



MACHINE LEARNING FOR ASTROPHYSICS

2ND EDITION

CATANIA, 8-12 JULY, 2024

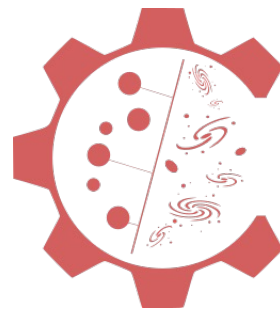
Extracting optimal information from cosmological surveys *with field-level inference and joint analyses*

Adrian Bayer

Princeton University / Simons Foundation

Catania
11 July 2024





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FOR ASTROPHYSICS**
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Translate

with an Italian doctor



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The right Ok, go away Tiger again. Purulent tonsillitis Purlo in tonsillitis
jokes because Forlan Translate Ok we need antibiotics, ok?



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I'm a singer 97 with 96 of frequencies 96 six9ine FC 90 oxygen 96
Epression snormann This is Twenty hundred 8.16pm, okay? He landed in
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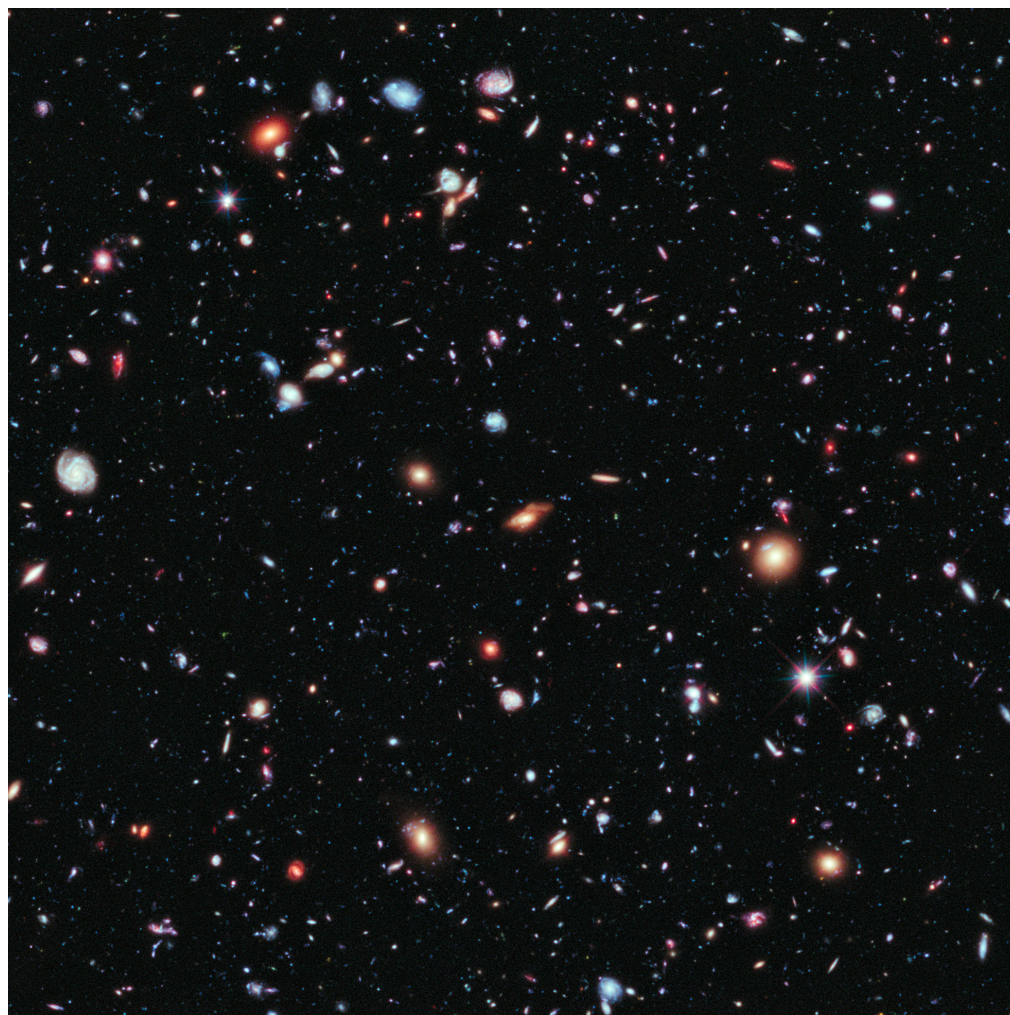
Should I point out Cold or Sud? Just don't talk and if not Speak to Filly.
Don't talk so much.



Cosmological
Field-Level Inference
with
Microcanonical
Langevin Monte Carlo



Cosmological
Field-Level Inference
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Langevin Monte Carlo



S_8

cosmological tensions?

 H_0 Ω_Λ

dark energy

 f_{NL}

primordial NG

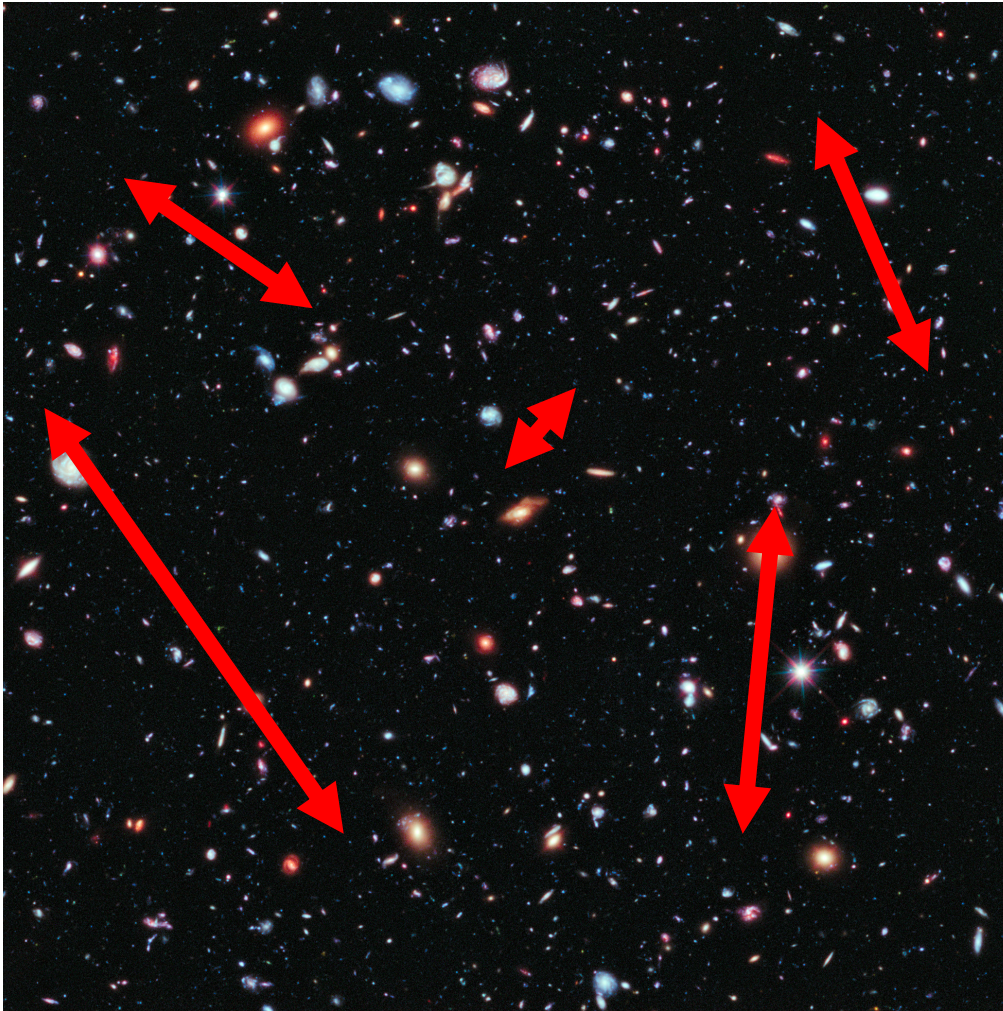
 M_ν

neutrino mass



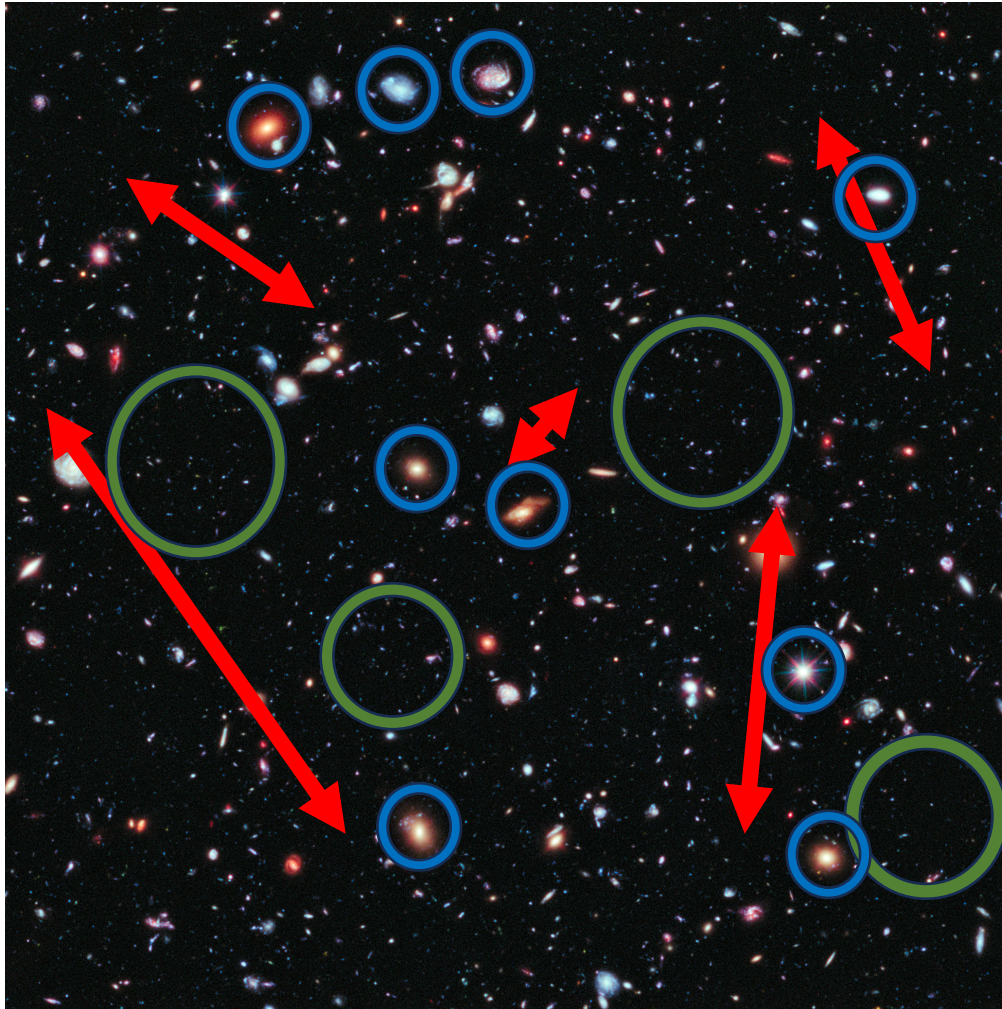
Traditional cosmology uses 2-pt information

but this is no longer optimal as we probe smaller scales



Higher-order statistics

can provide information beyond the 2-pt



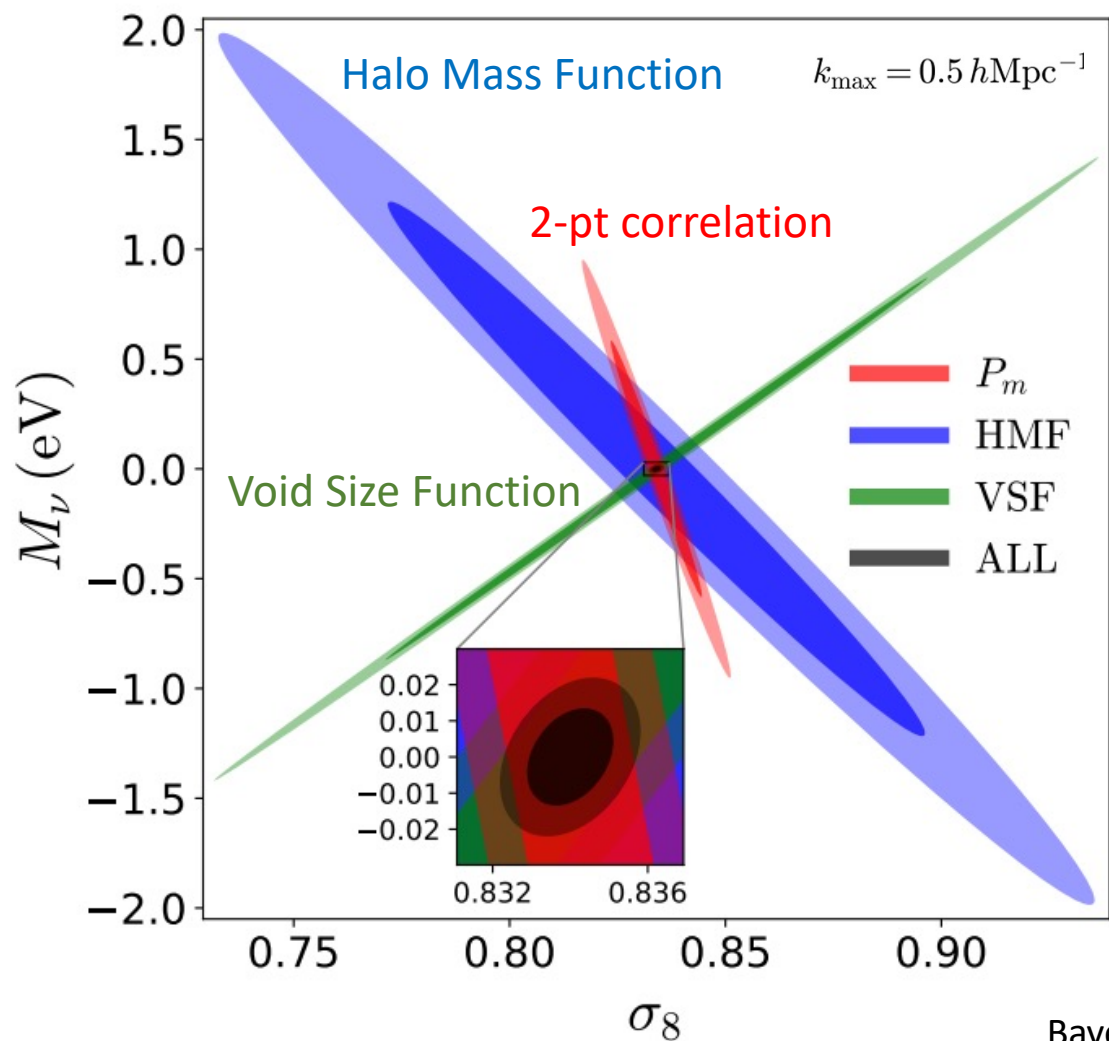
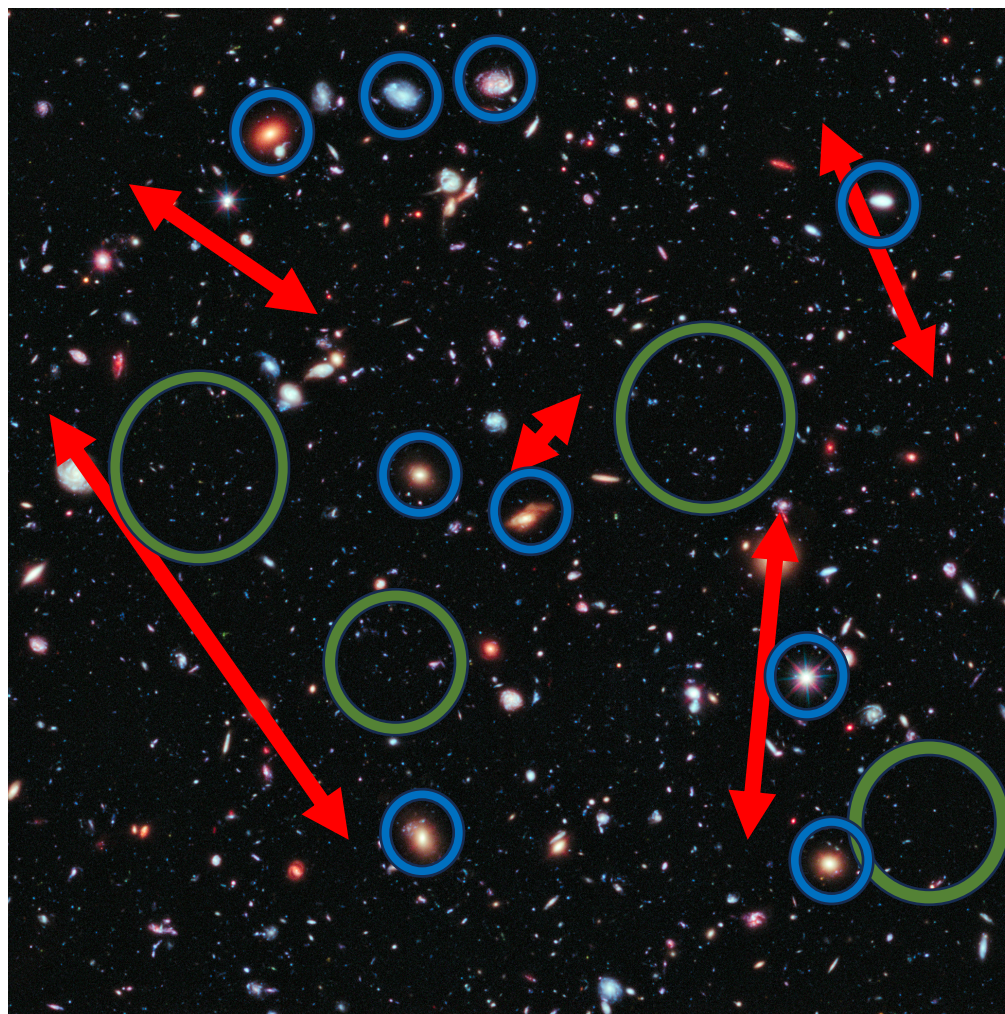
Halo Mass Function

2-pt correlation

Void Size Function

Higher-order statistics

can provide information beyond the 2-pt

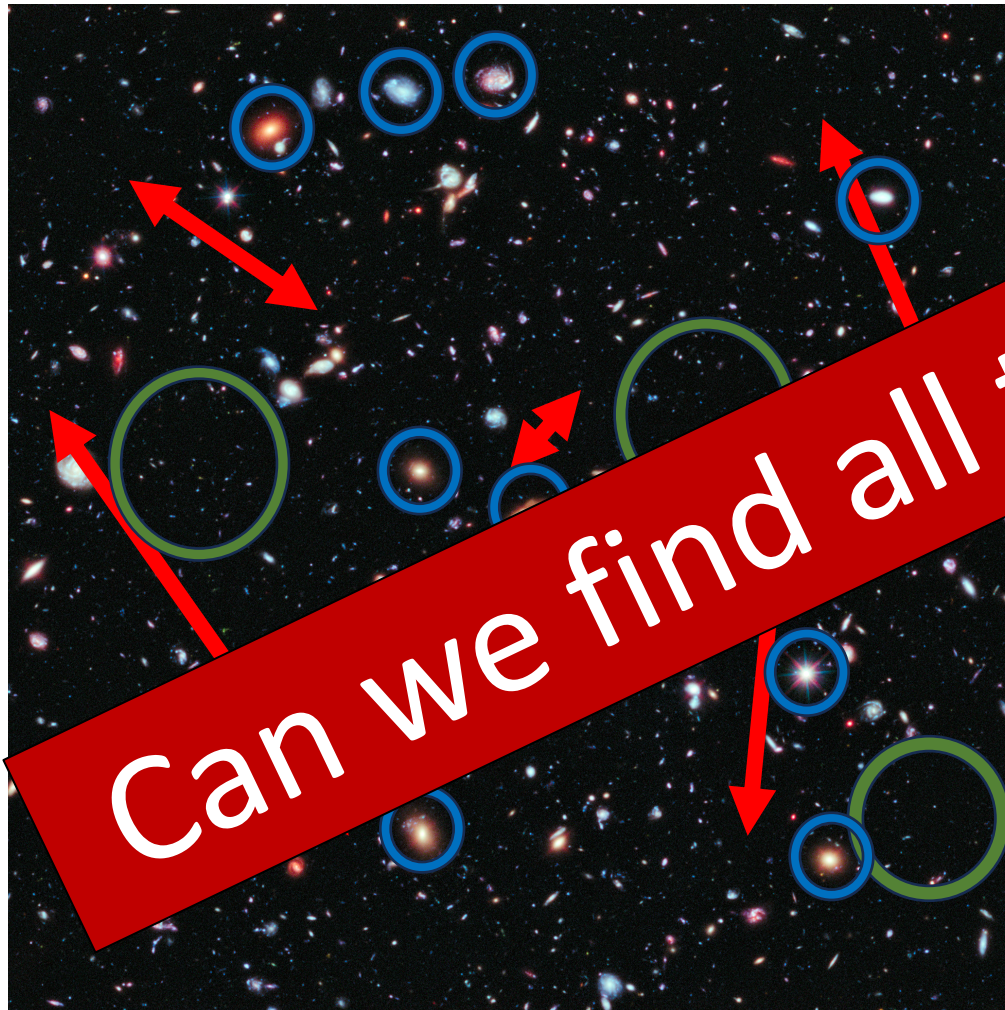


Bayer+ (2021)

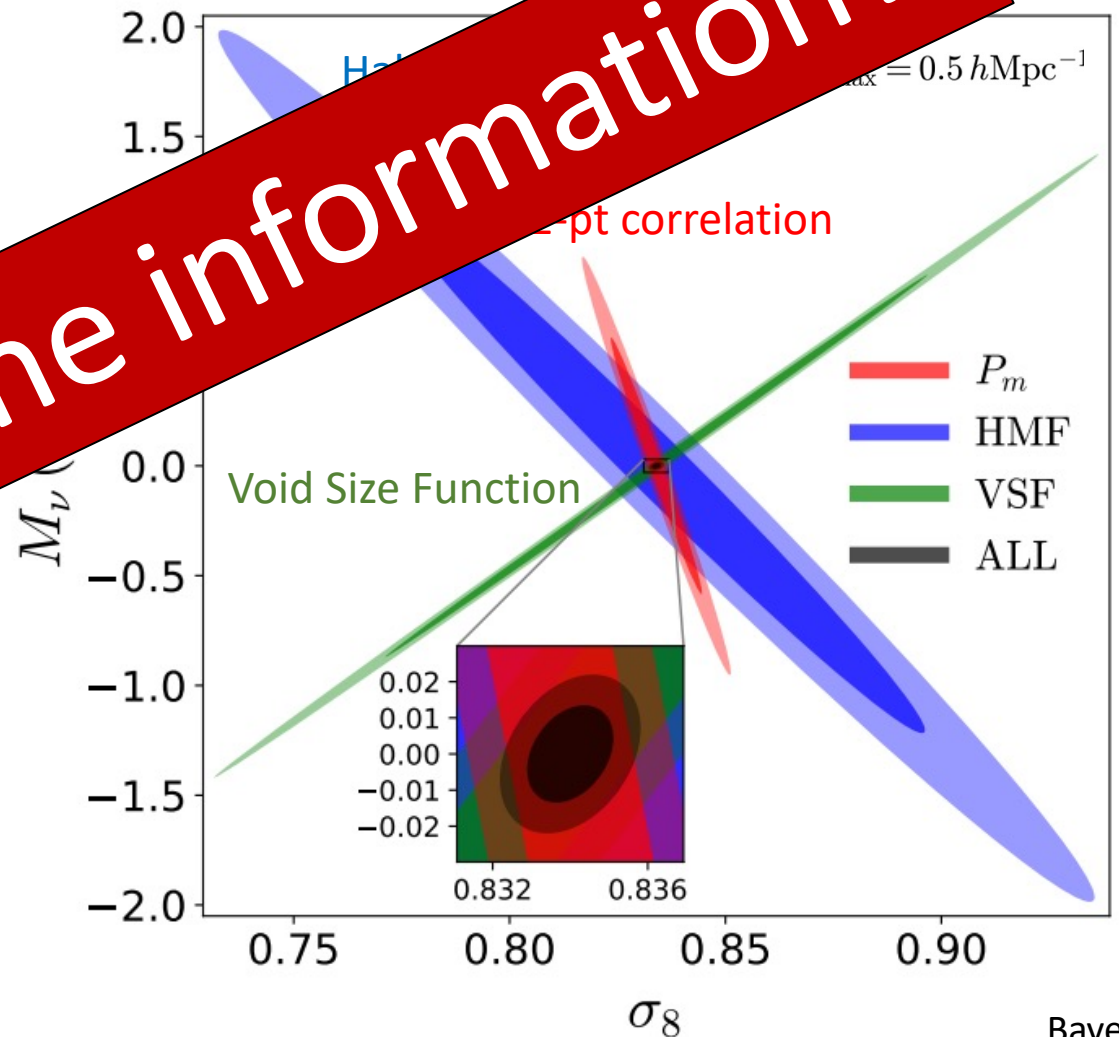
Fake vs? Bayer, Banerjee, Seljak (2022)

Higher-order statistics

can provide information beyond the 2-pt



Can we find all the information?



