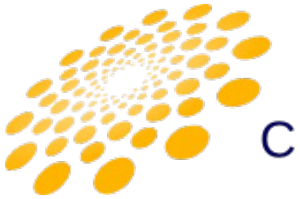


BERKELEY CENTER *for*
COSMOLOGICAL PHYSICS

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

Based on 2307.09504

Adrian Bayer

Princeton University / Simons Foundation

IAP/CCA ML Debate

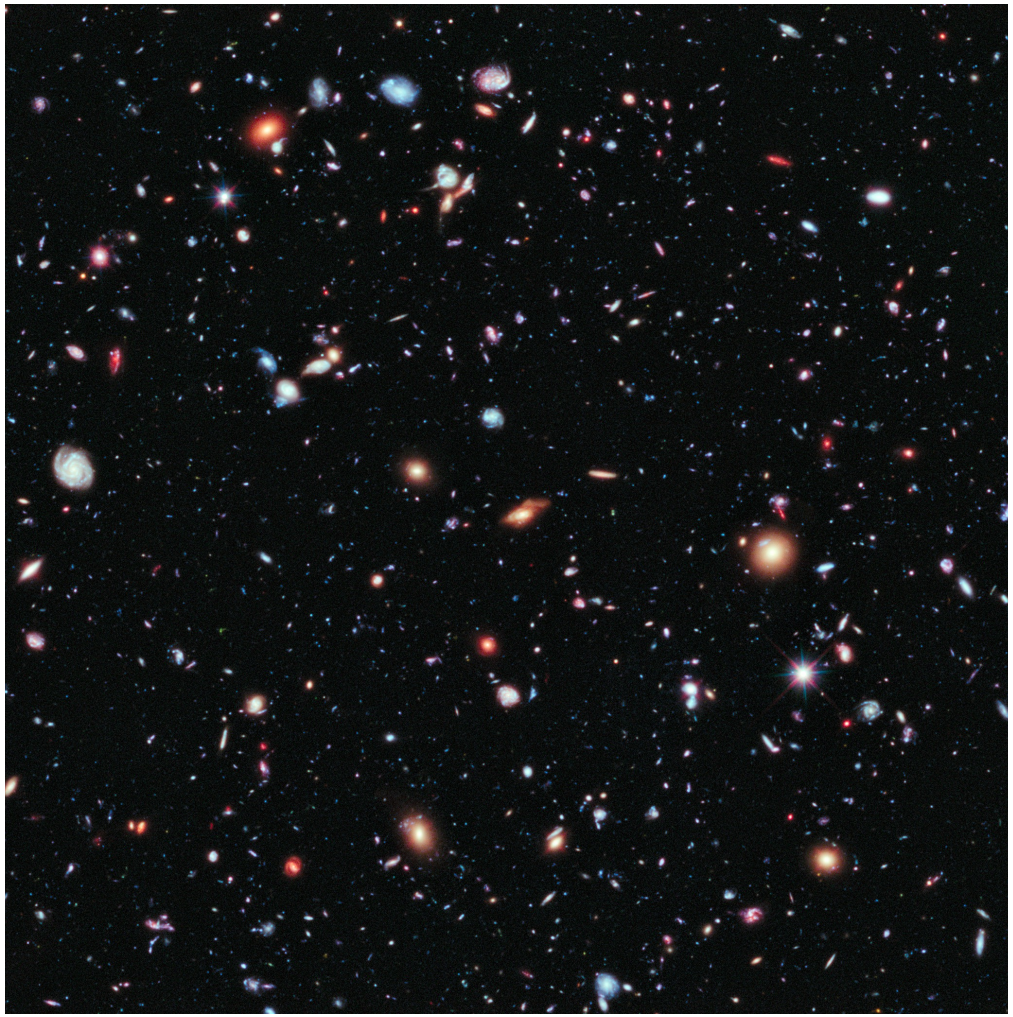
