction to LPT displacements
2. **Halonet (2018)** - Berger, Stein
 - CNN to find Lagrangian halos + 2LPT



Which method to use?

Comparing approximate methods for mock catalogues and covariance matrices

300 $1.5h^{-1}\text{Gpc}$, 1000^3 particles $z=1$ simulations

- I: correlation function [1806.09477](#)
- II: power spectrum multipoles [1806.09497](#)
- III: Bispectrum [1806.09499](#)



Which method to use?

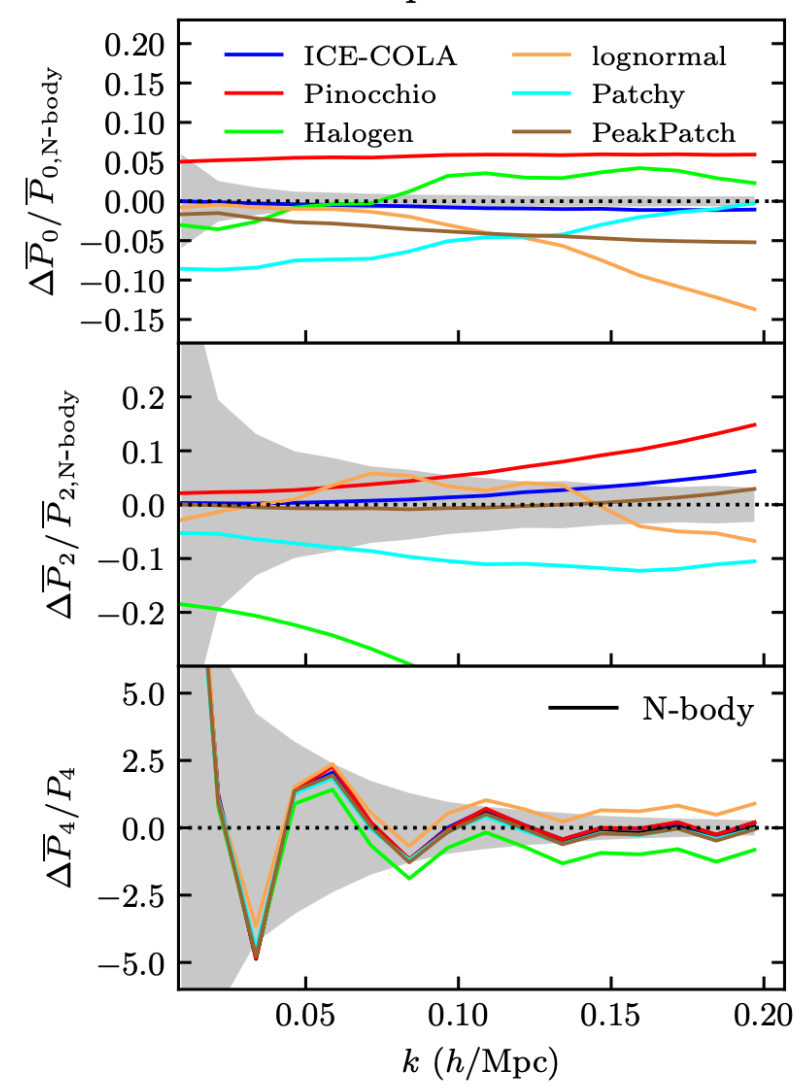
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- Power spectrum multipoles see ~20/40/50% difference between methods

Sample 2



Which method to use?

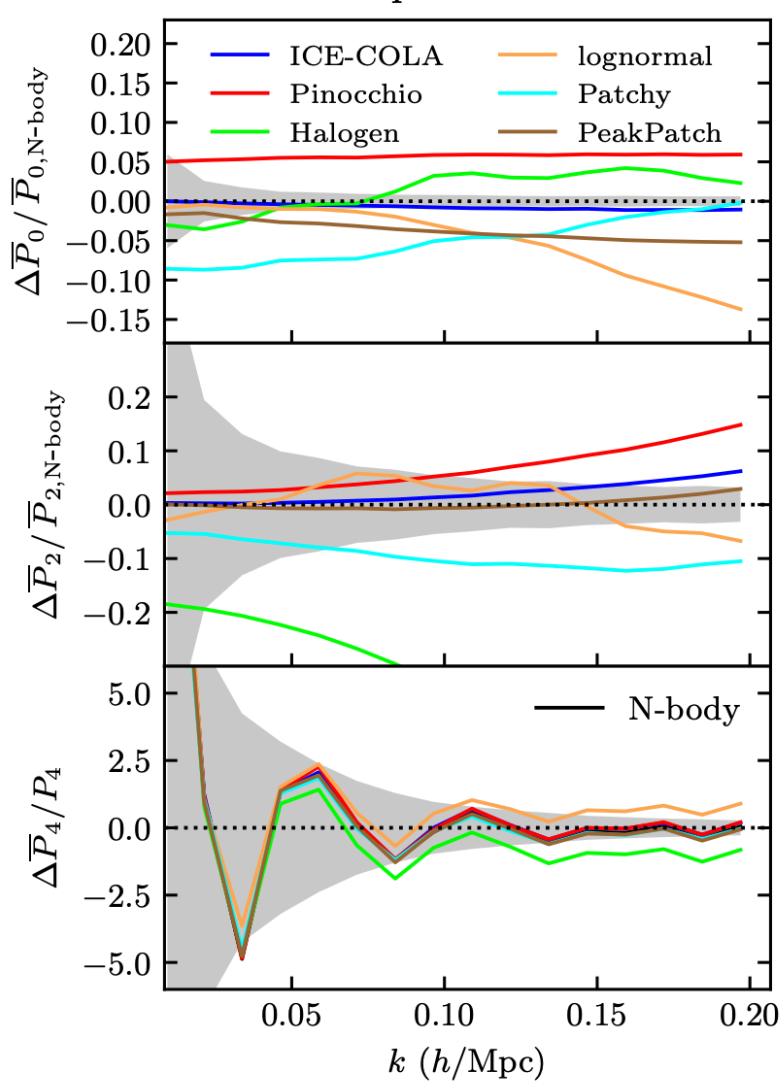
Comparing approximate methods for mock catalogues and covariance matrices

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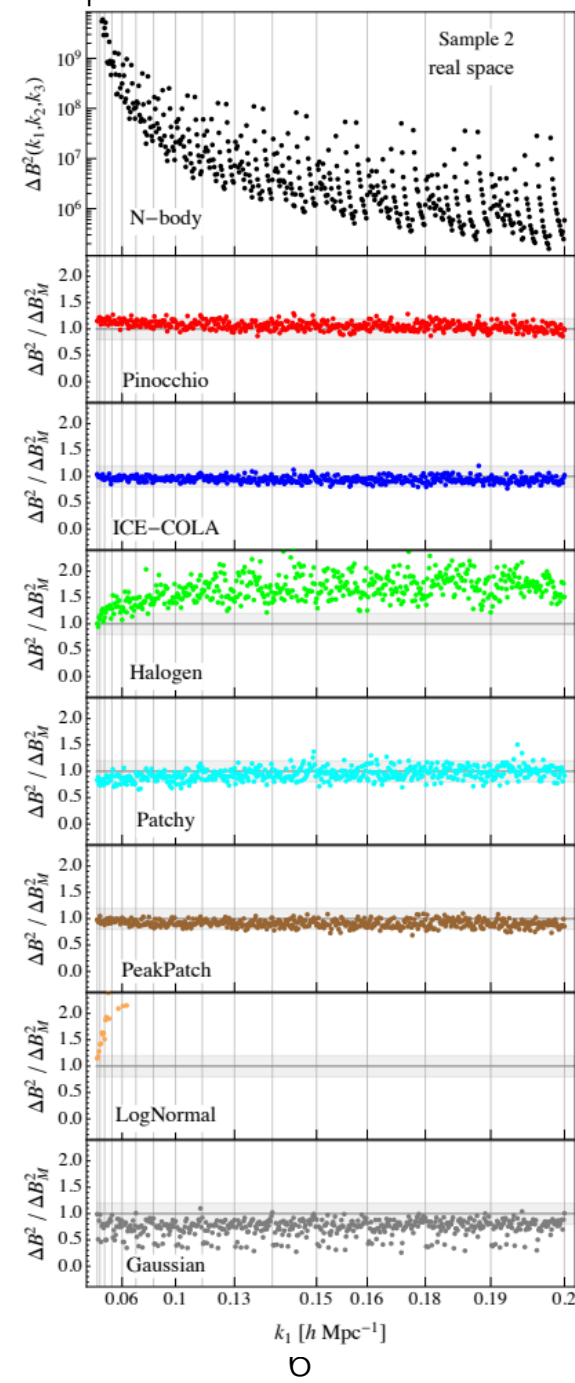
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Sample 2



- Methods fit to reproduce power spectrum do not reproduce bispectrum



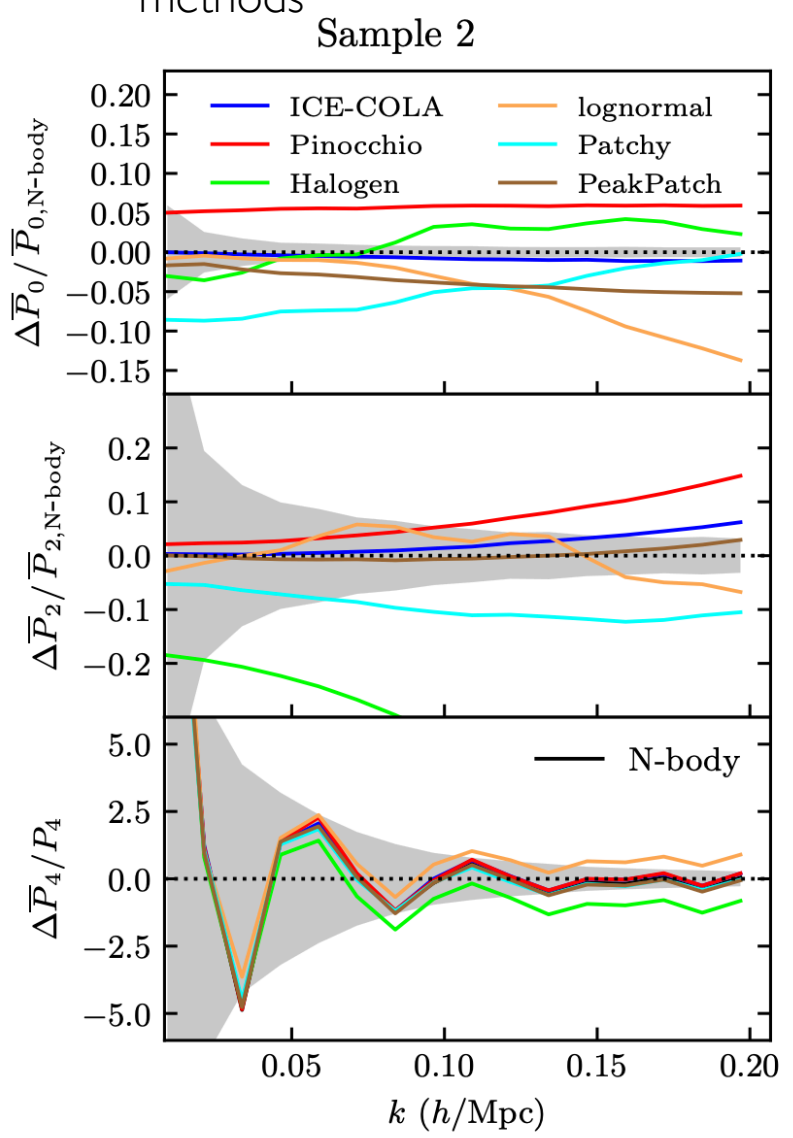
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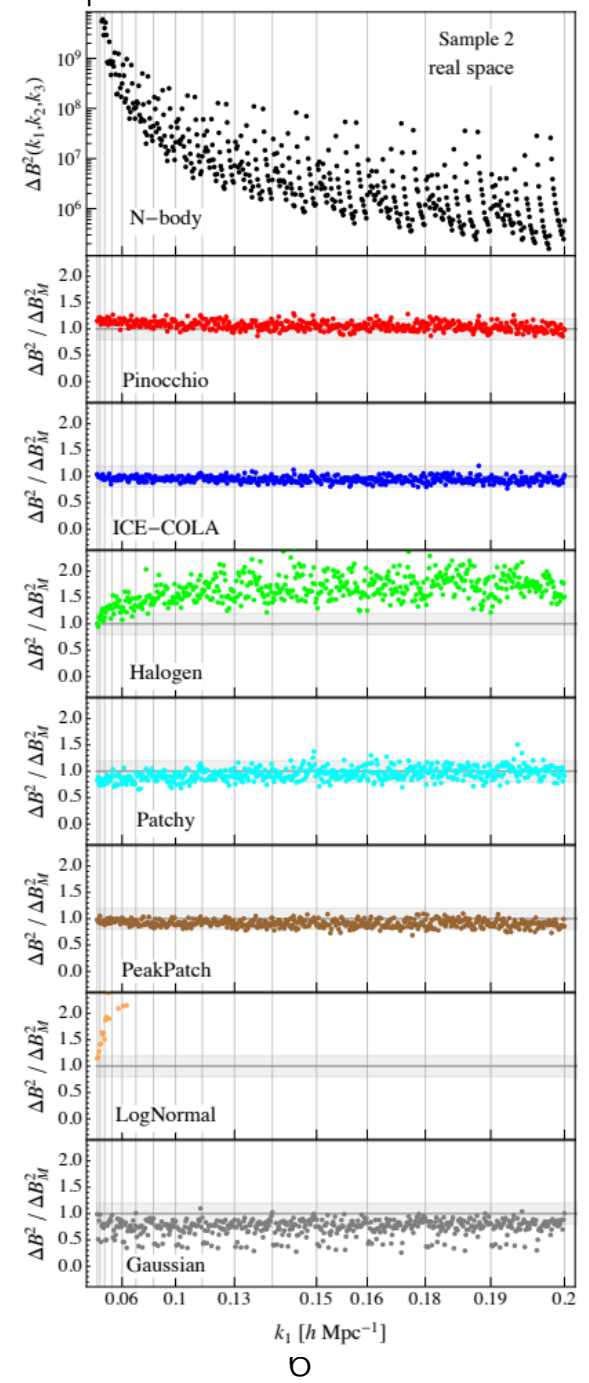
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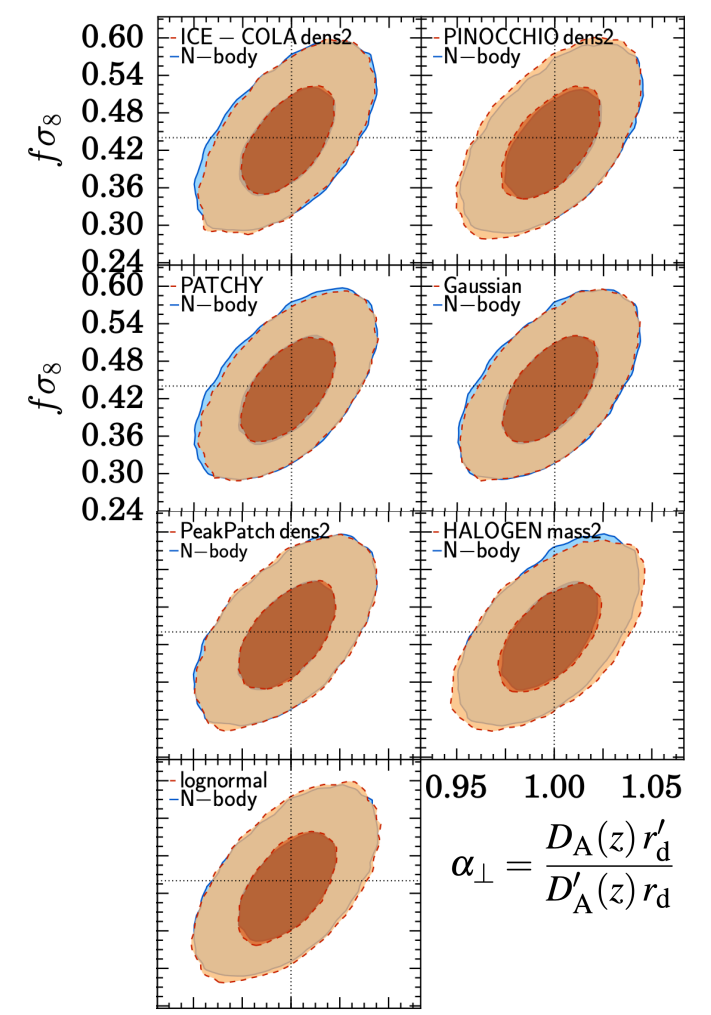
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- covariance matrices produce similar cosmological parameter constraints



Approximate Cosmological simulations

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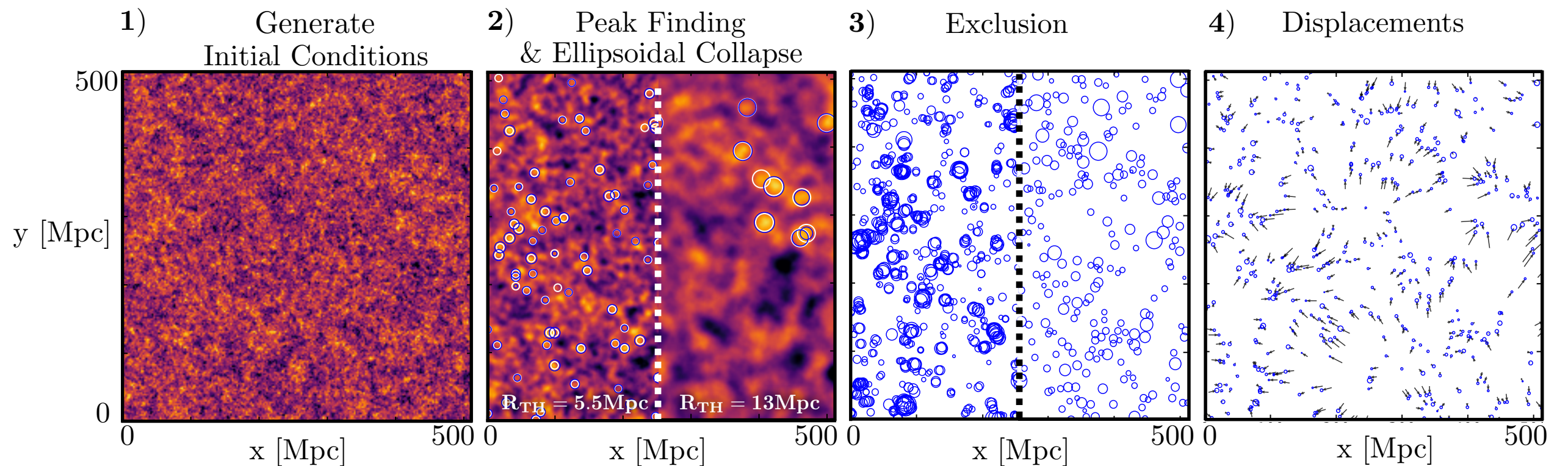
mass-Peak Patch

Stein, Alvarez, Bond, [1810.07727](#)

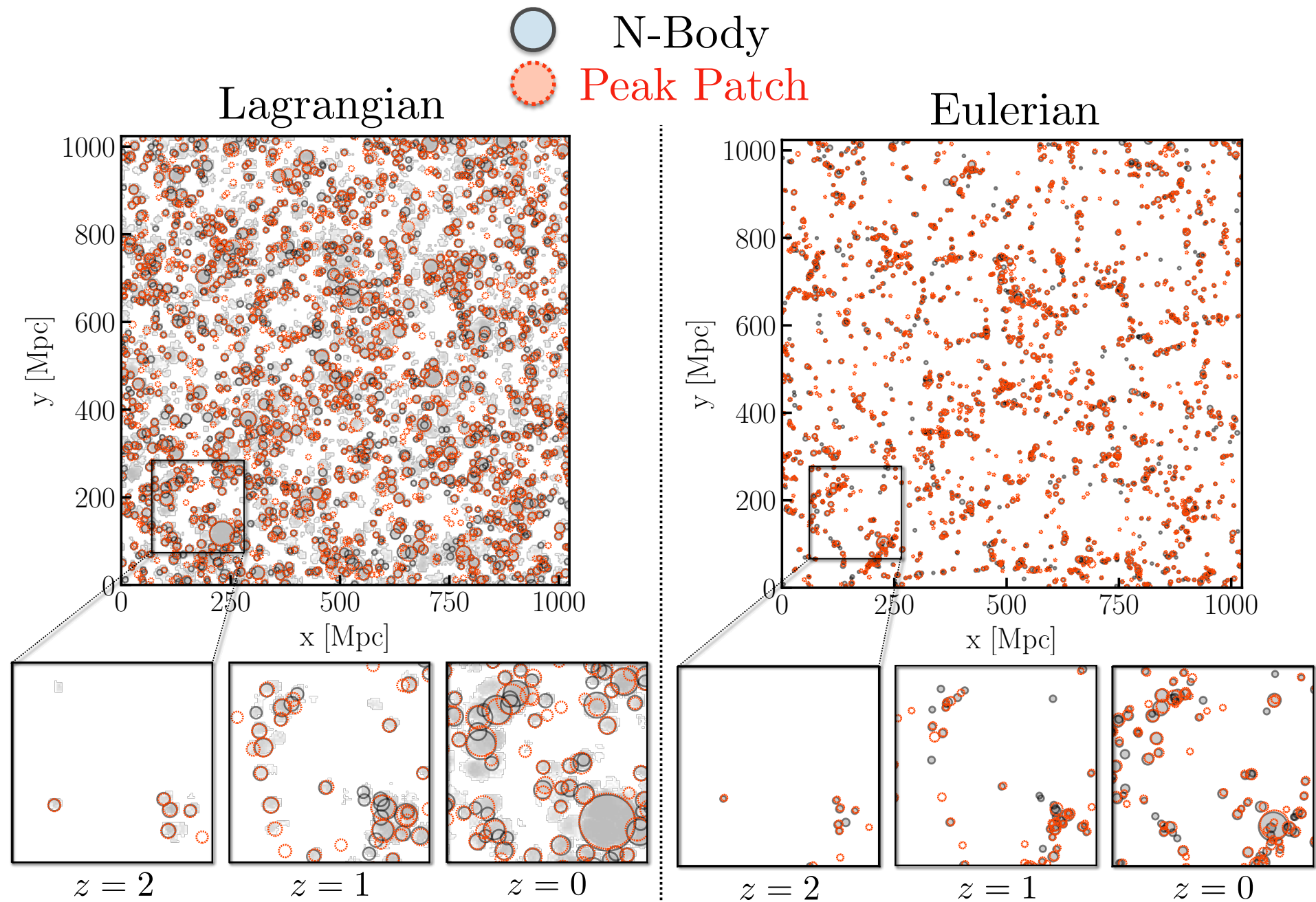
Bond & Myers [1996ApJS..103....1B](#), [1996ApJS..103...41B](#), [1996ApJS..103...63B](#)

Based on Homogeneous Ellipsoid Collapse

$$\frac{\ddot{x}_i}{x_i} = \frac{\ddot{a}}{a} - \frac{1}{2}\Omega_m H^2 [b_i \bar{\delta} + c_i \bar{\delta}_{\text{lin}}]$$



Comparisons to N-Body simulations

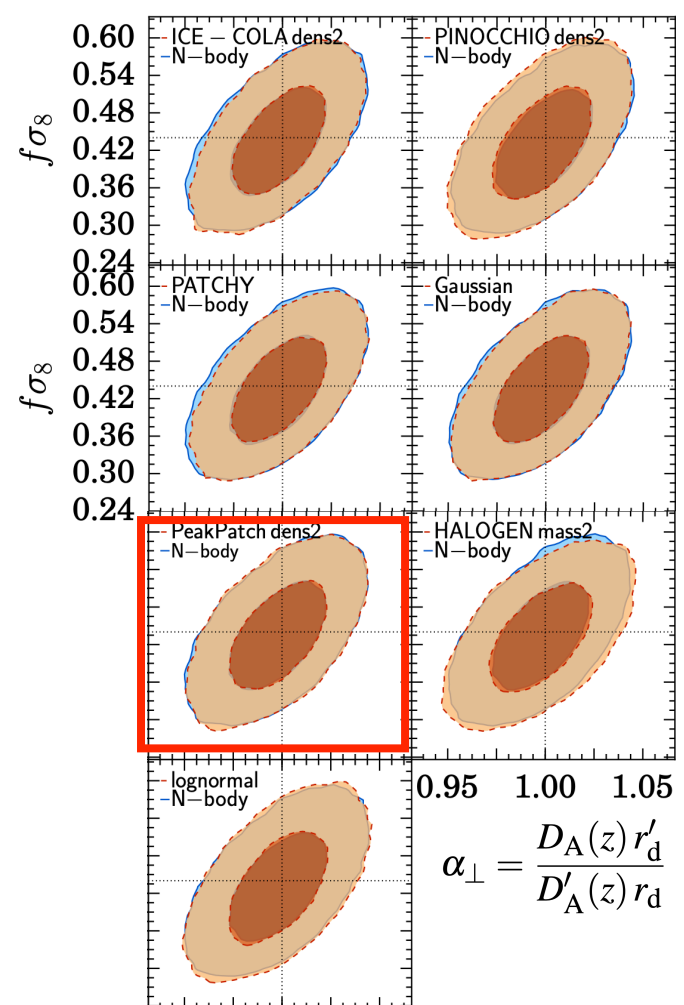


Which method to use?