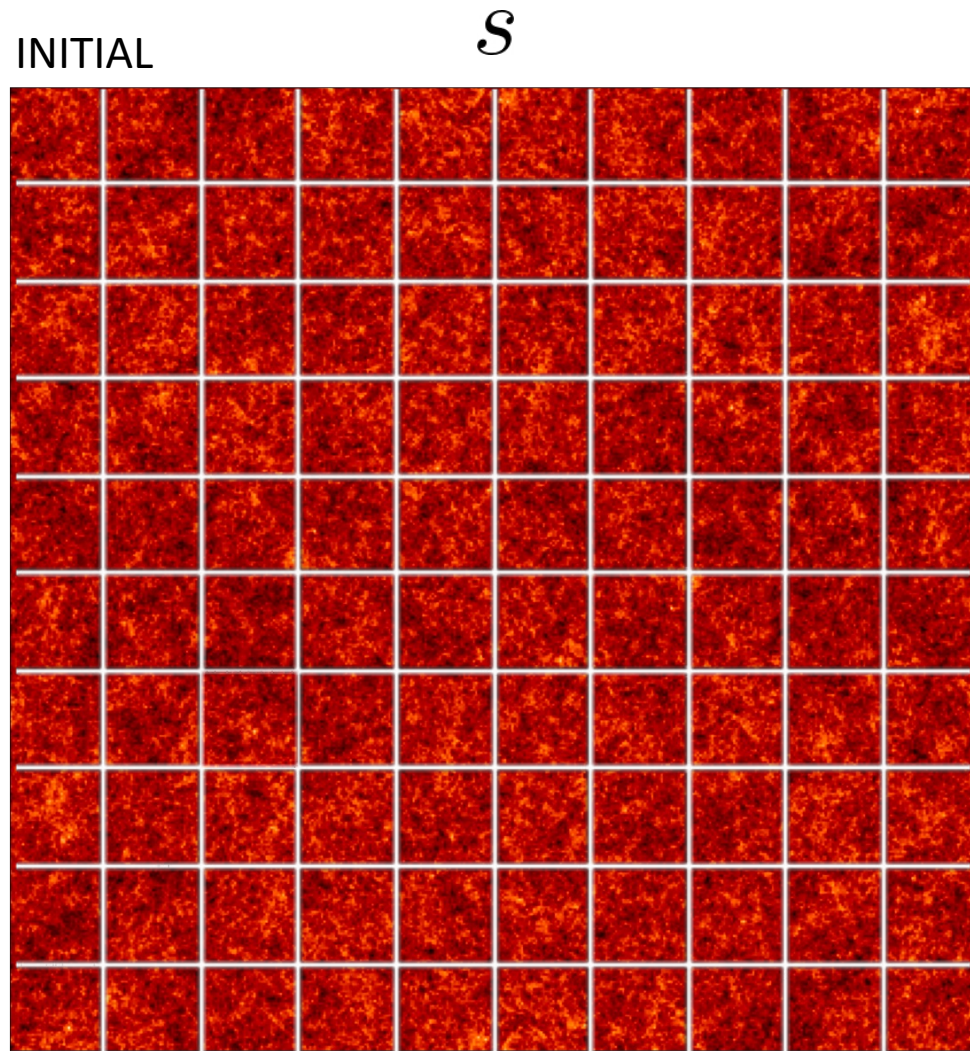
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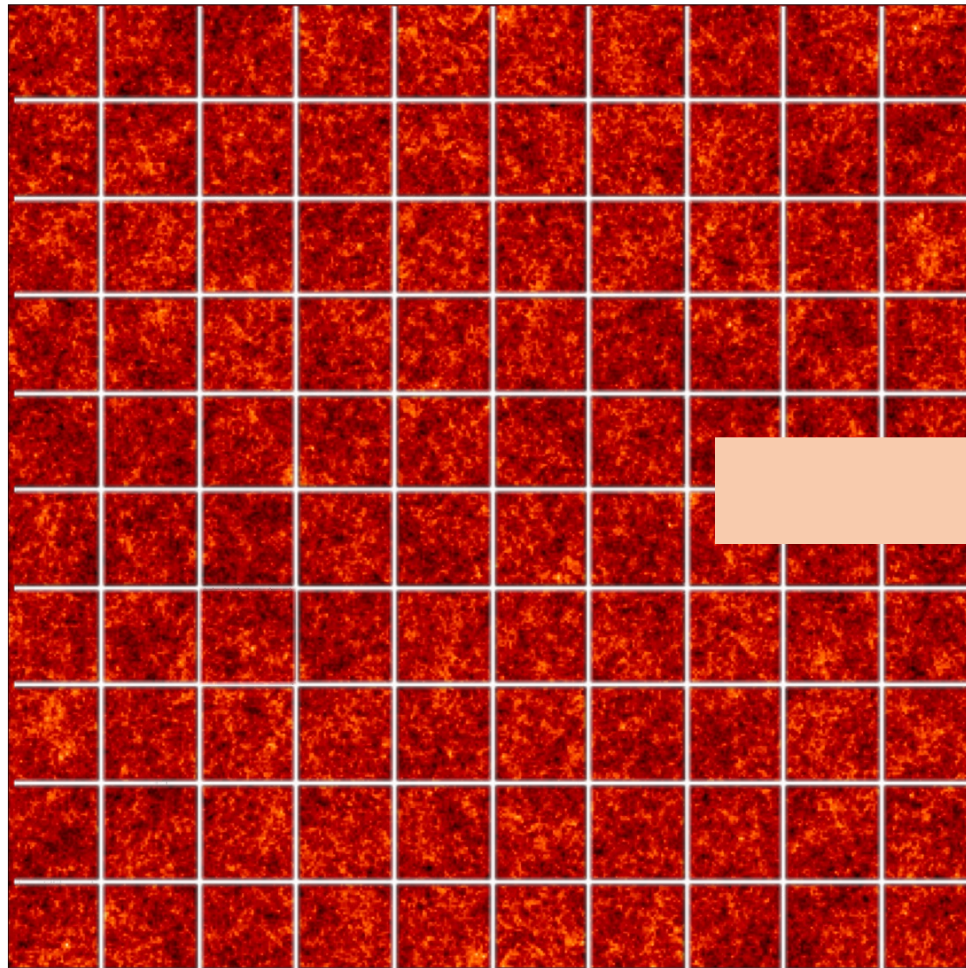
Cosmological
Field-Level Inference
with
Microcanonical
Langevin Monte Carlo

Forward modeling



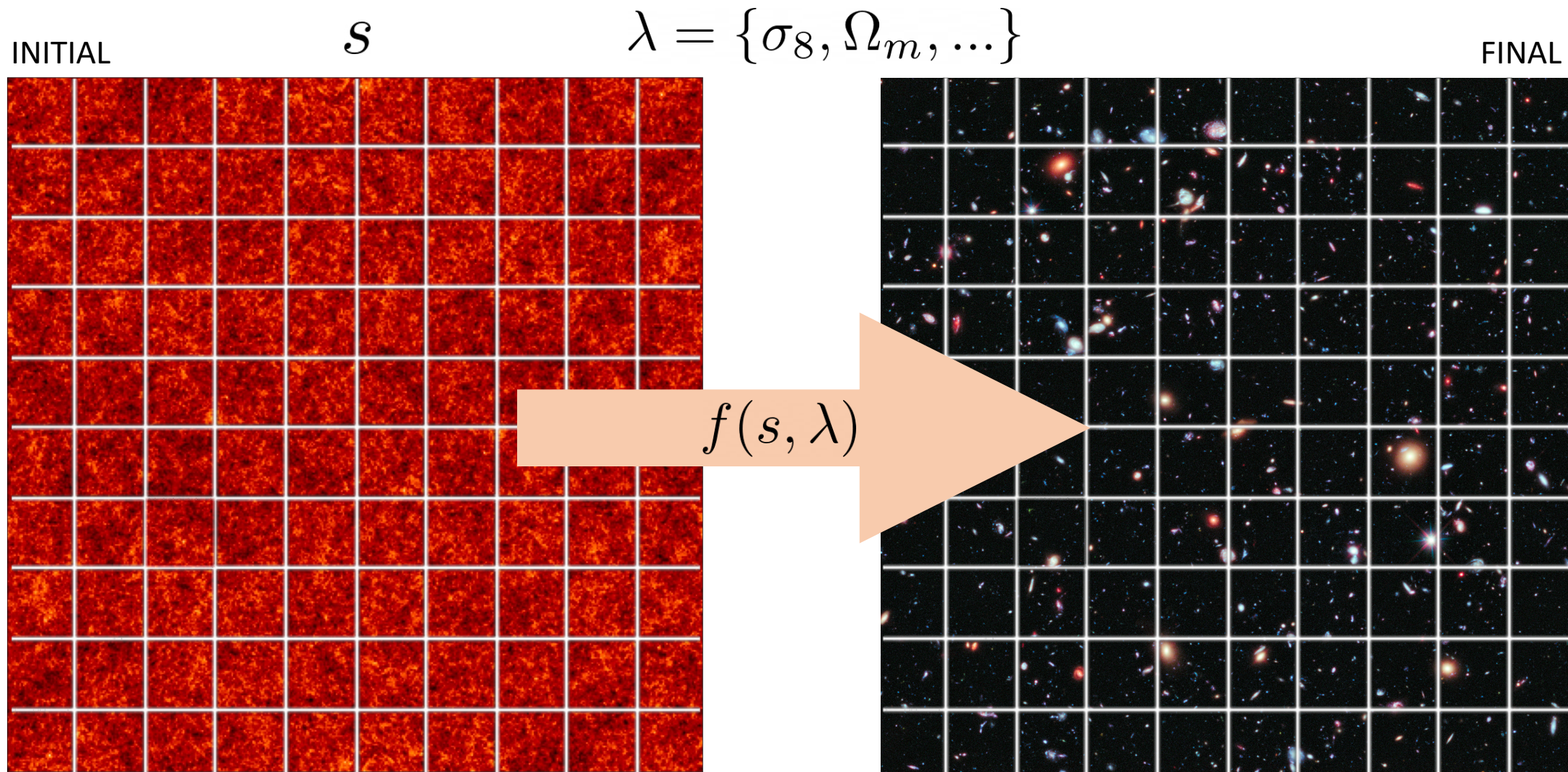
Forward modeling

INITIAL s $\lambda = \{\sigma_8, \Omega_m, \dots\}$

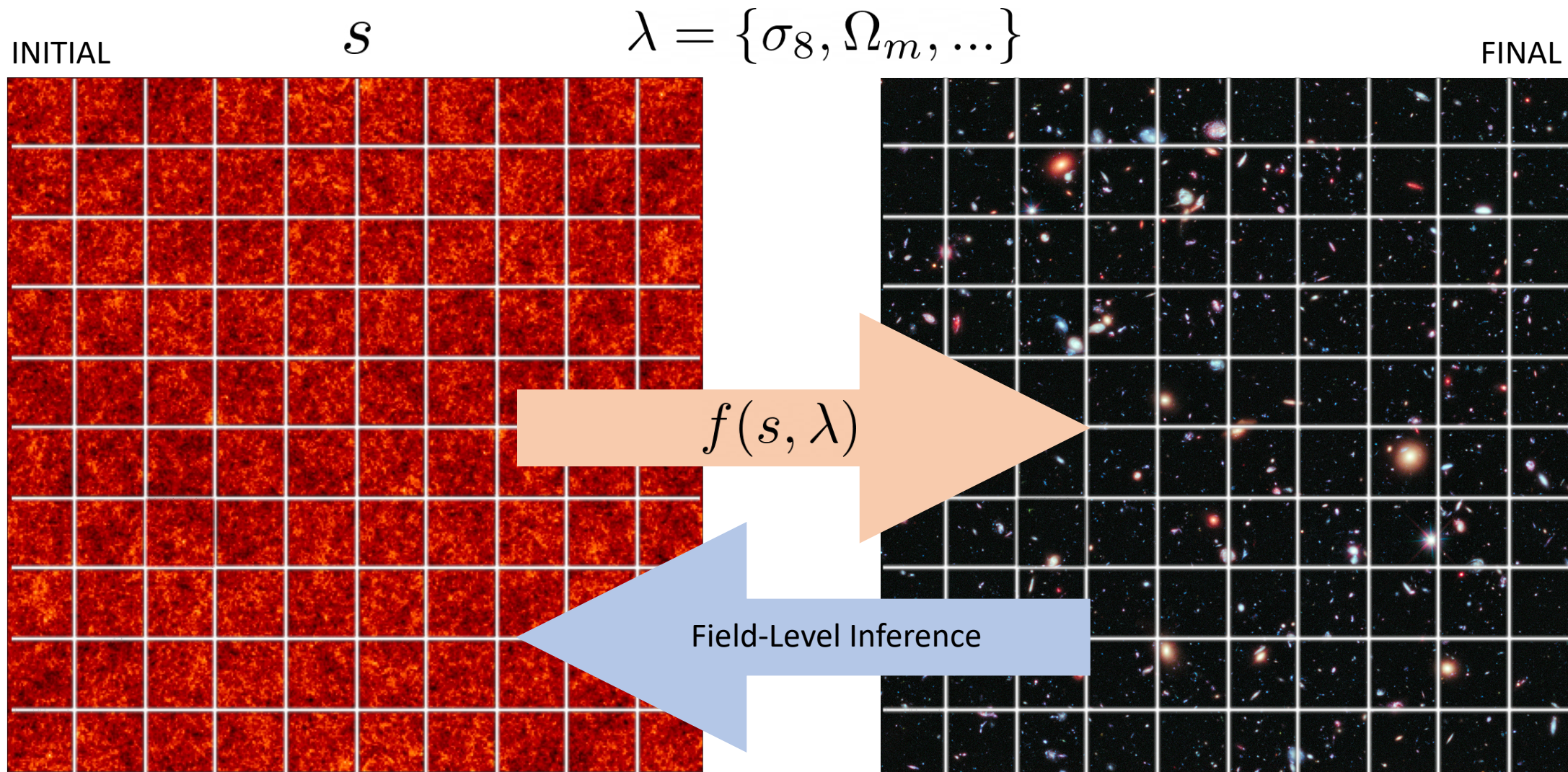


$f(s, \lambda)$

Forward modeling



Forward modeling



Field-Level Inference

Given field data d and forward model f infer
initial modes s and cosmological parameters λ

$$-2 \log P(\mathbf{s}, \lambda | d) = \sum_{\vec{k}} \left[\frac{|d - f(\mathbf{s}, \lambda)|^2}{N} + \frac{|\mathbf{s}|^2}{\mathcal{P}(\lambda)} \right]_{\vec{k}}$$

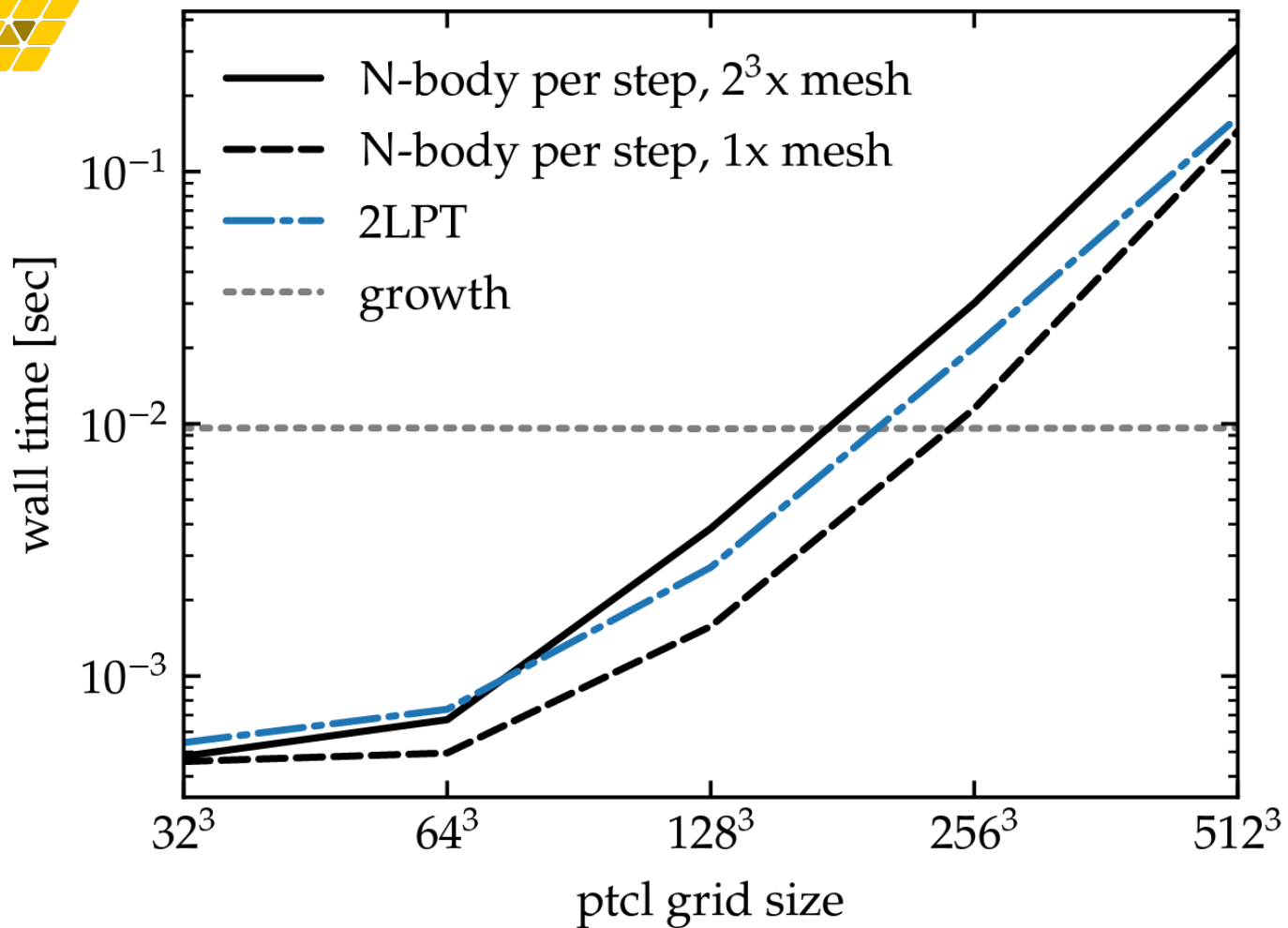
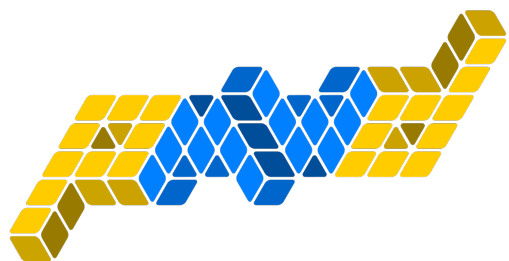
posterior likelihood prior

CHALLENGE: Multimillion dimensional parameter space!

1. Need fast forward model

2. Need differentiable forward model

3. Need fast sampler



1. Fast forward model



2. Differentiable forward model

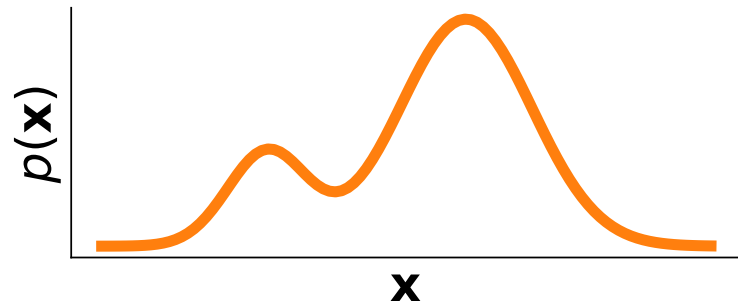


3. Need fast sampler

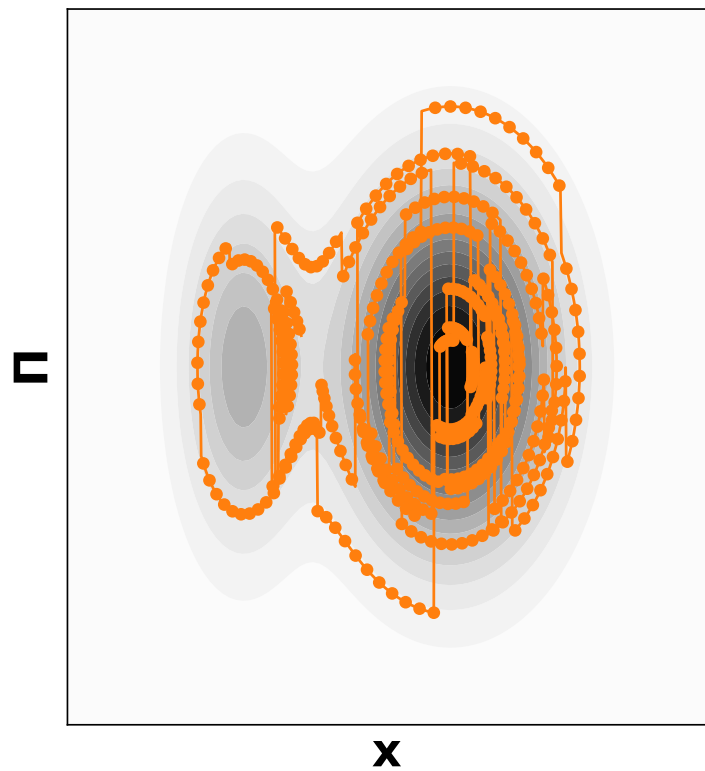


Cosmological
Field-Level Inference
with
**Microcanonical
Langevin Monte Carlo**

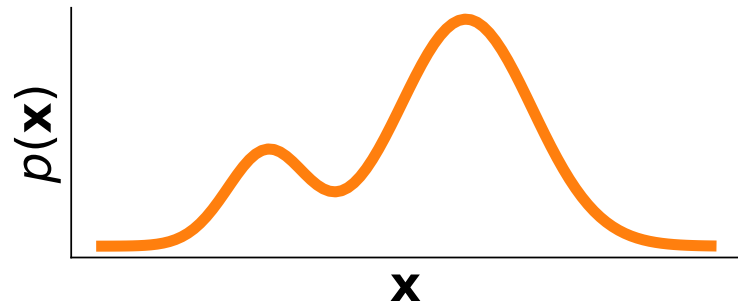
Canonical HMC



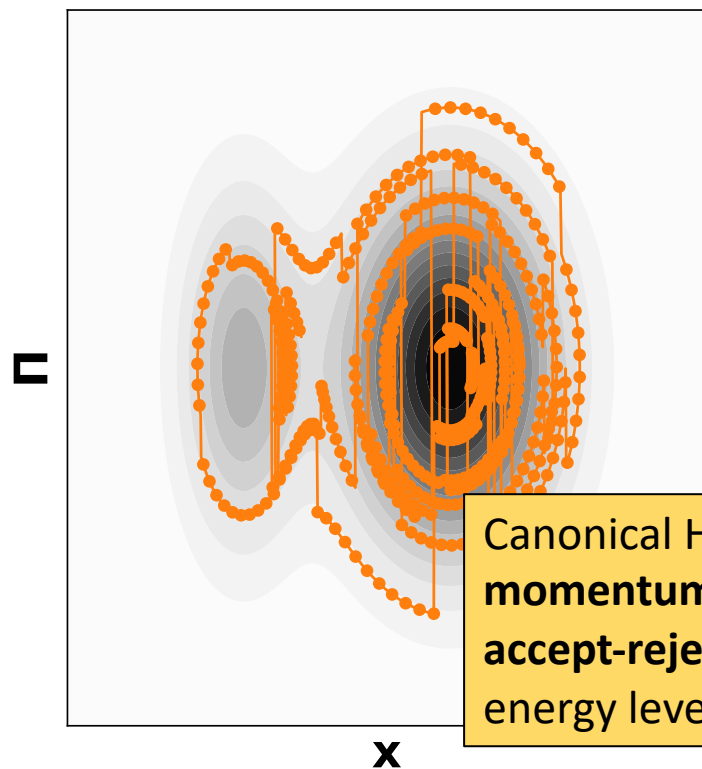
$$p(\mathbf{x}, \boldsymbol{\pi}) \propto e^{-H(\mathbf{x}, \boldsymbol{\pi})}$$



Canonical HMC

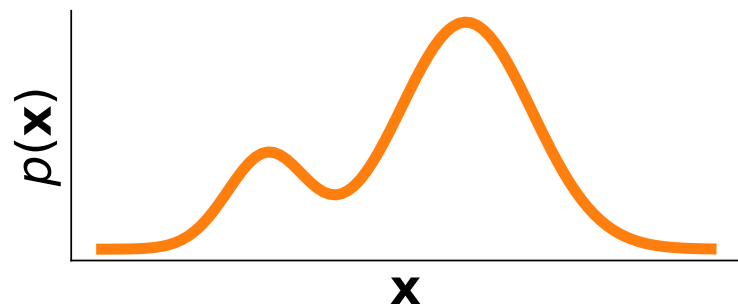


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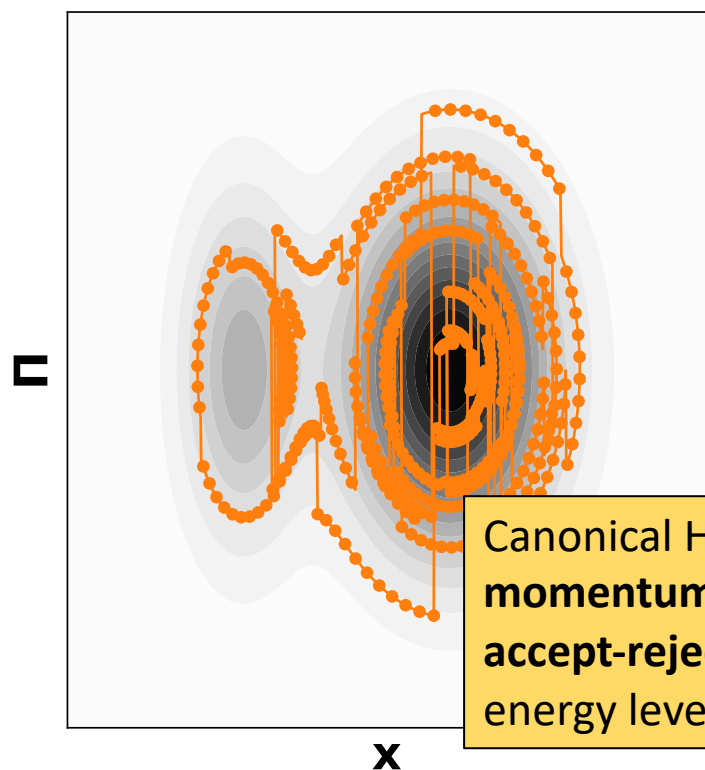


Canonical HMC requires **momentum resampling** and **accept-reject step** to change energy levels and converge

Canonical HMC

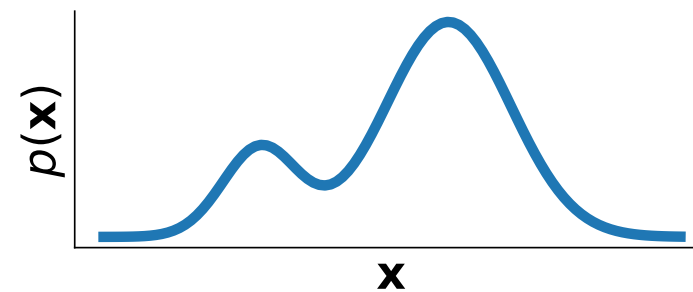


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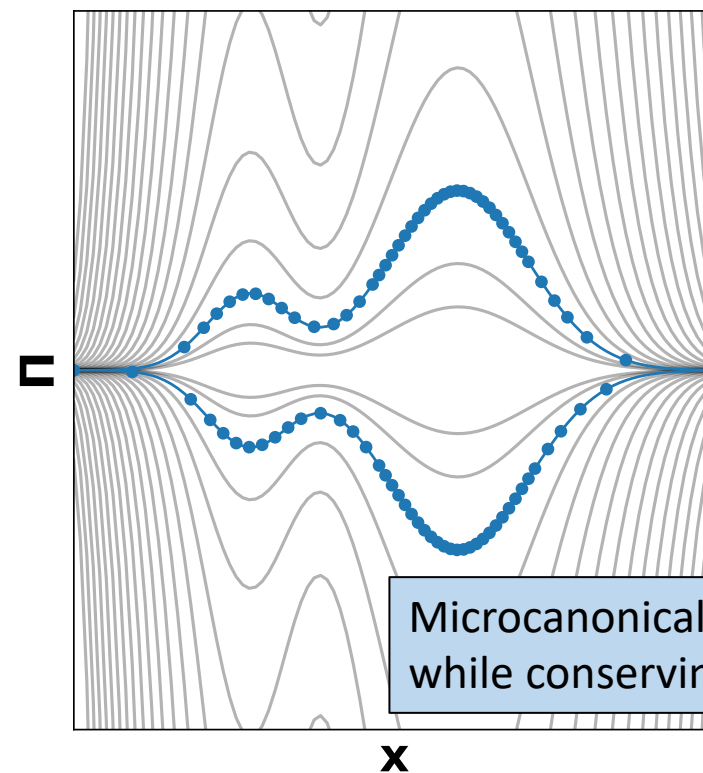