27 November 2023

PRINCETON
UNIVERSITY

SIMONS
FOUNDATION

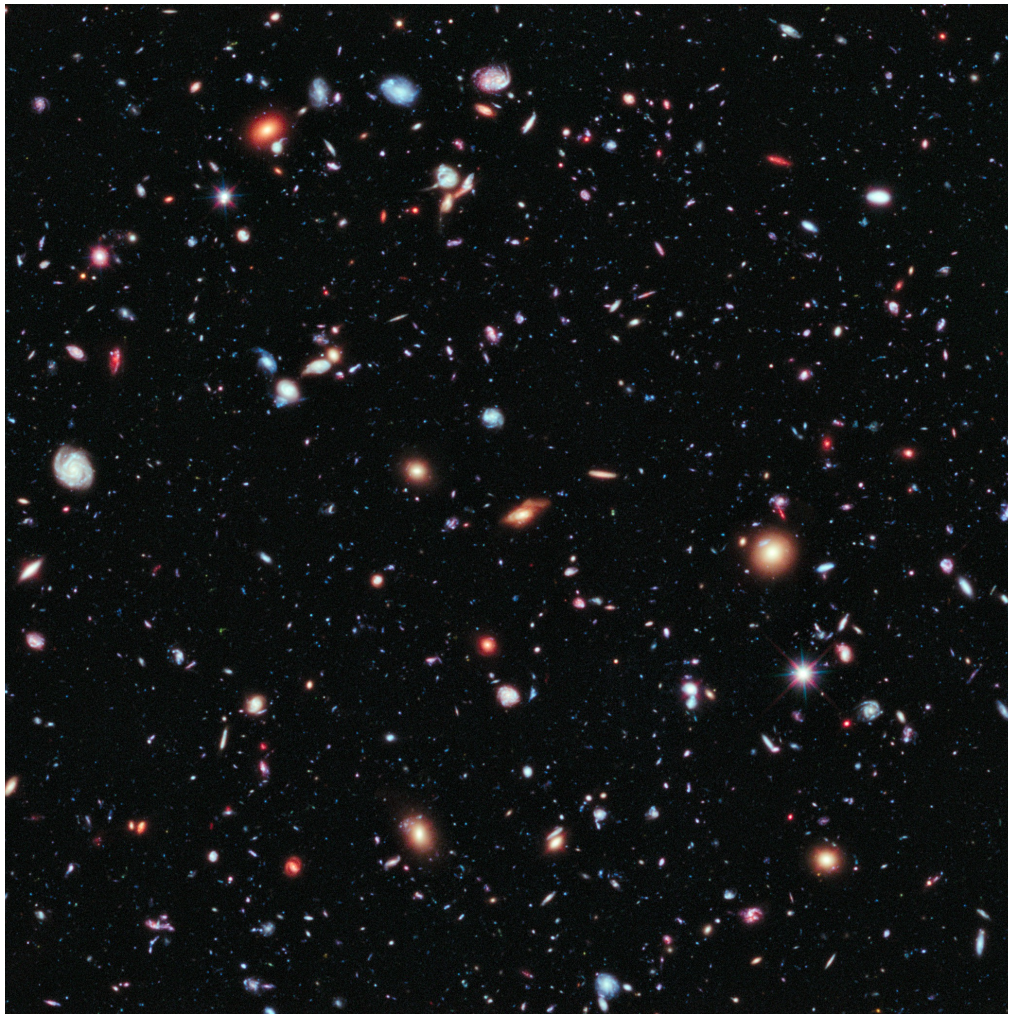
FLATIRON
INSTITUTE

Cosmological
Field-Level Inference
with
Microcanonical
Langevin Monte Carlo



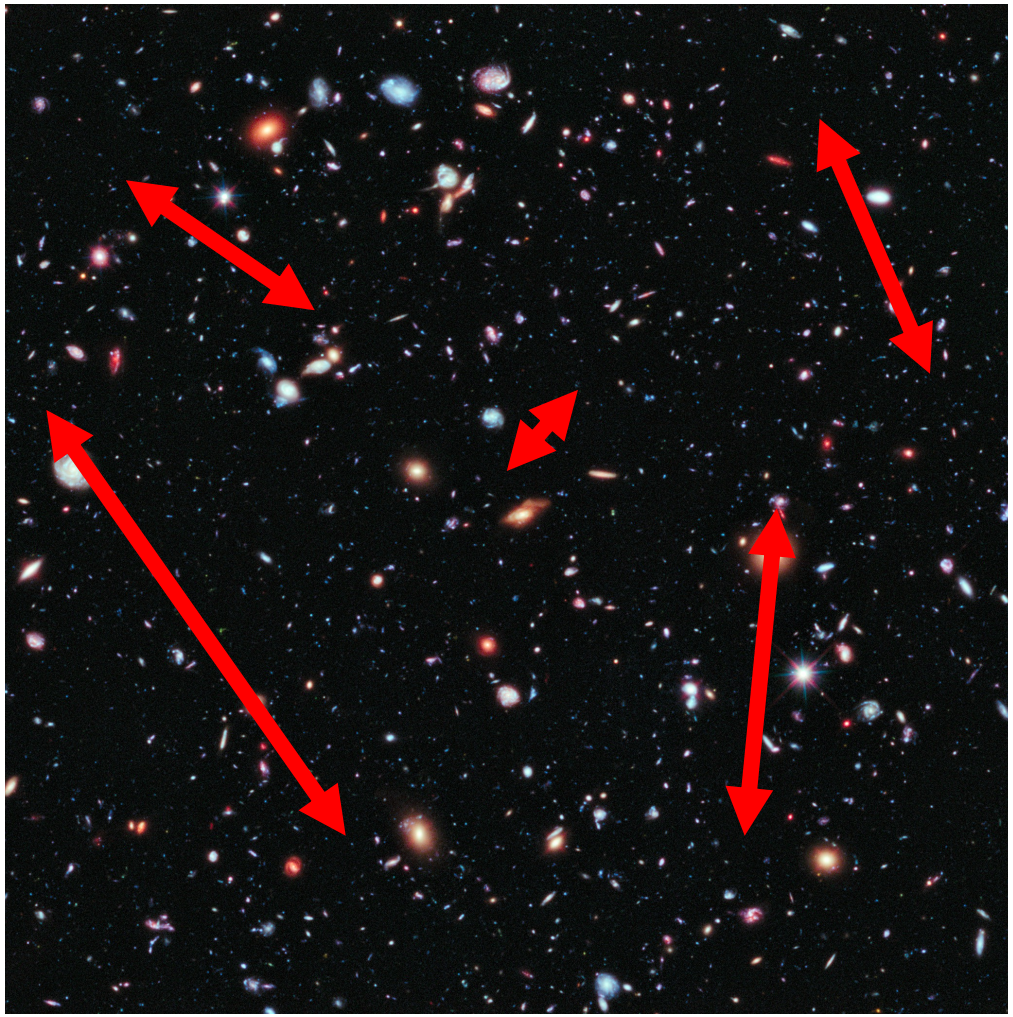
S_8 H_0 Ω_Λ $f_{\rm NL}$ M_ν