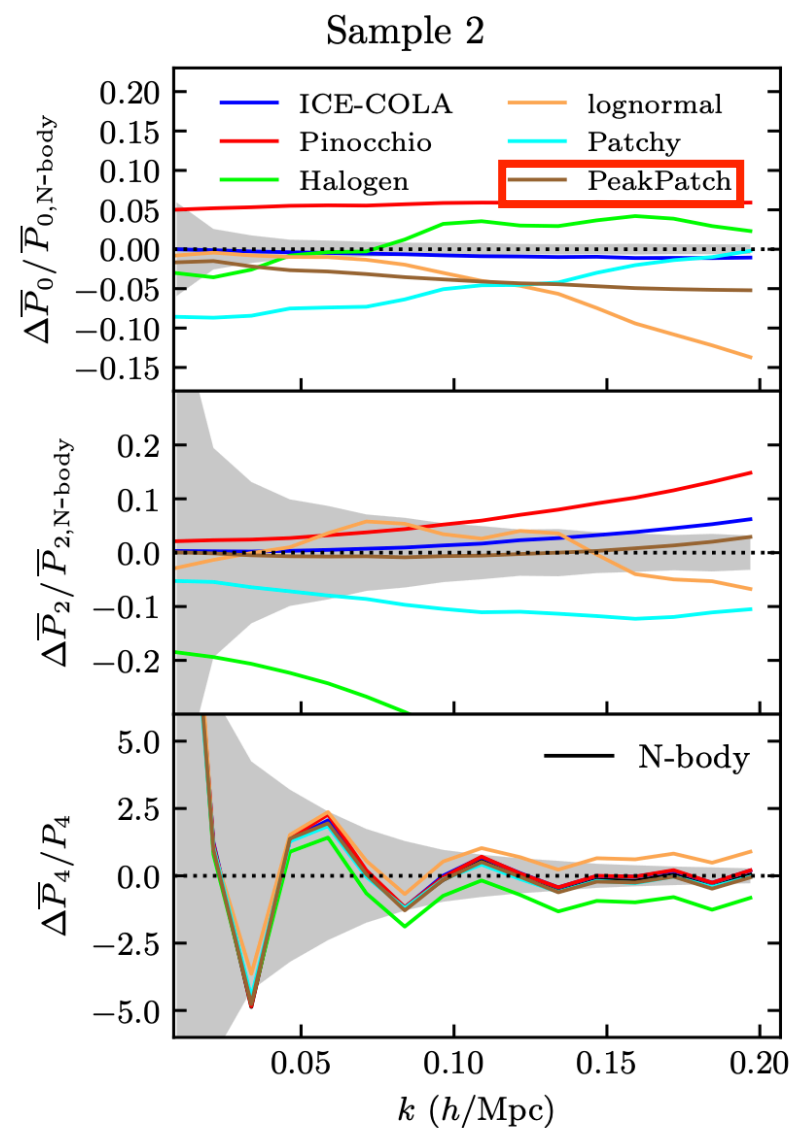
Comparing approximate methods for mock catalogues and covariance matrices

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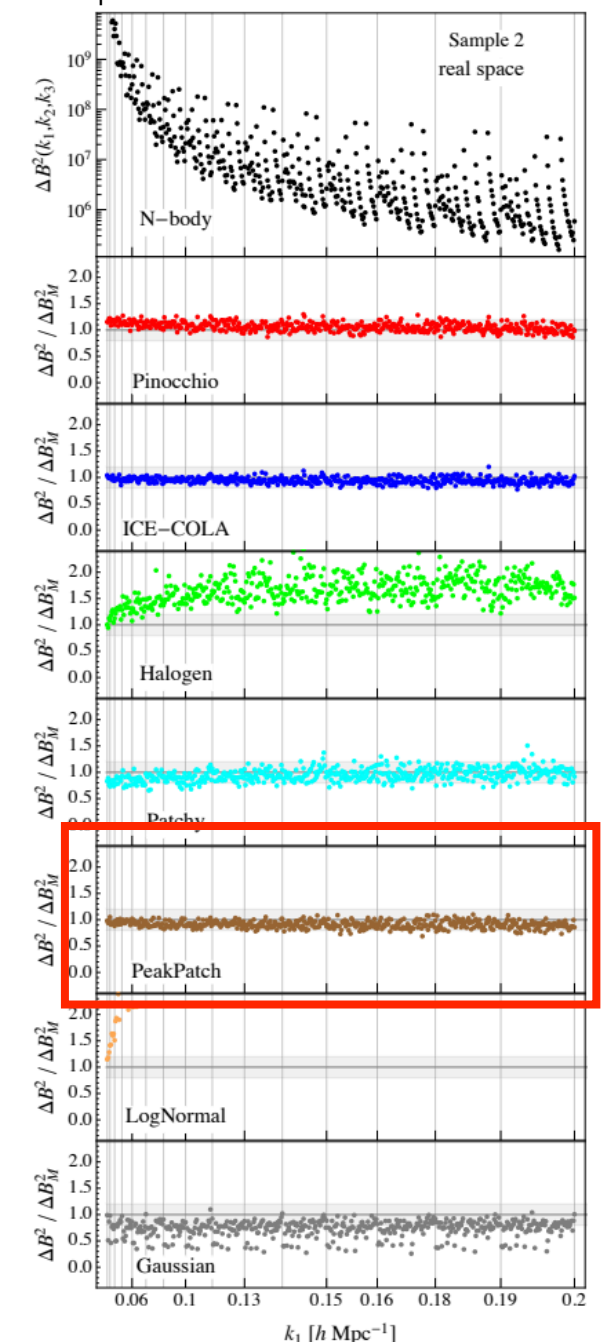
- covariance matrices produce similar cosmological parameter constraints



- Power spectrum multipoles see ~15% difference between methods



- Methods fit to reproduce power spectrum do not reproduce bispectrum



Constructing the Microwave Sky

Desired CMB Mock:

Fullsky out to $z \sim 5$

capable of resolving halos above $\sim 1 \times 10^{12} M_{\odot}$

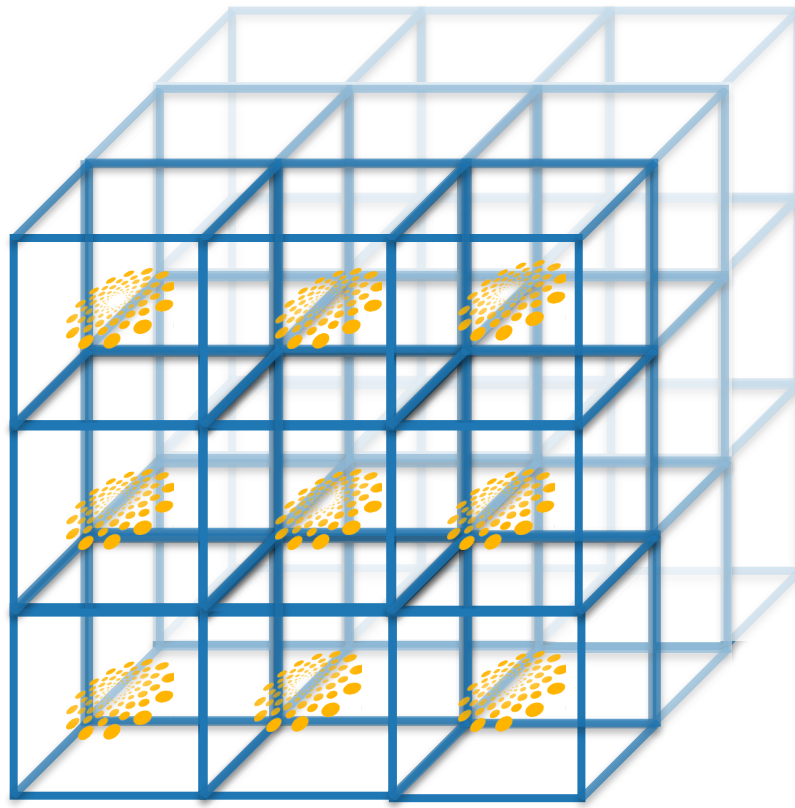
Requires:

$\sim 13,000^3$ particle simulation in a box size of ~ 16 Gpc.

~ 1 billion halos



Computational Approaches

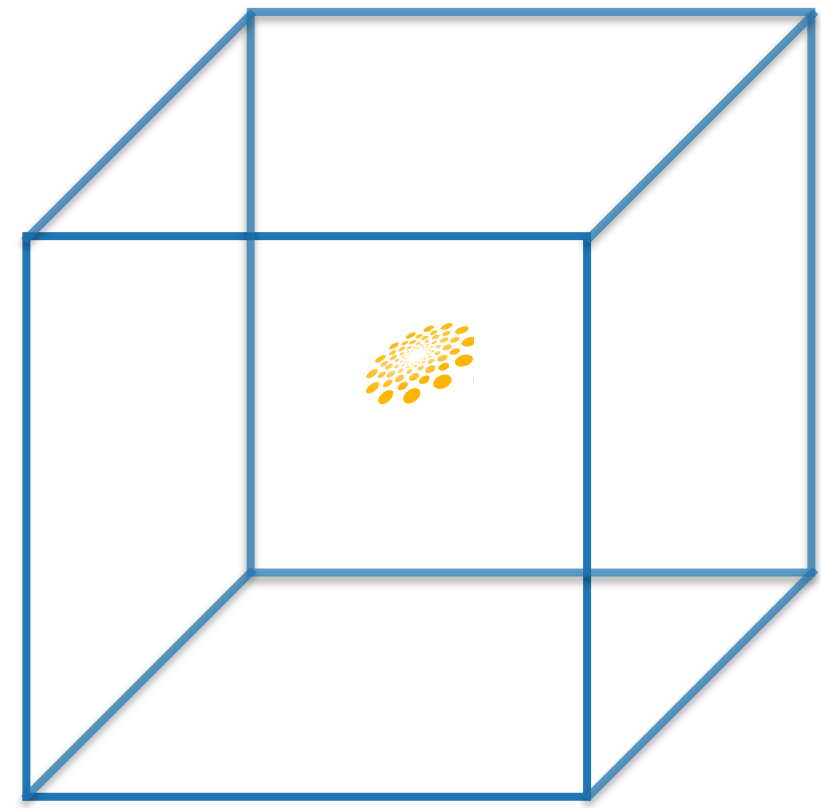


Small Box & Repeat

Repeats structures

Miss large scale density/velocity fluctuations
& rare objects in the universe

Computationally less demanding



Large Box

Includes large scale density/velocity fluctuations
& rare objects in the universe

Computationally more demanding



Dark Matter Lightcone

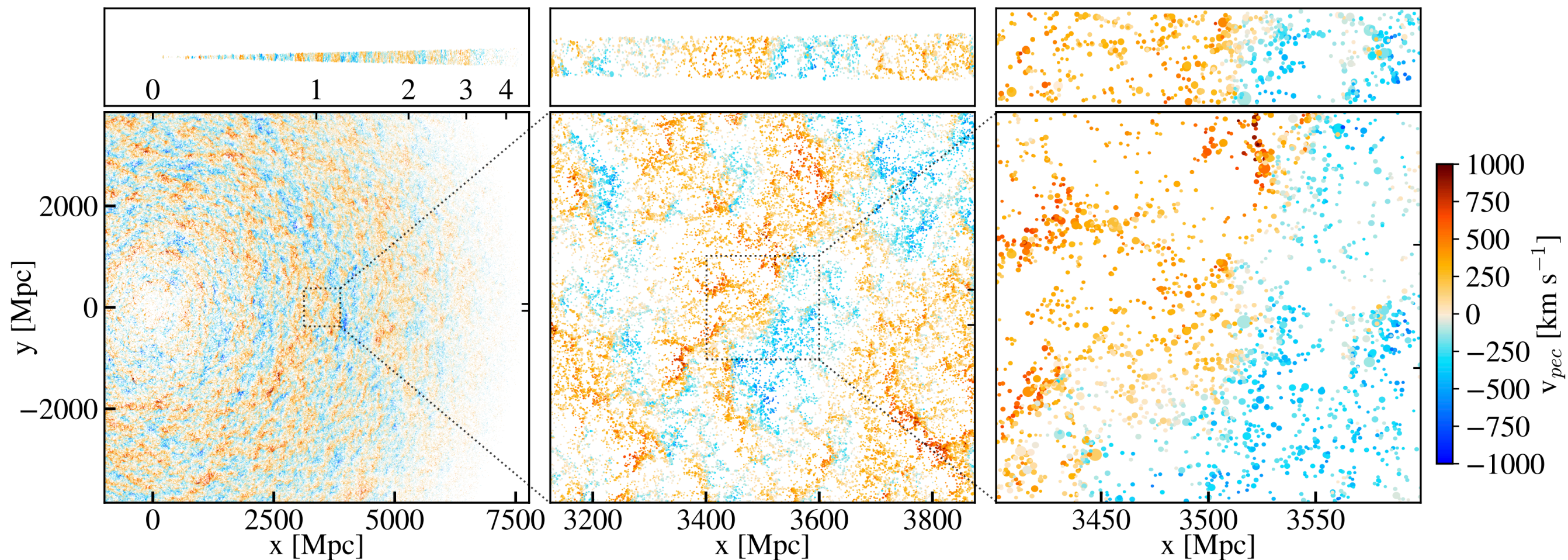
Simulation details:

Created using the **mass-Peak Patch** method [Stein, Alvarez, Bond - 1810.07727](#)

fullsky $z < 4.6$, 9×10^8 halos,

effective **12,288** particles, **1900 Gpc³** volume, from octants

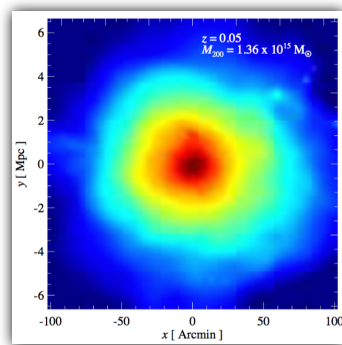
4336 CPU hours, **7.67 TB**



Dark Matter to Baryonic Observables

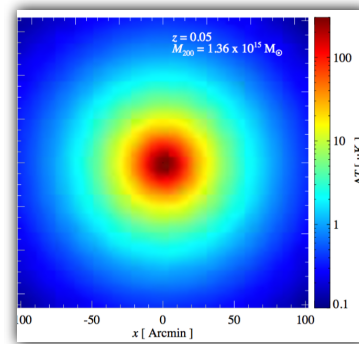
- Use spherical halo profiles fit to small box hydrodynamical simulations

Full Simulation

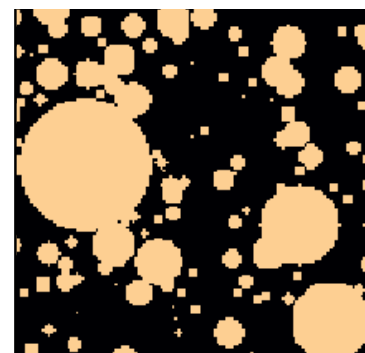


Hydro

Measure Fitting Functions

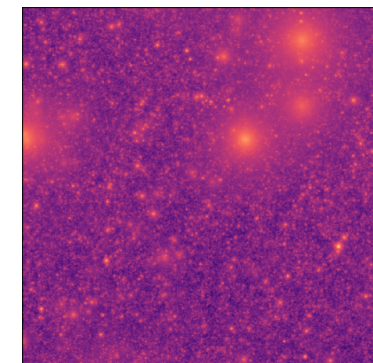


Fast Simulation



mass-Peak Patch

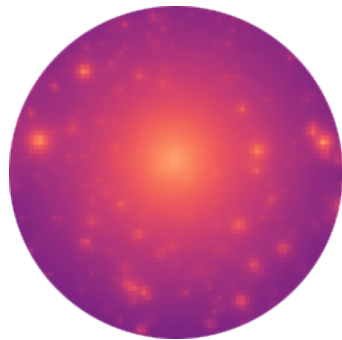
Mock Observation



Painting the Extragalactic Sky

thermal Sunyaev-Zel'dovich (tSZ)

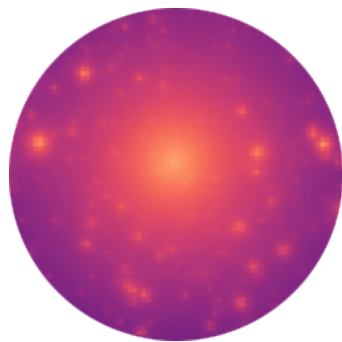
$$\propto \frac{k_B \sigma_T}{m_e c^2} \int d\chi (1+z)^{-1} P_{th}(\chi \hat{n})$$



Painting the Extragalactic Sky

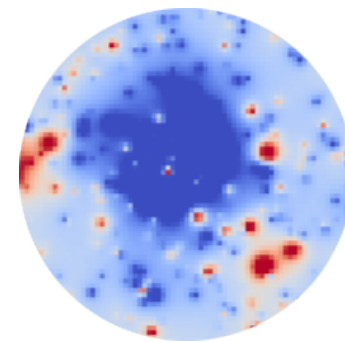
thermal Sunyaev-Zel'dovich (tSZ)

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kinetic Sunyaev-Zel'dovich (kSZ)

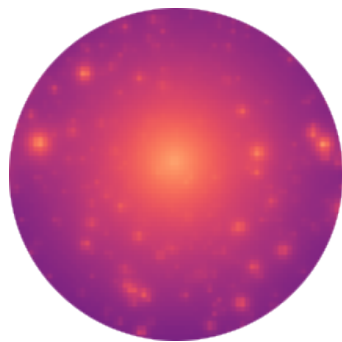
$$\propto \frac{\rho_{b,0} \sigma_T}{\mu_e m_p} \int d\chi (1+z)^2 \Delta_g(\chi \hat{n}) \mathbf{v}(\chi \hat{n}) \cdot \hat{n}$$



Painting the Extragalactic Sky

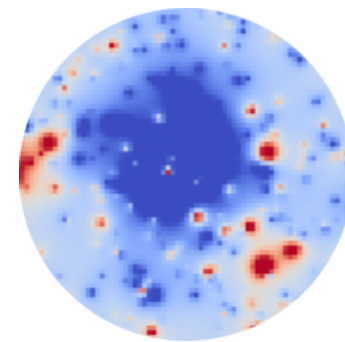
thermal Sunyaev-Zel'dovich (tSZ)

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$$\propto \frac{\rho_{b,0} \sigma_T}{\mu_e m_p} \int d\chi (1+z)^2 \Delta_g(\chi \hat{n}) \mathbf{v}(\chi \hat{n}) \cdot \hat{n}$$



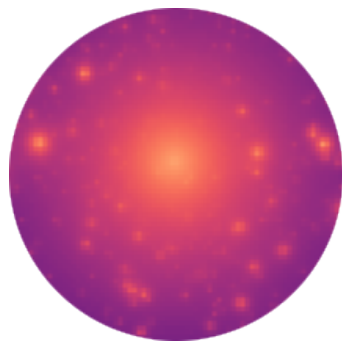
using gNFW profiles from
*Battaglia, Bond, Pfrommer,
Sievers (2012)*



Painting the Extragalactic Sky

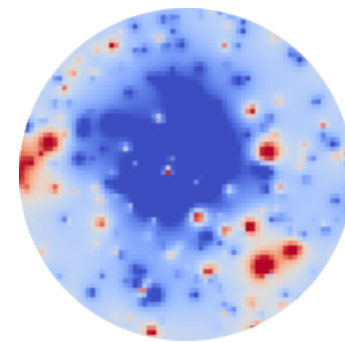
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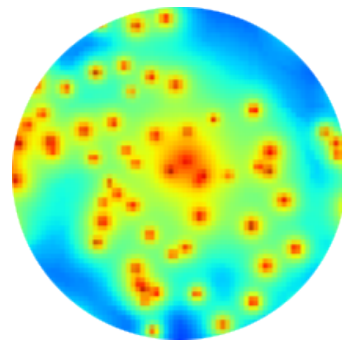
$$\propto \frac{\rho_{b,0} \sigma_T}{\mu_e m_p} \int d\chi (1+z)^2 \Delta_g(\chi \hat{n}) \mathbf{v}(\chi \hat{n}) \cdot \hat{n}$$



using gNFW profiles from
*Battaglia, Bond, Pfrommer,
Sievers (2012)*

Weak Lensing

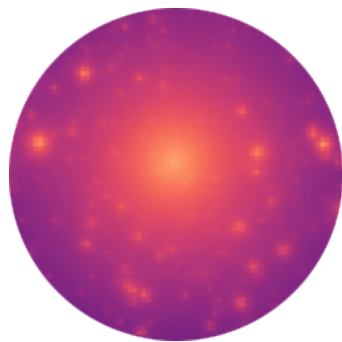
$$= \int d\chi W_{\kappa}(\chi) \delta(\chi \hat{n})$$



Painting the Extragalactic Sky

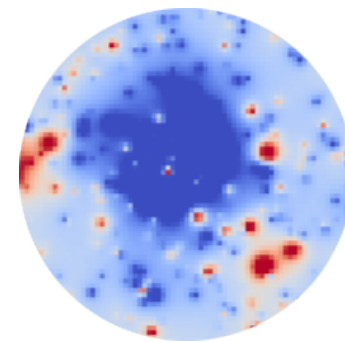
thermal Sunyaev-Zel'dovich (tSZ)

$$\propto \frac{k_B \sigma_T}{m_e c^2} \int d\chi (1+z)^{-1} P_{th}(\chi \hat{n})$$



kinetic Sunyaev-Zel'dovich (kSZ)