Canonical HMC requires **momentum resampling** and **accept-reject step** to change energy levels and converge

Microcanonical HMC



$$p(\mathbf{x}, \boldsymbol{\Pi}) \propto \delta(H(\mathbf{x}, \boldsymbol{\Pi}) - E)$$



Microcanonical HMC converges while conserving energy

Microcanonical Hamiltonian Monte Carlo

$$dz = u dt$$

$$du = - (d - 1)^{-1} (1 - uu^T) \nabla \mathcal{L}(z)$$

MCHMC

Microcanonical Langevin Monte Carlo

$$dz = u dt$$

$$du = - (d-1)^{-1} (1 - uu^T) [\nabla \mathcal{L}(z) + \eta dW]$$

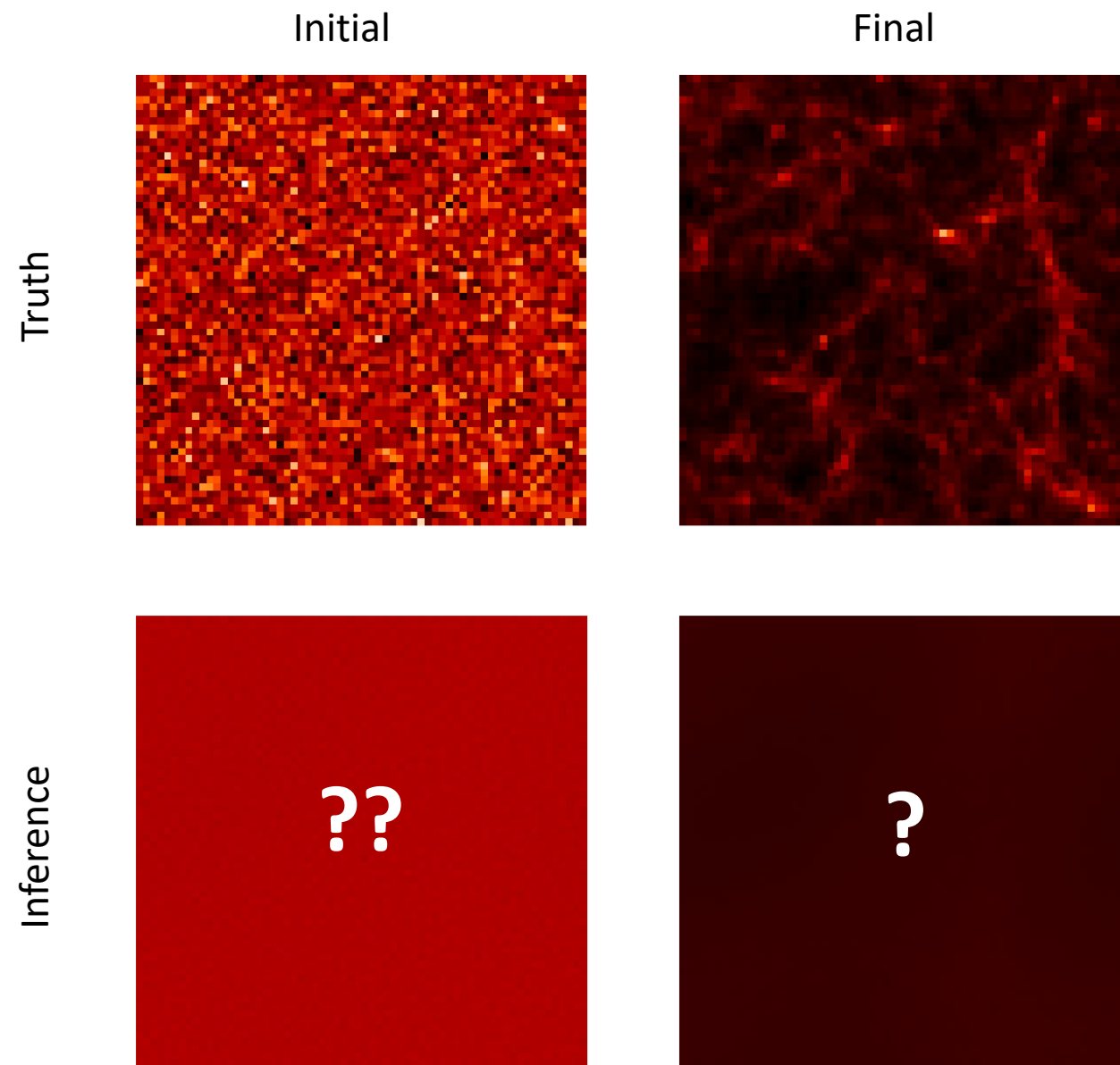
MCHMC

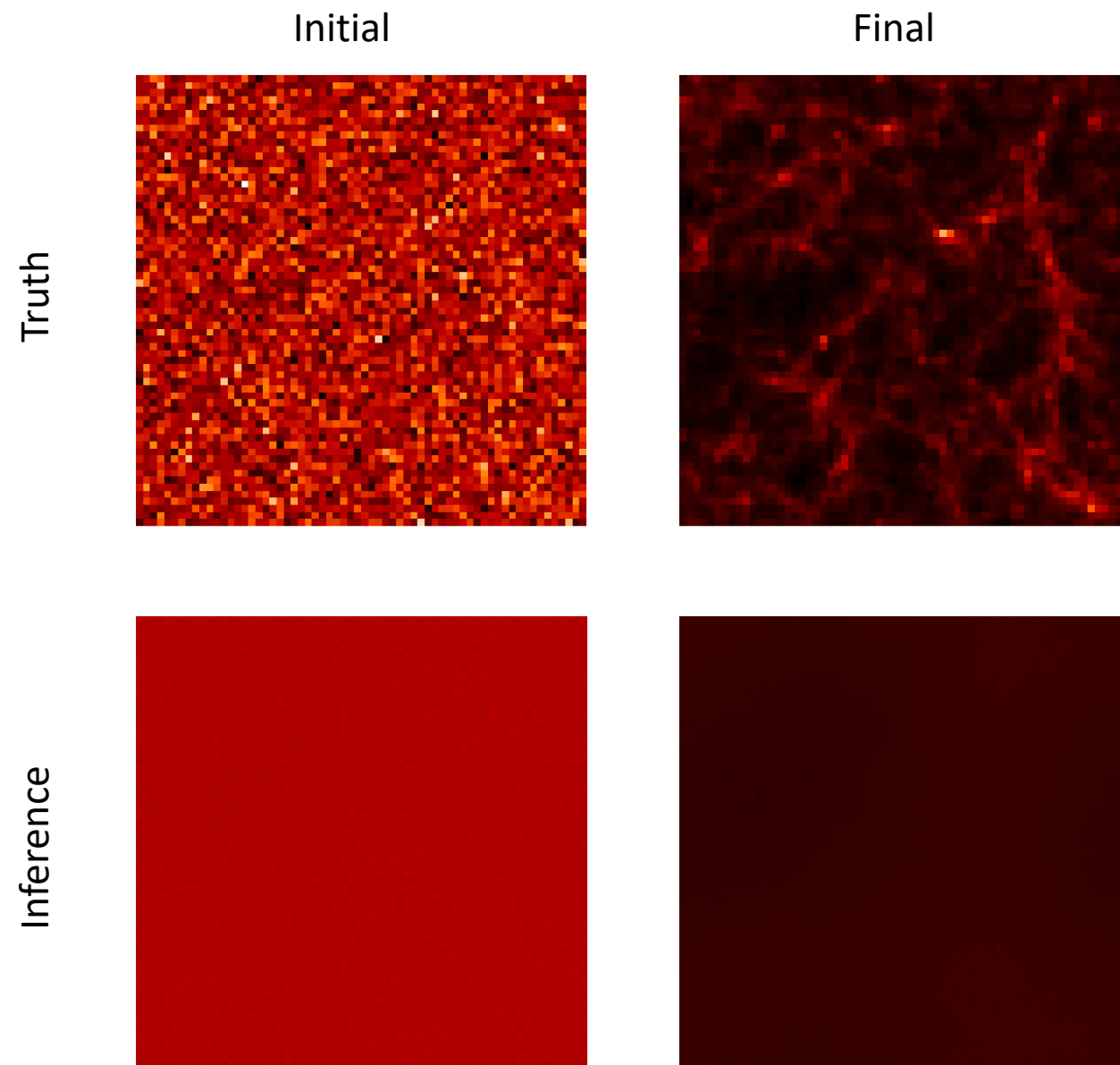
MCLMC

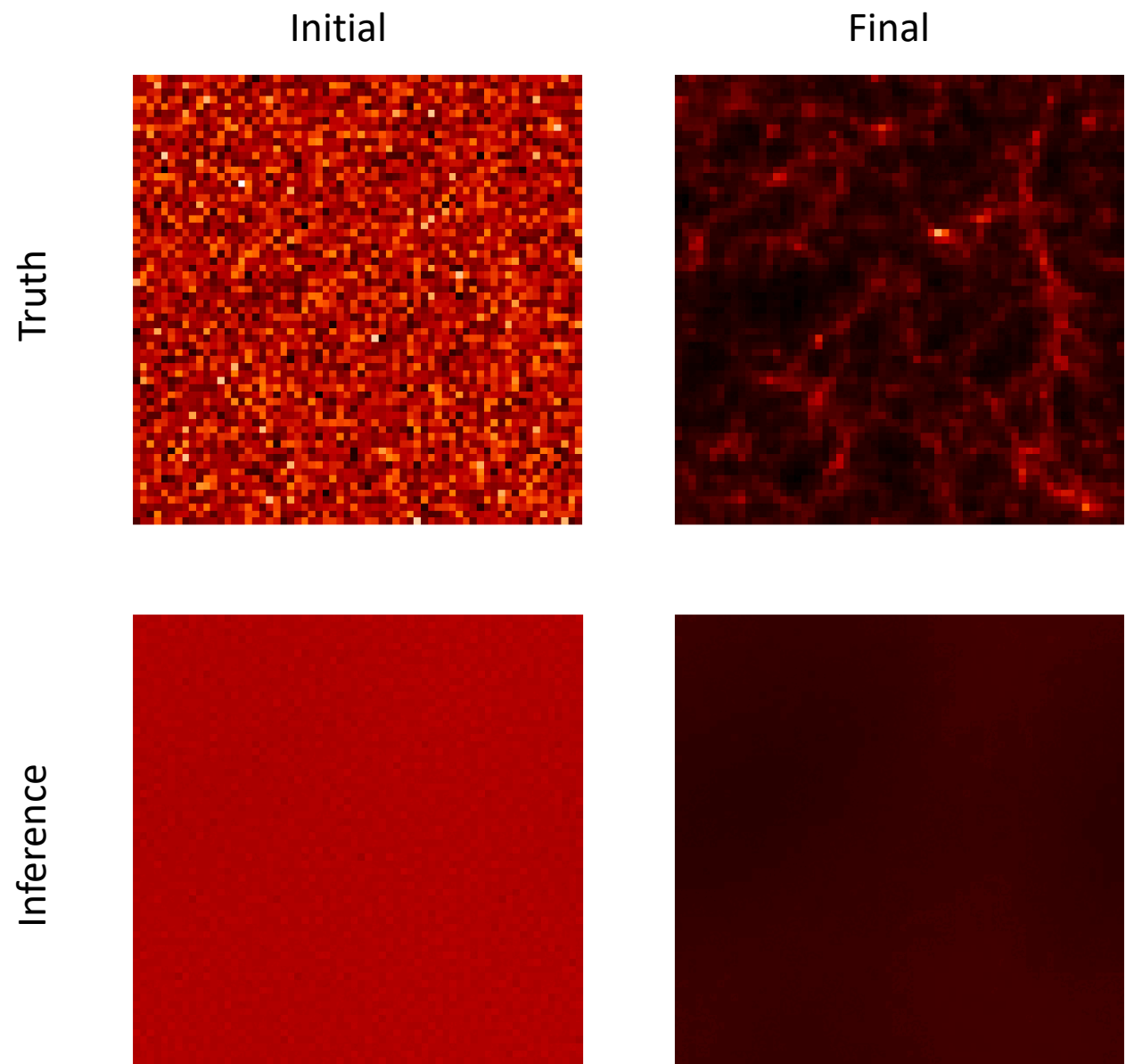
Improve ergodicity by including Langevin-like stochastic term

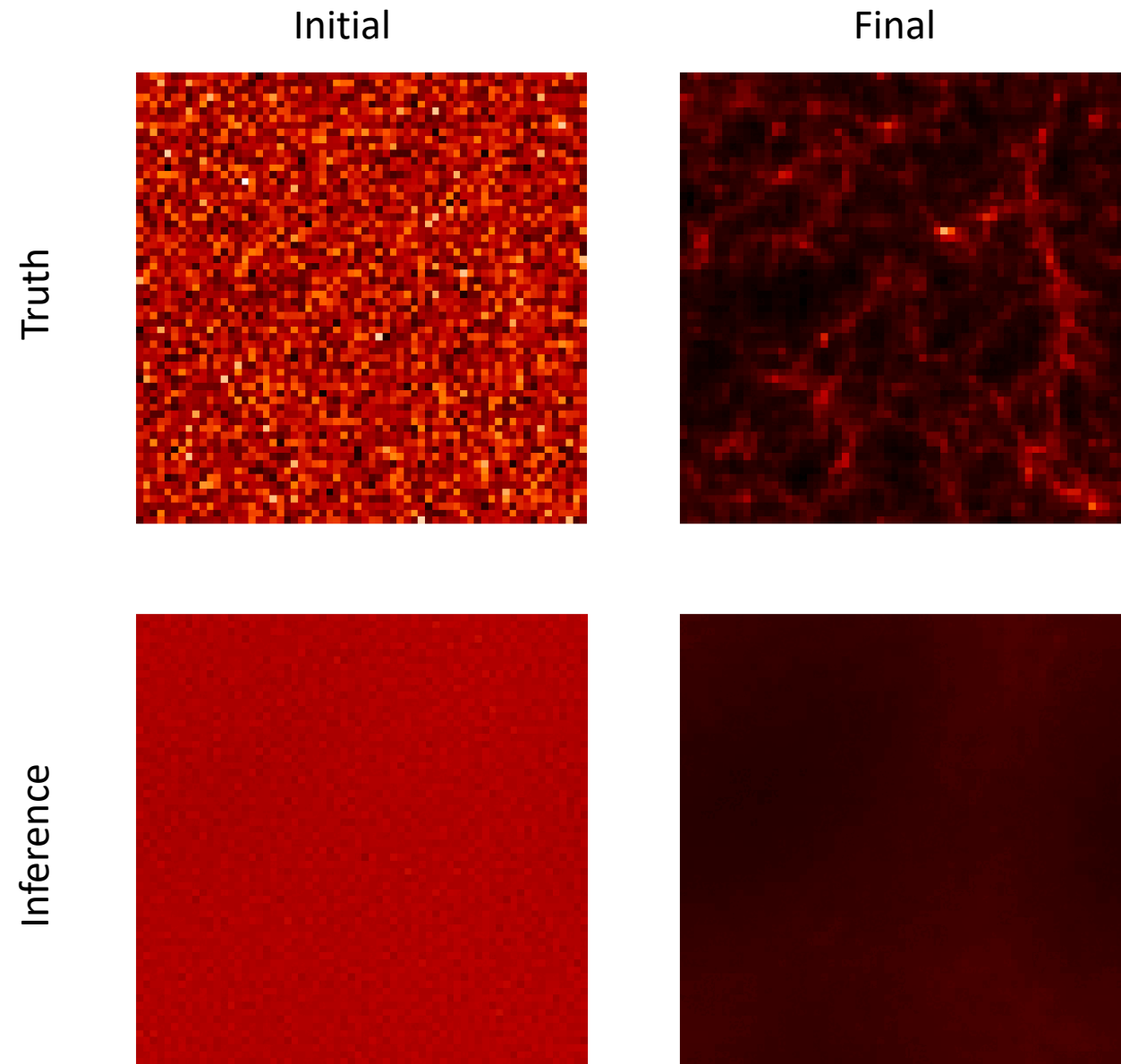


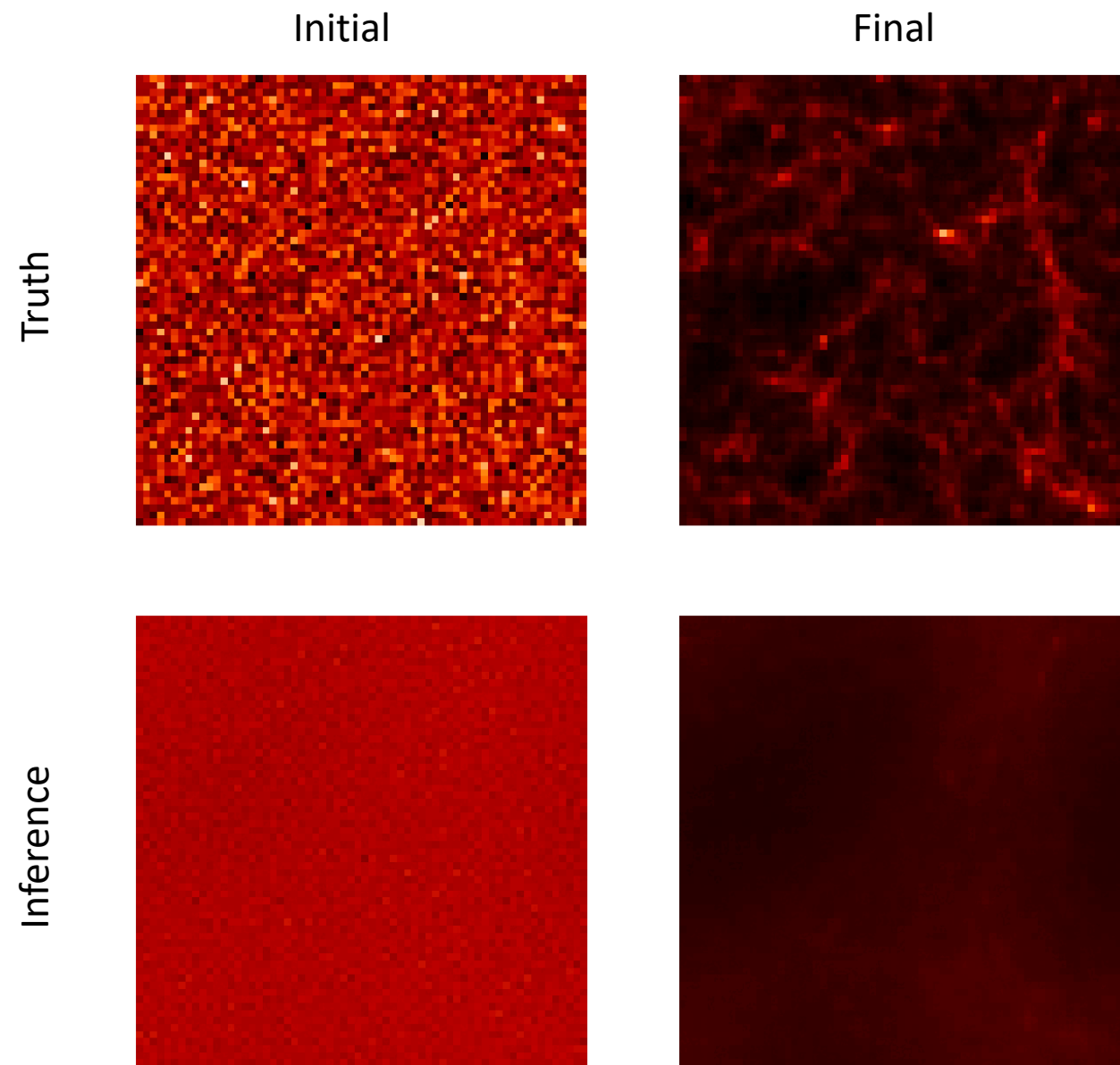
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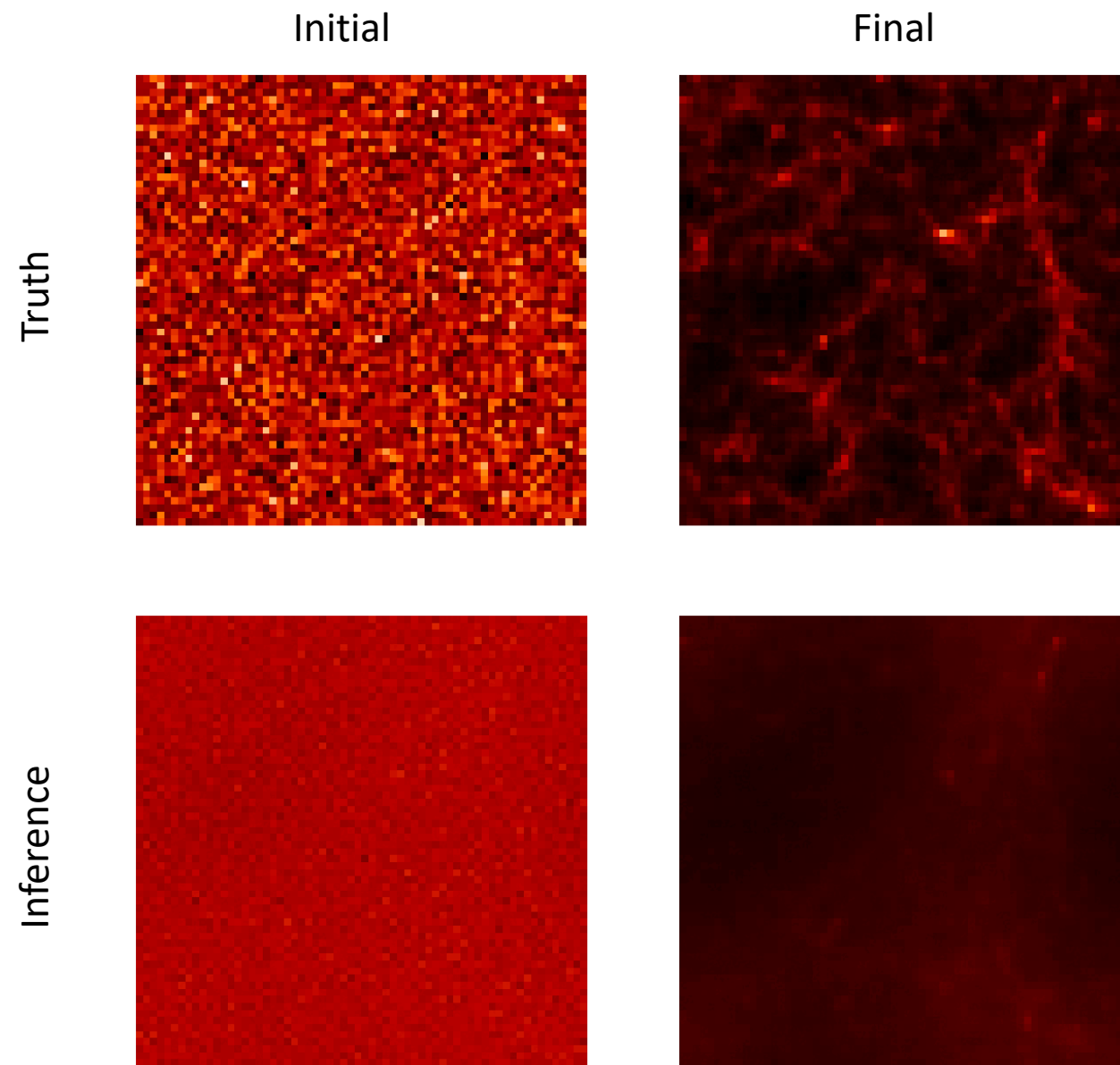


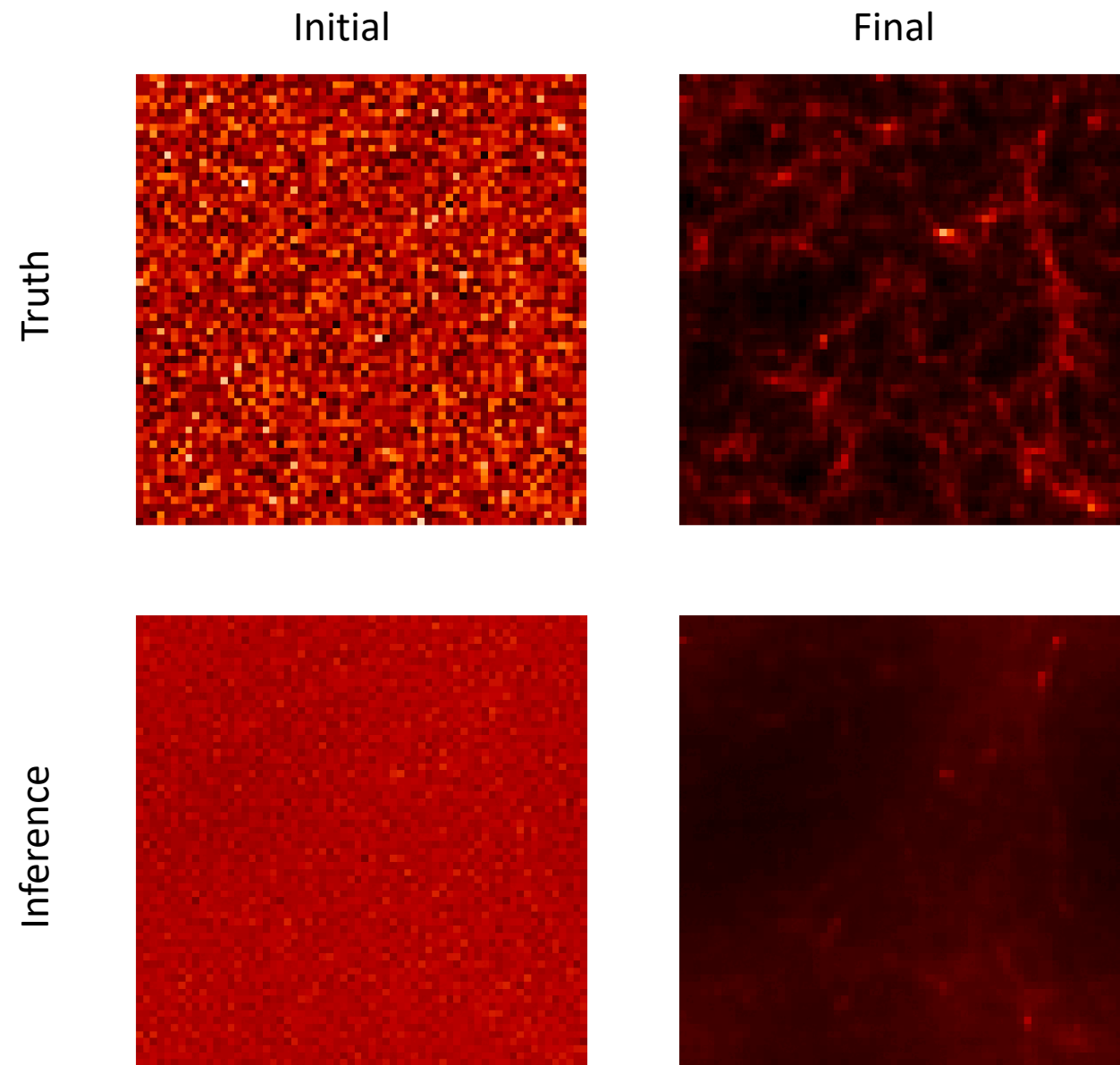


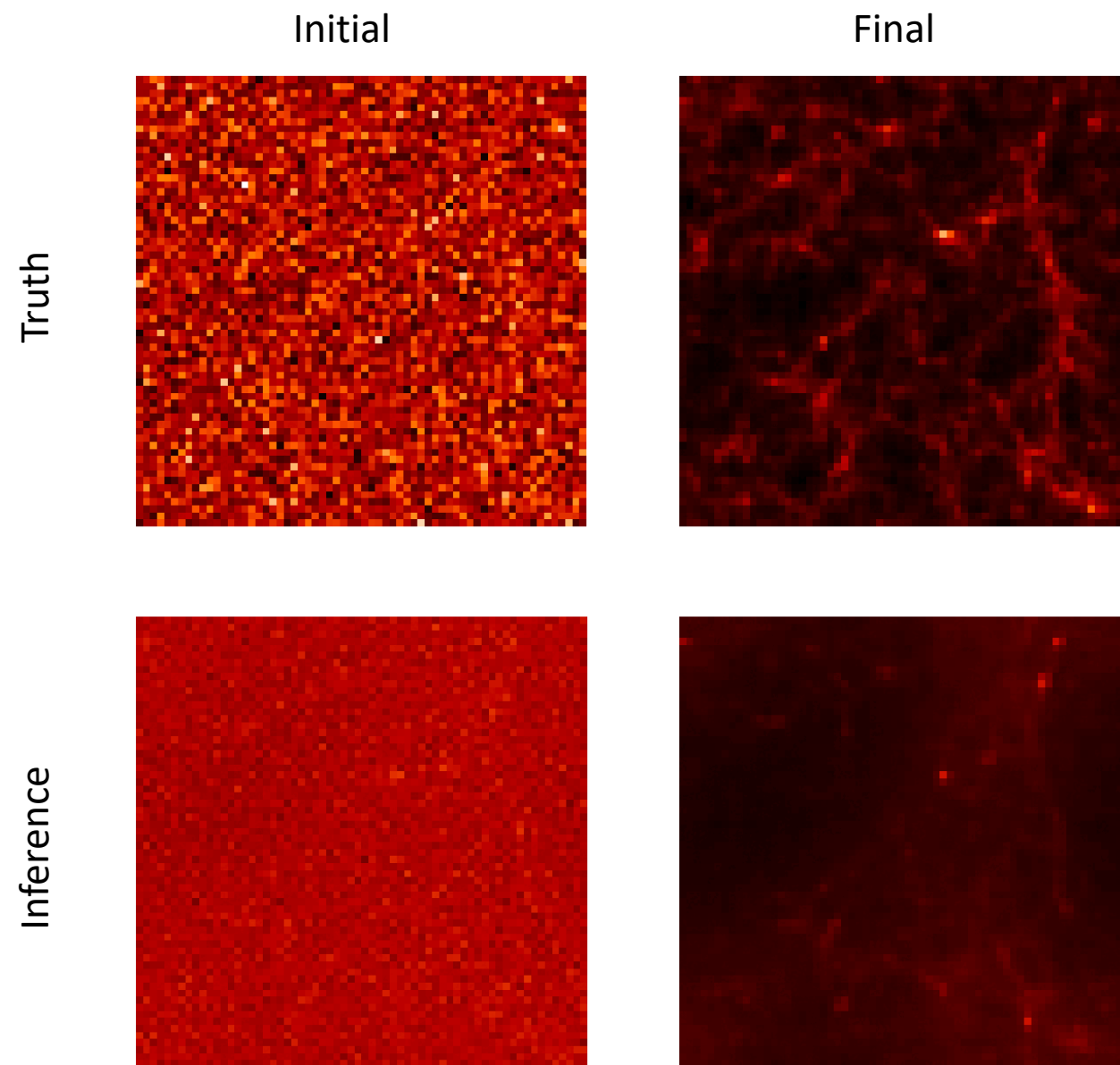


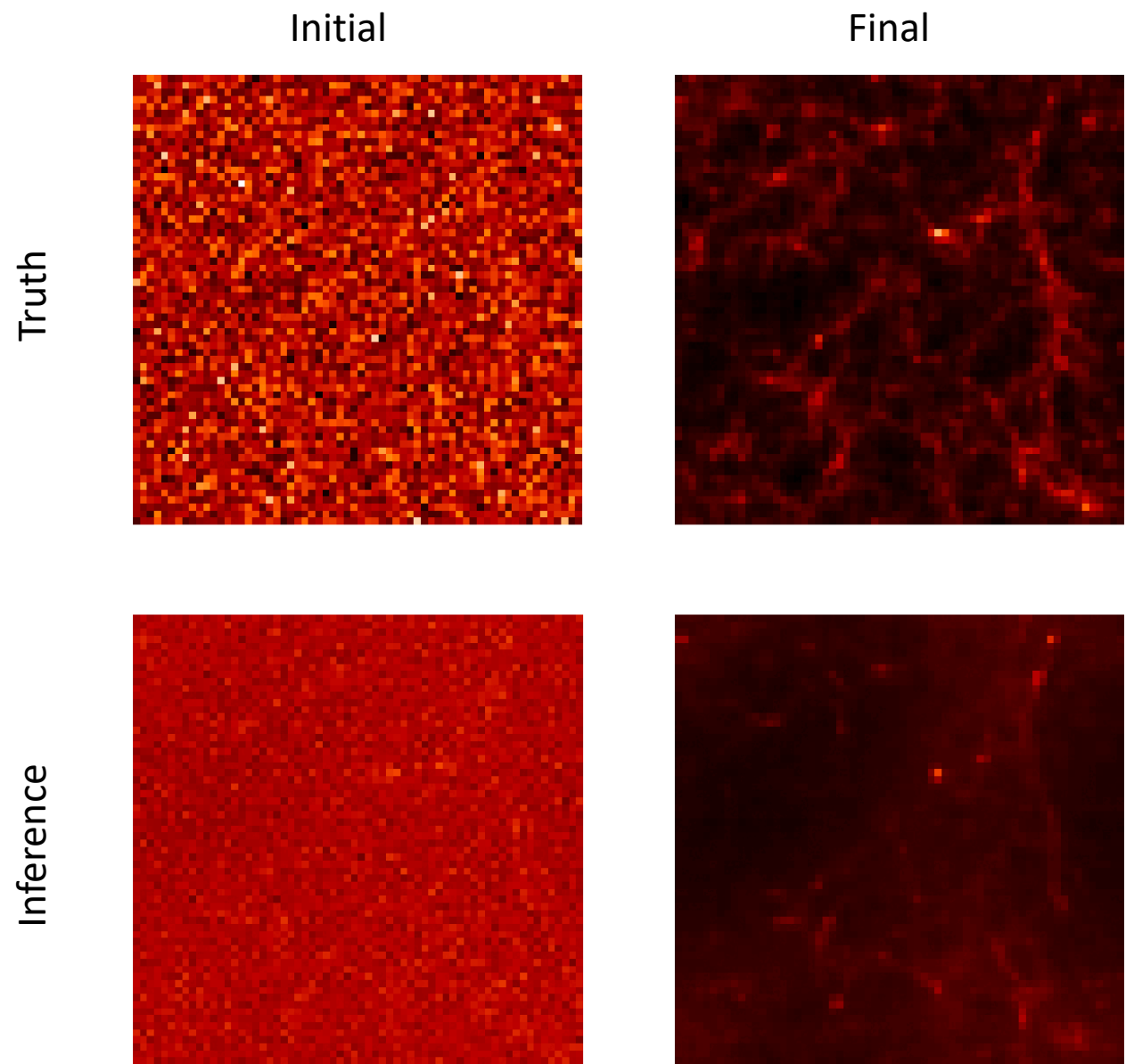


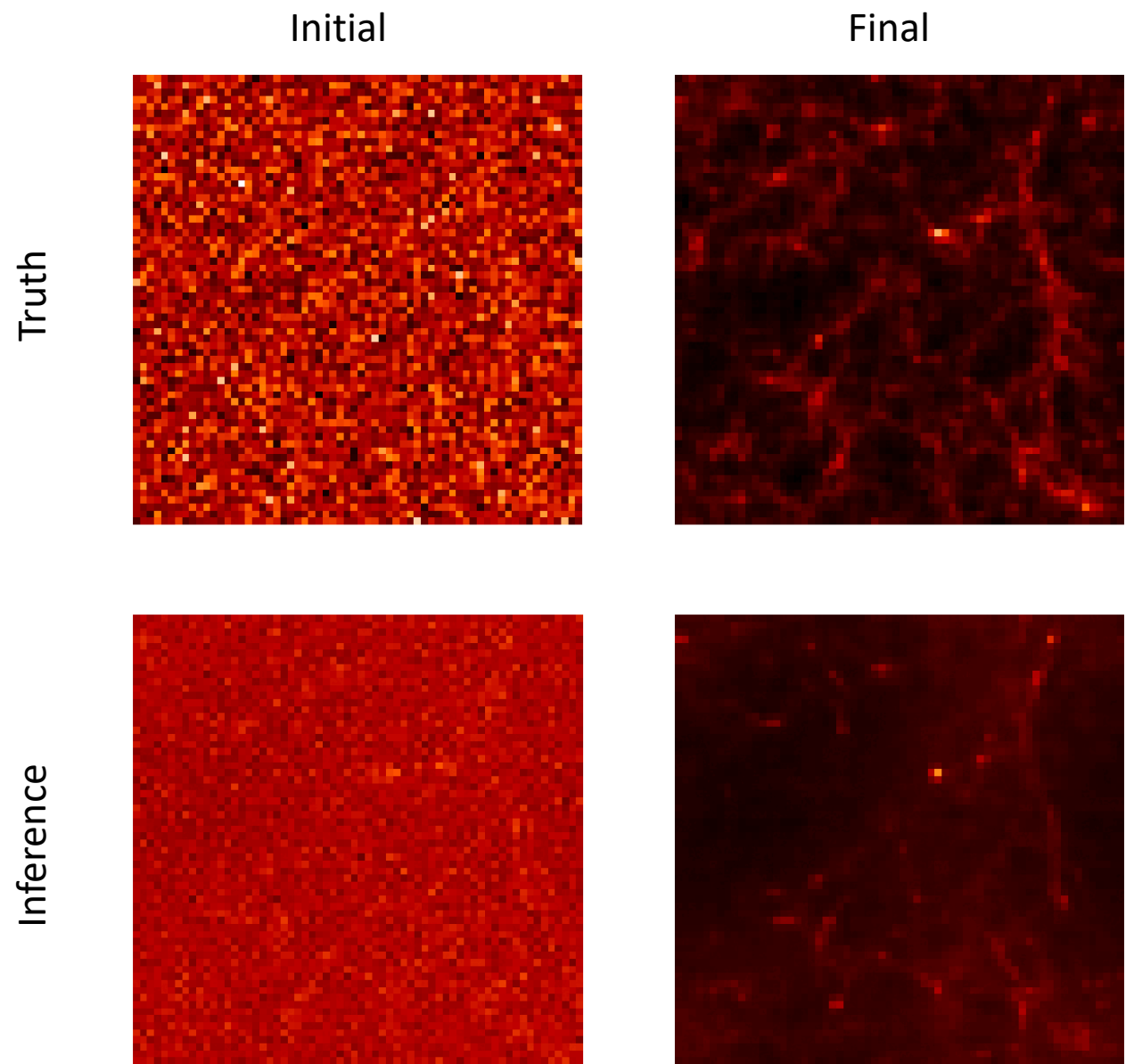


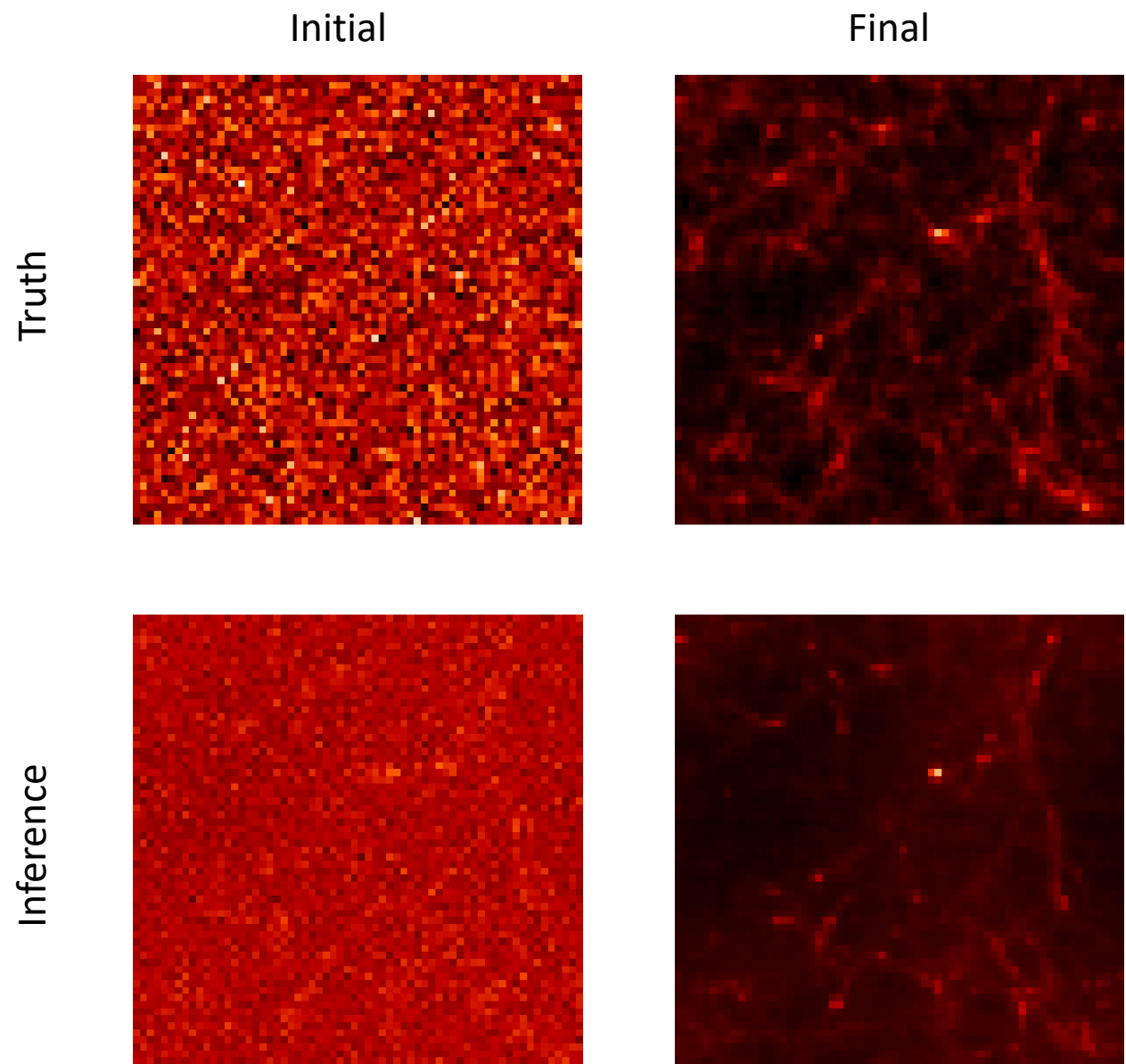


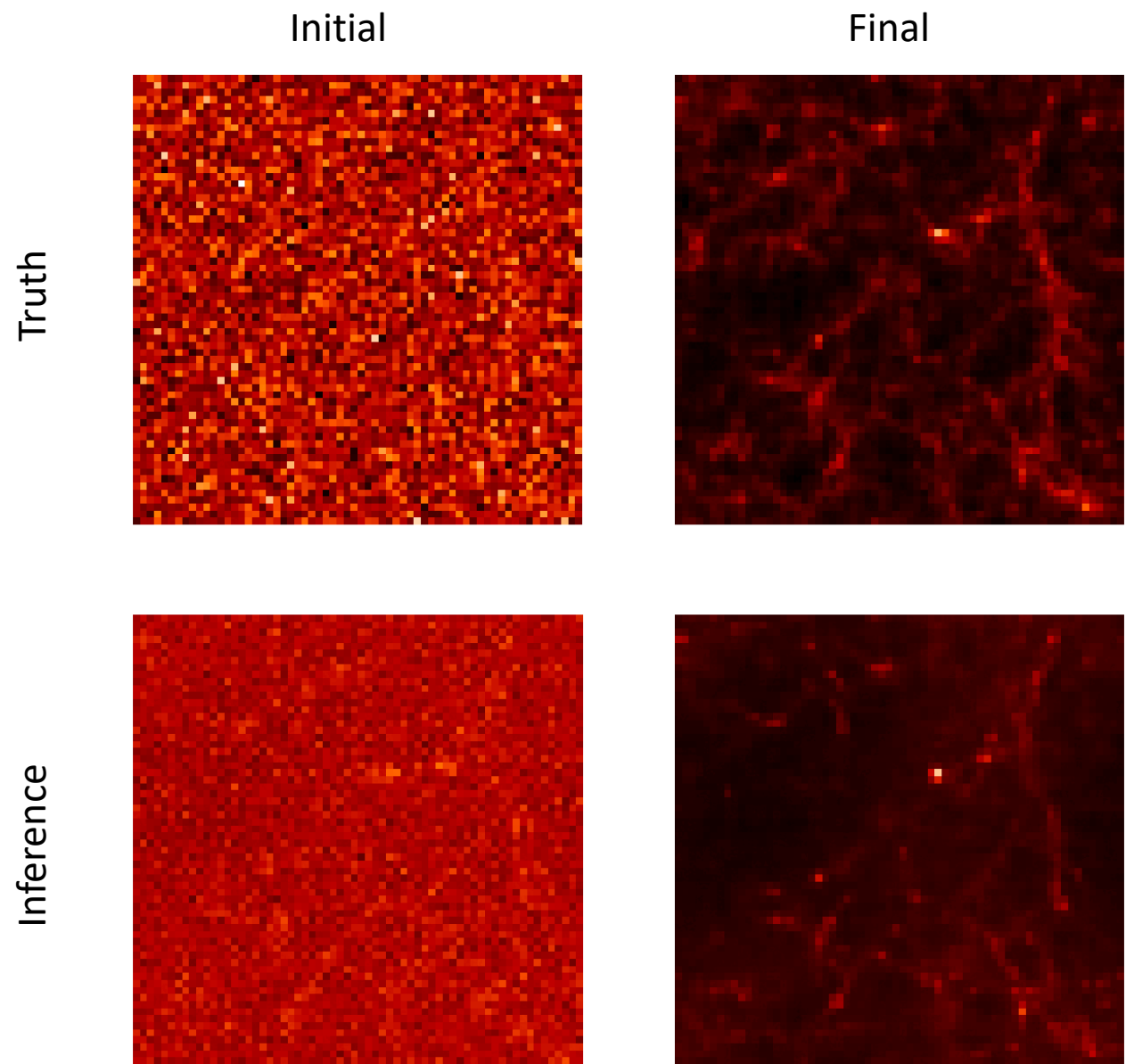


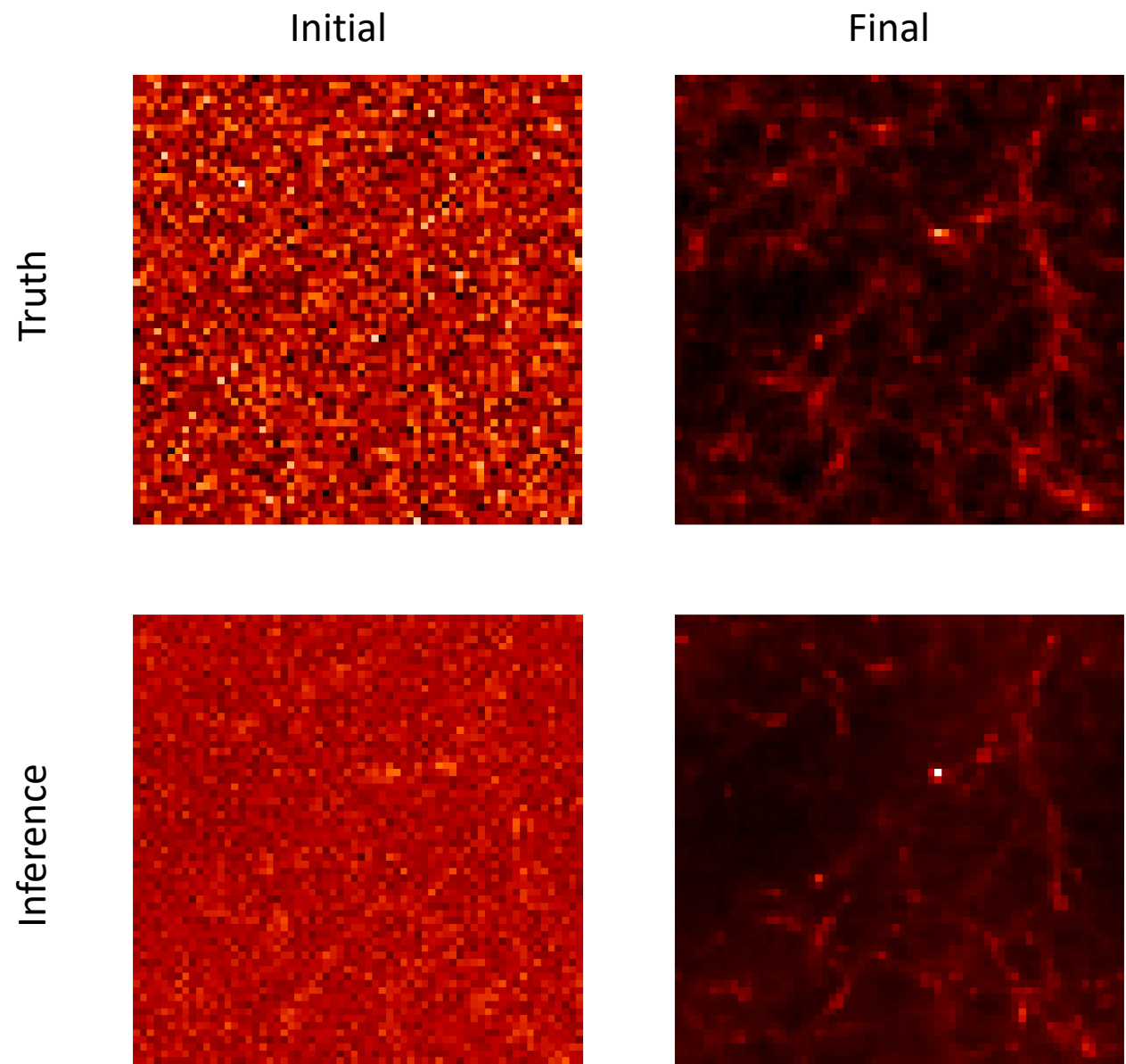