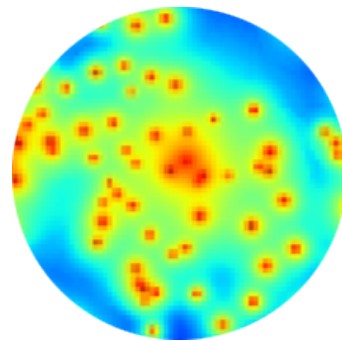
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using gNFW profiles from
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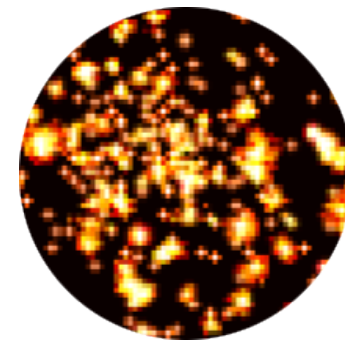
Weak Lensing

$$= \int d\chi W_\kappa(\chi) \delta(\chi \hat{n})$$



Cosmic Infrared Background (CIB)

$$L_{(1+z)\nu}(M, z) = L_0 \Phi(z) \Sigma(M, z) \Theta[(1+z)\nu, T_d(z)]$$

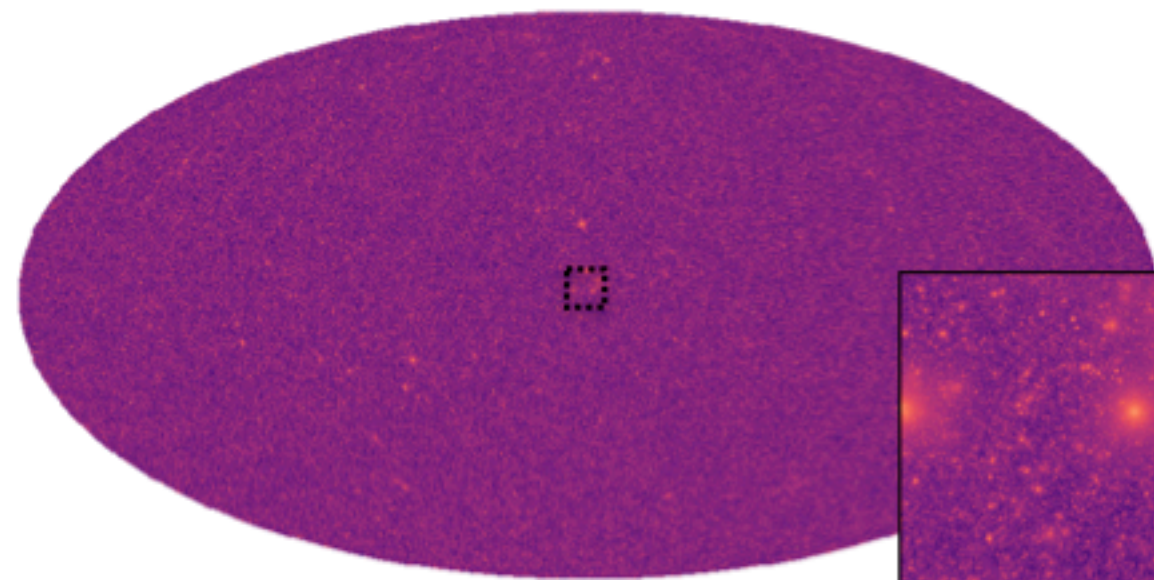


$\Phi(z)$: normalization of the L-M relation
 $\Sigma(M, z)$: dependence of the luminosity on halo mass
 $\Theta[(1+z)\nu, T_d(z)]$: spectral energy distribution



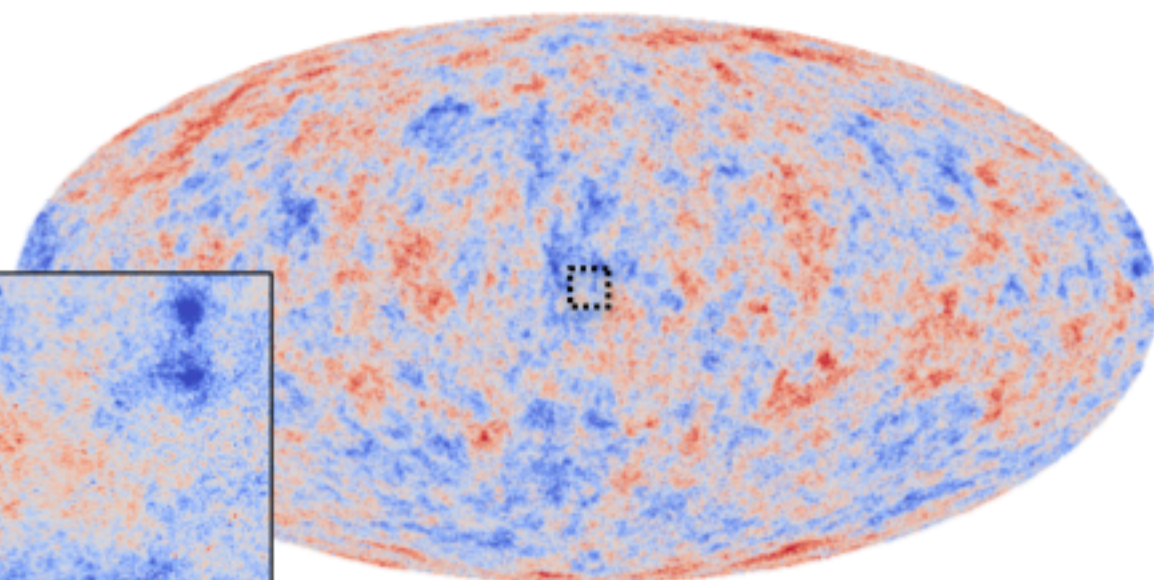
The Websky Extragalactic Maps

tSZ

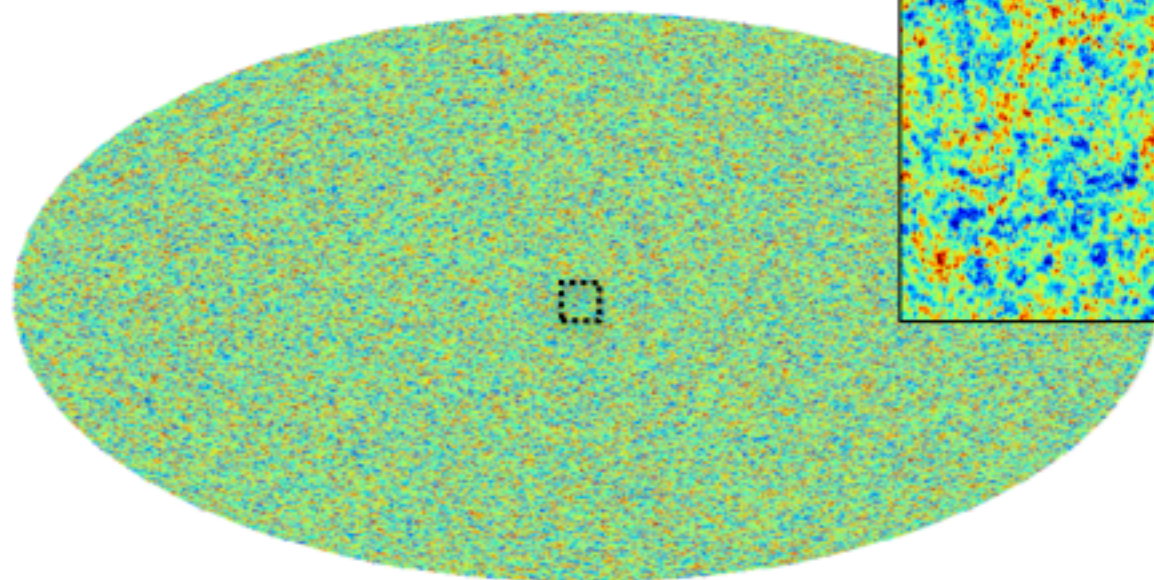


-7.2 -6.4 -5.6 -4.8 -4.0
 \log_{10} Compton-y

kSZ

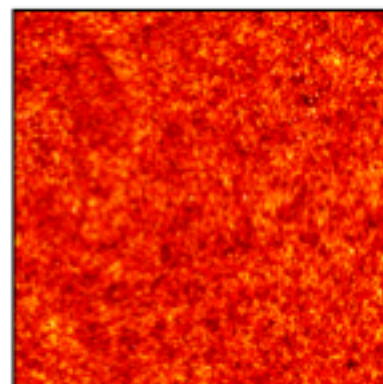
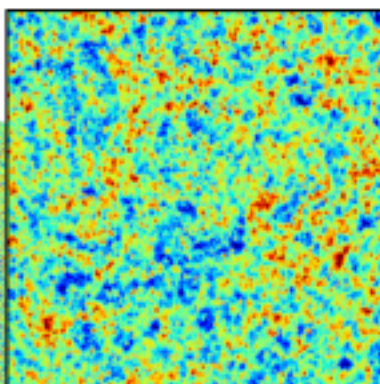
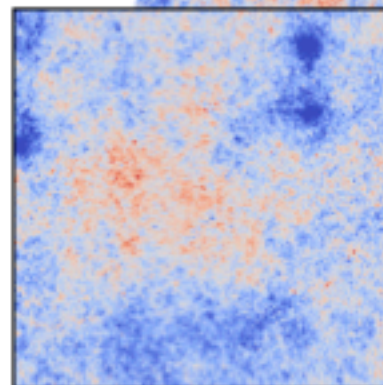
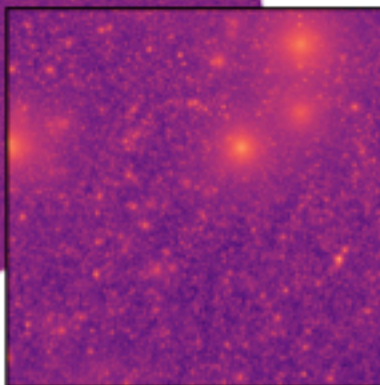