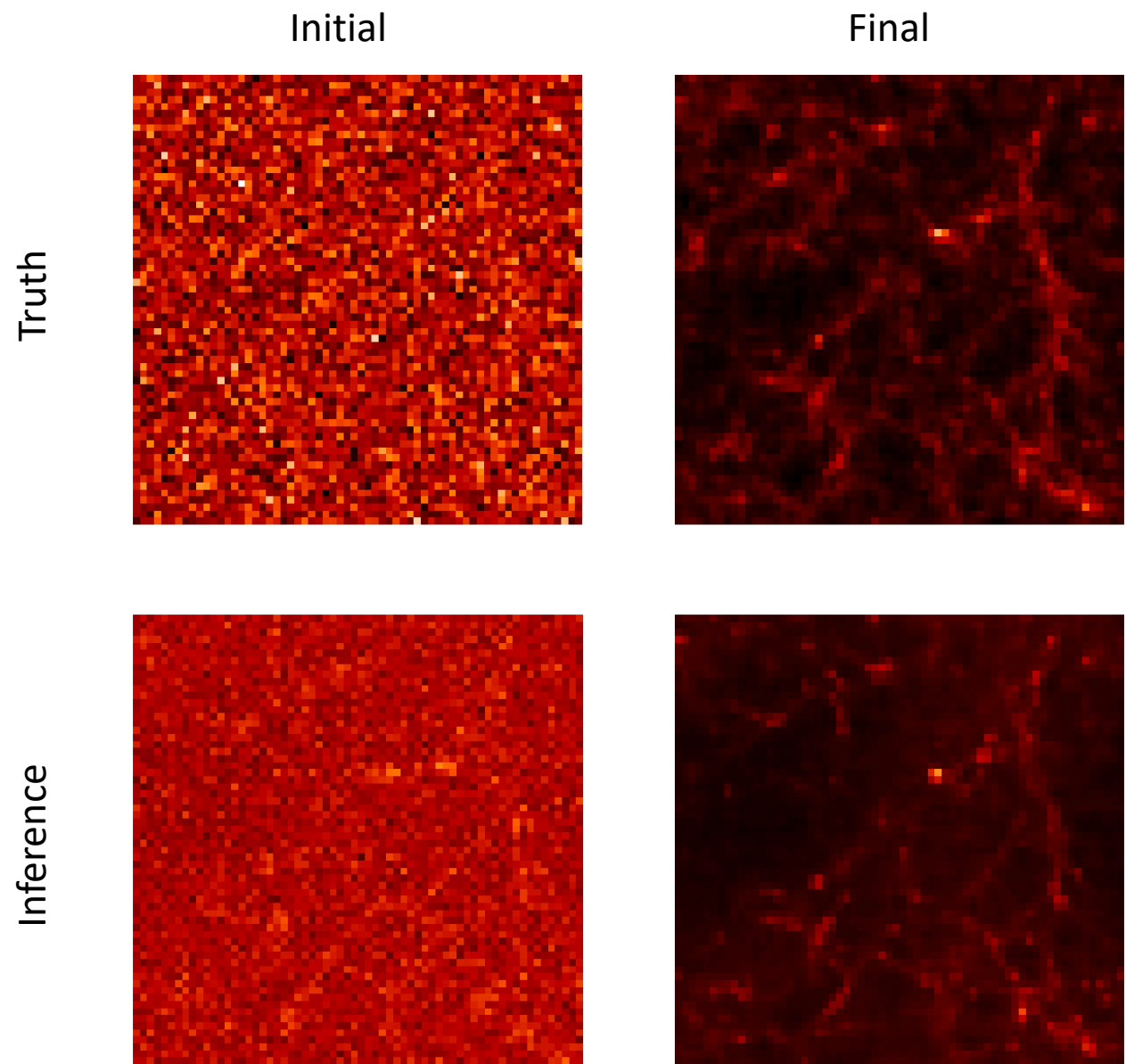


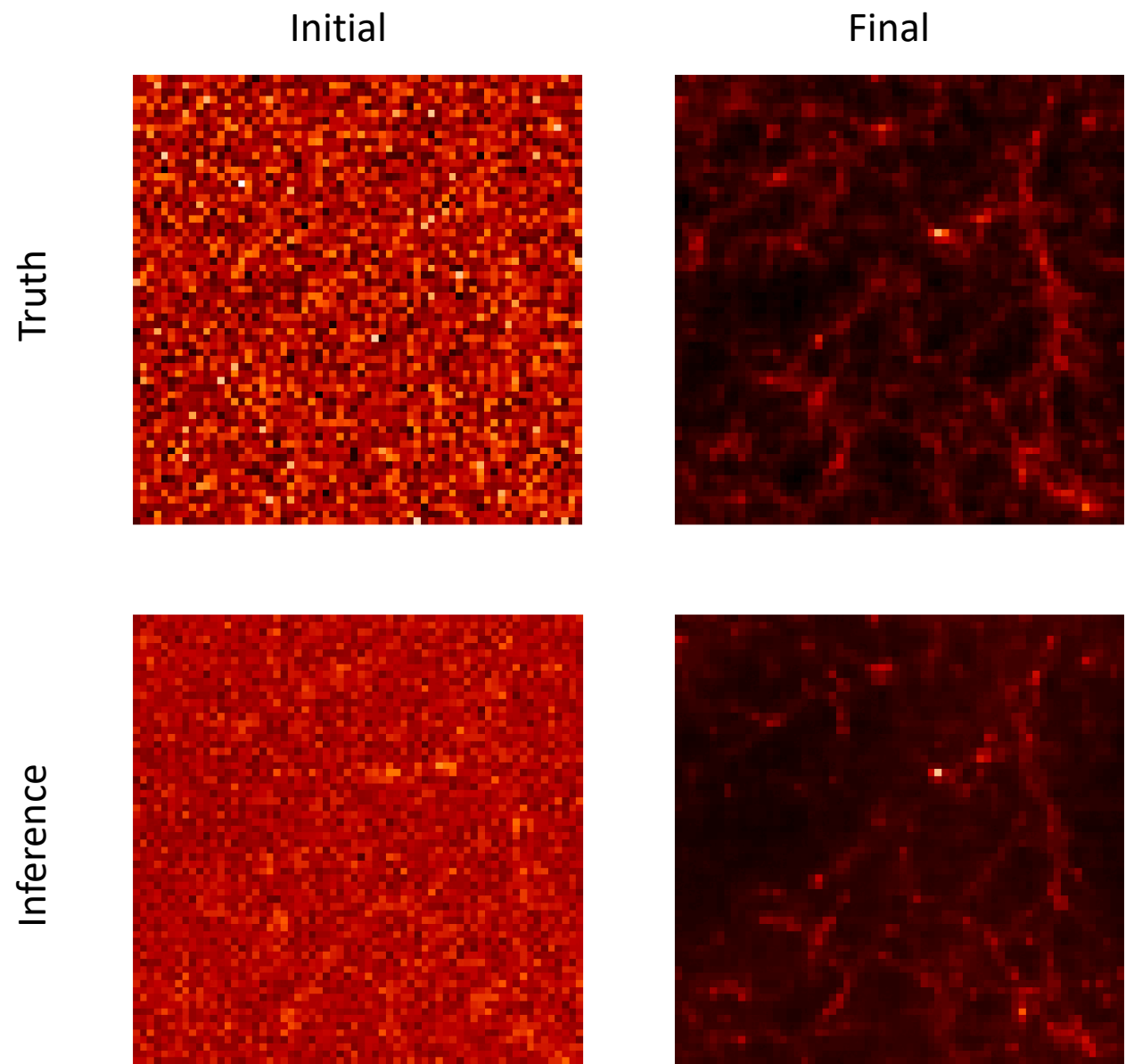


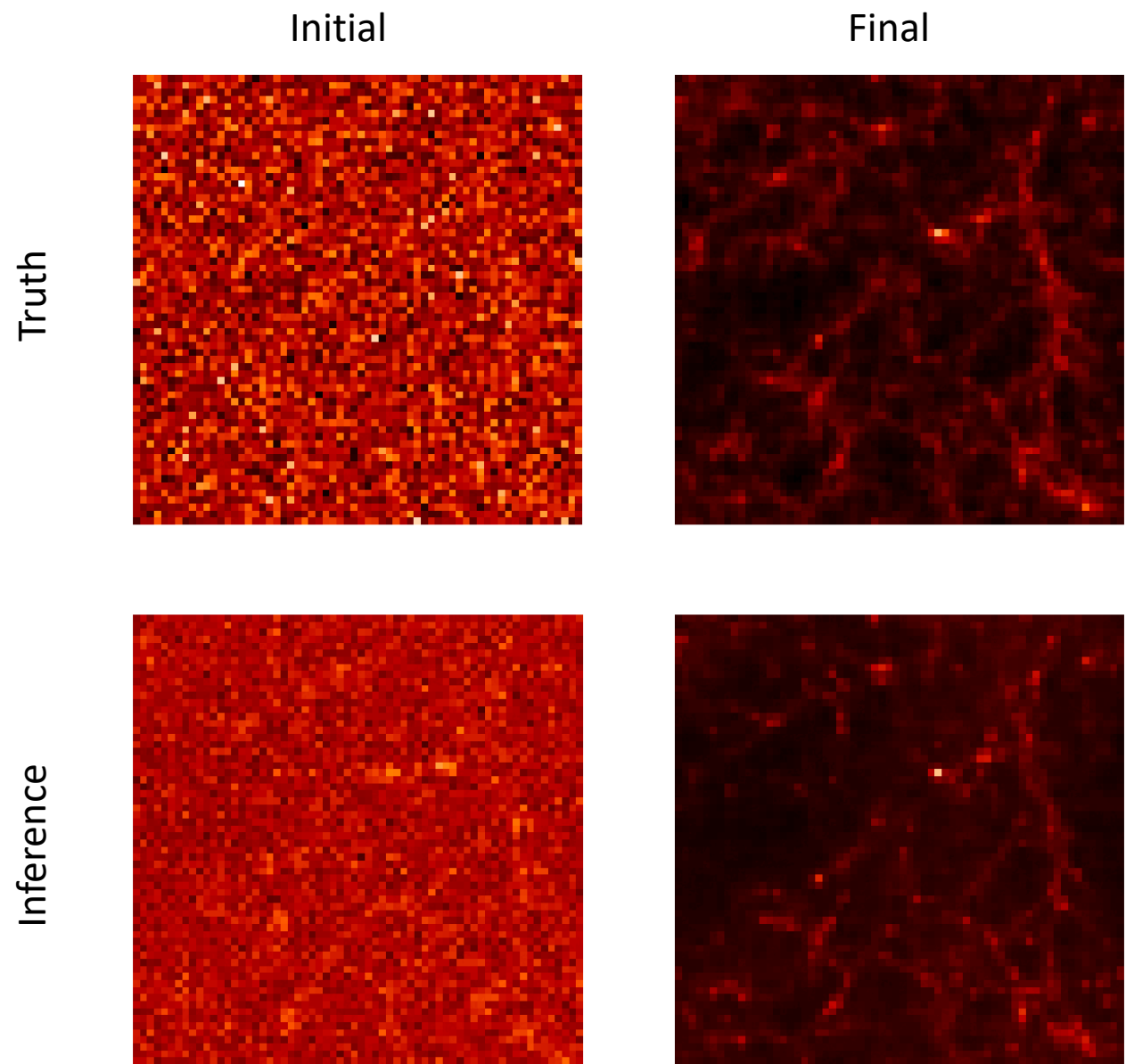


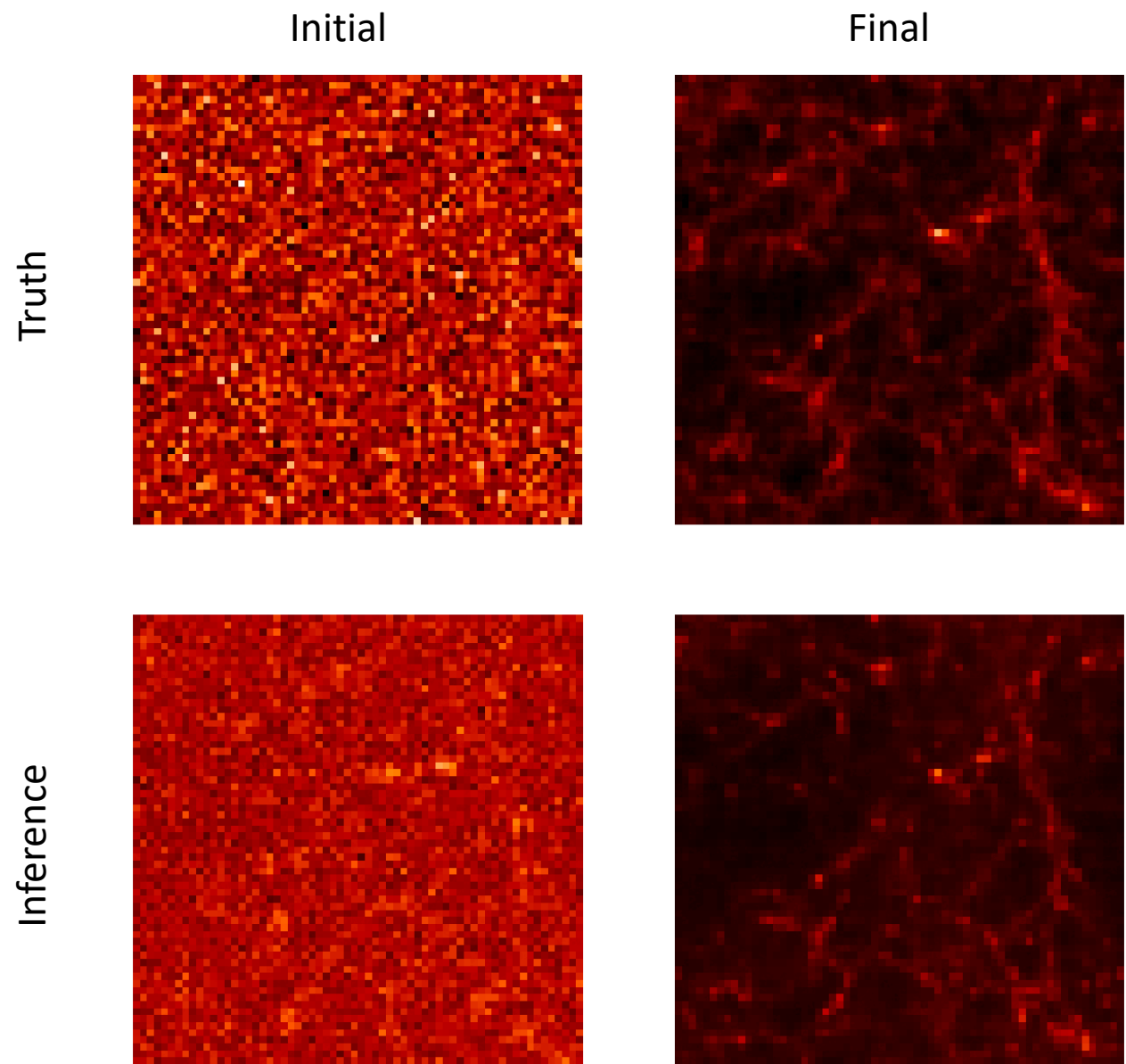


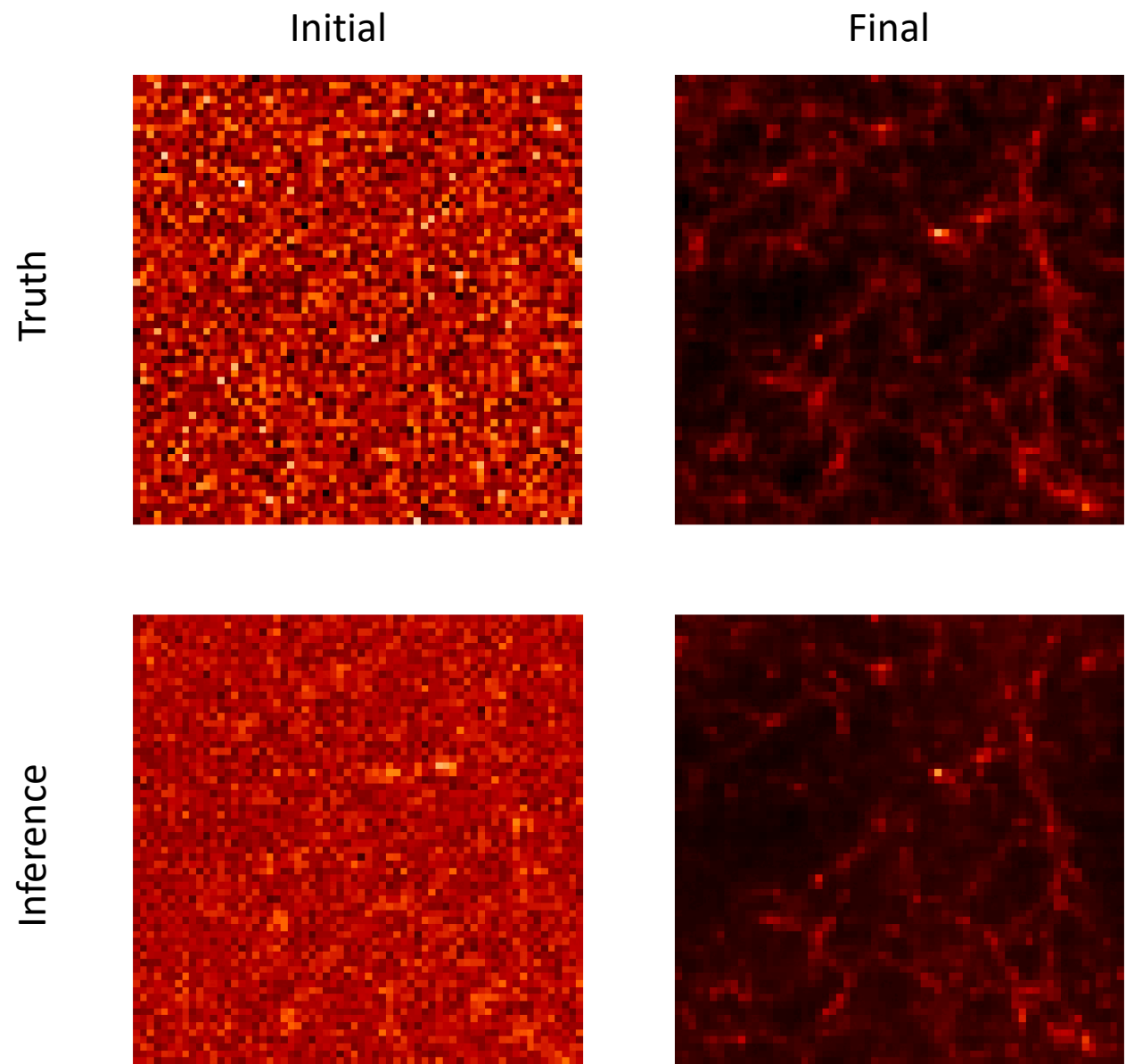


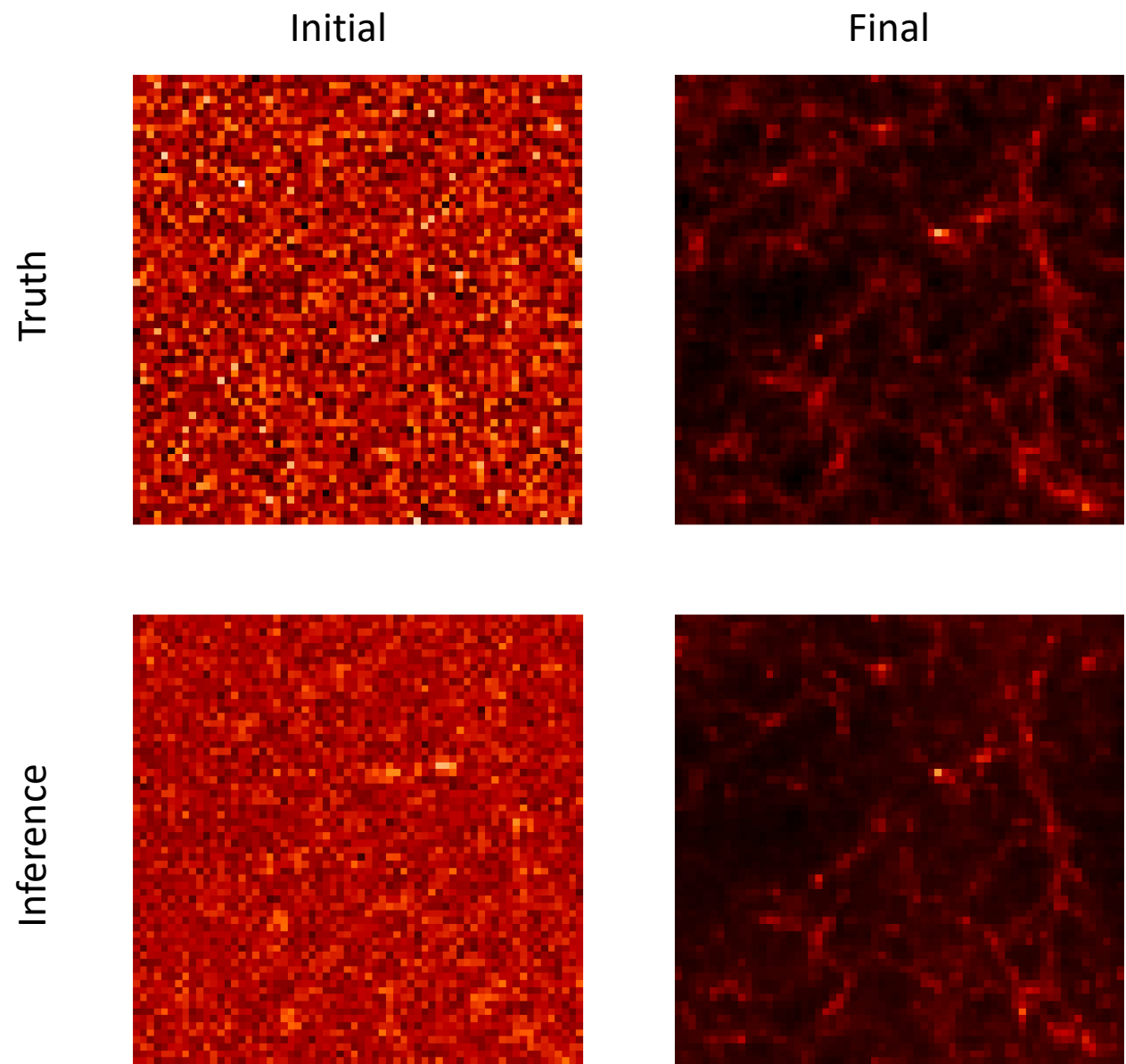


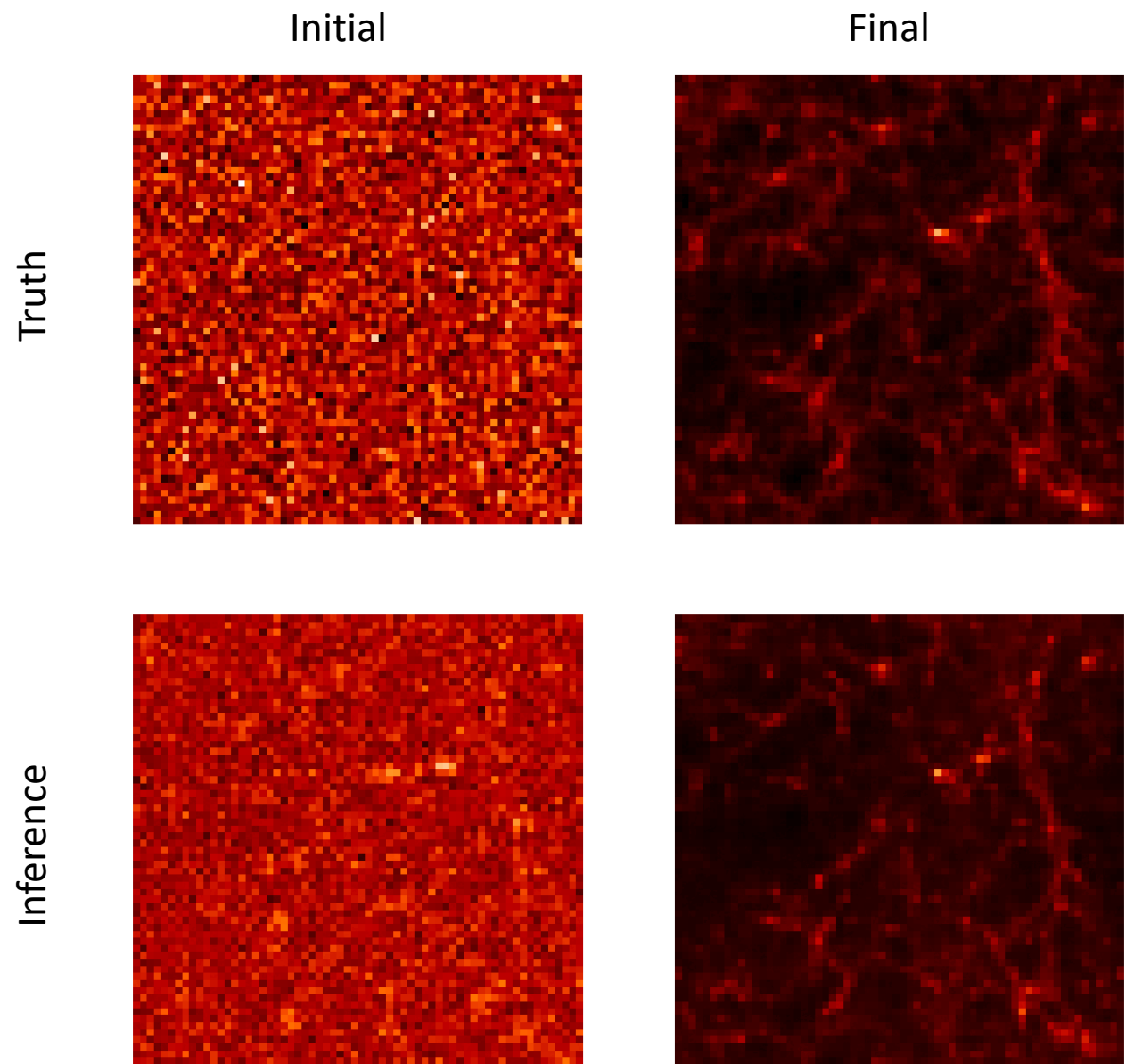


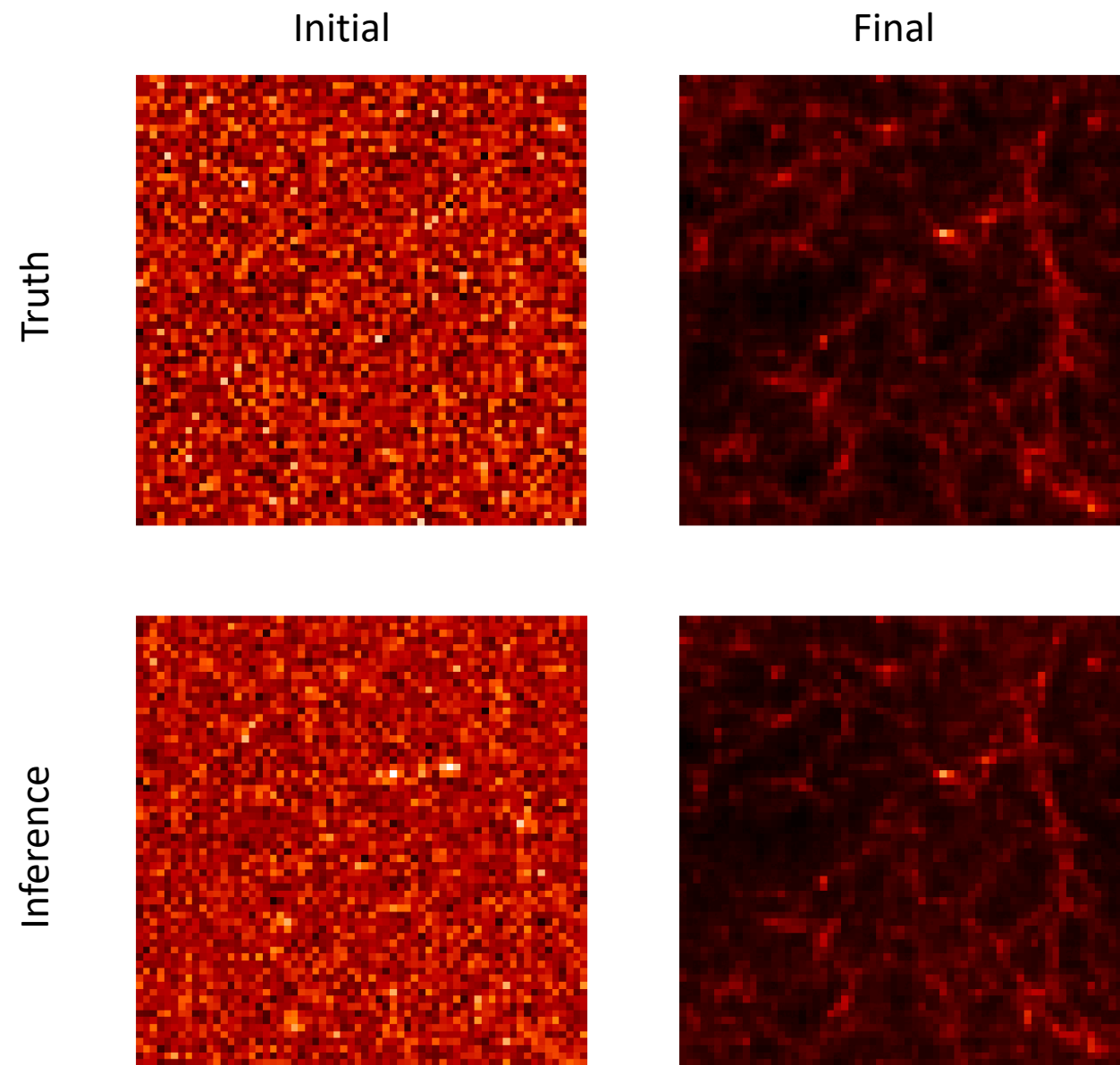


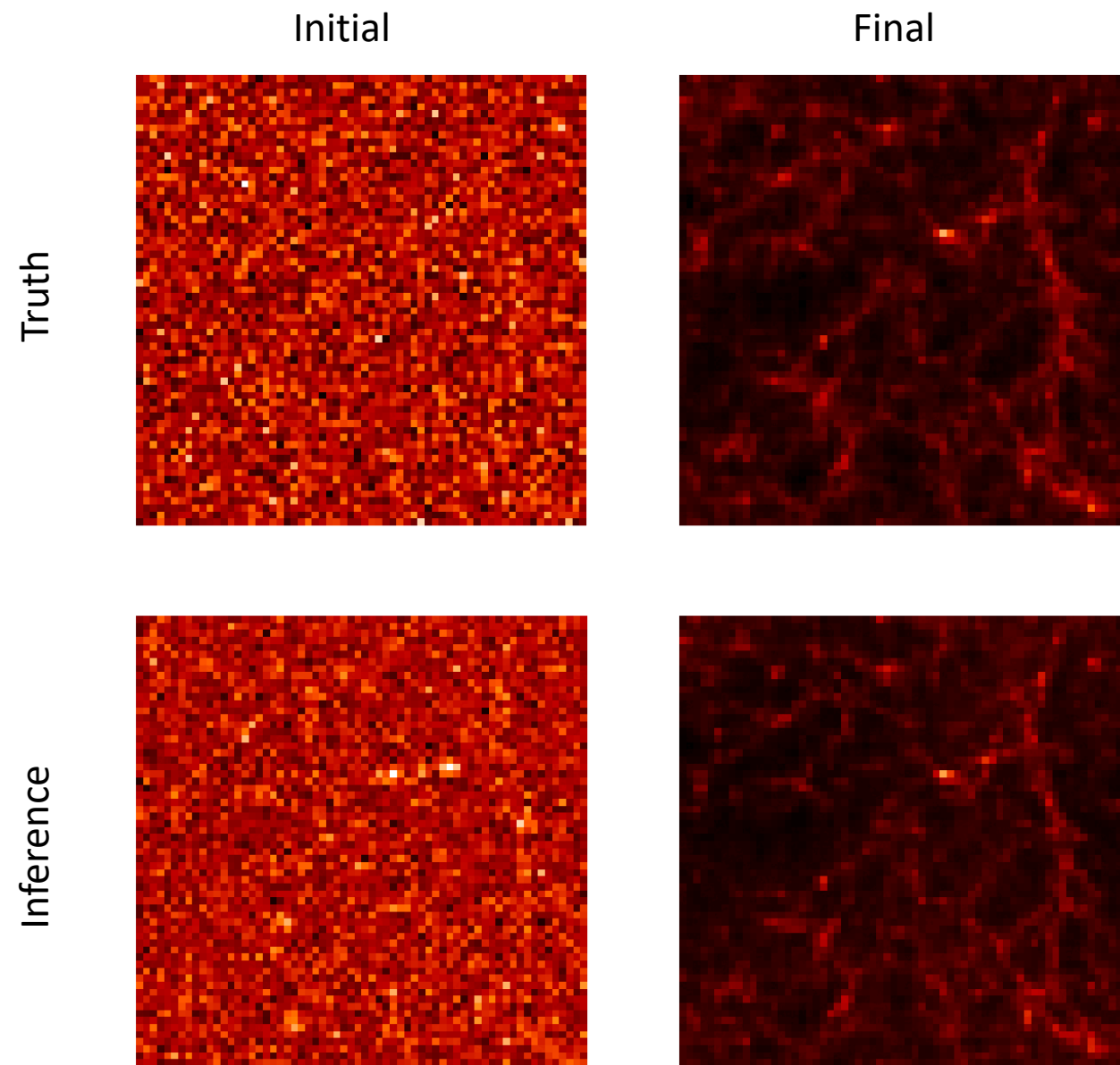


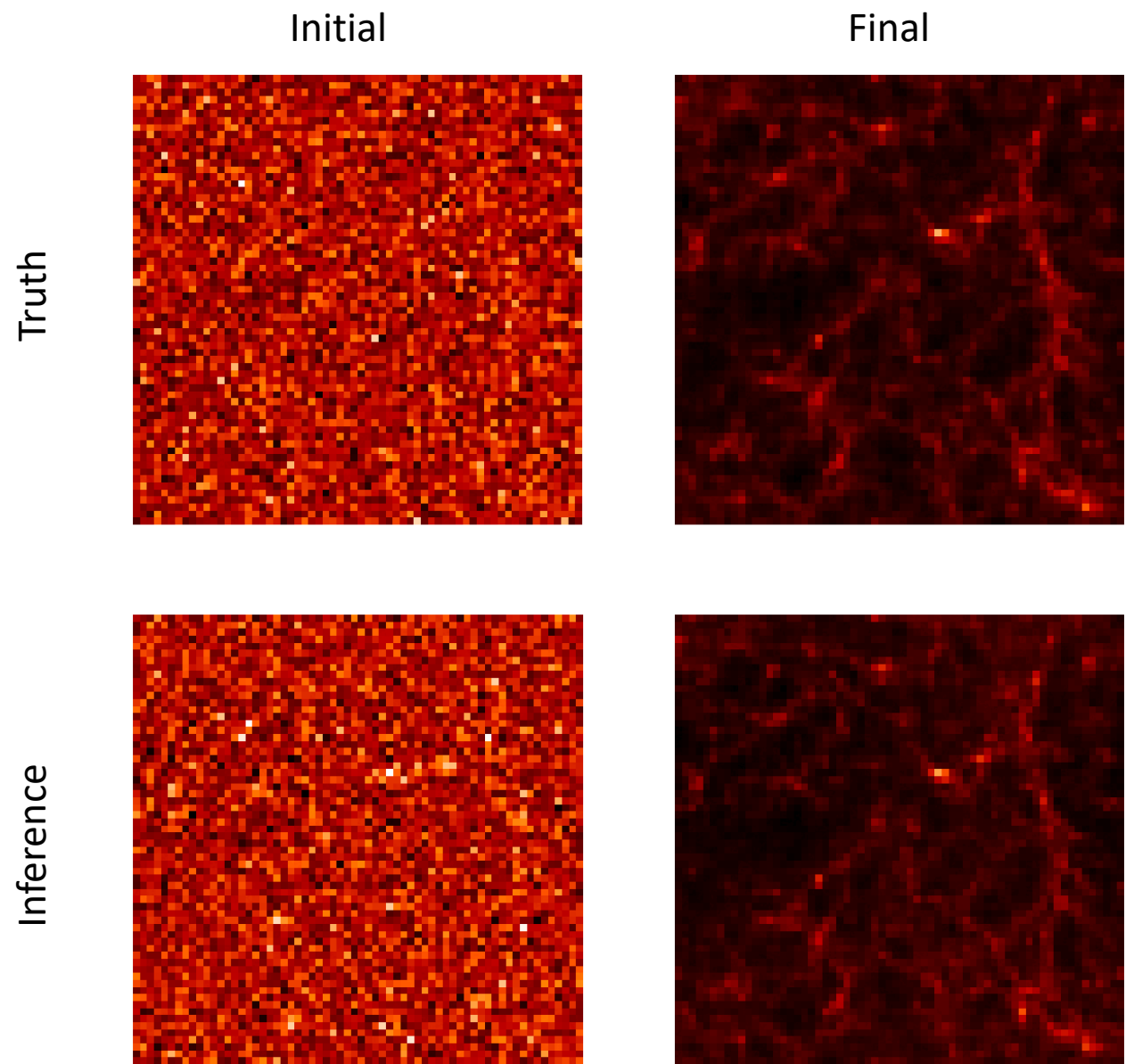


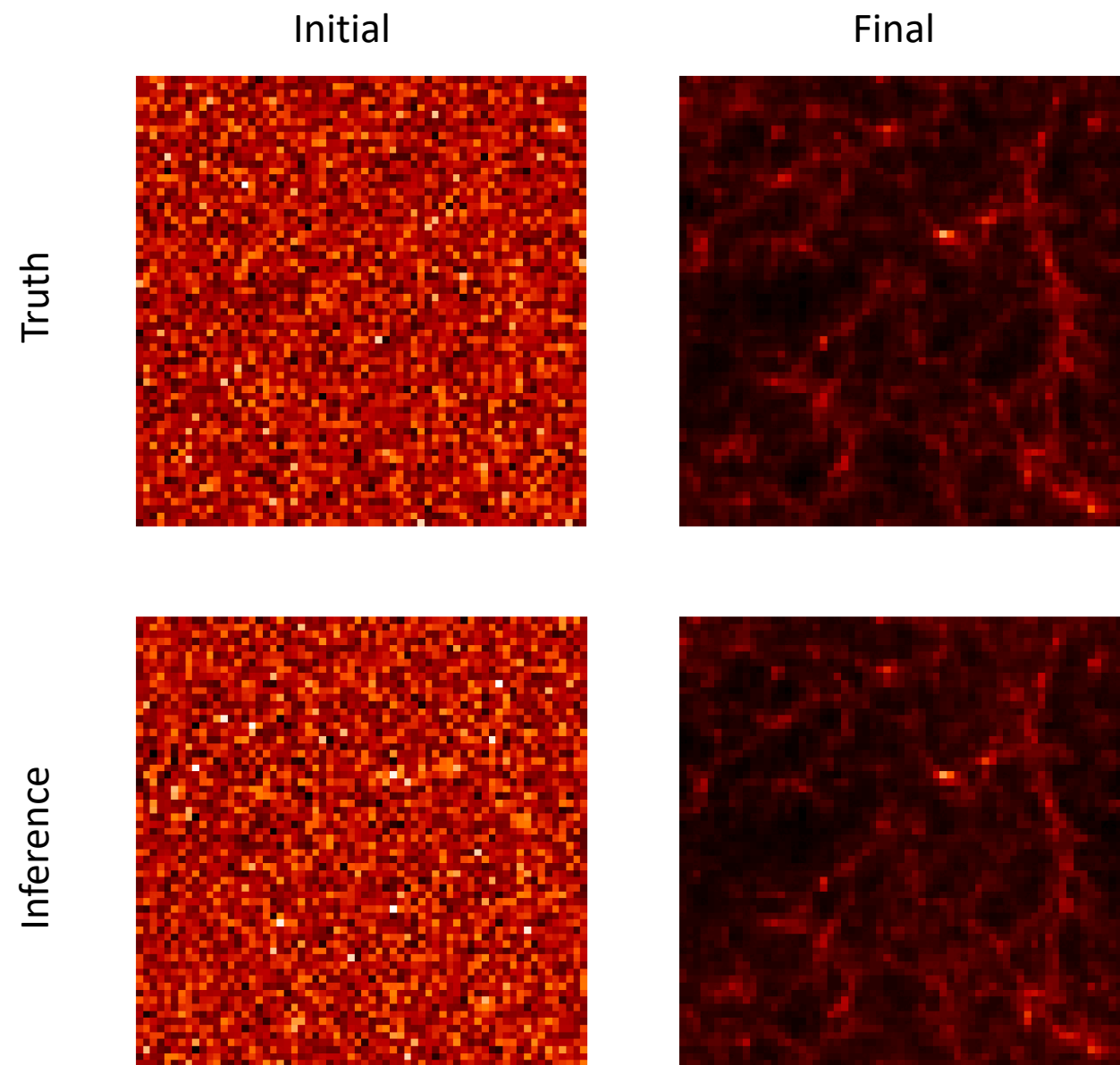


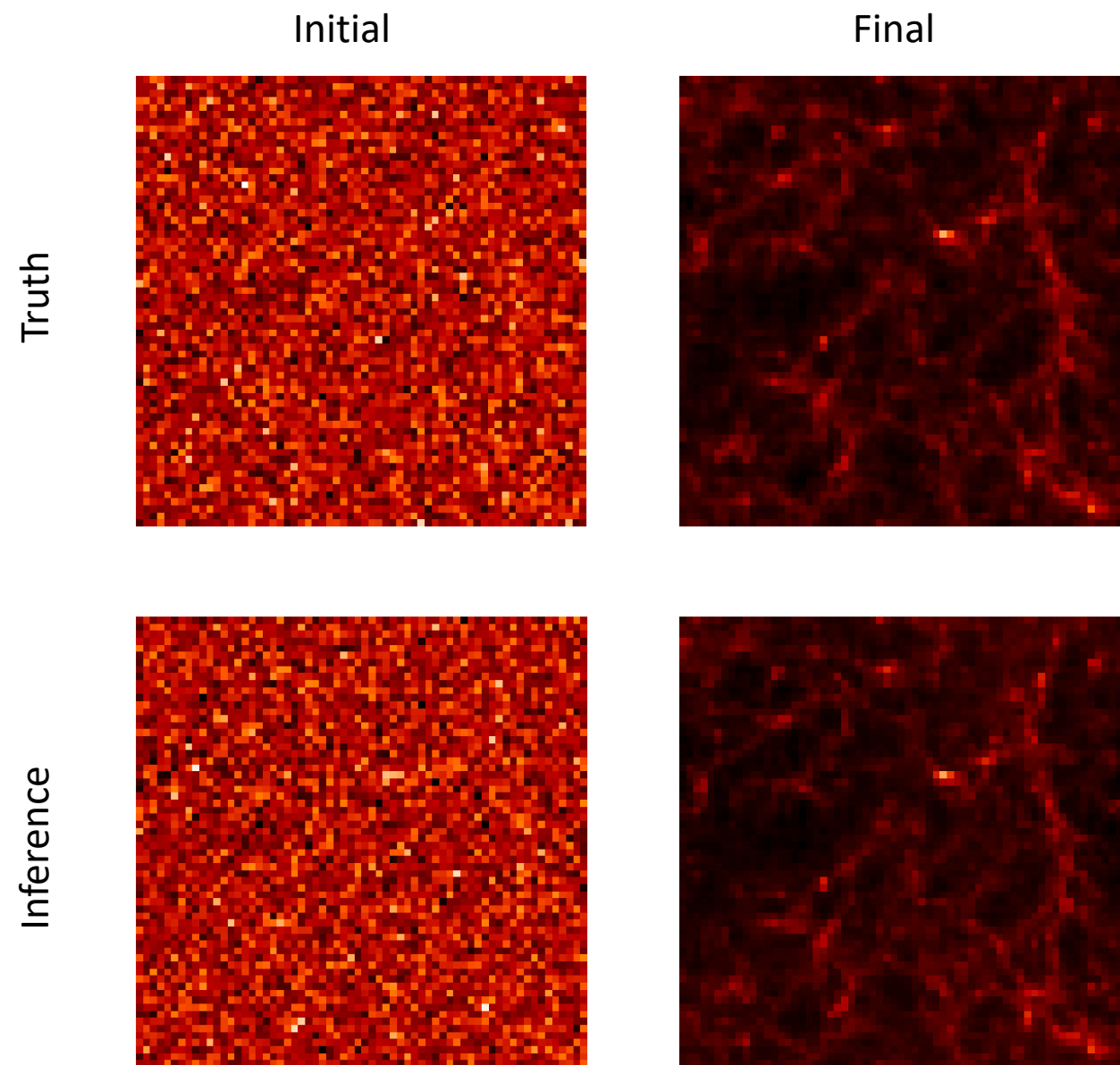






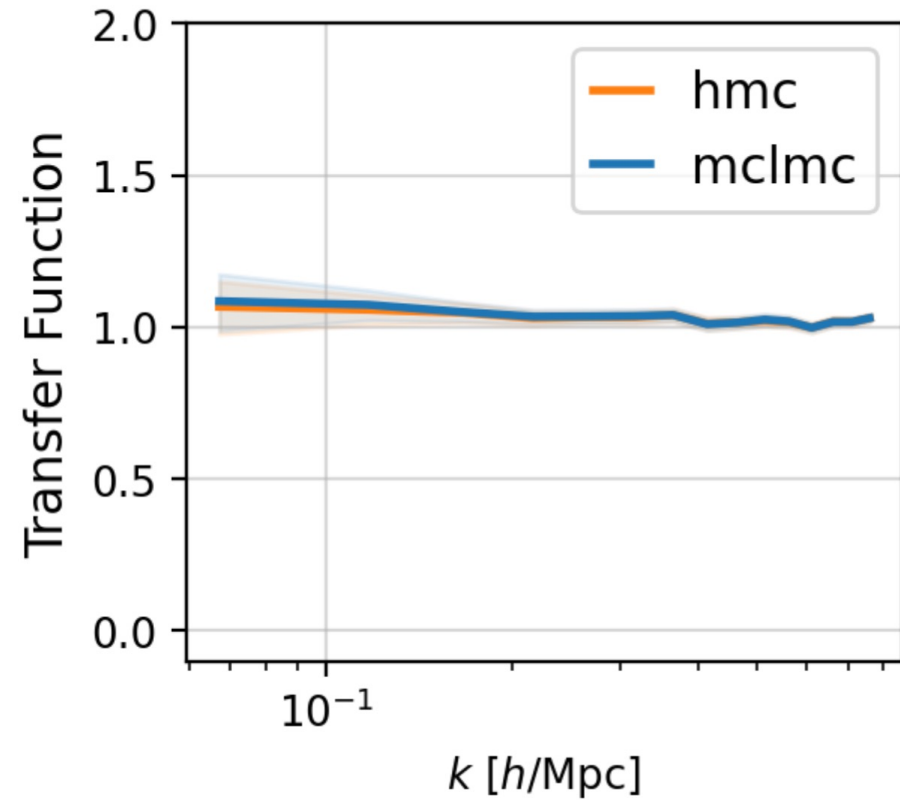
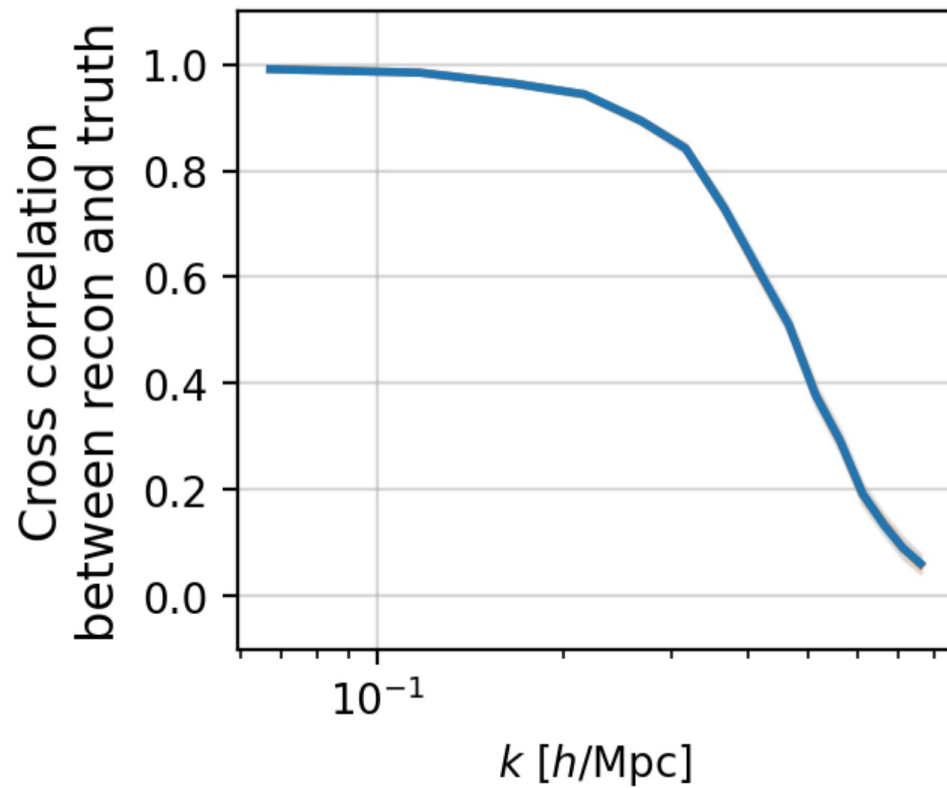