-8 -4 0 4 8
 $\Delta T_{\text{kSZ}} [\mu\text{K}]$

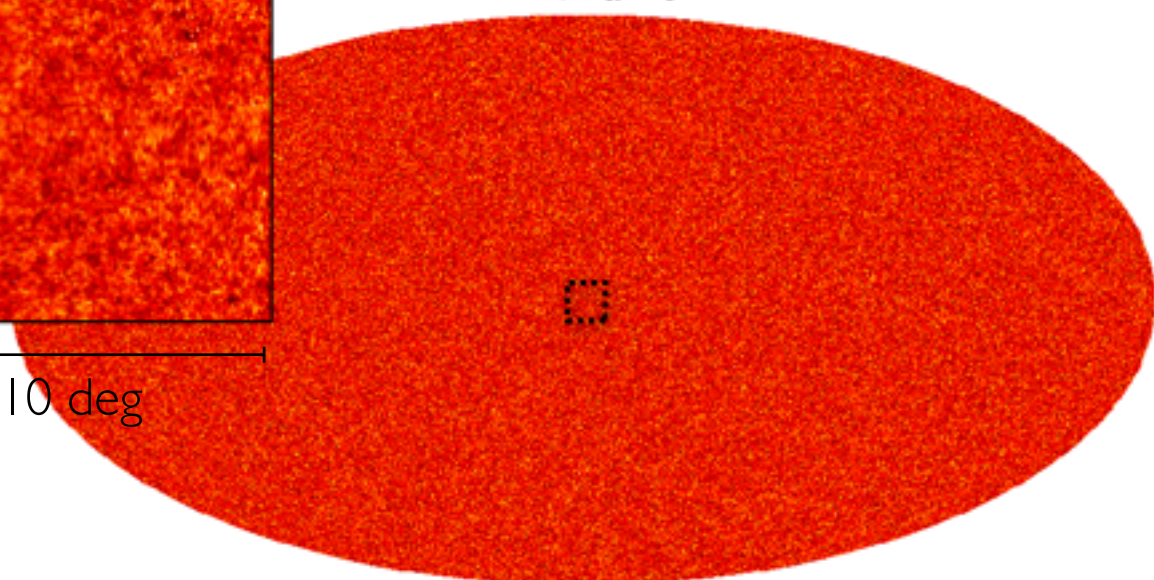


-0.10 -0.05 0.00 0.05 0.10
 κ

weak lensing



10 deg

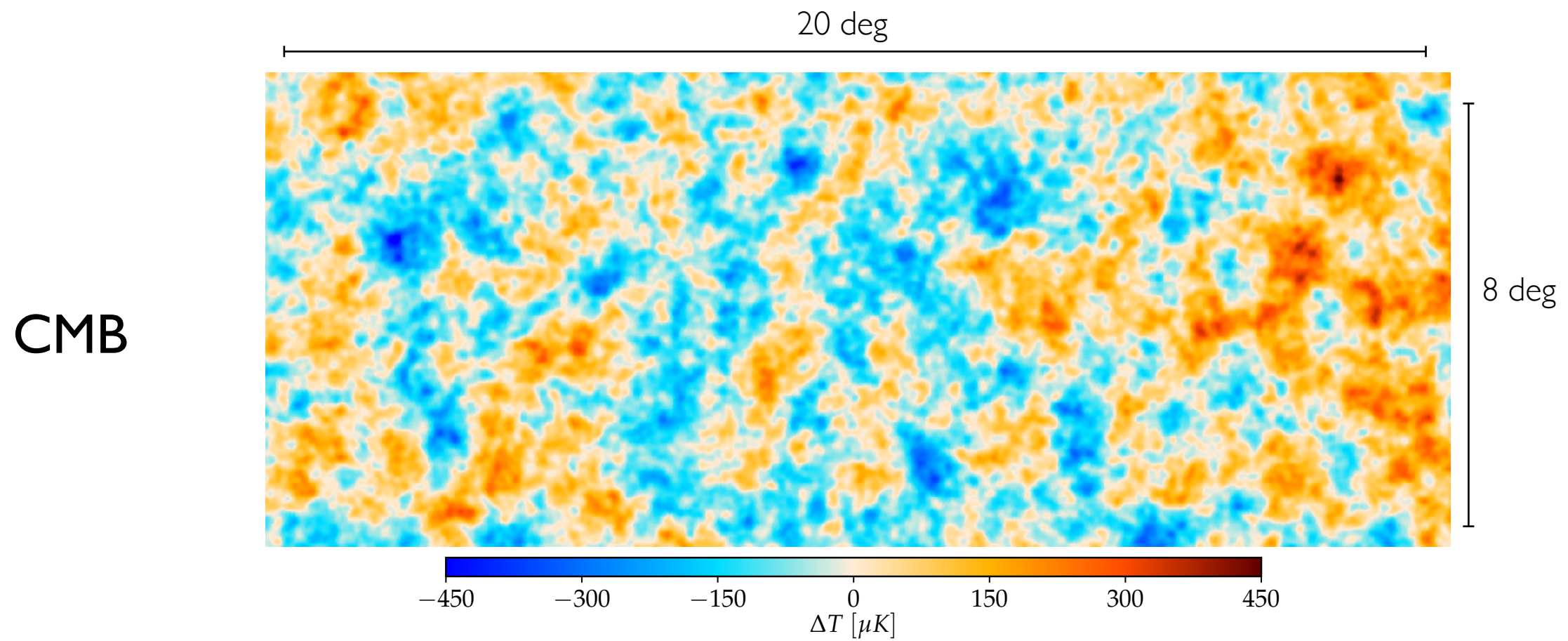


-0.15 0.00 0.15 0.30
 $\Delta I_{\nu}^{545\text{GHz}} [\text{MJy/sr}]$

CIB

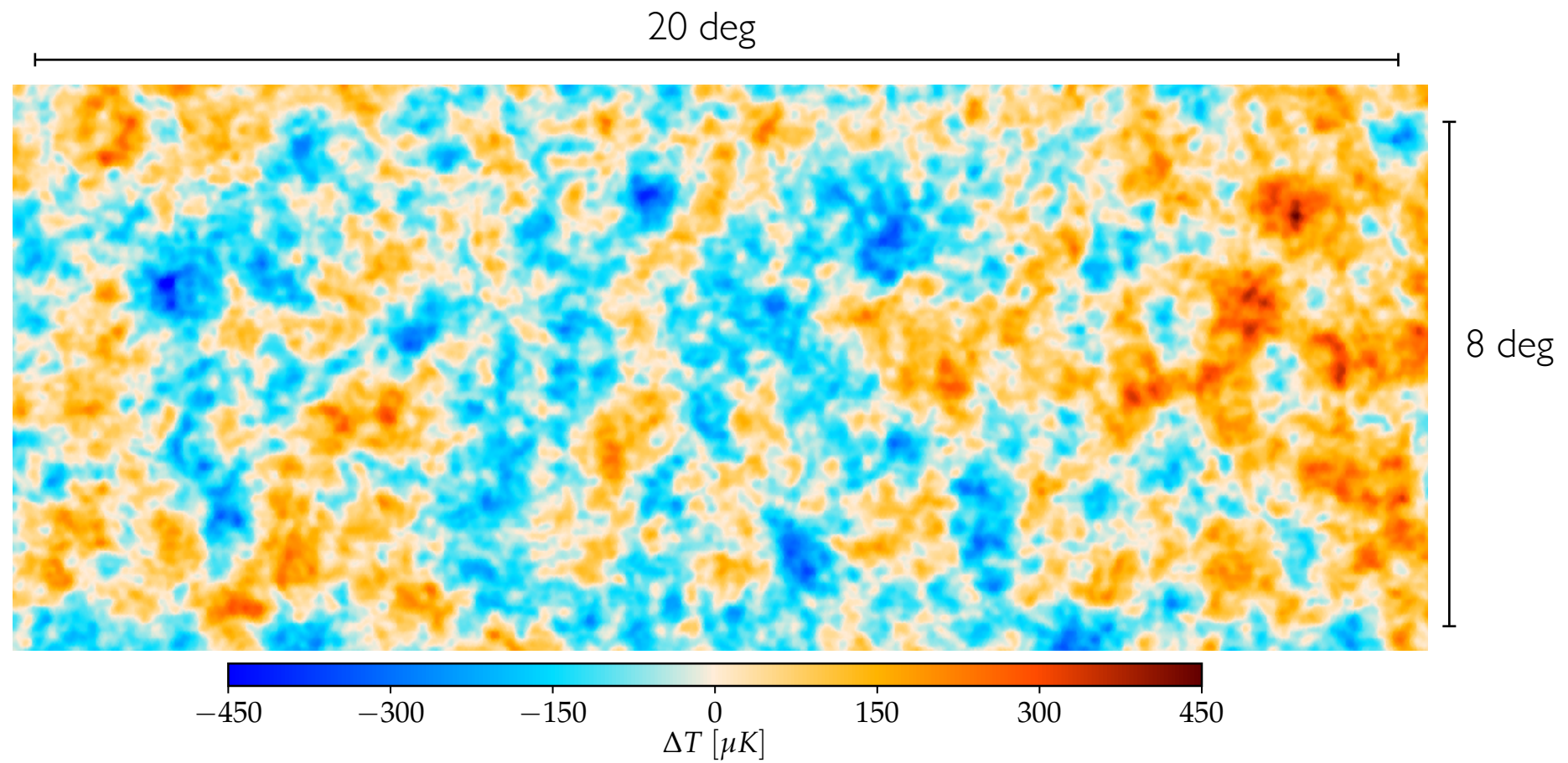


Extragalactic Foregrounds

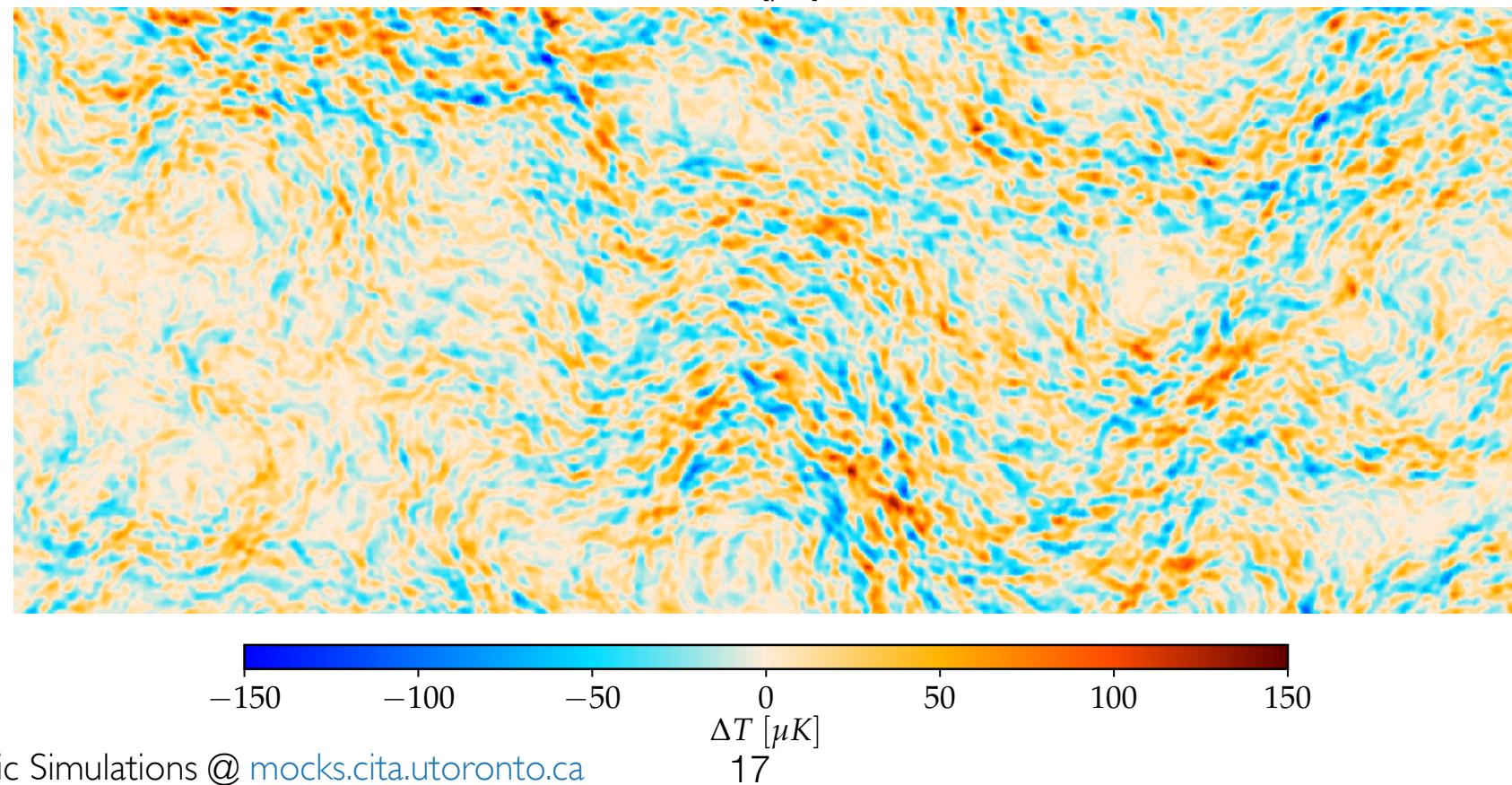


Extragalactic Foregrounds

Observed
CMB

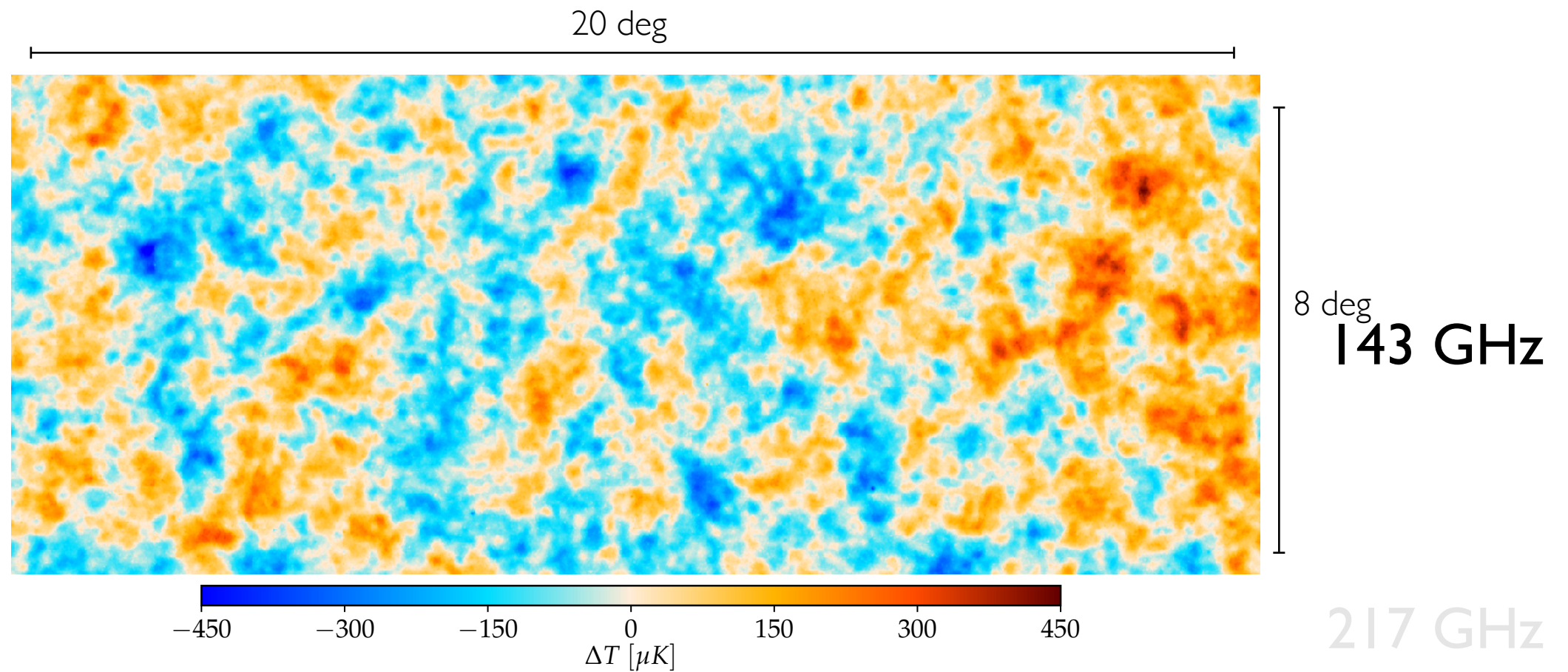


Lensing

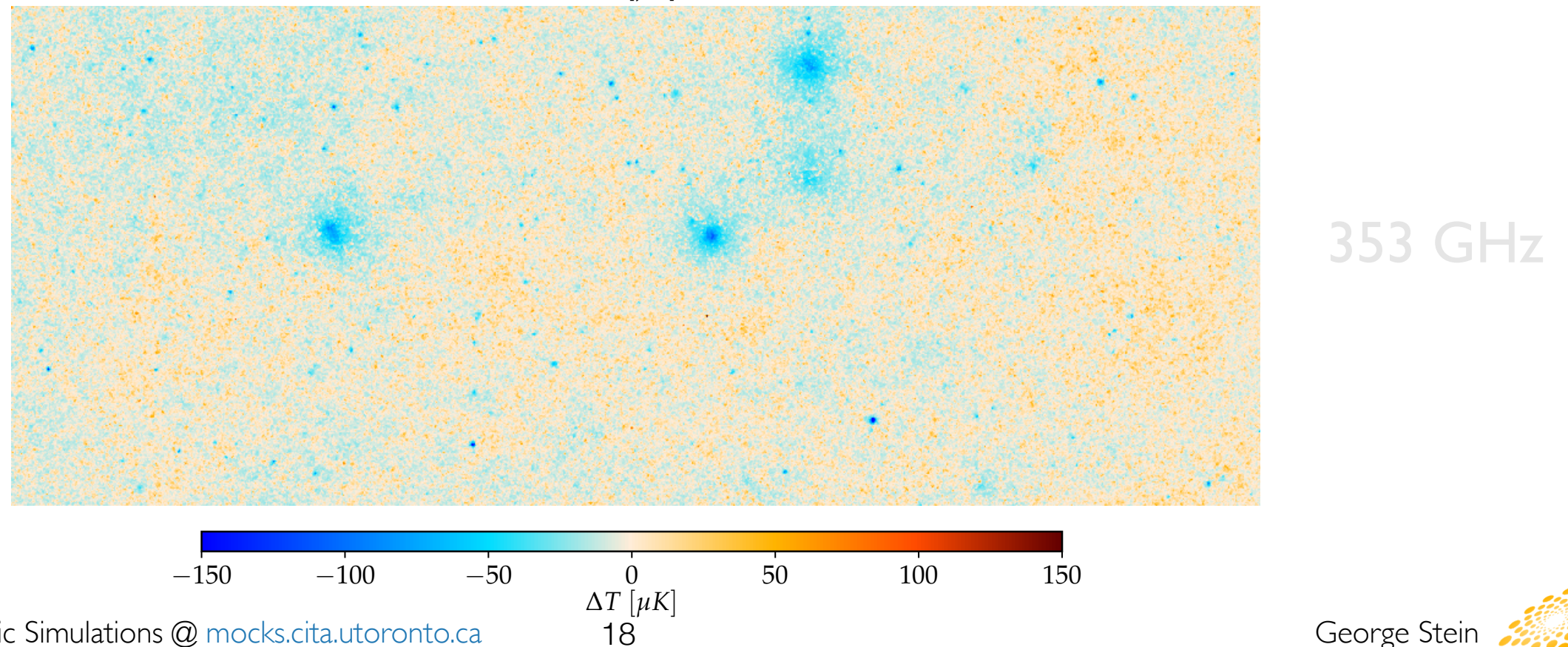


Extragalactic Foregrounds

Observed
CMB

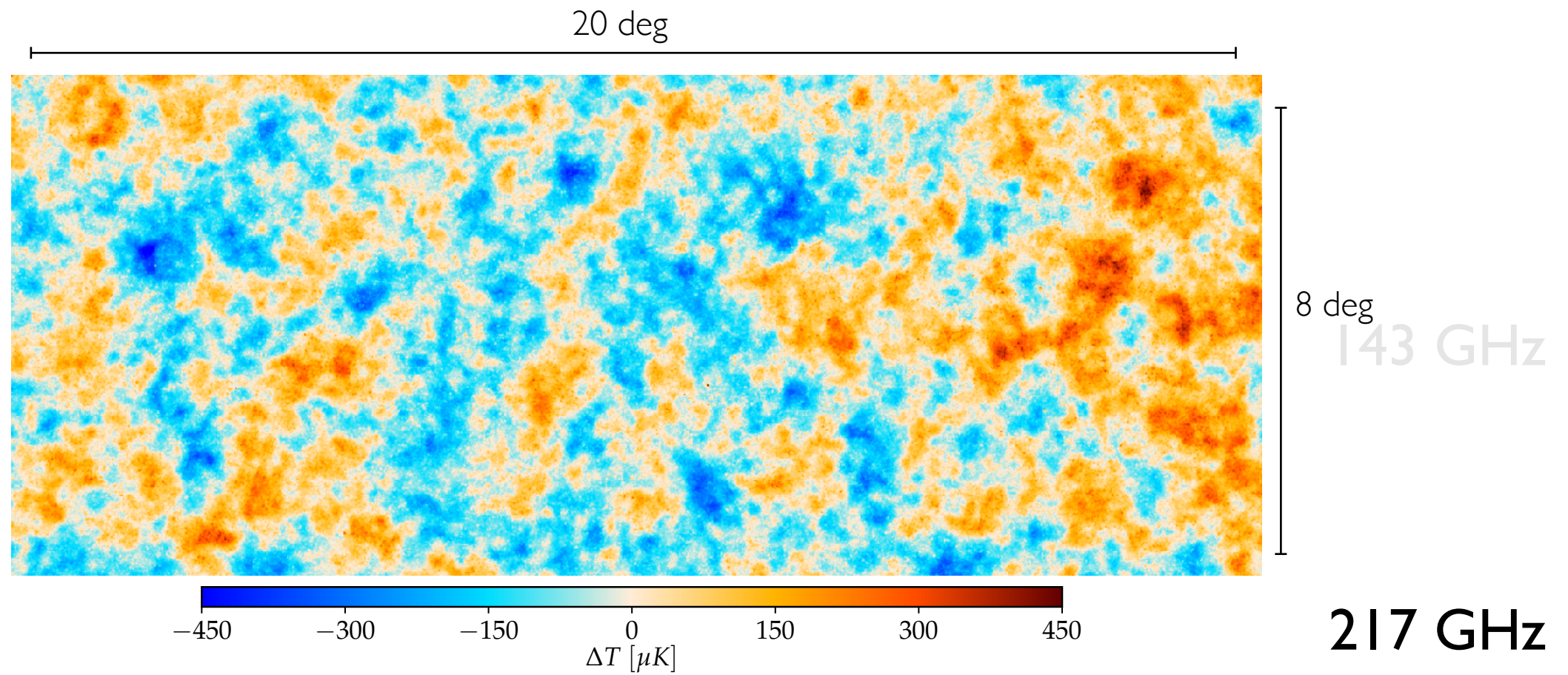


tSZ + kSZ
+ CIB

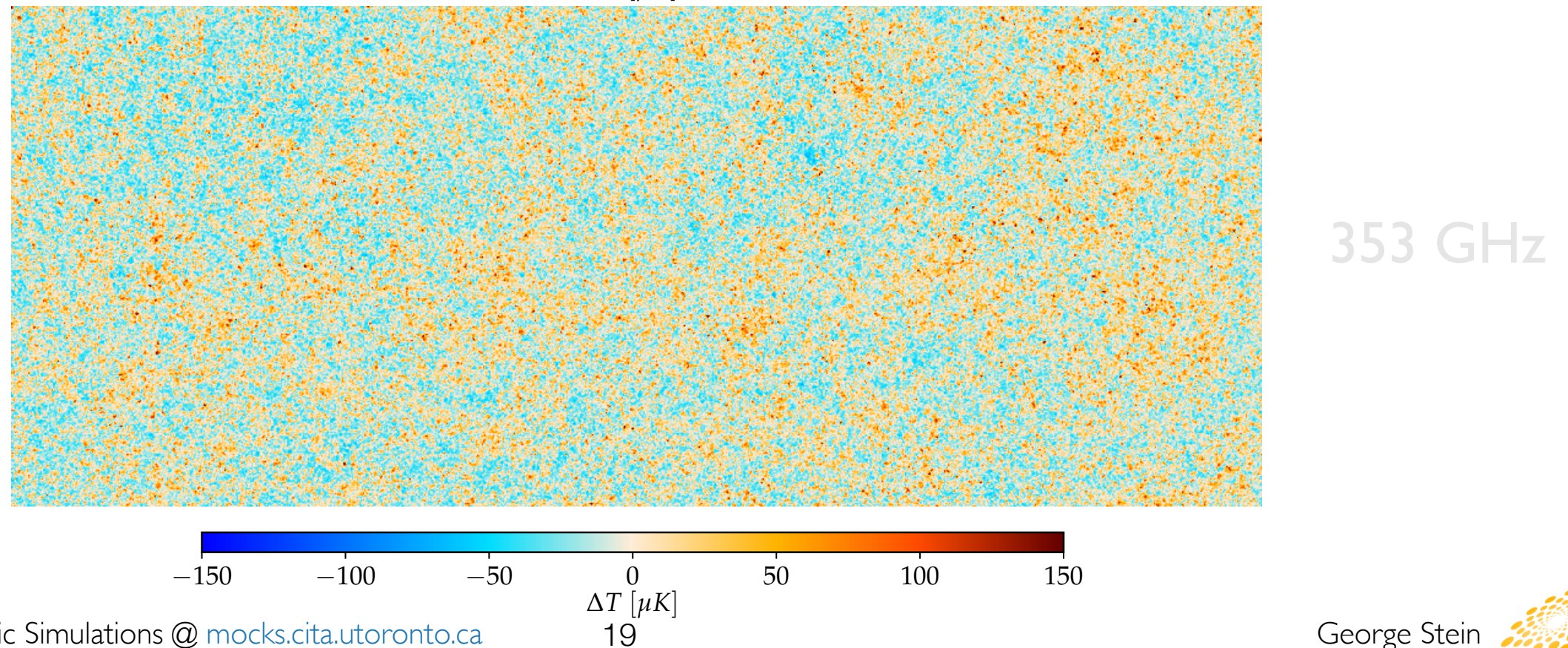


Extragalactic Foregrounds

Observed
CMB

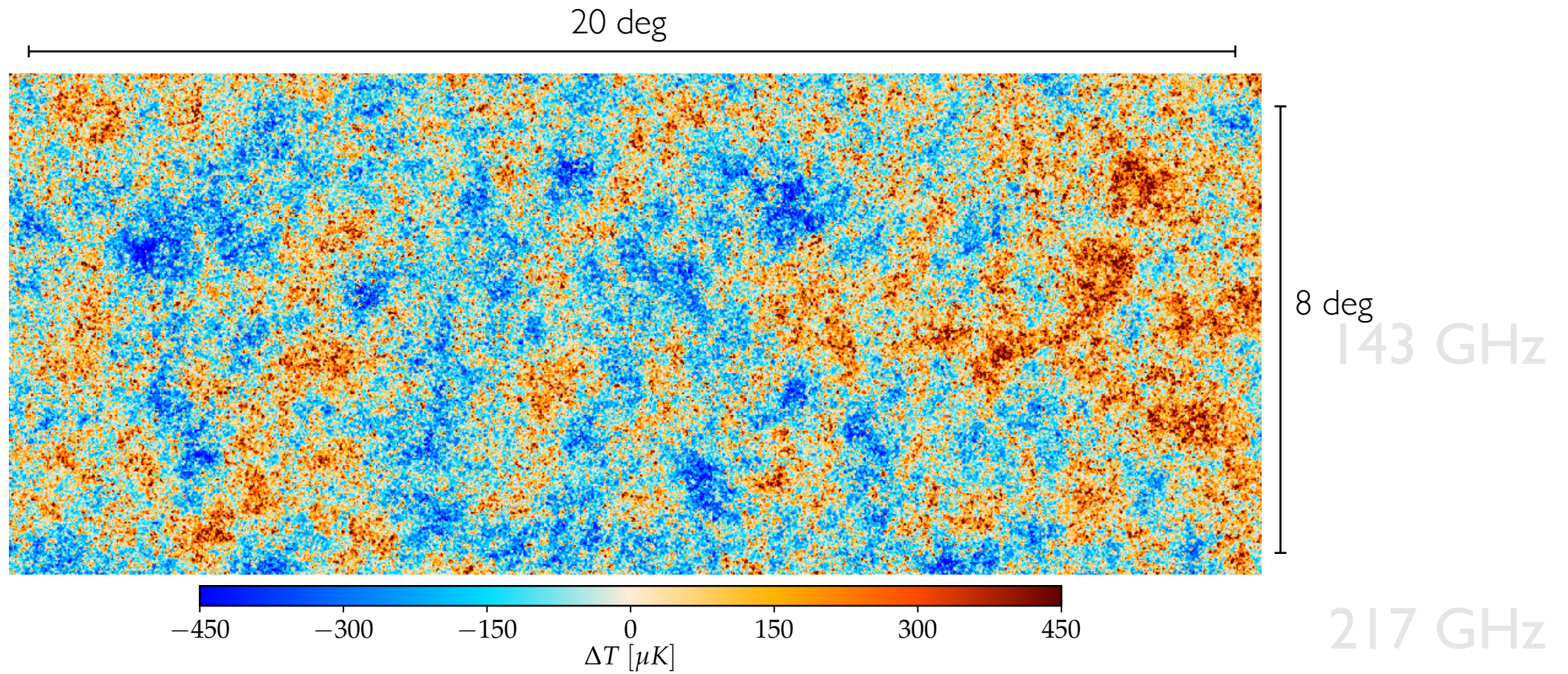


tSZ + kSZ
+ CIB

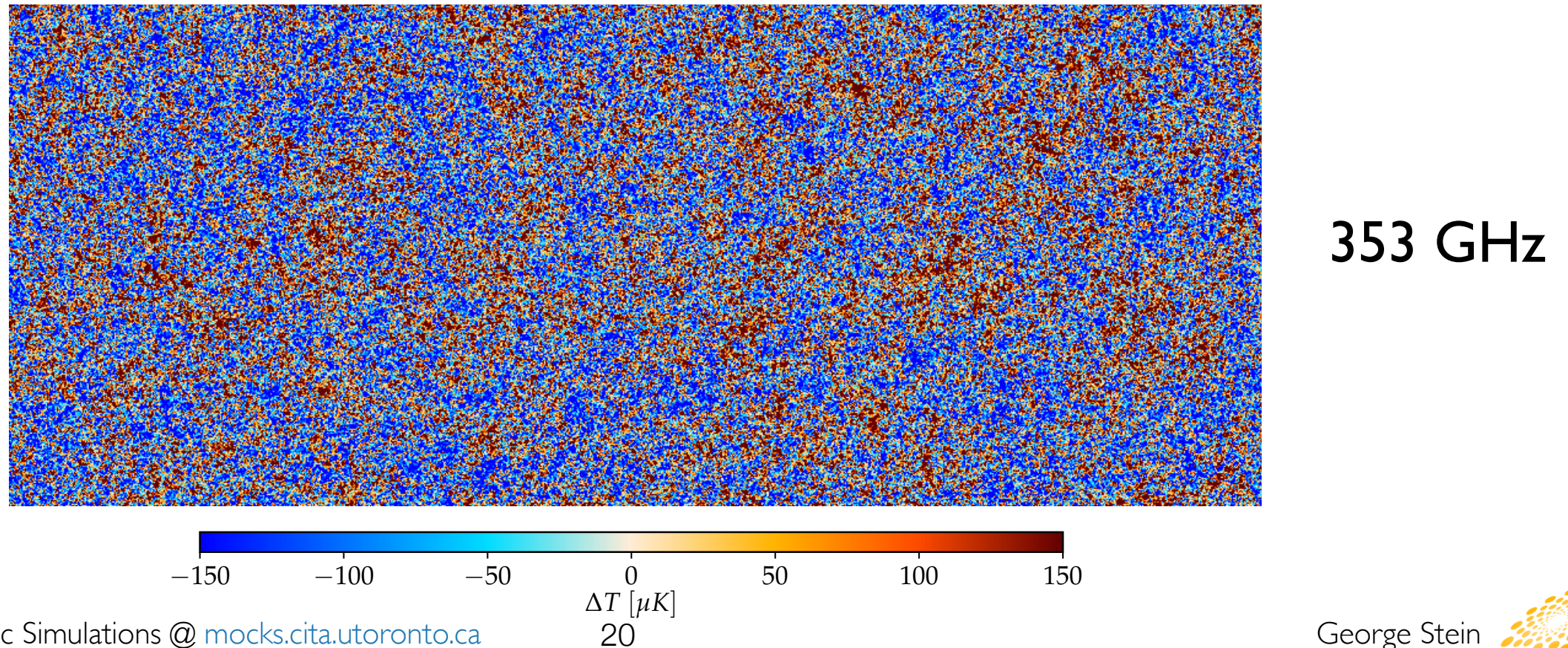


Extragalactic Foregrounds

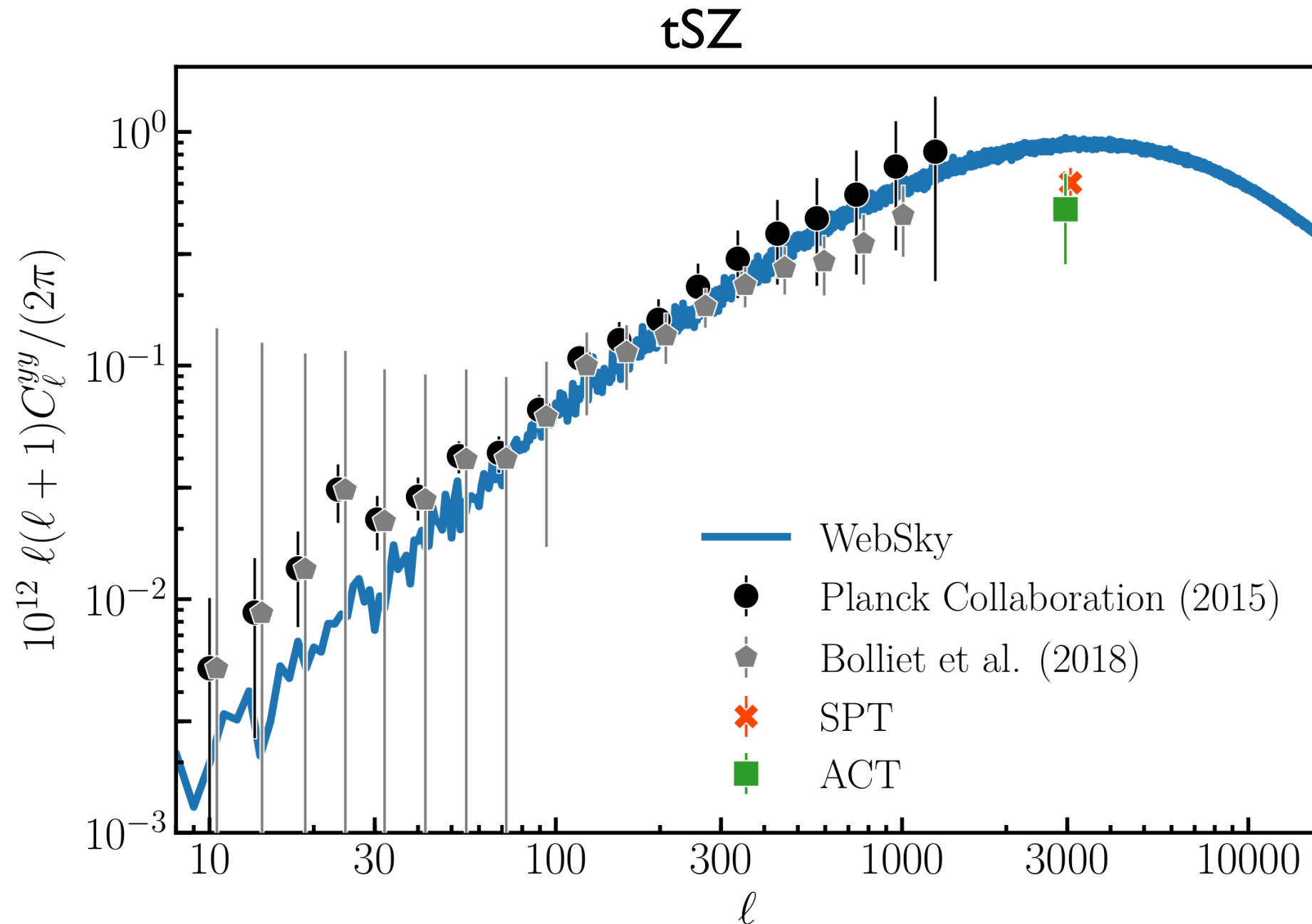
Observed
CMB



tSZ + kSZ
+ CIB



Validations: tSZ



- Matches well with Planck
- ~30% disagreement with ACT and SPT
 - small-scale suppression in the tSZ power?
 - systematic effects in the SPT and ACT measurements?