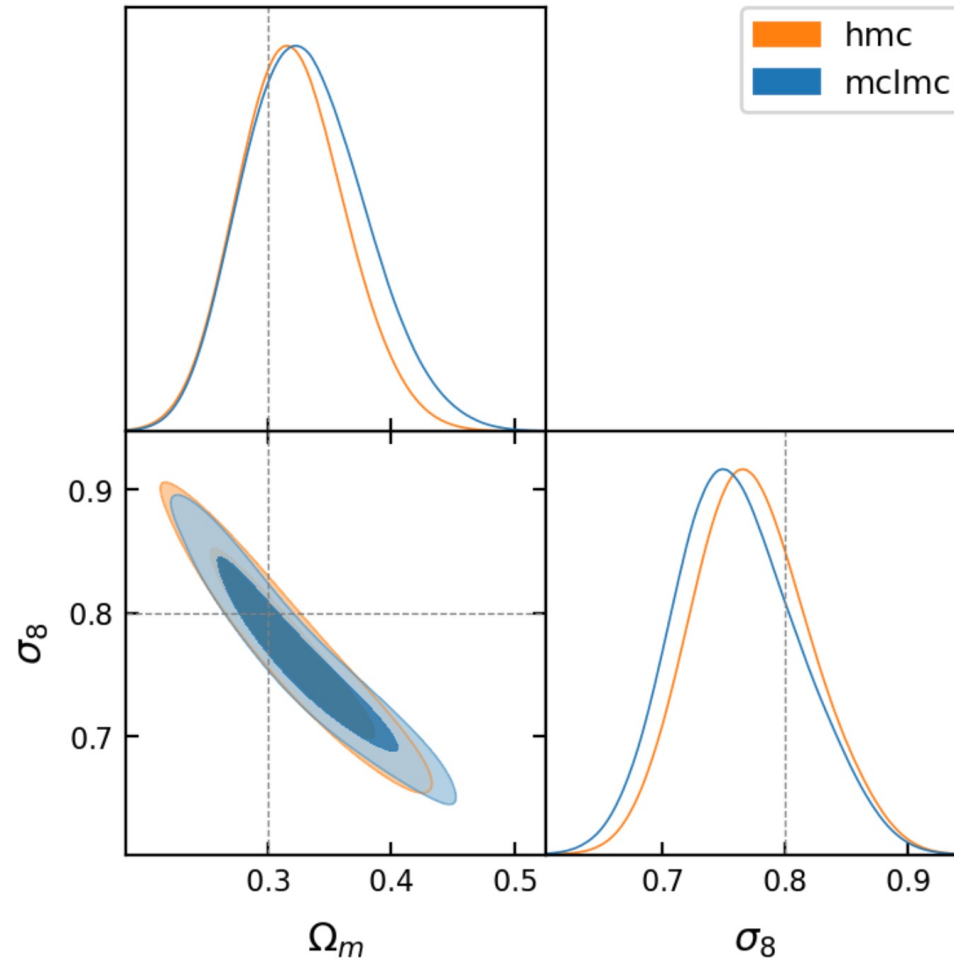
Samples of Initial Modes

$$d = 32^3 + 2 = 32,770$$

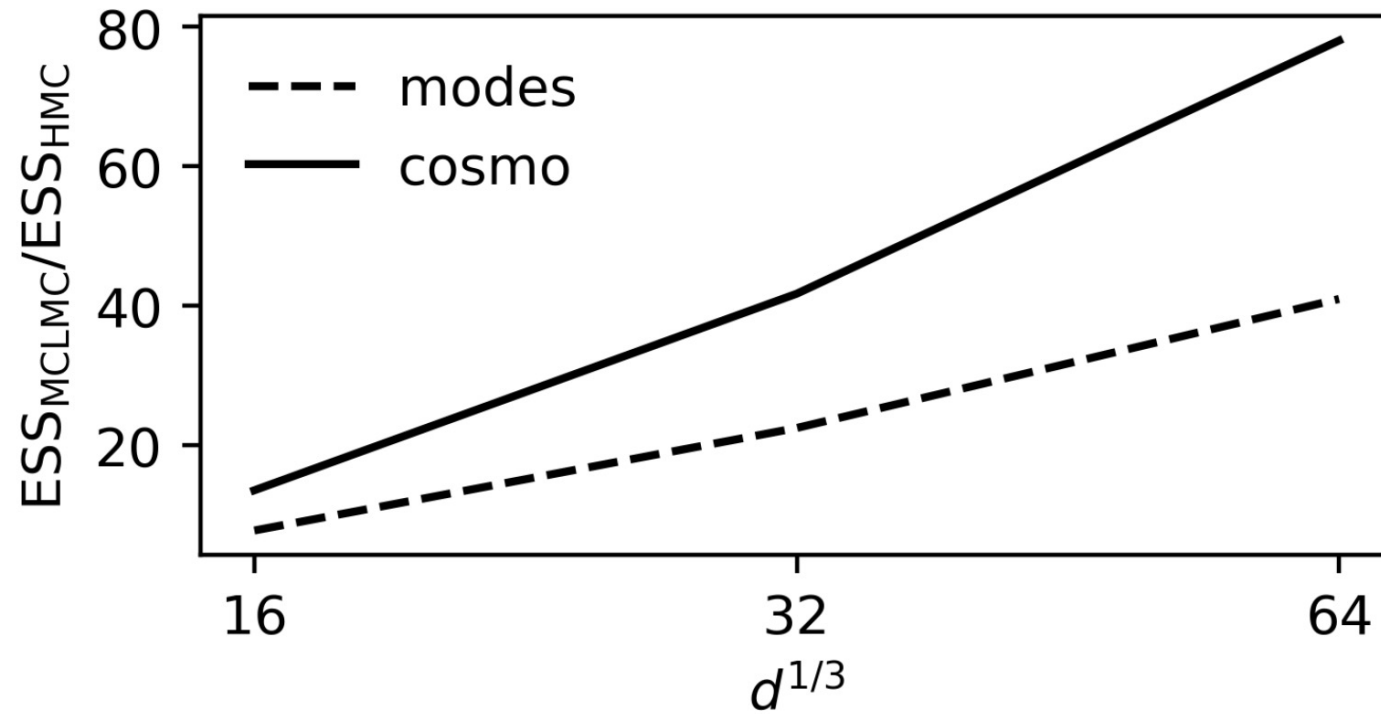


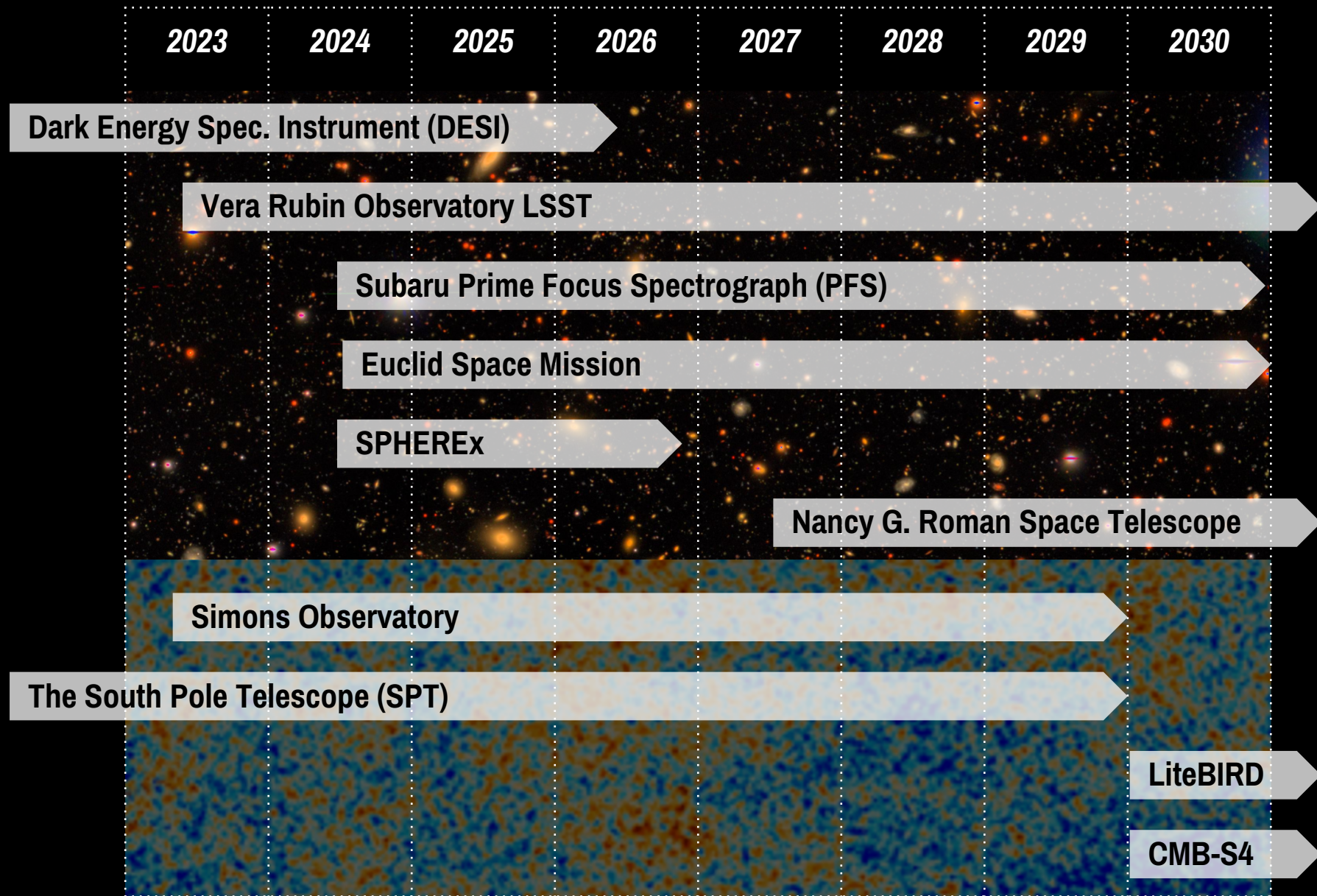
Samples of Cosmological Parameters

$$d = 32^3 + 2 = 32,770$$

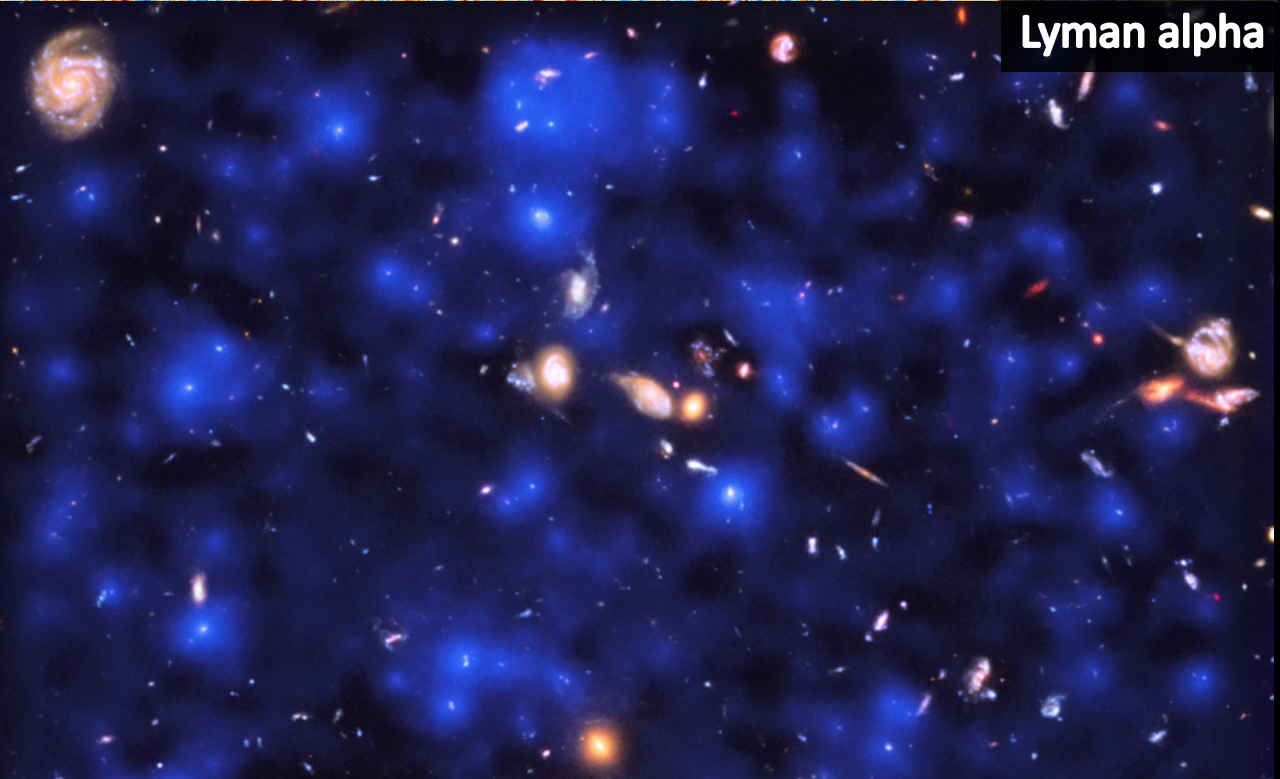
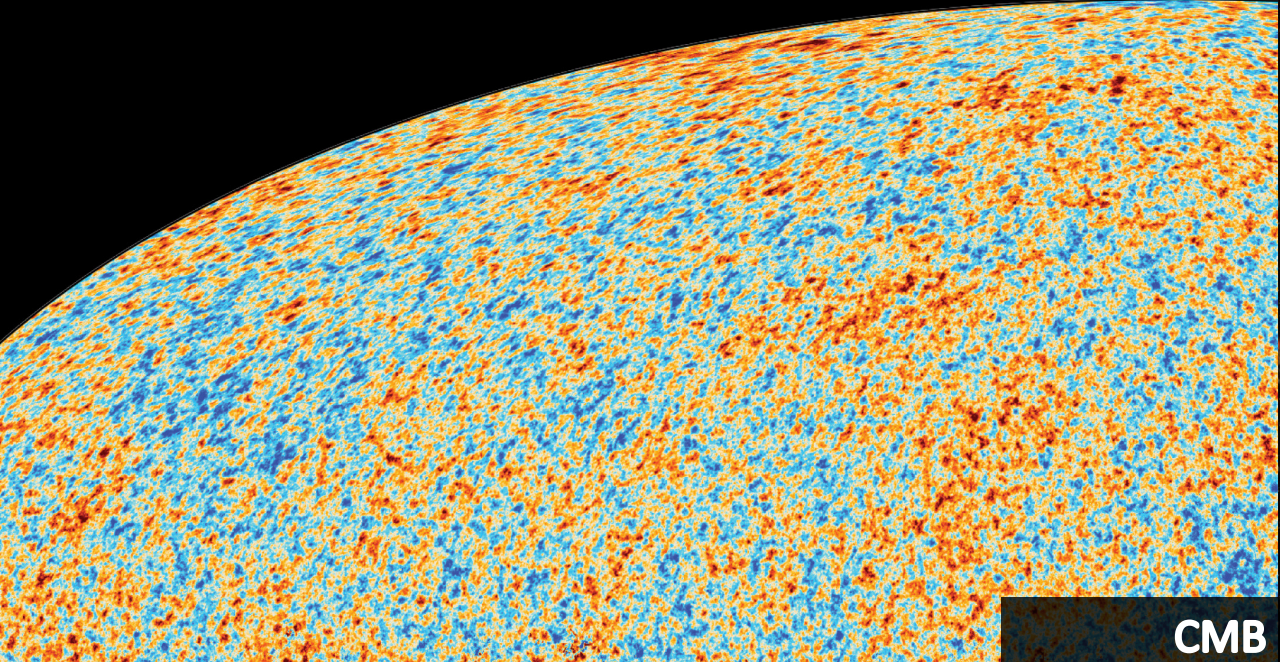


Efficiency improves with dimensionality!

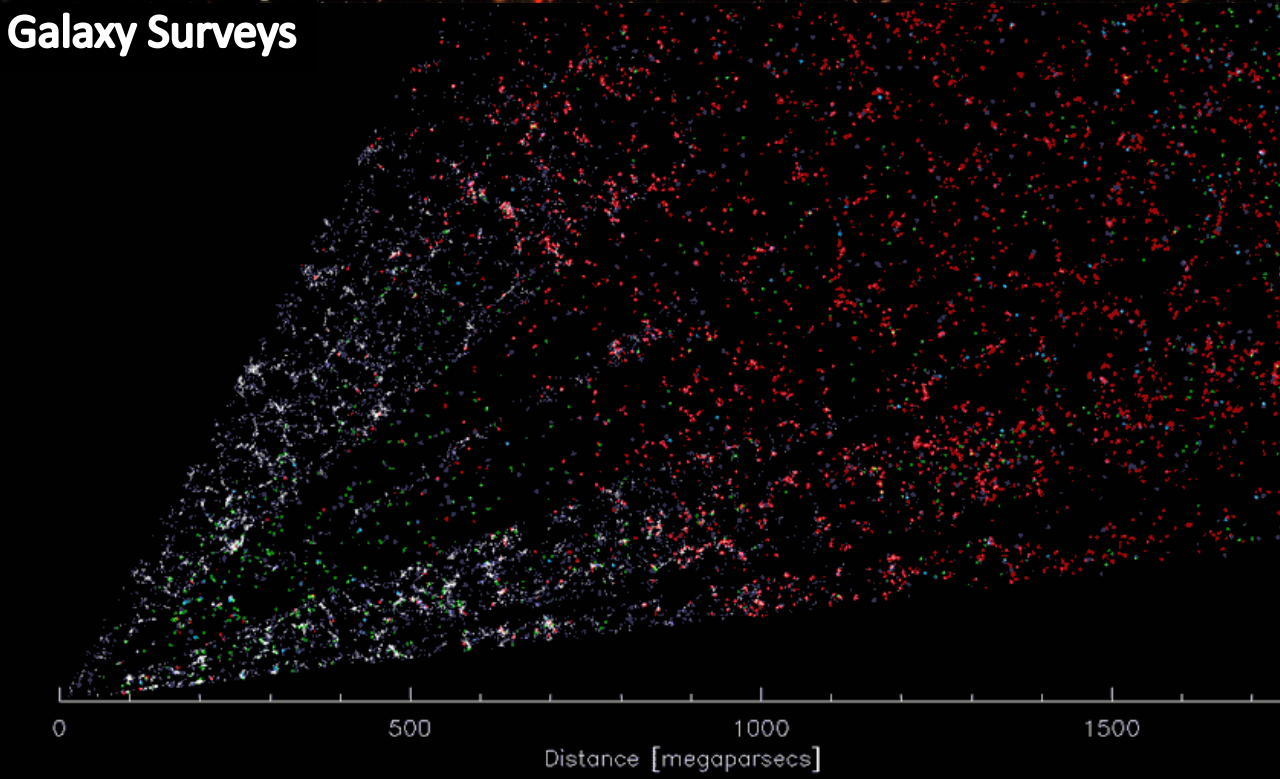


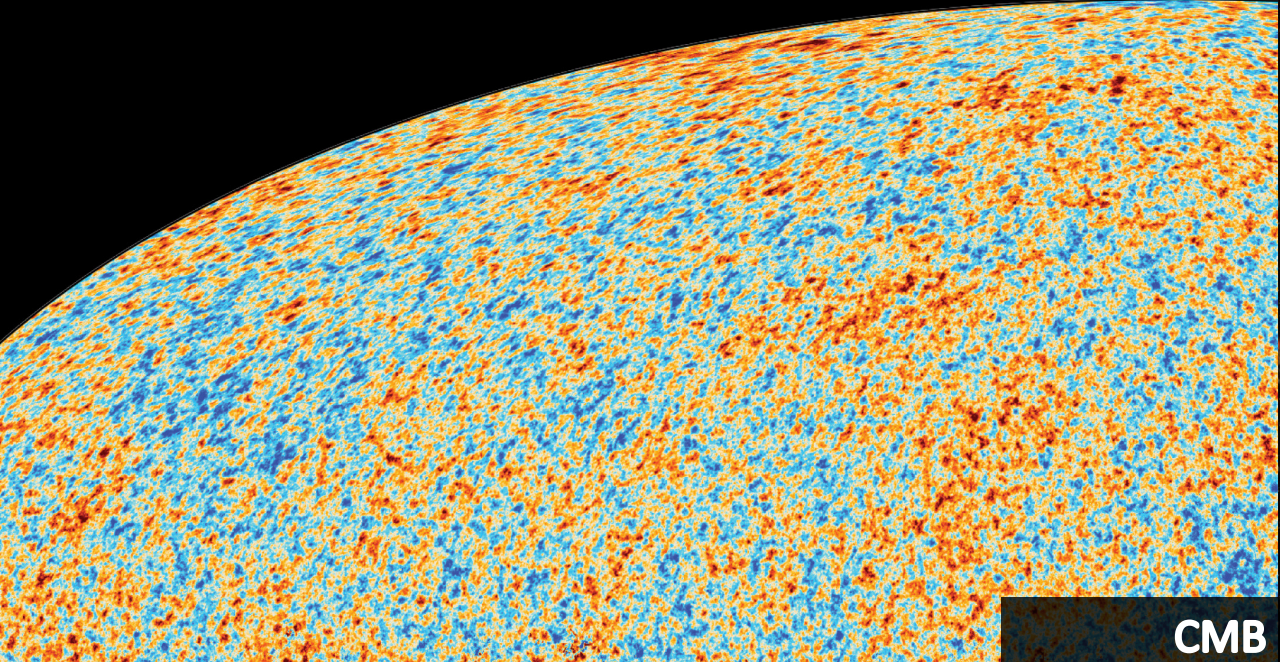


$$d \sim 512^3$$



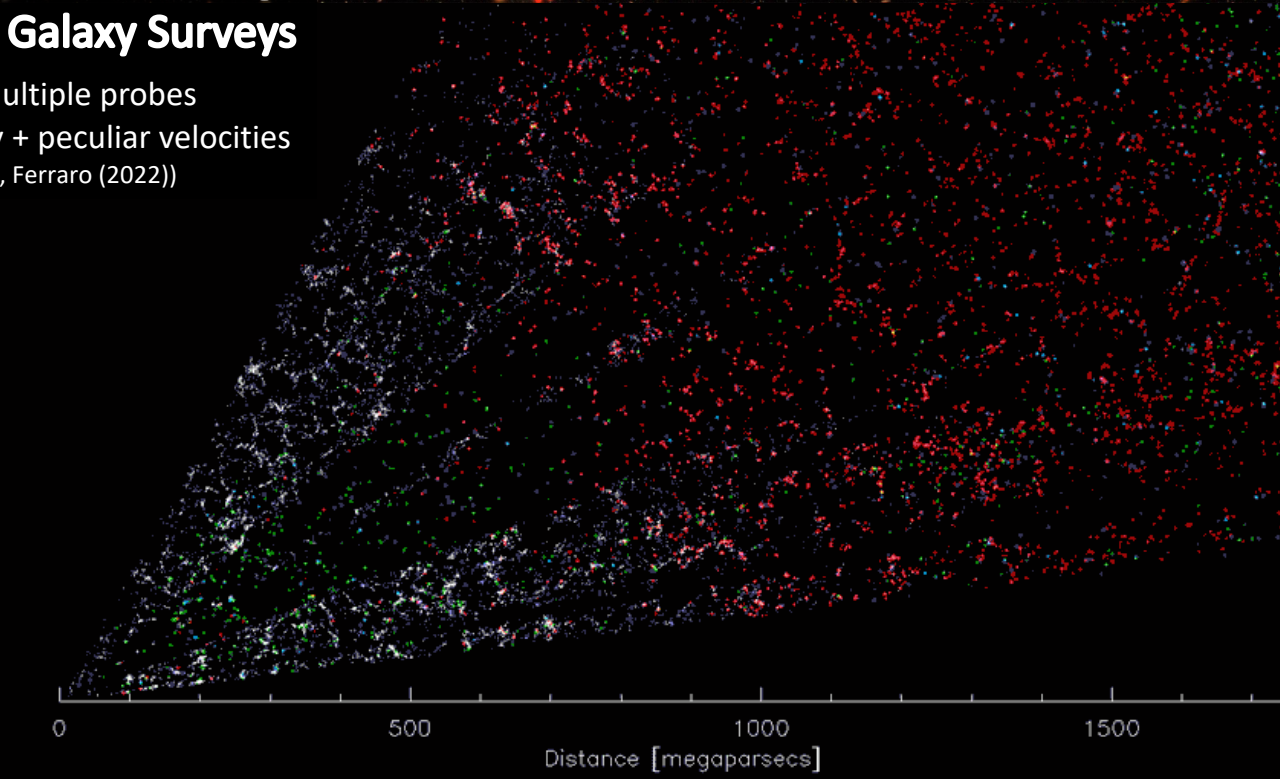
CMB Weak Lensing
Lyman alpha Galaxy Surveys

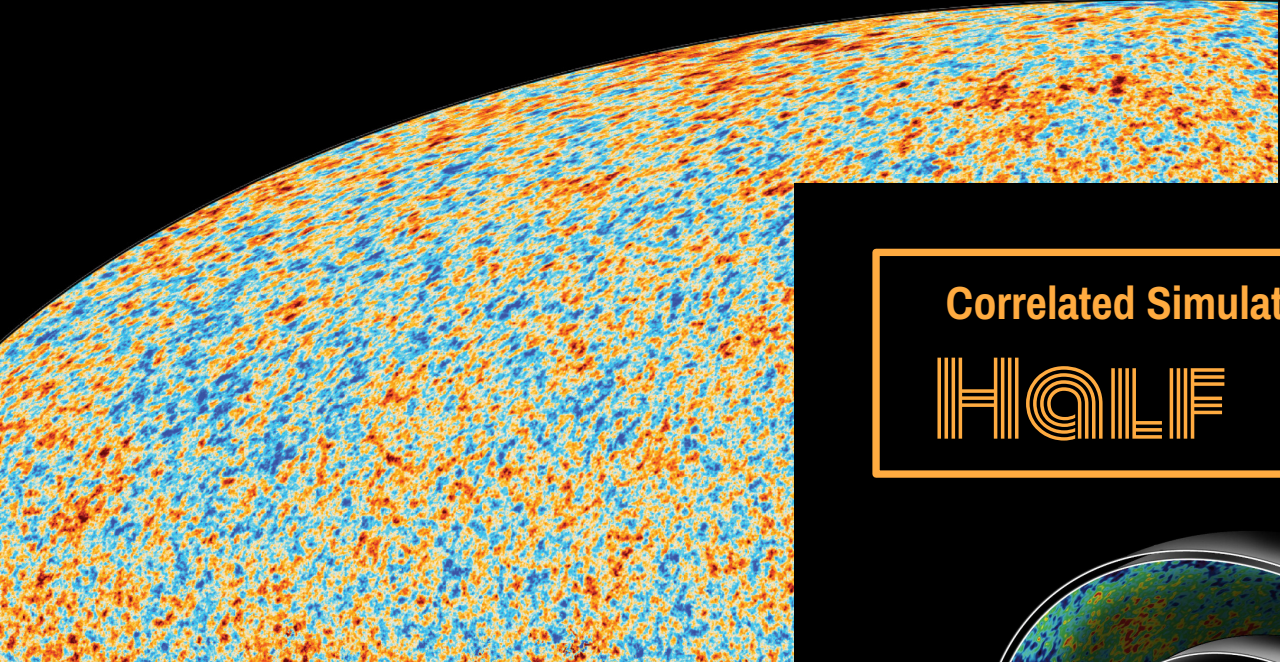




**CMB Weak Lensing
Lyman alpha Galaxy Surveys**

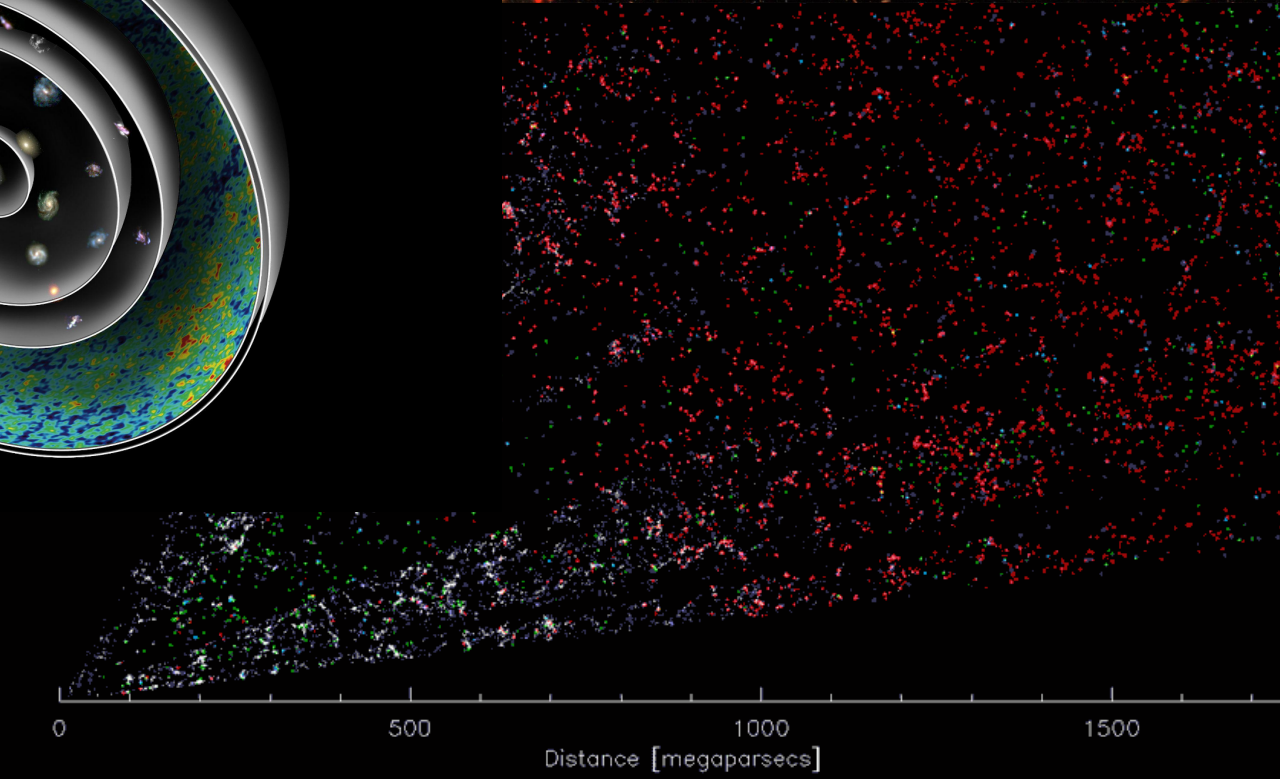
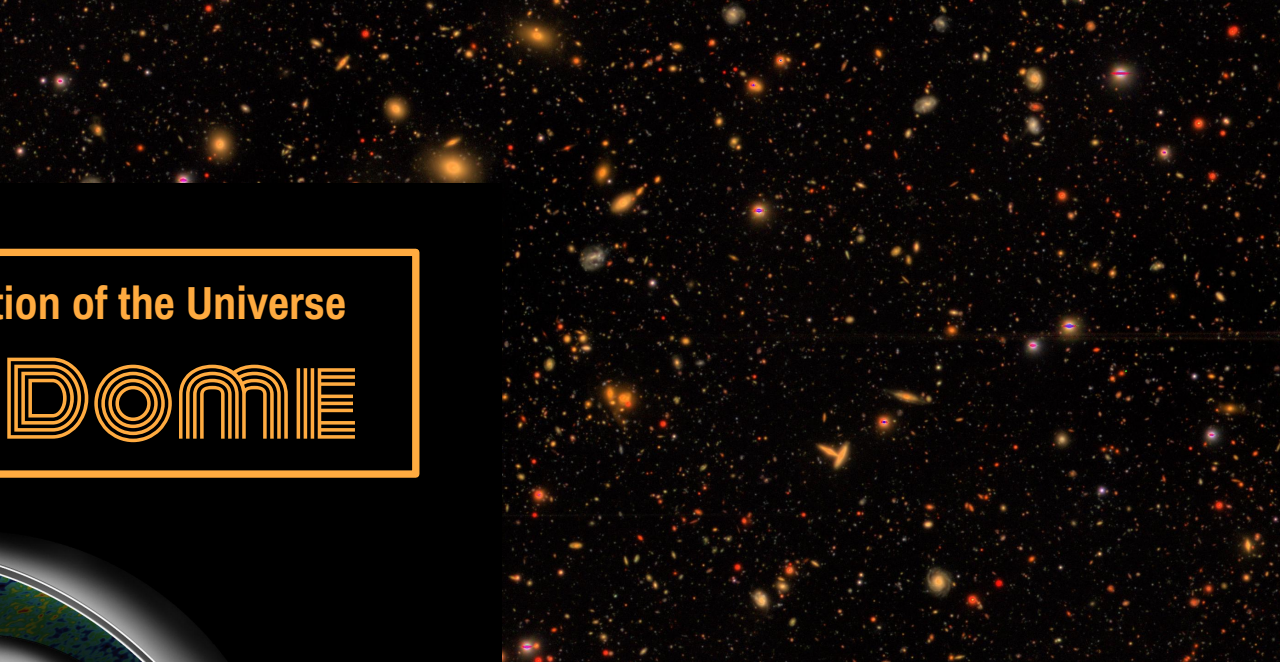
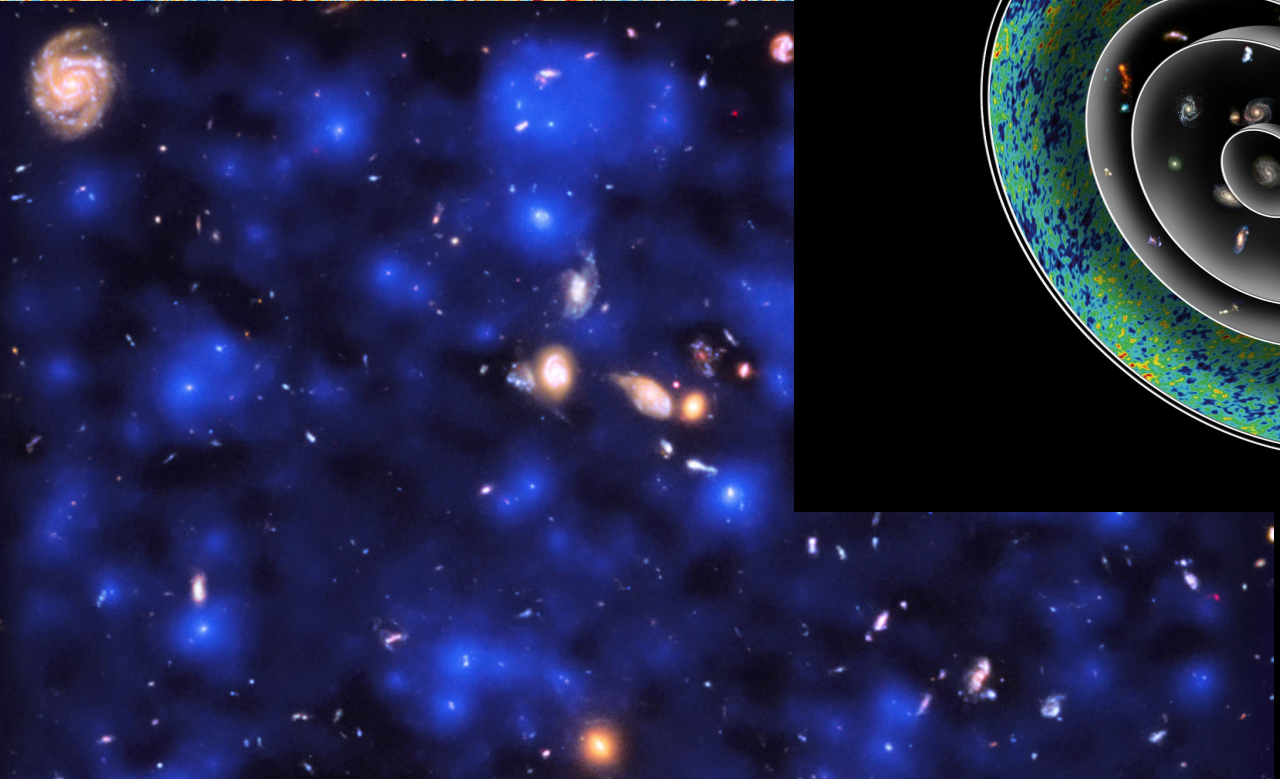
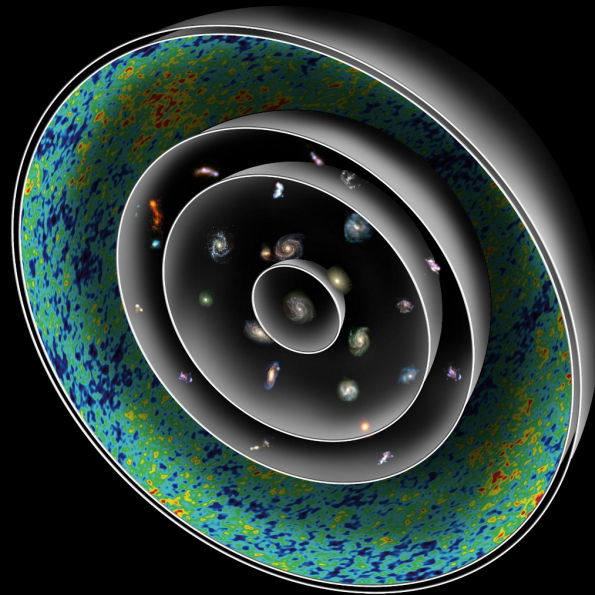
Combine multiple probes
e.g. galaxy density + peculiar velocities
(Bayer, Modi, Ferraro (2022))