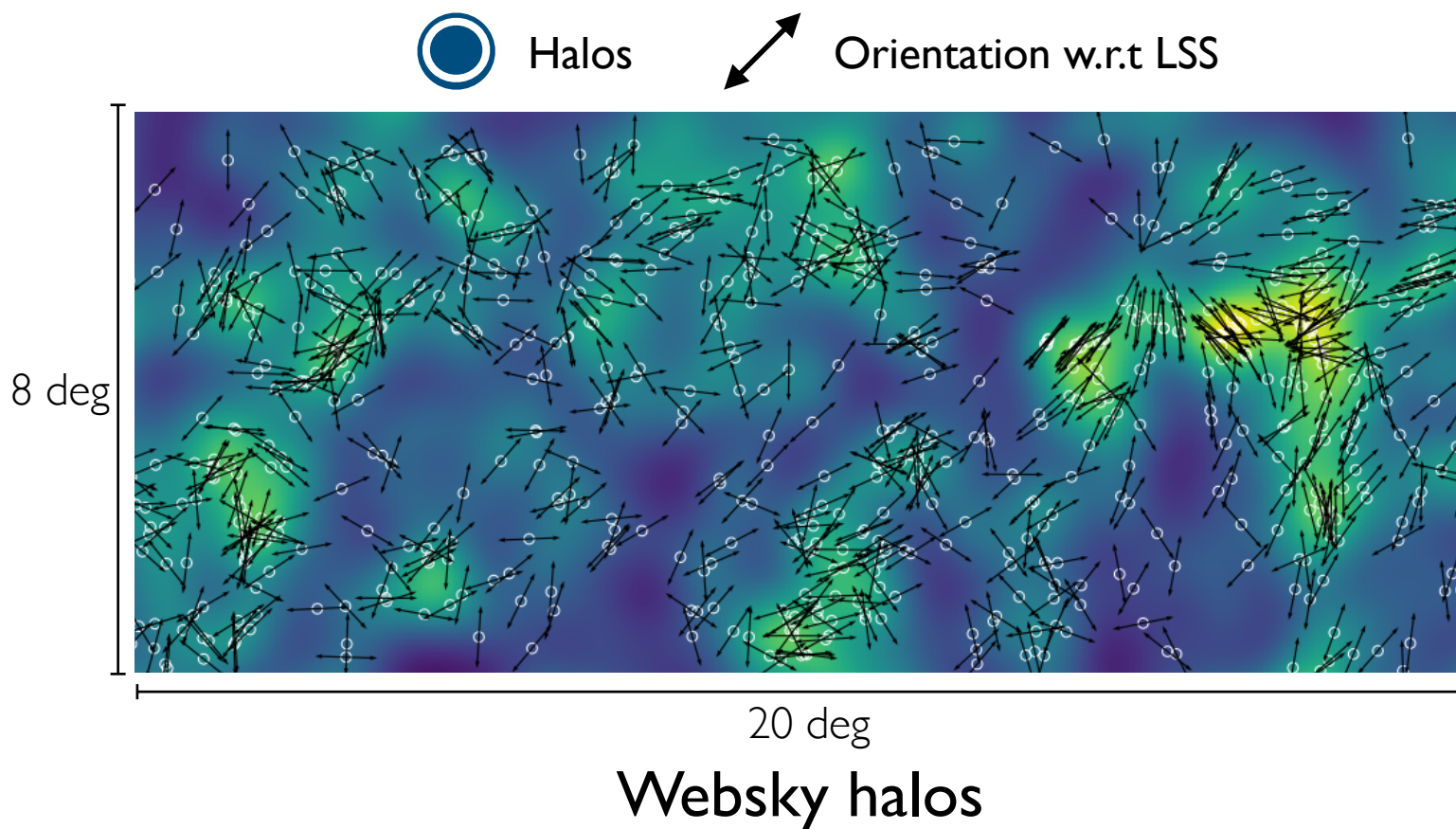


Cluster applications: tSZ stacking on DES Clusters

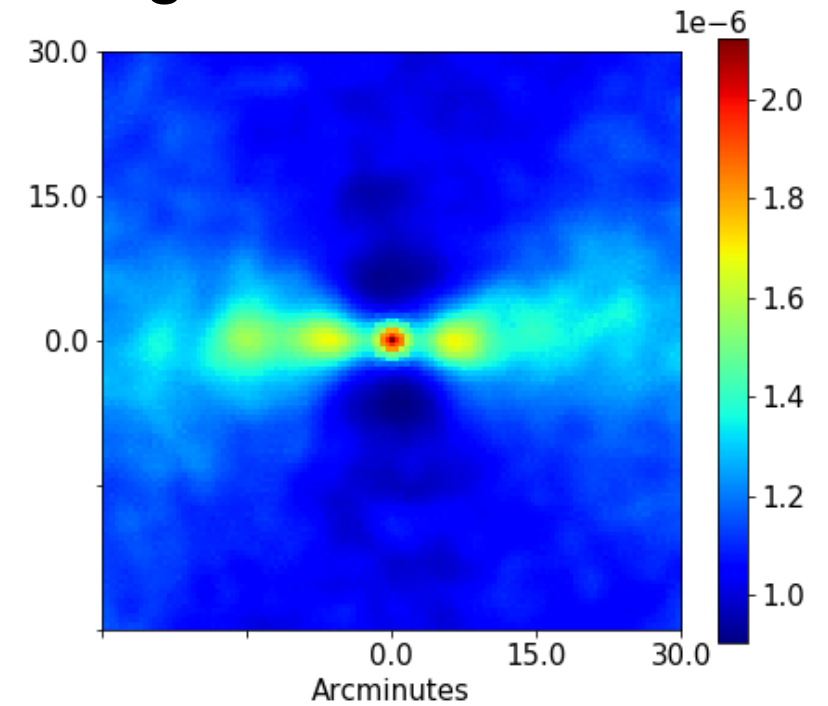
Preliminary



Martine Lokken, Mat Madhavacheril, Renee Hlozek, ...

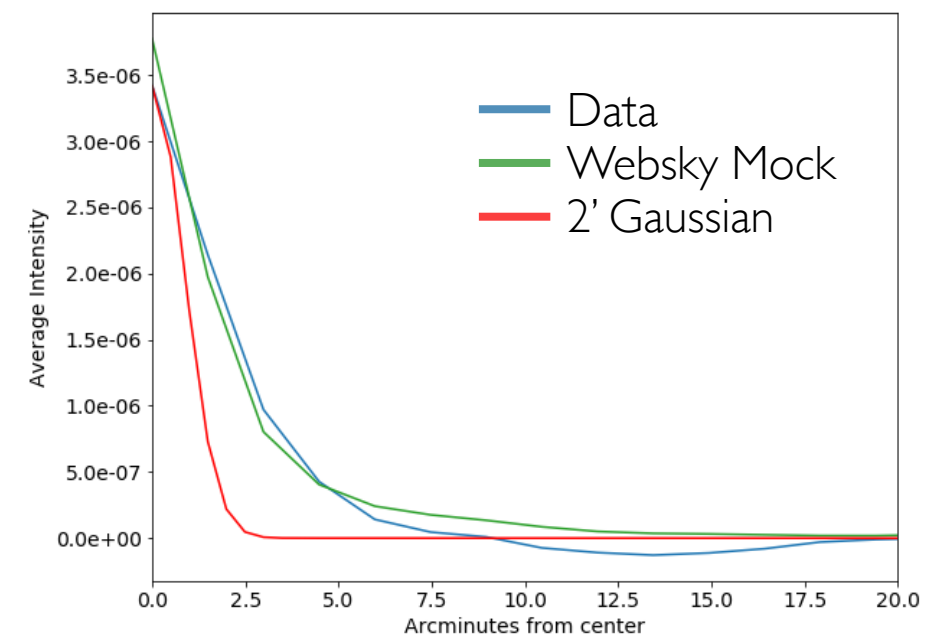


tSZ signal of Oriented Stack

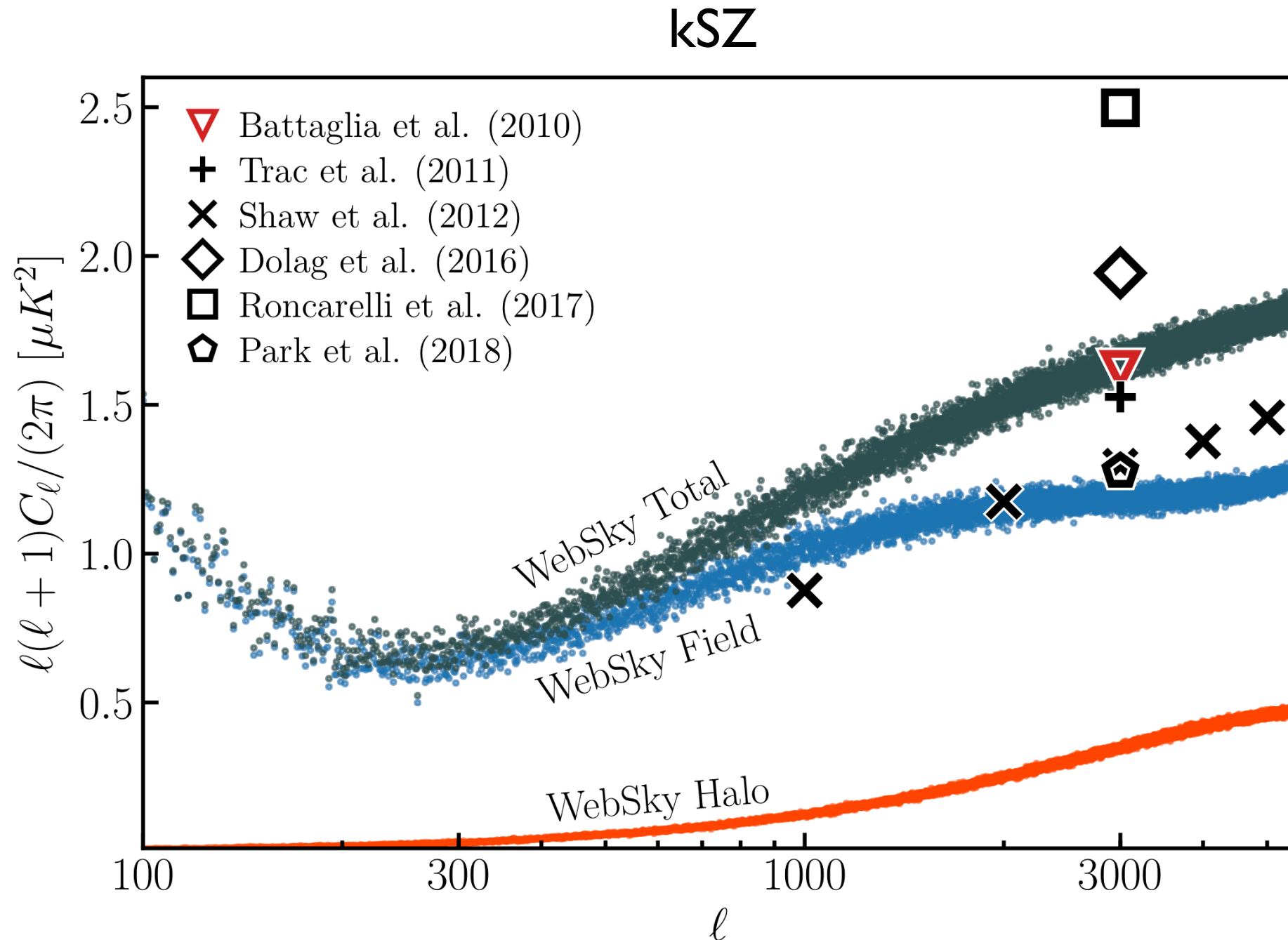


Radial profile compared to data

$20 < \lambda < 1000$, $0.10 < z < 0.34$



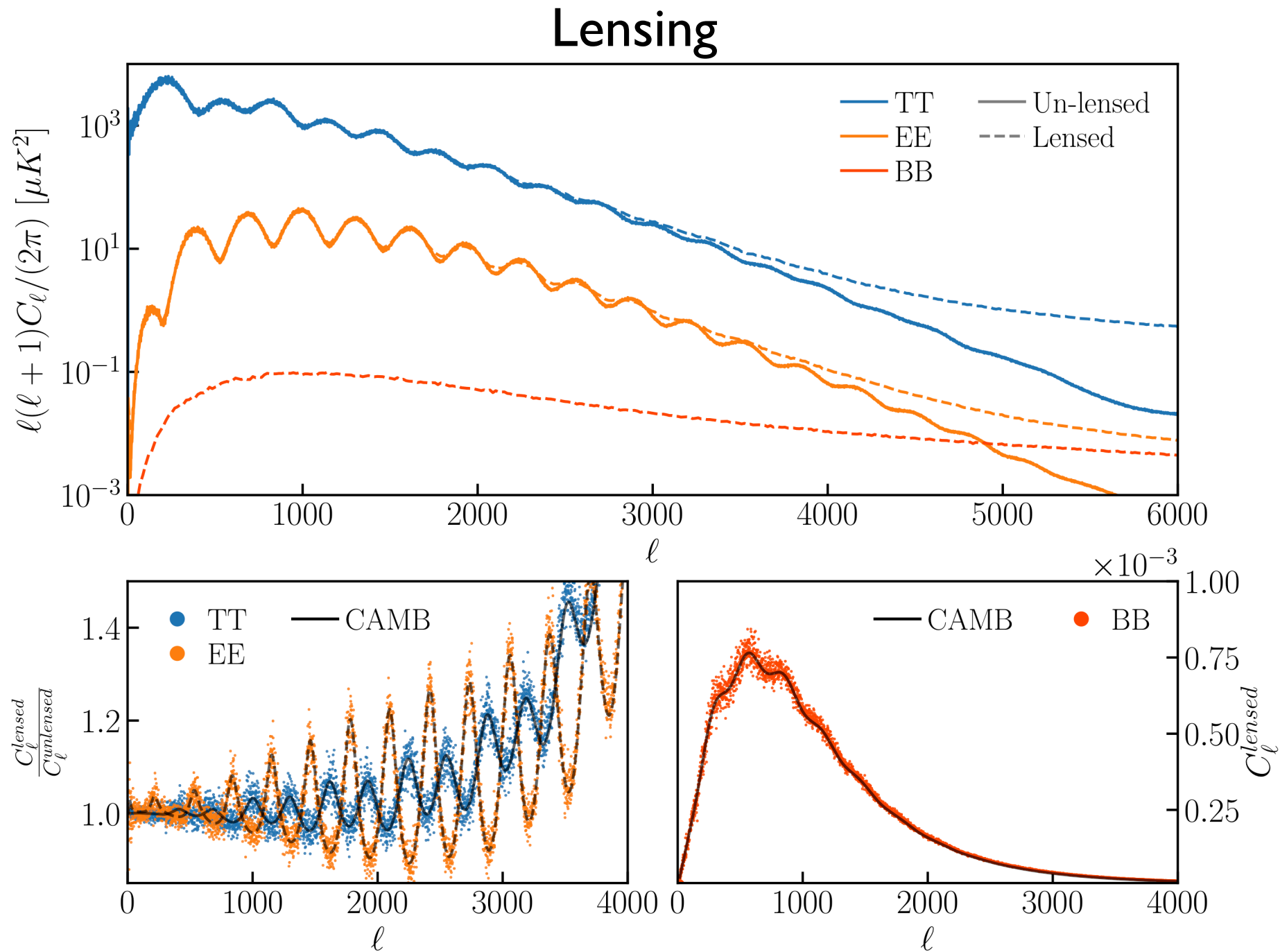
Validations: kSZ



- Agrees with various hydrodynamical studies
- Includes late-time contribution only. Early time kSZ can be added independently



Validations: Weak Lensing

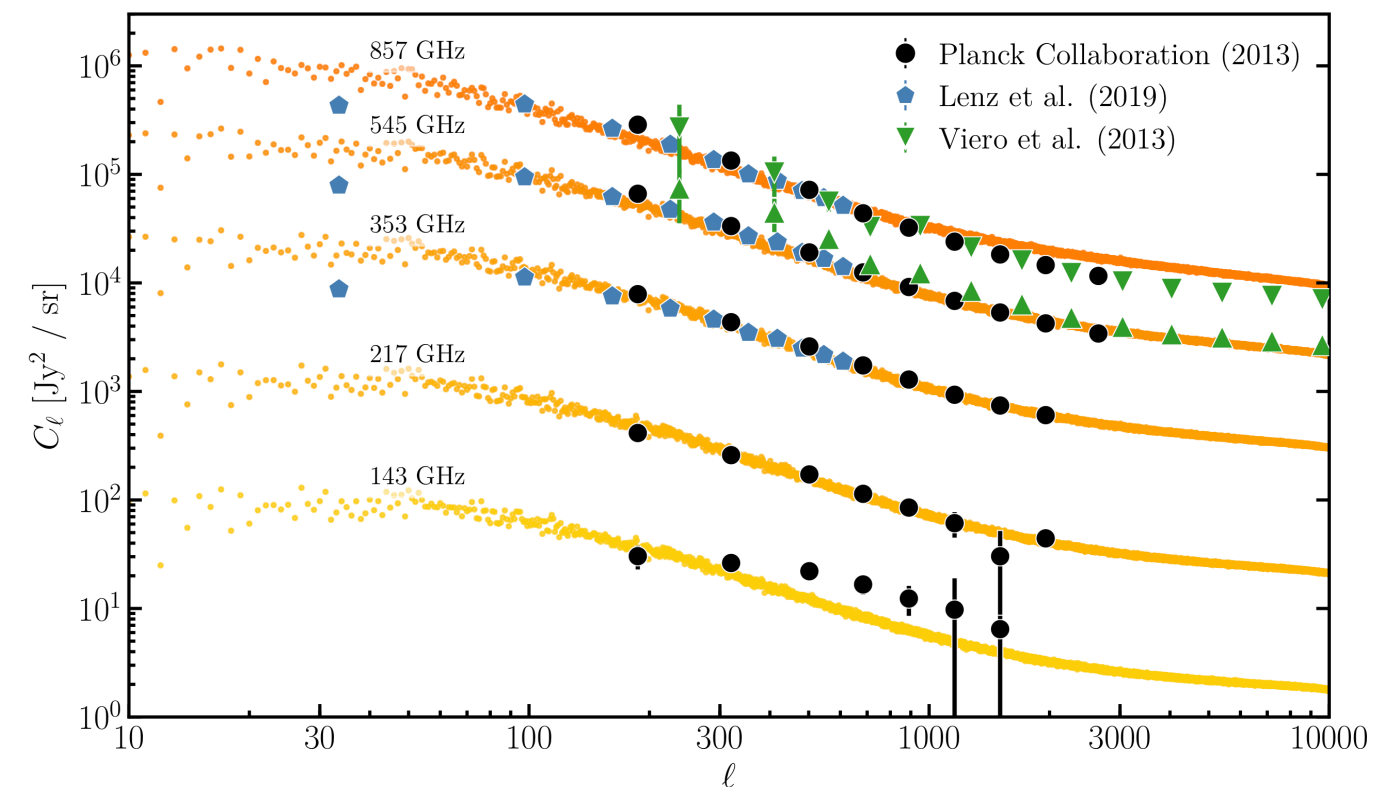


- Peak Smearing well reproduced
- $r=0$ in input CMB - feel free to lens your own with the convergence map



Validations: CIB

CIB Powerspectra

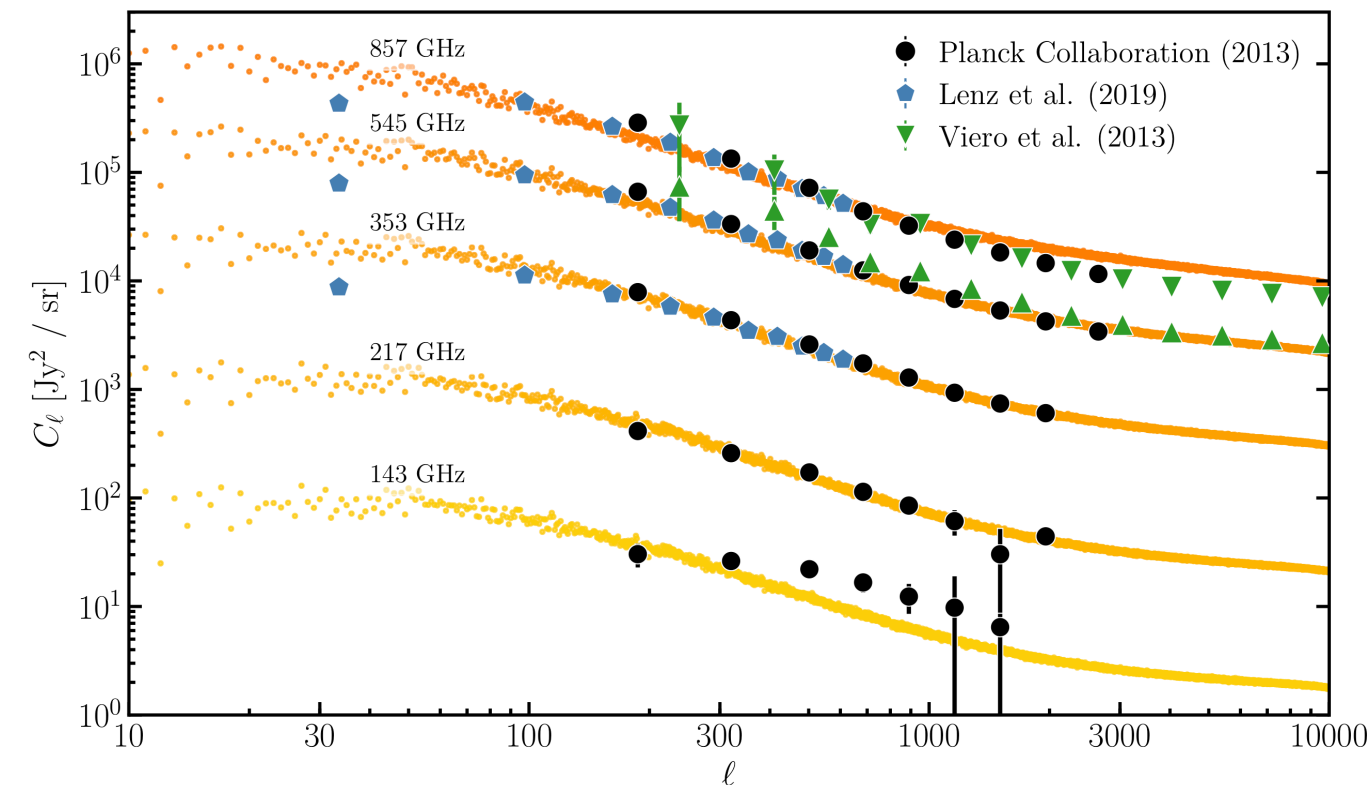


- Slight excess in small scale power at 857 GHz
 - $M_{h,\min} \sim 1 \times 10^{12} M_\odot$



Validations: CIB

CIB Powerspectra



- Slight excess in small scale power at 857 GHz
 - $M_{h,min} \sim 1 \times 10^{12} M_{\odot}$

CIB Decoherence

		857	545	353	217
857	<i>Websky</i>	1	0.933 ± 0.017	0.882 ± 0.021	0.838 ± 0.026
	<i>Planck</i>	1	0.949 ± 0.005	0.911 ± 0.003	0.85 ± 0.05
	<i>Lenz et al.</i>	1	0.96 ± 0.01	0.91 ± 0.01	0.85 ± 0.05
545	<i>Websky</i>	...	1	0.960 ± 0.014	0.935 ± 0.018
	<i>Planck</i>	...	1	0.983 ± 0.007	0.90 ± 0.05
	<i>Lenz et al.</i>	...	1	0.98 ± 0.01	
353	<i>Websky</i>	1	0.968 ± 0.014
	<i>Planck</i>	1	0.91 ± 0.05
	<i>Lenz et al.</i>	1	

Table 1. Frequency decoherence of the CIB measured by averaging $C_{\ell}^{vv'}/(C_{\ell}^{vv}C_{\ell}^{v'v'})^{1/2}$ over the range $150 < \ell < 1000$. Error bars correspond to the standard deviation in this range. We include the Planck measurements of [16] and the Lenz et al. measurements of [100].