Correlated Simulation of the Universe

HALF DOME



Simulation Comparison

	Sehgal+2010	Websky Stein+2020 Li+2022	Agora Omori 2022	Stage IV requirements*
Box Size $N_{\text{particles}}$	1 Gpc/h 1024^3	7.7 Gpc 6144^3	1 Gpc/h 3840^3	a few Gpc/h
Min. M_{halo}	$10^{13} M_{\odot}$	$1.2 \times 10^{13} M_{\odot}$	$1.5 \times 10^9 M_{\odot}/h$	$10^{12} M_{\odot}/h$
LSS observables	None	None	κ , clusters, LIM, +more to come	κ , galaxies, clusters
Number of realizations	1	1	1	10–100

* Inputs from SO, CMB-S4, LSST, DESI, PFS, SPHEREx, Roman collaborators

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Box Size $N_{\text{particles}}$	1 Gpc/h 1024^3	7.7 Gpc 6144^3	1 Gpc/h 3840^3	a few Gpc/h	3.5 Gpc/h, 6144^3
Min. M_{halo}	$10^{13} M_{\odot}$	$1.2 \times 10^{13} M_{\odot}$	$1.5 \times 10^9 M_{\odot}/h$	$10^{12} M_{\odot}/h$	$10^{12} M_{\odot}/h$
LSS observables	None	None	κ , clusters, LIM, +more to come	κ , galaxies, clusters	κ , galaxies, clusters, +more
Number of realizations	1	1	1	10–100	11+ $1f_{\text{NL}}$ (more to come)

* Inputs from SO, CMB-S4, LSST, DESI, PFS, SPHEREx, Roman collaborators

The Team



[Adrian Bayer](#)

Princeton/CCA



[Jia Liu](#)

Kavli IPMU



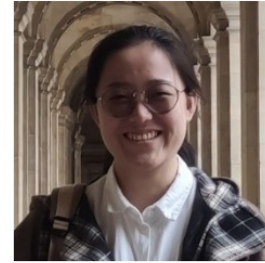
[Zack Li](#)

UC Berkeley/LBL



[Joe DeRose](#)

UC Berkeley/LBL



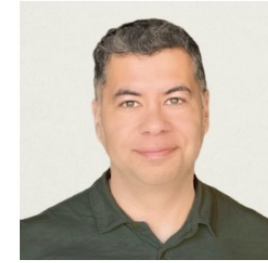
[Yici Zhong](#)

U Tokyo



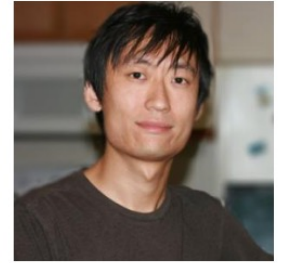
[Linda Blot](#)

Kavli IPMU



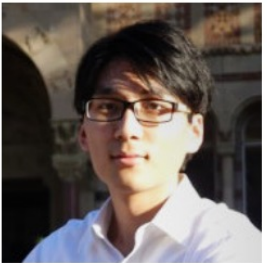
[Marcelo Alvarez](#)

LBL



[Yu Feng](#)

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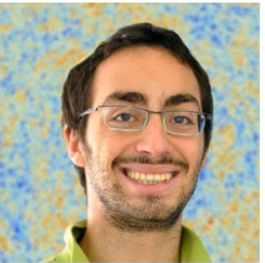
[Alex Laguë](#)

U Penn



[Will Coulton](#)

Cambridge



[Giuseppe Puglisi](#)

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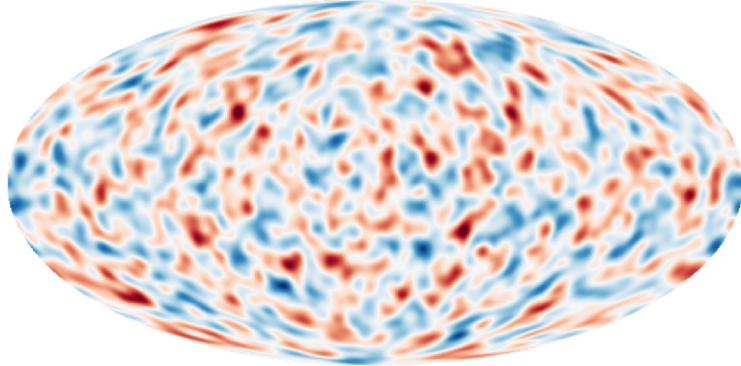
[Mathew Madhavacheril](#)

U Penn

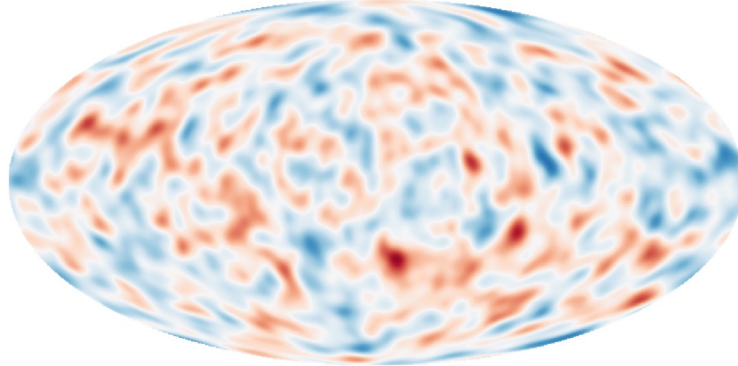
Preliminary Maps

stay tuned for more!

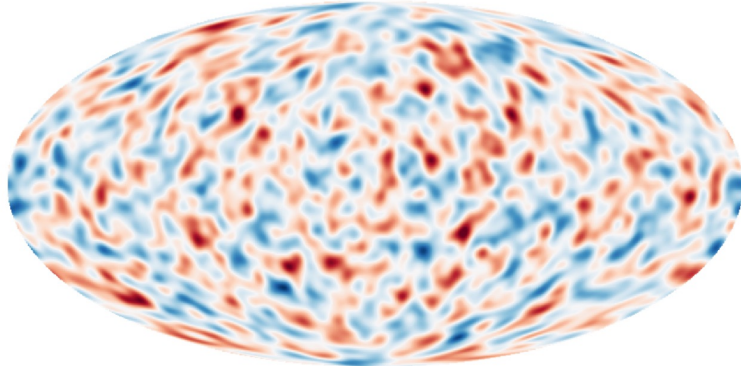
Matter Density



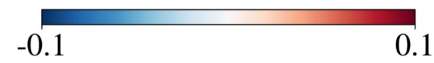
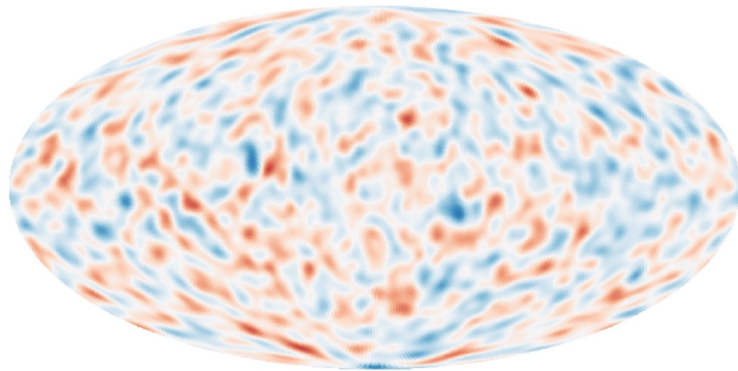
Velocity Sheet



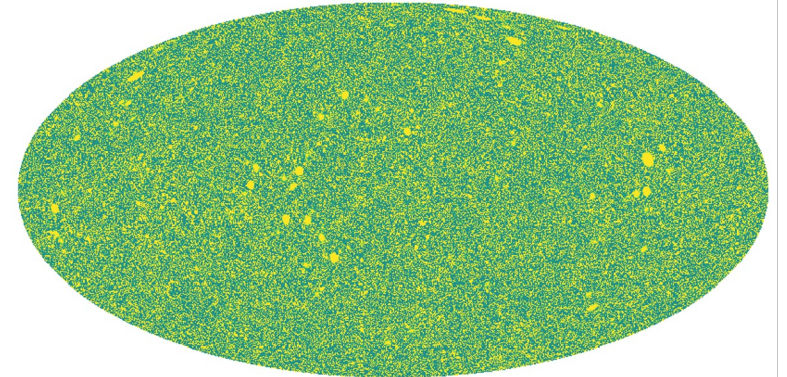
Mass Sheet



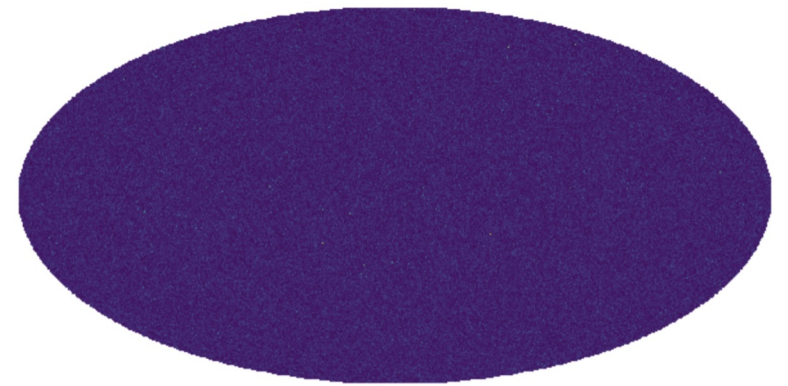
Halo Density

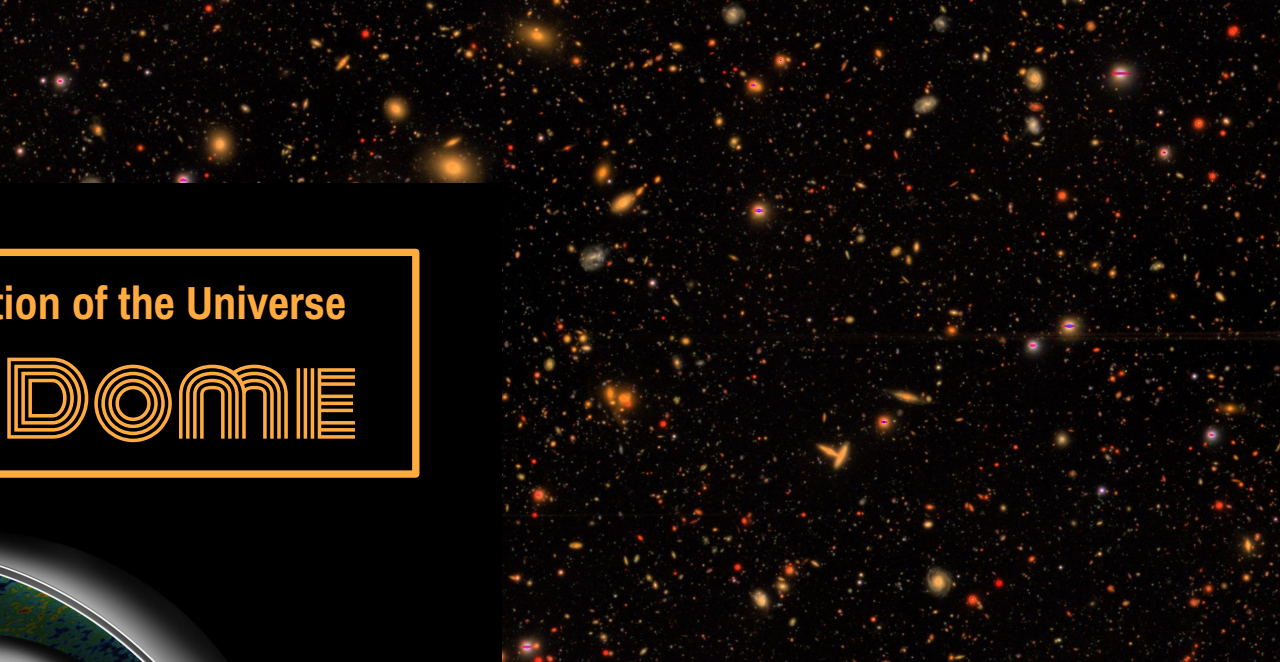
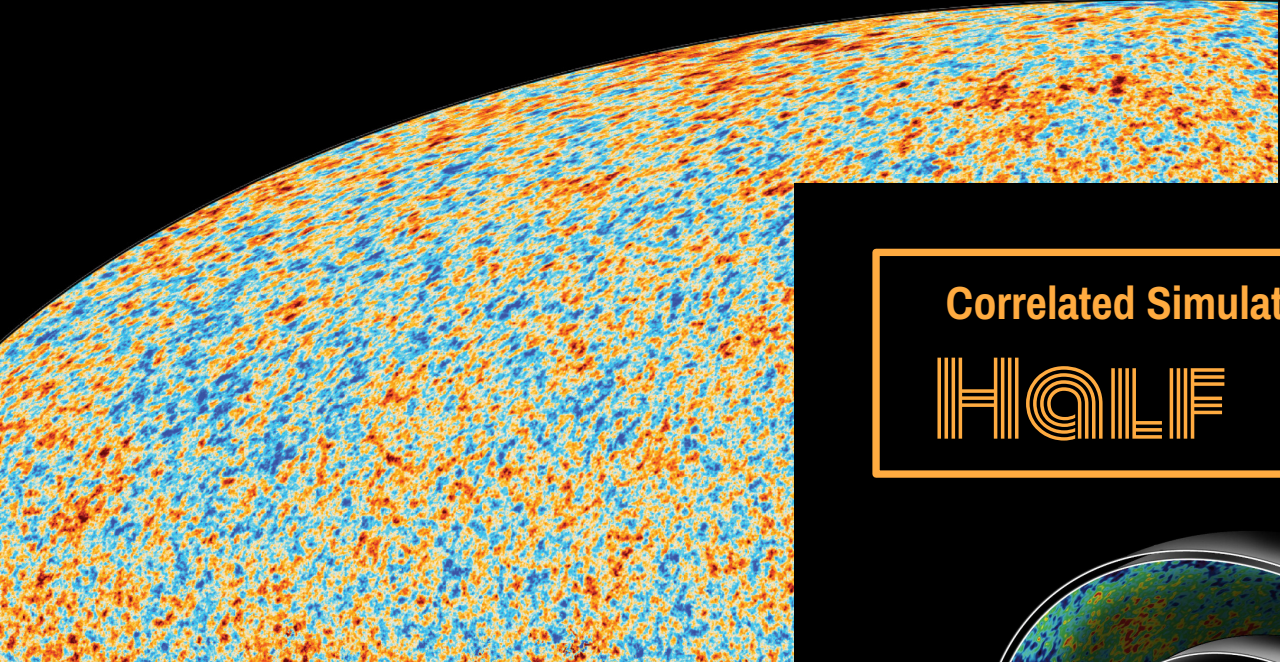


tSZ



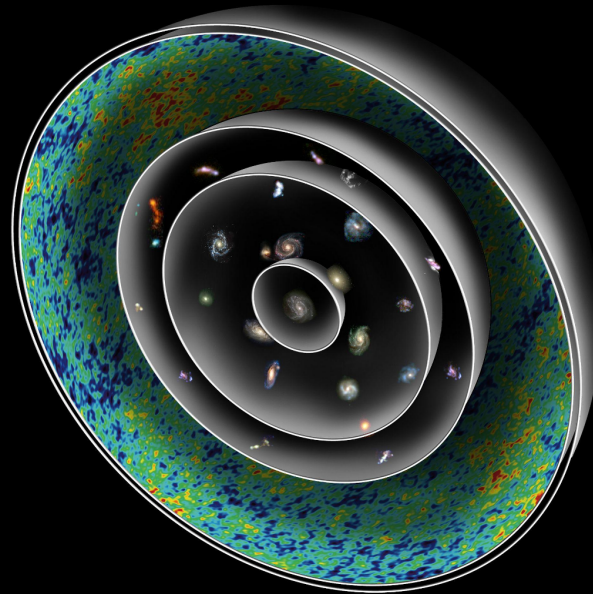
$z_s=3$ lensing map





Correlated Simulation of the Universe

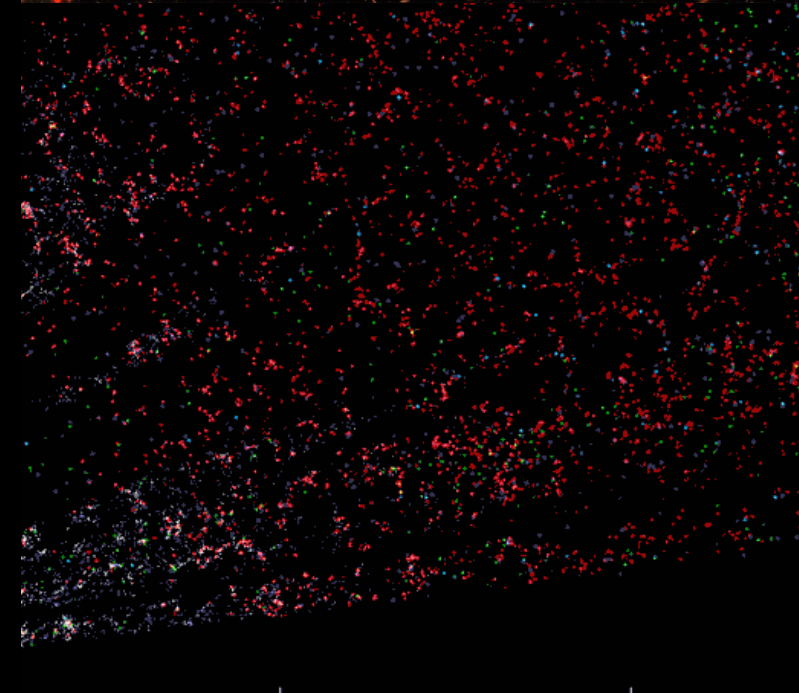
HALF DOME



Thank you!

Adrian Bayer

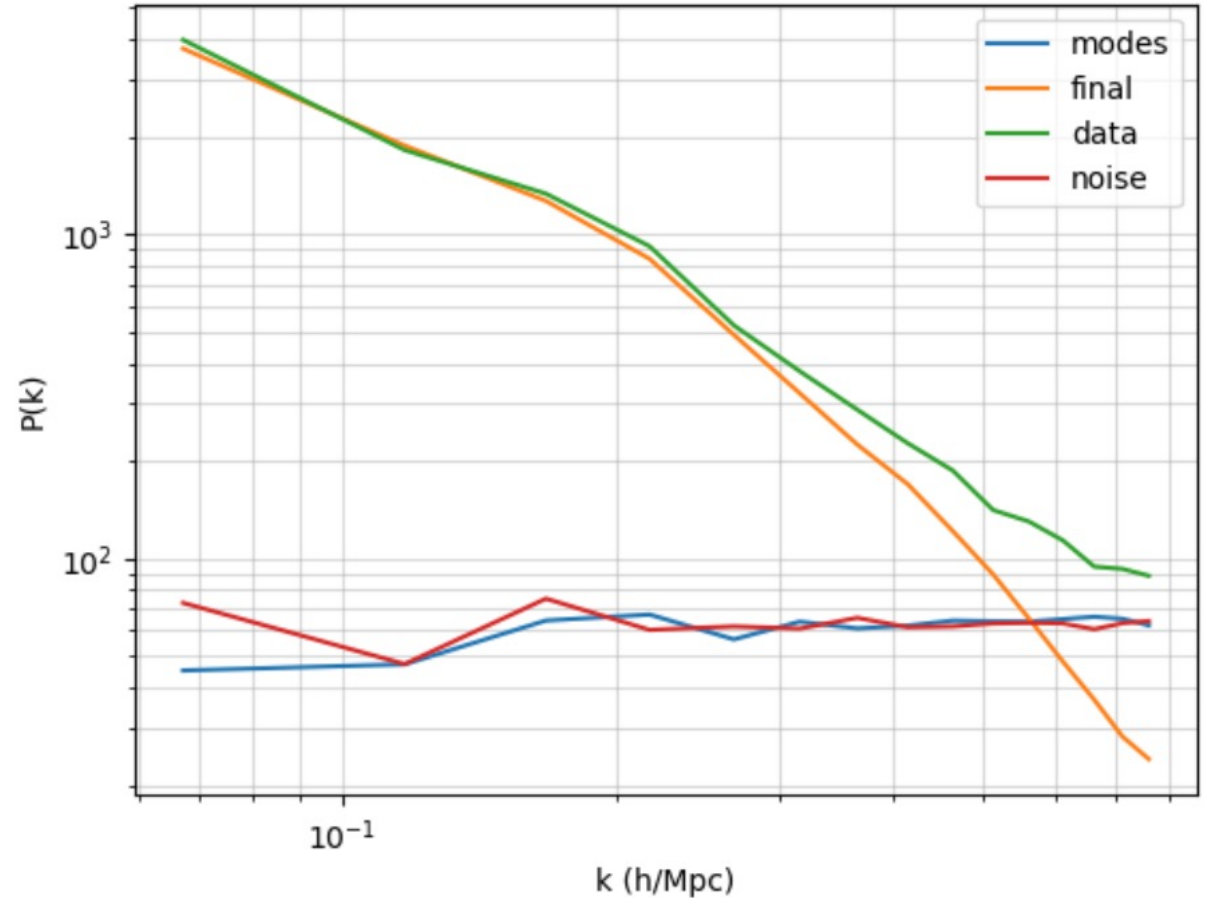
<http://adrianbayer.github.io>



Distance [megaparsecs]
1000 1500

Experiments

- Nonlinear dark matter
 - 1LPT, 2LPT, 5-step PM
- Dimensionality
 - 16^3 , 32^3 , 64^3
- Voxel size 4 Mpc/h
- Inject noise



2.2. Hamiltonian Monte Carlo

The traditional approach for sampling in the context of field-level inference is HMC (Duane et al., 1987; Neal et al., 2011; Betancourt, 2017). Given a d -dimensional target distribution $p(z) \propto e^{-\mathcal{L}(z)}$, where $z \in \mathbb{R}^d$, HMC uses the gradient $\nabla \mathcal{L}(z)$ to improve the sampling efficiency compared to gradient-free methods such as MH. It considers the Hamiltonian $H(z, \Pi)$, where Π is the canonical momentum, and samples the canonical ensemble in $2d$ -dimension phase space, denoted by $p(z, \Pi) \propto e^{-H(z, \Pi)}$. The success of HMC relies on the tuning of the Hamiltonian such that the marginal of $p(z, \Pi)$ over Π converges to the target distribution,

$$p(z) \propto \int_{\mathbb{R}^d} d\Pi e^{-H(z, \Pi)}. \quad (2)$$

The most popular choice is the Hamiltonian of a free particle, $H(z, \Pi) = \frac{1}{2}\Pi^2(z) + \mathcal{L}(z)$, for which the solution is the set of ODEs,

$$\begin{aligned} dz &= u dt, \\ du &= -\nabla \mathcal{L}(z) dt, \end{aligned} \quad (3)$$

where t is time and u is velocity. Following Hamiltonian dynamics ensures the trajectory conserves the Hamiltonian, or energy, allowing efficient exploration at a fixed energy level. Different energy levels must be explored to obtain an accurate set of samples in HMC, which is achieved by resampling the momentum Π according to its marginal distribution (a normal distribution) and results in inefficiencies (Betancourt, 2017). Moreover, to ensure the target distribution is converged to, HMC additionally requires an MH accept-reject step, which in turn requires a sufficiently small step size to ensure a frequent rate of acceptance.

2.3. Microcanonical Hamiltonian Monte Carlo

Unlike HMC which considers the marginal of the canonical distribution, the approach of MCHMC is to tune the Hamiltonian such that the microcanonical distribution marginalized over the momentum variables gives the target distribution, as follows

$$p(z) \propto \int_{\mathbb{R}^d} d\Pi \delta(H(z, \Pi) - E), \quad (4)$$

where $\delta(\cdot)$ denotes the delta function, and E is the energy. The motion of a particle under this Hamiltonian can be written as a set of ODEs as follows

$$\begin{aligned} dz &= u dt, \\ du &= P(u) f(z) dt, \end{aligned} \quad (5)$$

where we have introduced the projection $P(u) \equiv (I - uu^T)$ and force $f(z) \equiv -\nabla \mathcal{L}(z)/(d-1)$ (Ver Steeg & Galstyan, 2021; De Luca & Silverstein, 2022; Robnik et al., 2022). The key difference to the HMC ODEs in Eqn. (3) is the projection operator. Unlike HMC, the MCHMC dynamics converges to the target distribution while maintaining a constant energy.

2.4. Microcanonical Langevin Monte Carlo

To further speed up reaching ergodicity, the ODEs can be modified by considering Langevin dynamics (Grenander & Miller, 1994; Girolami & Calderhead, 2011) such that,

$$dz = u dt, \quad (6)$$

$$du = P(u) [f(z) dt + \eta dW], \quad (7)$$

where η is a hyperparameter and W is a standard normal random vector. This additional term proportional to η can be understood physically as a diffusion term which enforces better exploration of the target, in turn boosting ergodicity.

MCLMC has two hyperparameters, the step size and the amount of noise η . Both of these parameters can be tuned during a burn-in stage by monitoring fluctuations in the energy and ensuring they are below a certain threshold.

Many other applications

- Lattice Field Theory (Robnik+2023)
- CMB (Bonici+2023)
- CMB lensing (Ruiz-Zapatero+, in prep)
- ...

- Have an application? Let's chat!

	NUTS	MCLMC
Stochastic Volatility	0.006	0.023
German Credit	0.001	0.01
Neal's funnel	0.006	0.021
Critical ϕ^4 field theory (8×8 lattice)	0.016	0.2
(64×64 lattice)	0.005	0.16
CMB lensing d = 12288	0.0001	0.006

Talk structure: the audience is from diverse academic backgrounds, so we request that your talk addresses 3 aspects:

- (1) the key scientific question you are trying to answer;
- (2) why is AI/ML suitable for this question;
- (3) performance comparison to previous (non-AI) methods.