- Frequency dependence **not** just an amplitude scaling

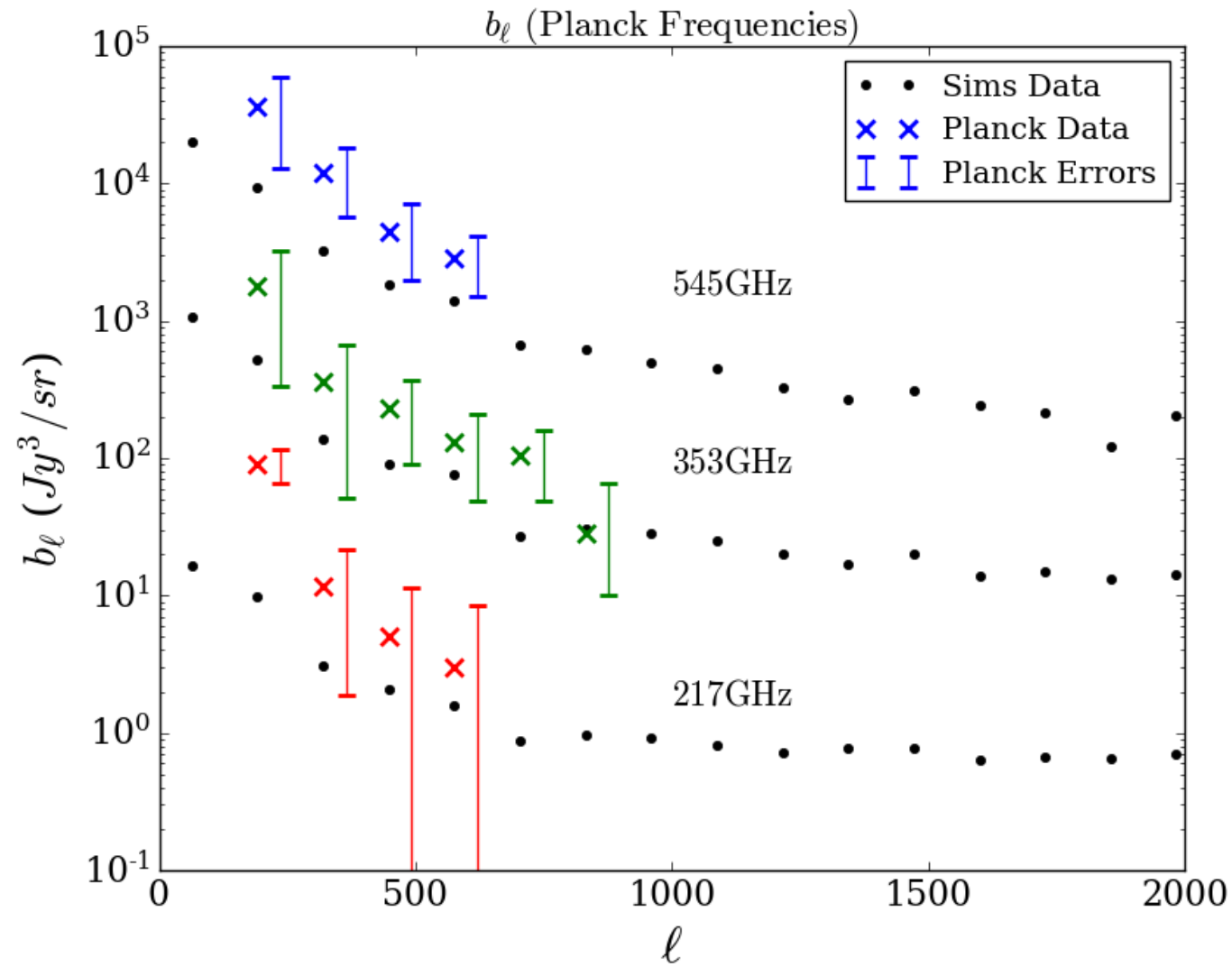


Validations: CIB Bispectrum

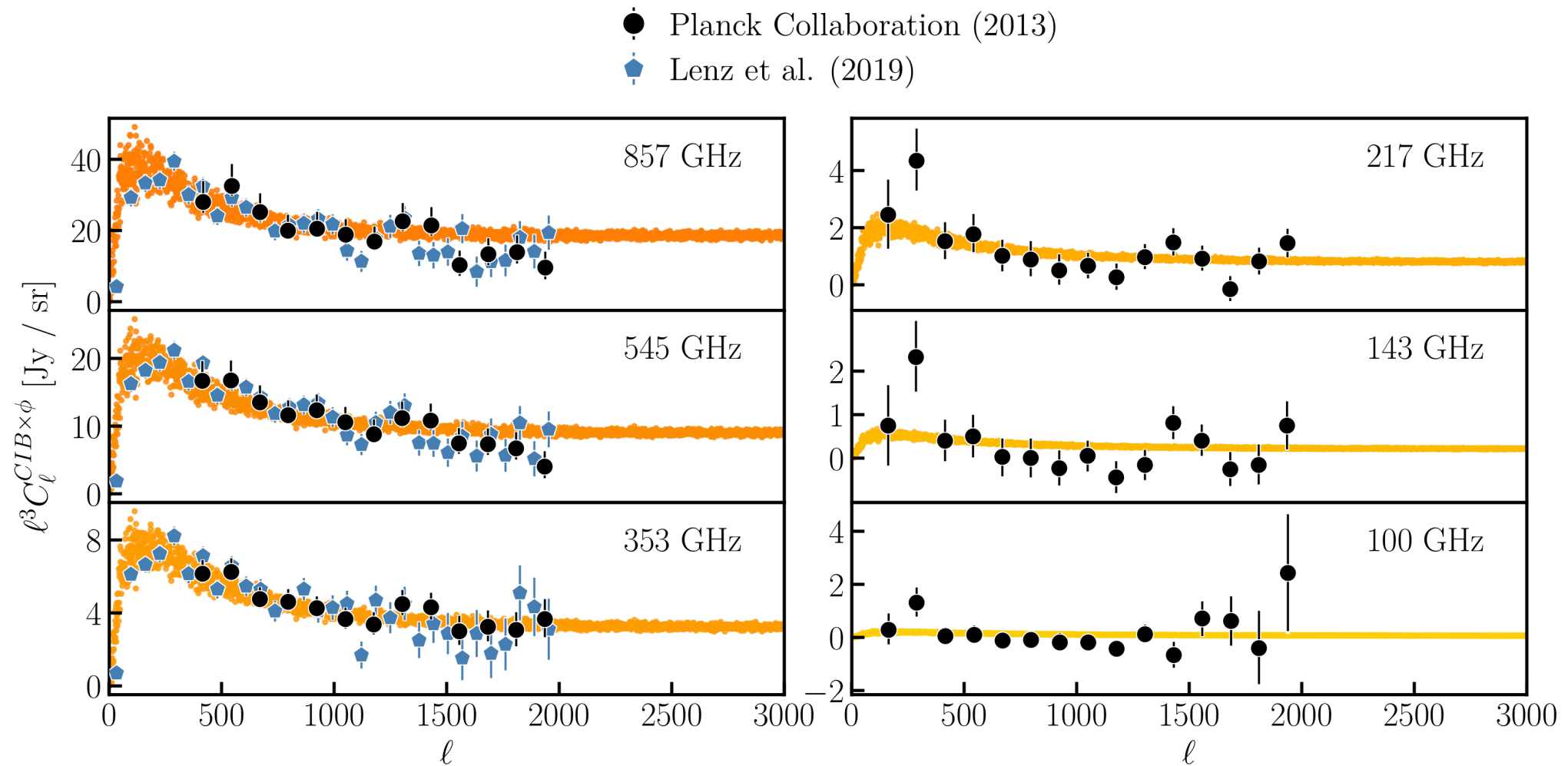
Preliminary



Jason Lee, Pavel Motloch, ...



Validations: CIB x lensing



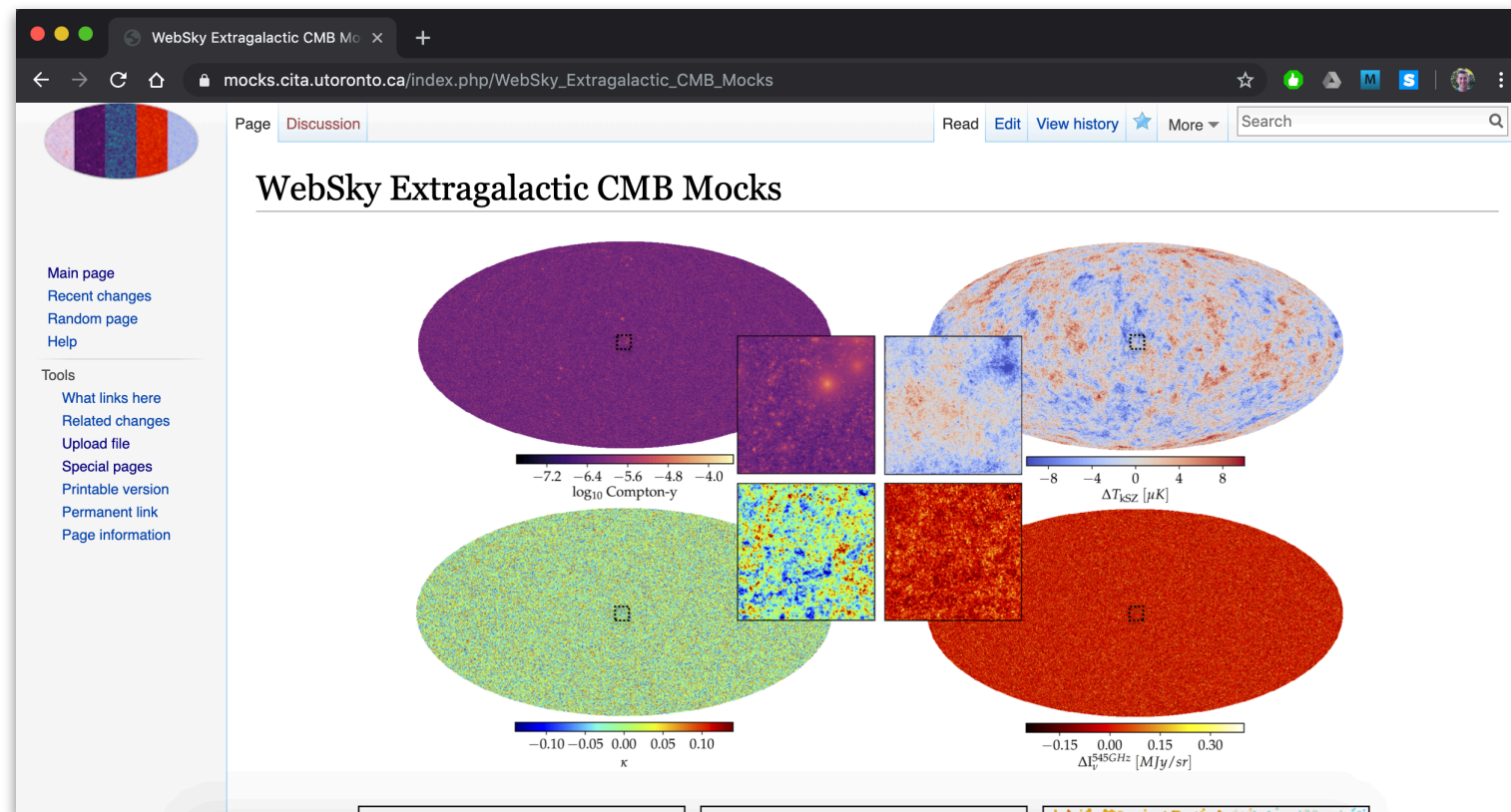
- Cross correlations to date look good



The Current Generation of CMB Extragalactic Simulations

All data publicly available @
mocks.cita.utoronto.ca

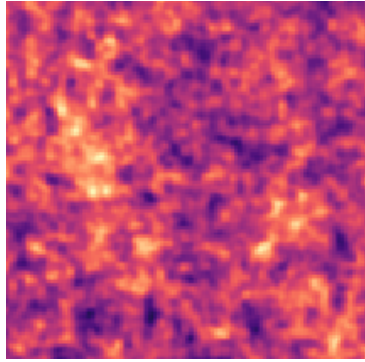
Ask away @
[websky-cmb](https://webchat.slack.com/#C0138888888)



The Current Generation of CMB Extragalactic Simulations

- Minimum halo mass of $\sim 1 \times 10^{12} M_{\odot}$ for full-sky simulation

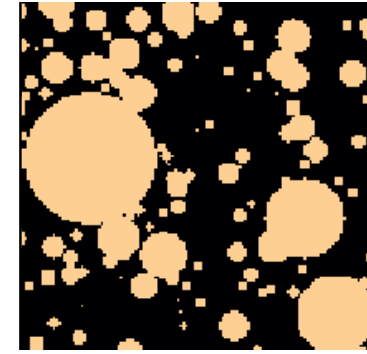
Initial Conditions



Physical Approximation



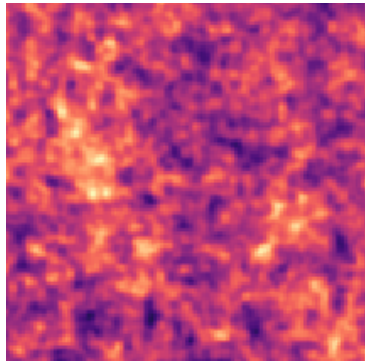
Final Halos/Matter Field



The Current Generation of CMB Extragalactic Simulations

- Minimum halo mass of $\sim 1 \times 10^{12} M_{\odot}$ for full-sky simulation

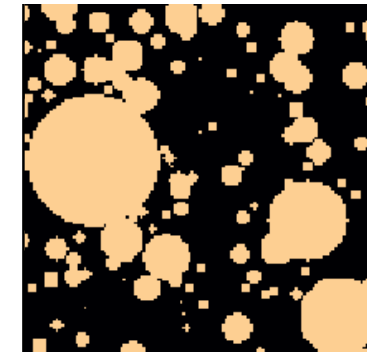
Initial Conditions



Physical Approximation

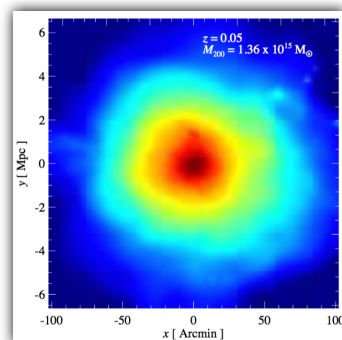


Final Halos/Matter Field

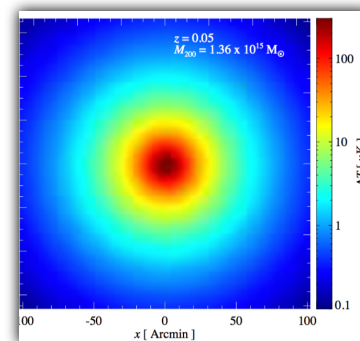


- Spherical halo profiles fit to small box hydrodynamical simulations used

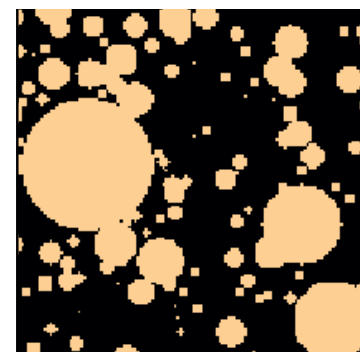
Full Simulation



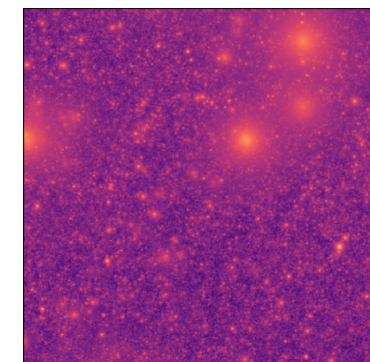
Measure Fitting Functions



Fast Simulation



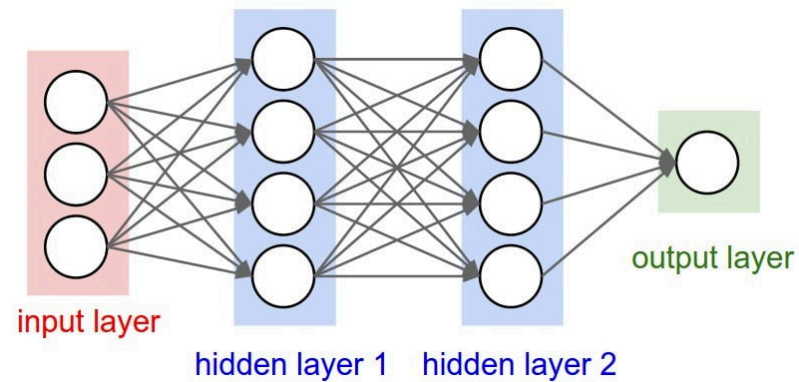
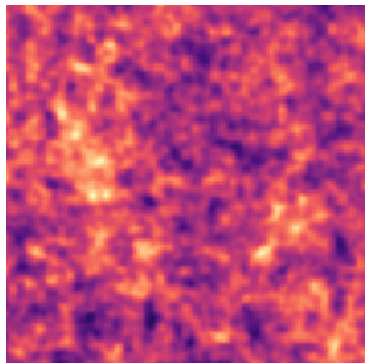
Mock Observation



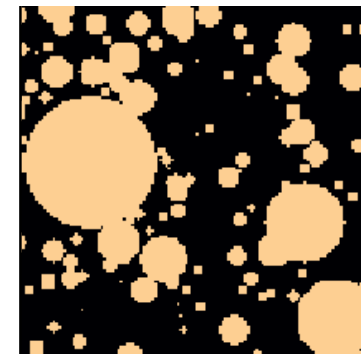
The **Next** Generation of Simulations?

- Minimum halo mass of $\ll 1 \times 10^{12} M_{\odot}$ for full-sky simulation

Initial Conditions



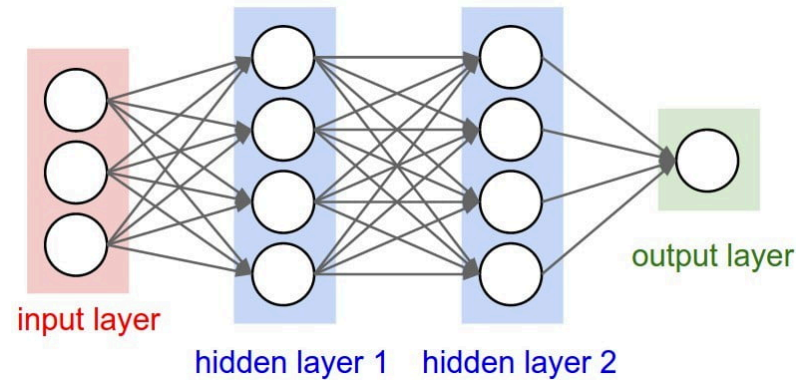
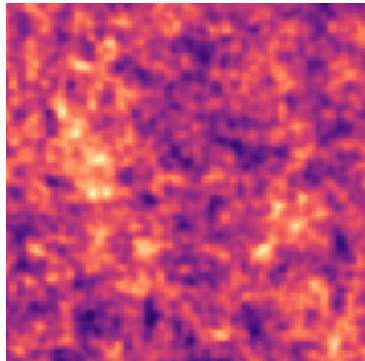
Final Conditions



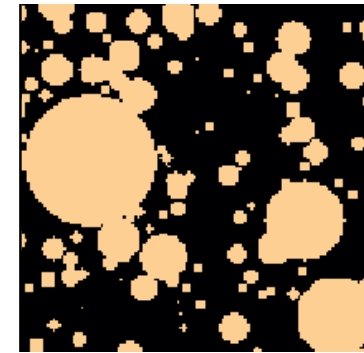
The **Next** Generation of Simulations?

- Minimum halo mass of $\ll 1 \times 10^{12} M_{\odot}$ for full-sky simulation

Initial Conditions

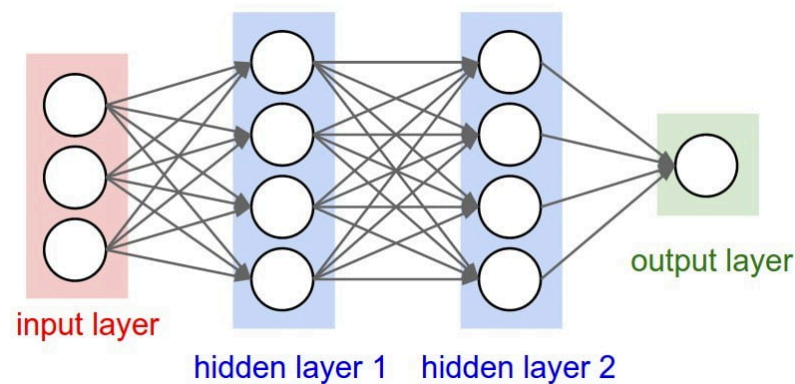
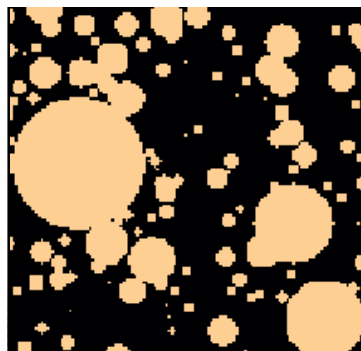


Final Conditions

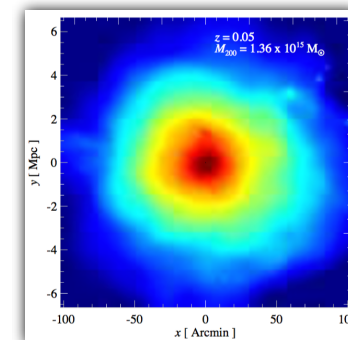


- Direct approximate method to mock observable mapping

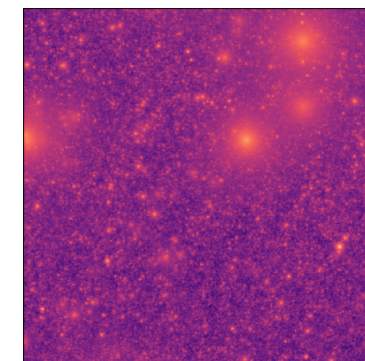
Fast Simulation



Full Simulation



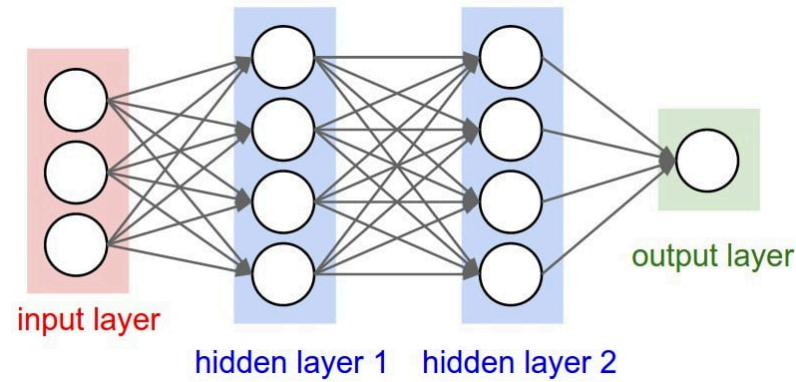
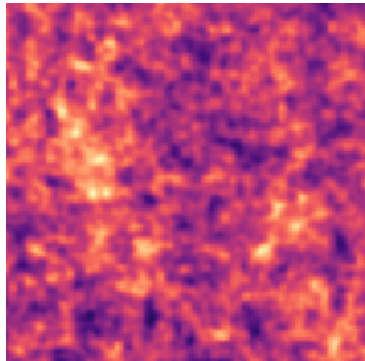
Mock Observation



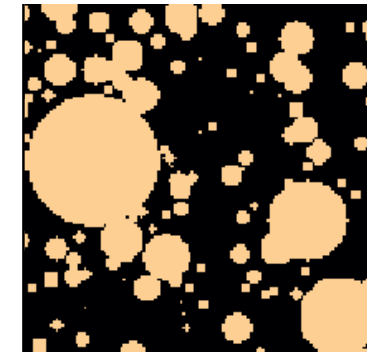
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- Minimum halo mass of $\ll 1 \times 10^{12} M_{\odot}$ for full-sky simulation

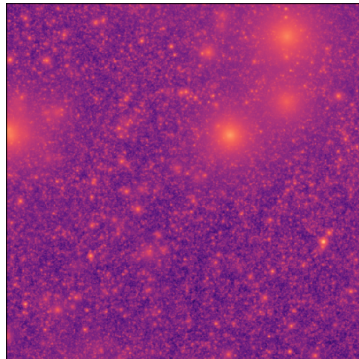
Initial Conditions



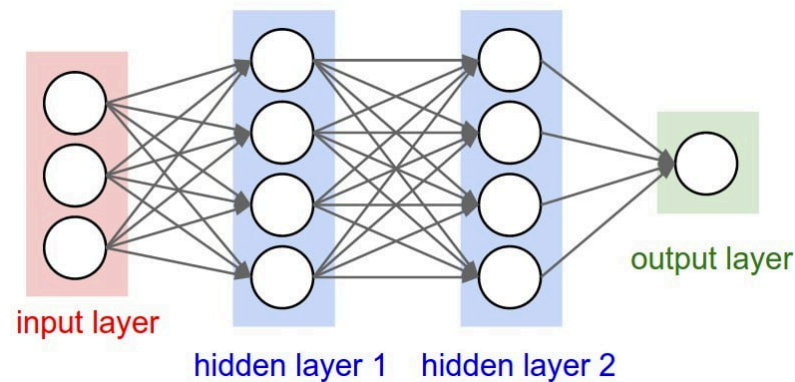
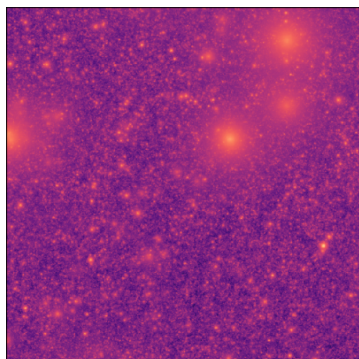
Final Conditions



Mock Observation



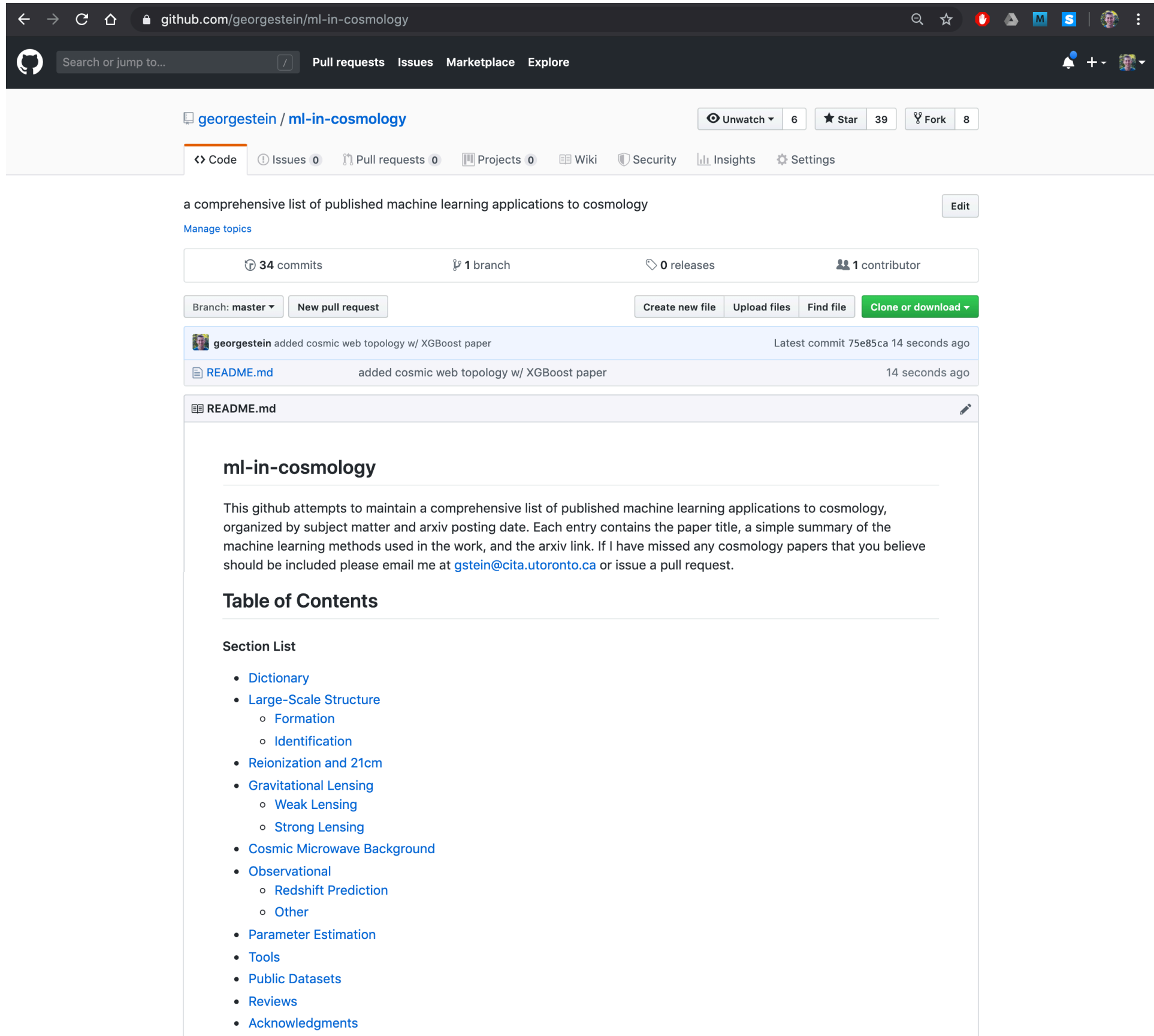
True Observation



Cosmological Information



Machine Learning in Cosmology <https://github.com/georgestein/ml-in-cosmology>



github.com/georgestein/ml-in-cosmology

georgestein / ml-in-cosmology

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a comprehensive list of published machine learning applications to cosmology

Manage topics

34 commits 1 branch 0 releases 1 contributor

Branch: master New pull request

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Commit	Message	Time
georgestein	added cosmic web topology w/ XGBoost paper	Latest commit 75e85ca 14 seconds ago
README.md	added cosmic web topology w/ XGBoost paper	14 seconds ago

README.md

ml-in-cosmology

This github attempts to maintain a comprehensive list of published machine learning applications to cosmology, organized by subject matter and arxiv posting date. Each entry contains the paper title, a simple summary of the machine learning methods used in the work, and the arxiv link. If I have missed any cosmology papers that you believe should be included please email me at gstein@cita.utoronto.ca or issue a pull request.

Table of Contents

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- [Reionization and 21cm](#)
- [Gravitational Lensing](#)
 - [Weak Lensing](#)
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 - [Redshift Prediction](#)
 - [Other](#)
- [Parameter Estimation](#)
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- [Public Datasets](#)
- [Reviews](#)
- [Acknowledgments](#)

~140 papers



Convolutional Neural Networks for LSS

HaloNet - First application of a volumetric deep Convolutional Neural Network (CNN) for large scale structure simulations

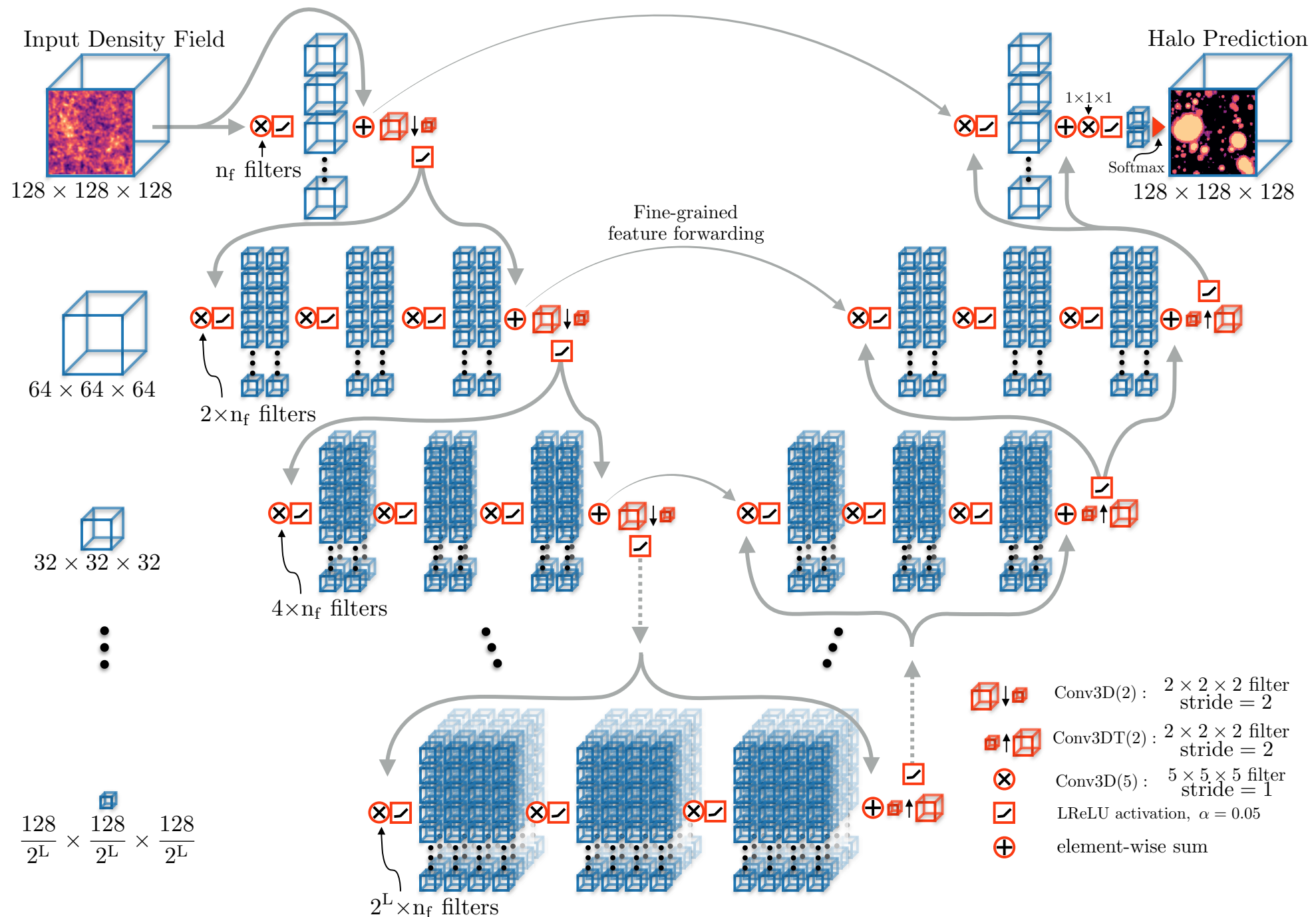
Berger & Stein - arXiv 1805.04537

V-Net = 3D U-Net

Milletari, Navab, Ahmadi: 1606.04797

U-Net

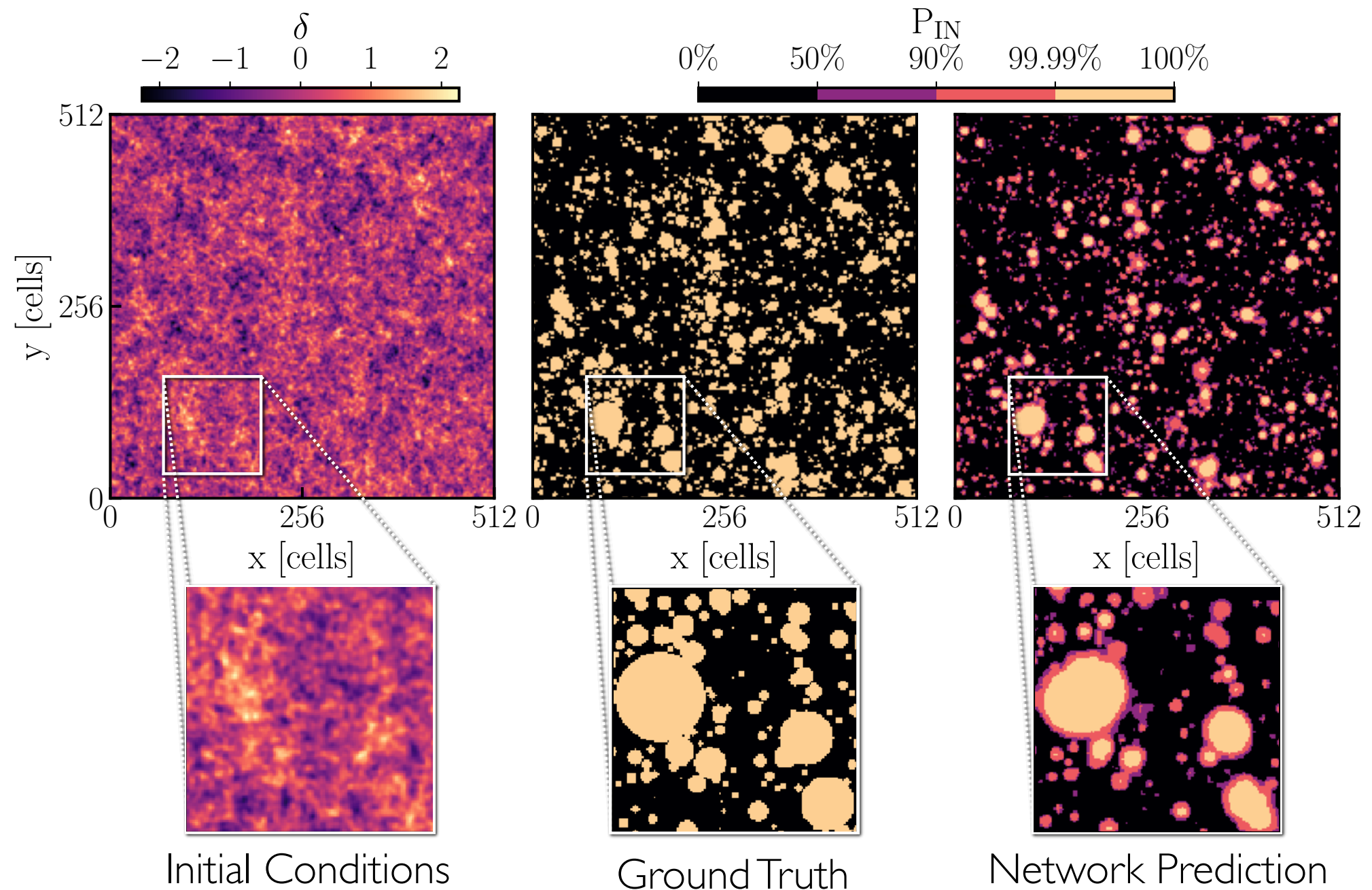
Ronneberger, Fischer, Brox: 1505.04597



Accurately find halos/collapsed regions in Lagrangian space

HaloNet - First application of a volumetric deep Convolutional Neural Network (CNN) for large scale structure simulations

Berger & Stein - arXiv 1805.04537

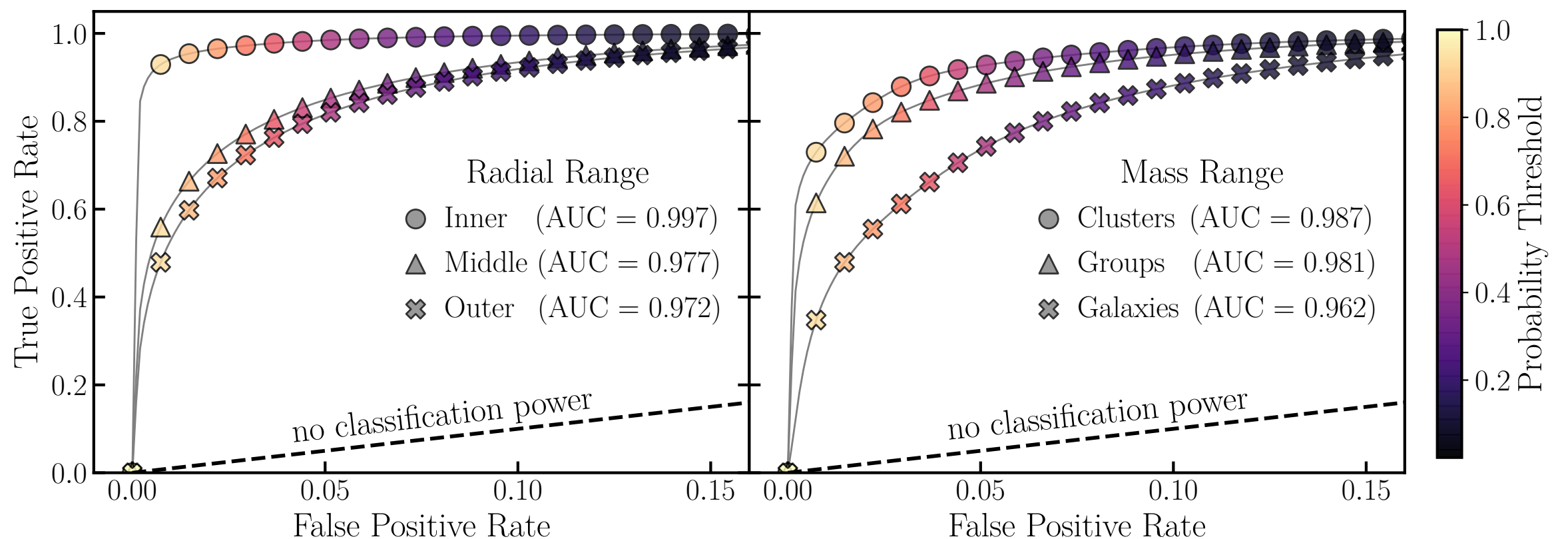


Quantifying the network accuracy

receiver operating characteristic (ROC) curve

$$\text{True Positive Rate} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}} \quad (\text{Sensitivity})$$

$$\text{False Positive Rate} = \frac{\text{False Positives}}{\text{False Positives} + \text{True Negatives}} \quad (1 - \text{Specificity})$$

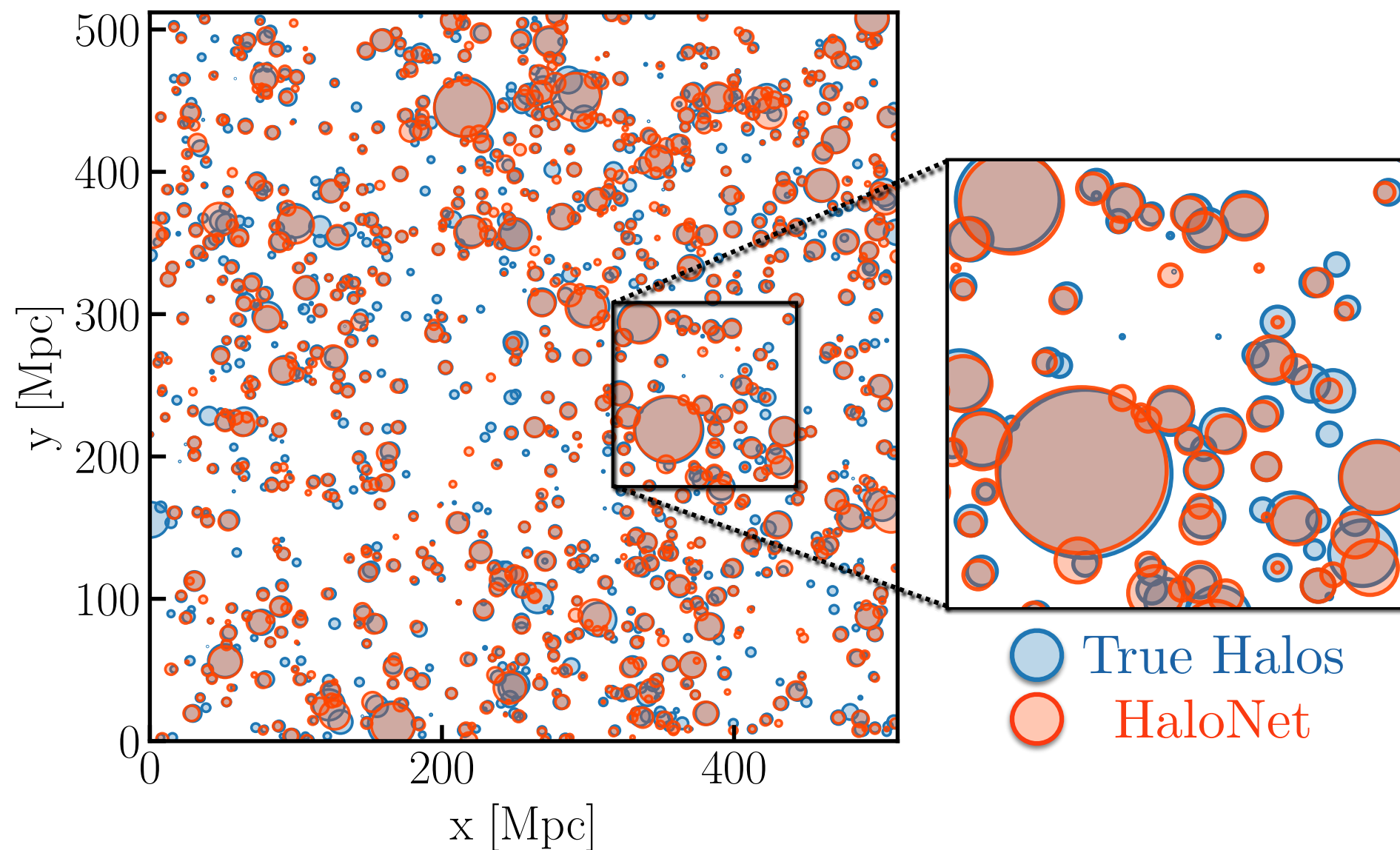


- Quick predictive halo finder, move halos with LPT for final halo catalogue, simple predictive method



Apply Lagrangian halo finder

- Developed simple Lagrangian halo finder
- Move halos with LPT for final halo catalogue,
= simple predictive method



Things to overcome for many current ML LSS methods

- Single (or low) simulation resolution
- Single redshift
- Single set of cosmological/astrophysical parameters

...

ICs to halos

corrections to LPT displacements

DM to galaxies

DM to halos

DM to pressure (2D)

HI cube generation

DM cube generation + resolution upscaling

<i>Cosmological Reconstruction From Galaxy Light: Neural Network Based Light-Matter Connection</i>	NN	https://arxiv.org/abs/1805.02247
<i>A volumetric deep Convolutional Neural Network for simulation of mock dark matter halo catalogues</i>	V-Net	https://arxiv.org/abs/1805.04537
<i>Learning to Predict the Cosmological Structure Formation</i>	V-Net	https://arxiv.org/abs/1811.06533
<i>deepCool: Fast and Accurate Estimation of Cooling Rates in Irradiated Gas with Artificial Neural Networks</i>	NN, RF, kNN	https://arxiv.org/abs/1901.01264
<i>From Dark Matter to Galaxies with Convolutional Networks</i>	V-Net	https://arxiv.org/abs/1902.05965
<i>Painting halos from 3D dark matter fields using Wasserstein mapping networks</i>	GAN	https://arxiv.org/abs/1903.10524
<i>Painting with baryons: augmenting N-body simulations with gas using deep generative models</i>	GAN, VAE	https://arxiv.org/abs/1903.12173
<i>HIGAN: Cosmic Neutral Hydrogen with Generative Adversarial Networks</i>	GAN	https://arxiv.org/abs/1904.12846
<i>A deep learning model to emulate simulations of cosmic reionization</i>	CNN	https://arxiv.org/abs/1905.06958
<i>An interpretable machine learning framework for dark matter halo formation</i>	BDT	https://arxiv.org/abs/1906.06339
<i>Cosmological N-body simulations: a challenge for scalable generative models</i>	GAN	https://arxiv.org/abs/1908.05519



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<i>deepCool: Fast and Accurate Estimation of Cooling Rates in Irradiated Gas with Artificial Neural Networks</i>	NN, RF, kNN	https://arxiv.org/abs/1901.01264
<i>From Dark Matter to Galaxies with Convolutional Networks</i>	V-Net	https://arxiv.org/abs/1902.05965
<i>Painting halos from 3D dark matter fields using Wasserstein mapping networks</i>	GAN	https://arxiv.org/abs/1903.10524
<i>Painting with baryons: augmenting N-body simulations with gas using deep generative models</i>	GAN, VAE	https://arxiv.org/abs/1903.12173
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<i>An interpretable machine learning framework for dark matter halo formation</i>	BDT	https://arxiv.org/abs/1906.06339
<i>Cosmological N-body simulations: a challenge for scalable generative models</i>	GAN	https://arxiv.org/abs/1908.05519

Simulation to Simulation

True answer known, full control, and ability to validate.

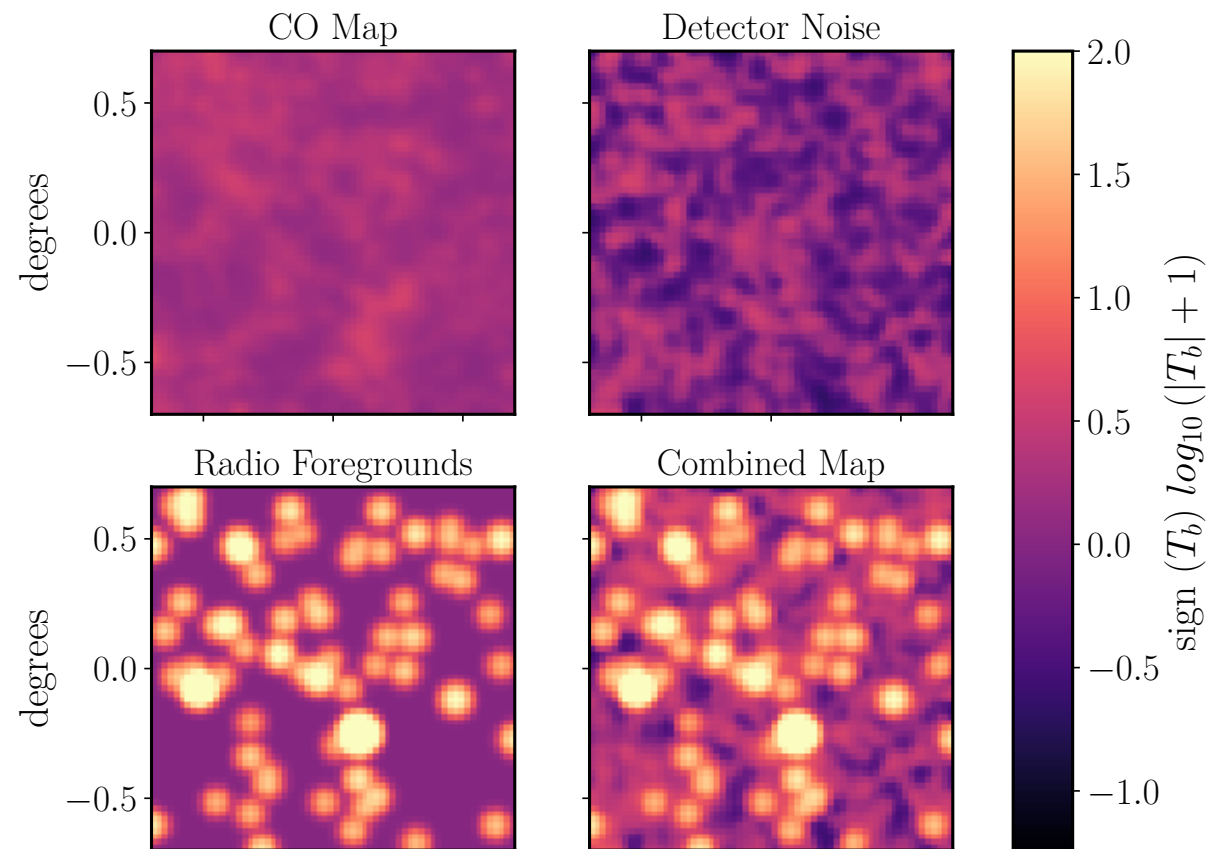


Simulation to Data to Parameters

Making the Network robust to input

Deconfusing Intensity Maps with Neural Networks
[Pfeffer, Breyse, Stein - arXiv 1905.10376](#)

I.) Construct suite of mock
CO intensity maps
using **one** luminosity model
and **various** levels of gaussian noise
and foregrounds



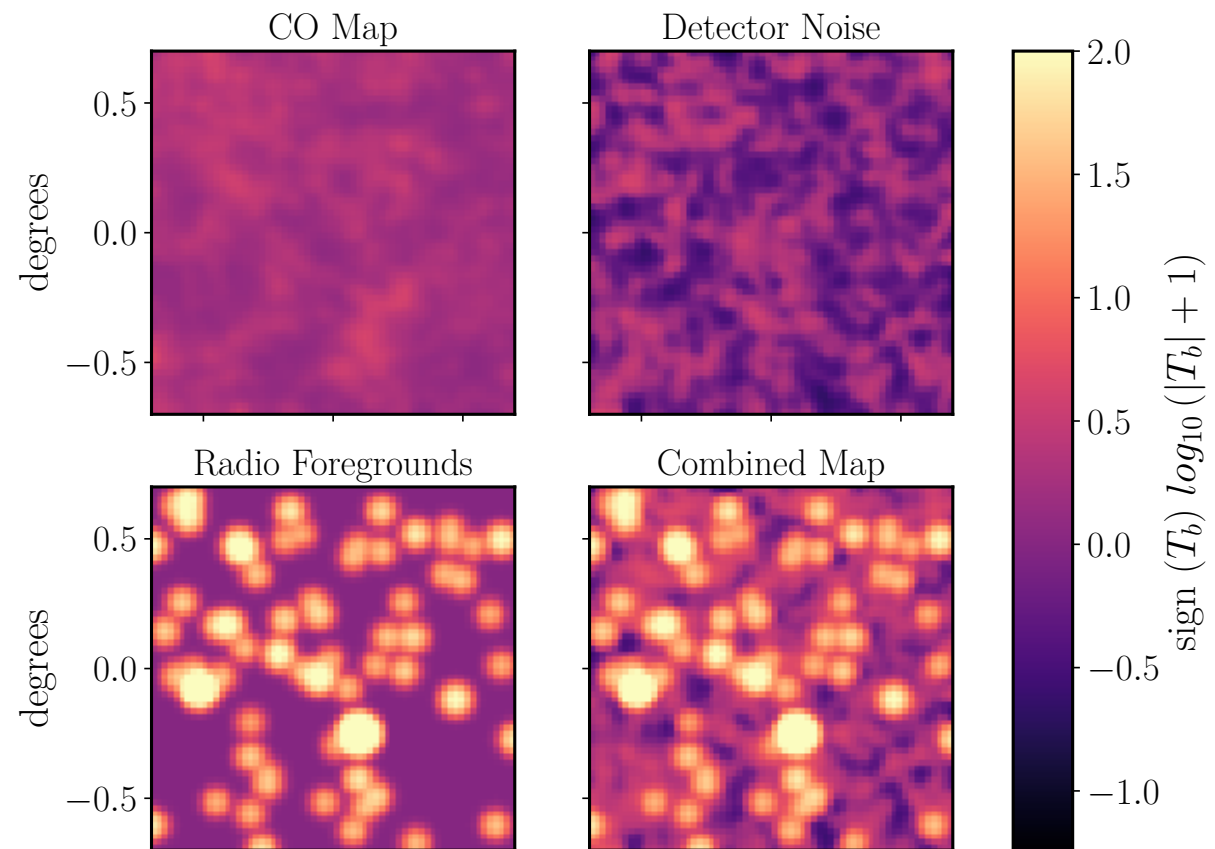
Simulation to Data to Parameters

Making the Network robust to input

Deconfusing Intensity Maps with Neural Networks
[Pfeffer, Breysse, Stein - arXiv 1905.10376](#)

1.) Construct suite of mock
CO intensity maps
using **one** luminosity model
and **various** levels of gaussian noise
and foregrounds

2.) Train ResNet to
pull out luminosity function
from mocks



Simulation to Data to Paramaters

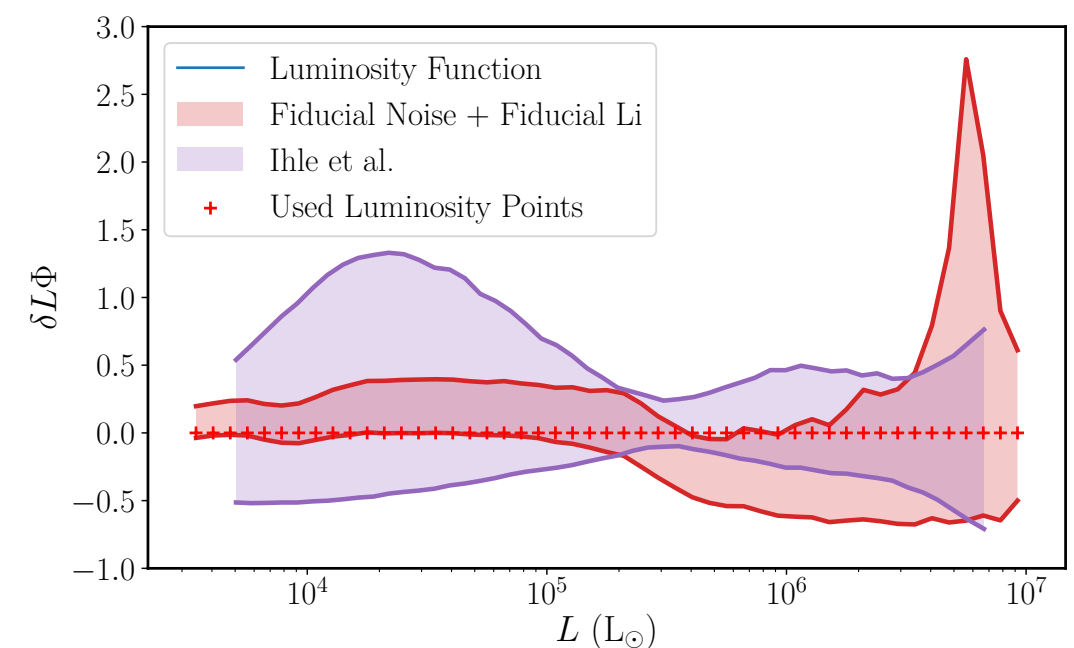
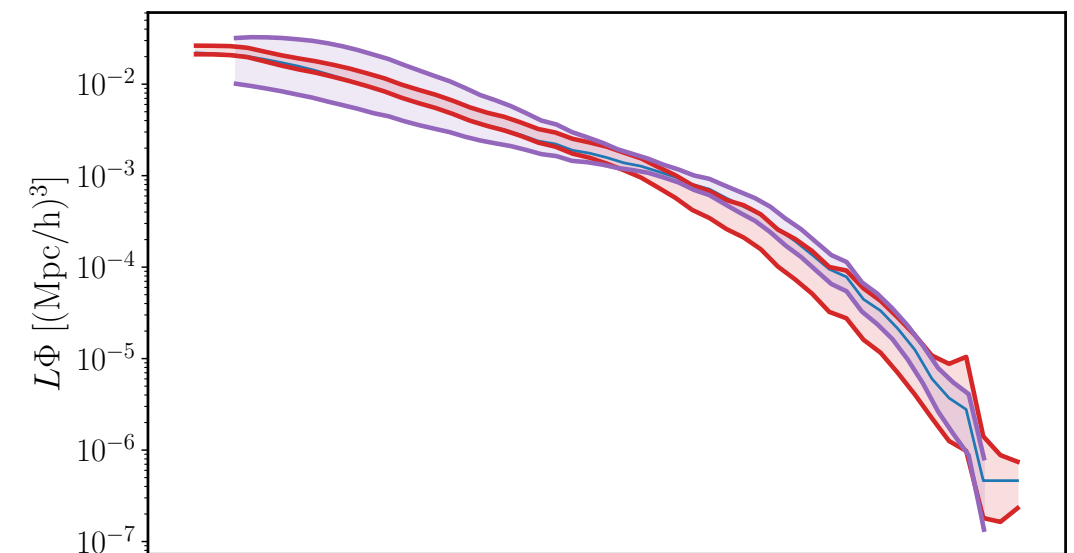
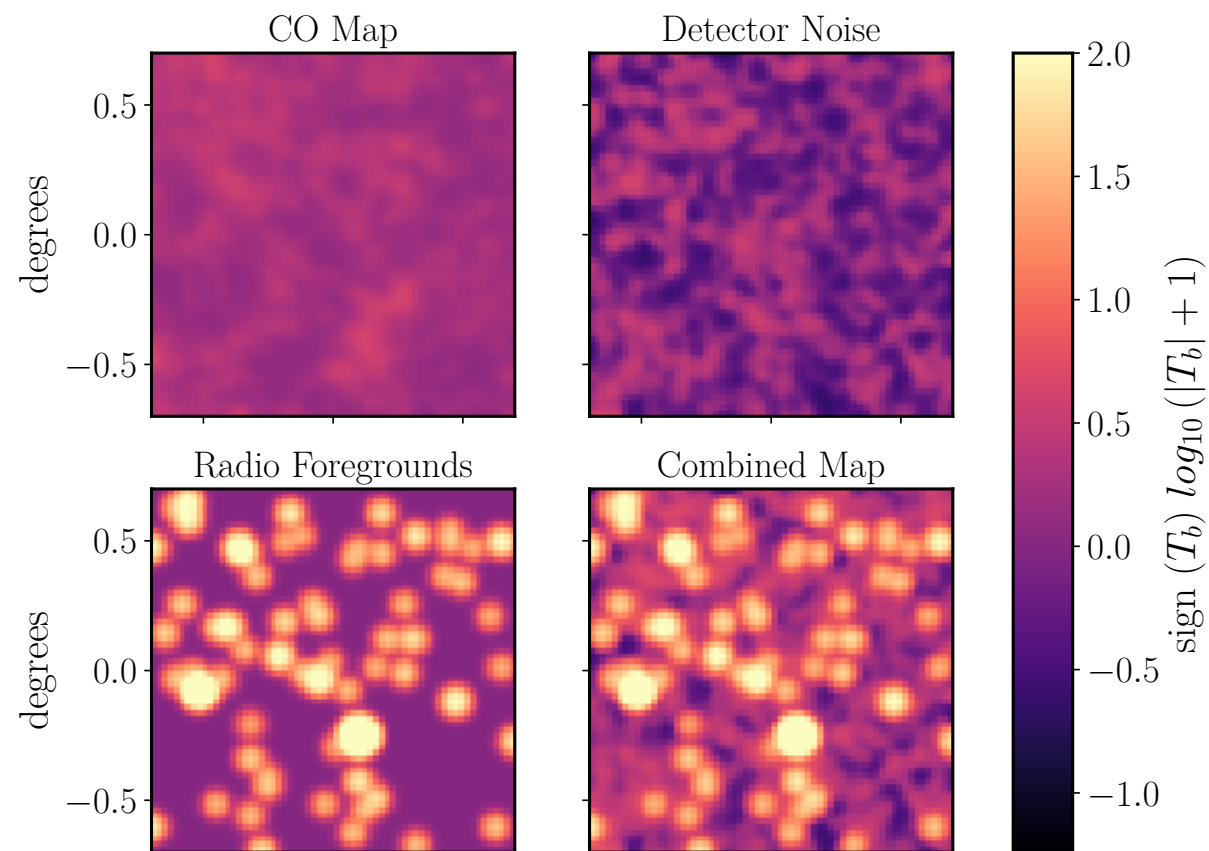
Making the Network robust to input

Deconfusing Intensity Maps with Neural Networks
Pfeffer, Breyse, Stein - arXiv 1905.10376

1.) Construct suite of mock CO intensity maps using **one** luminosity model and **various** levels of gaussian noise and foregrounds

2.) Train ResNet to pull out luminosity function from mocks

3.) Extract luminosity function from mocks



comparable with standard $P(k)$ + PDF methods

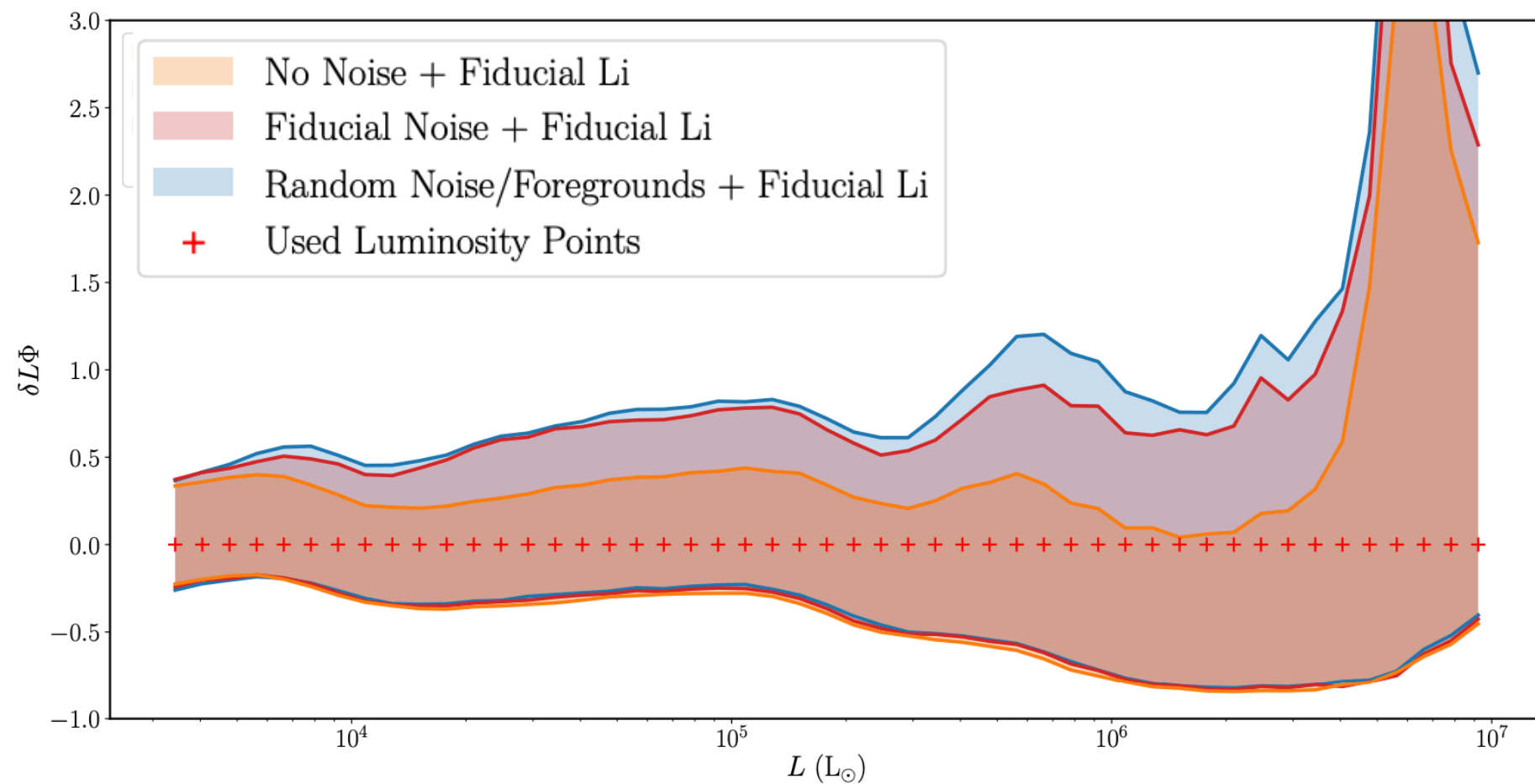


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Network can still perform with various levels of noise and foregrounds
that were **included in training set**

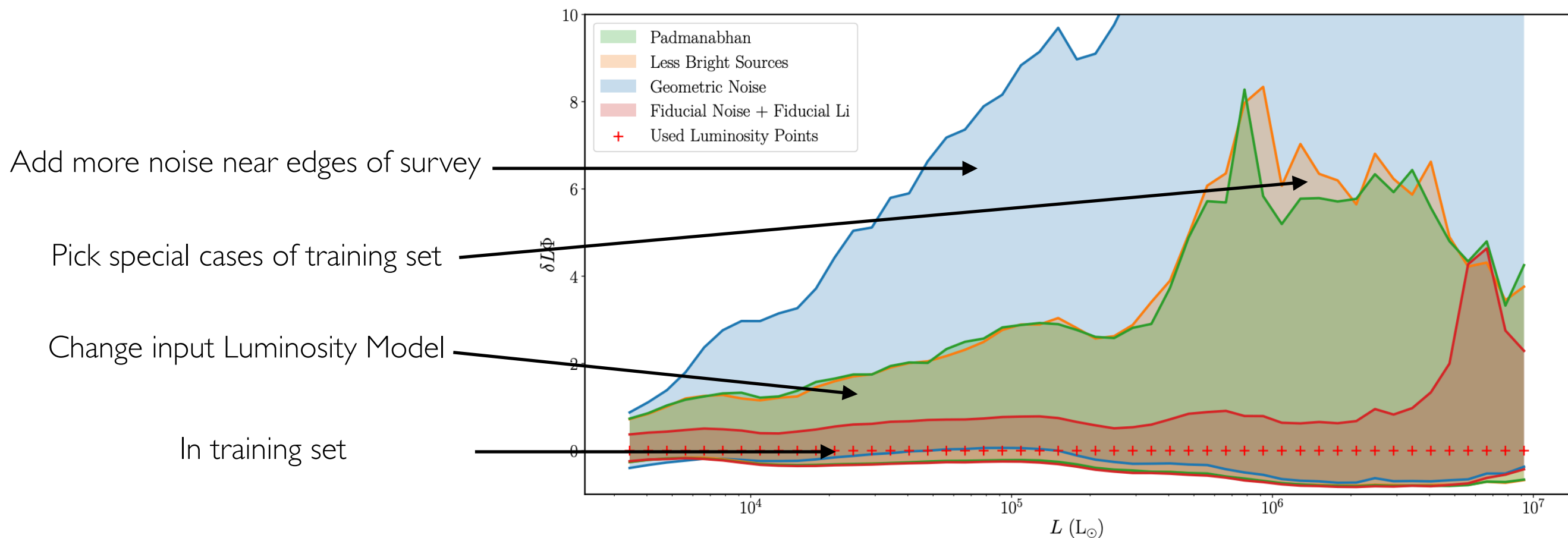


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Network completely fails for scenarios **not included in training set**

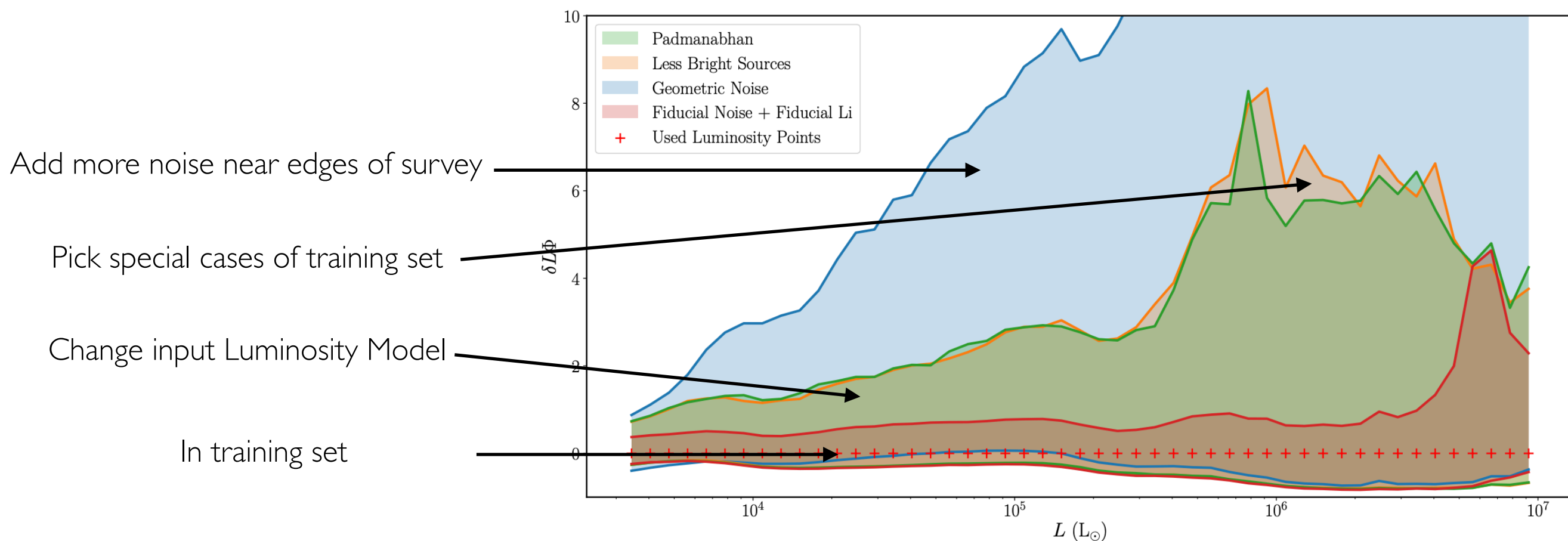


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Network completely fails for scenarios **not included in training set**



find that, in the ideal case where the mock data capture all of the features of the real data, the CNN performs comparably to or better than conventional analyses. However, the network's accuracy degrades considerably when tested on signals and systematics outside of those it was trained on. For both intensity mapping and cosmology as a whole, this motivates a broad-based study of whether simulated data can ever be generated with sufficient detail to realize the enormous potential of machine learning methods.



Come find me in office 341,
or email me at gstein@berkeley.edu