cosmological tensions? dark energy primordial NG neutrino mass



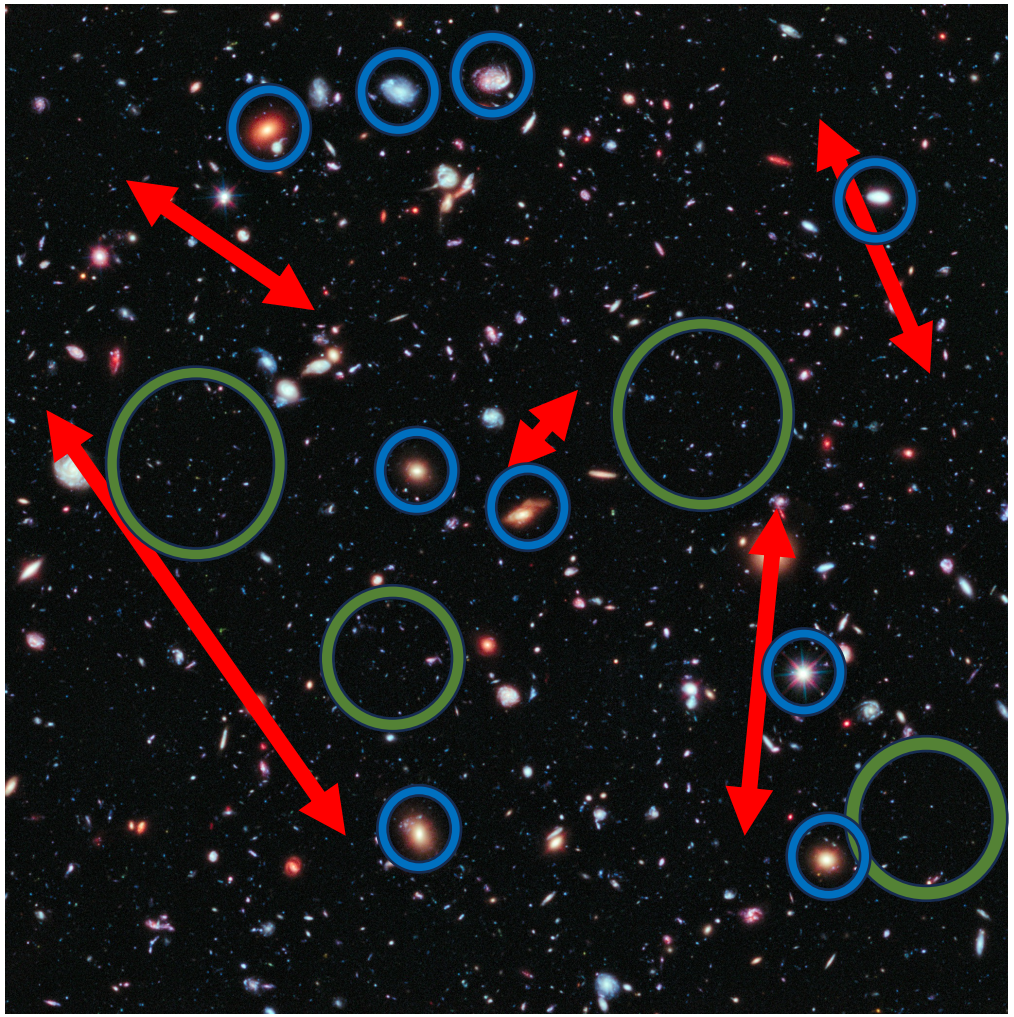
Traditional cosmology uses 2-pt information

but this is no longer optimal as we probe smaller scales



Higher-order statistics

can provide information beyond the 2-pt



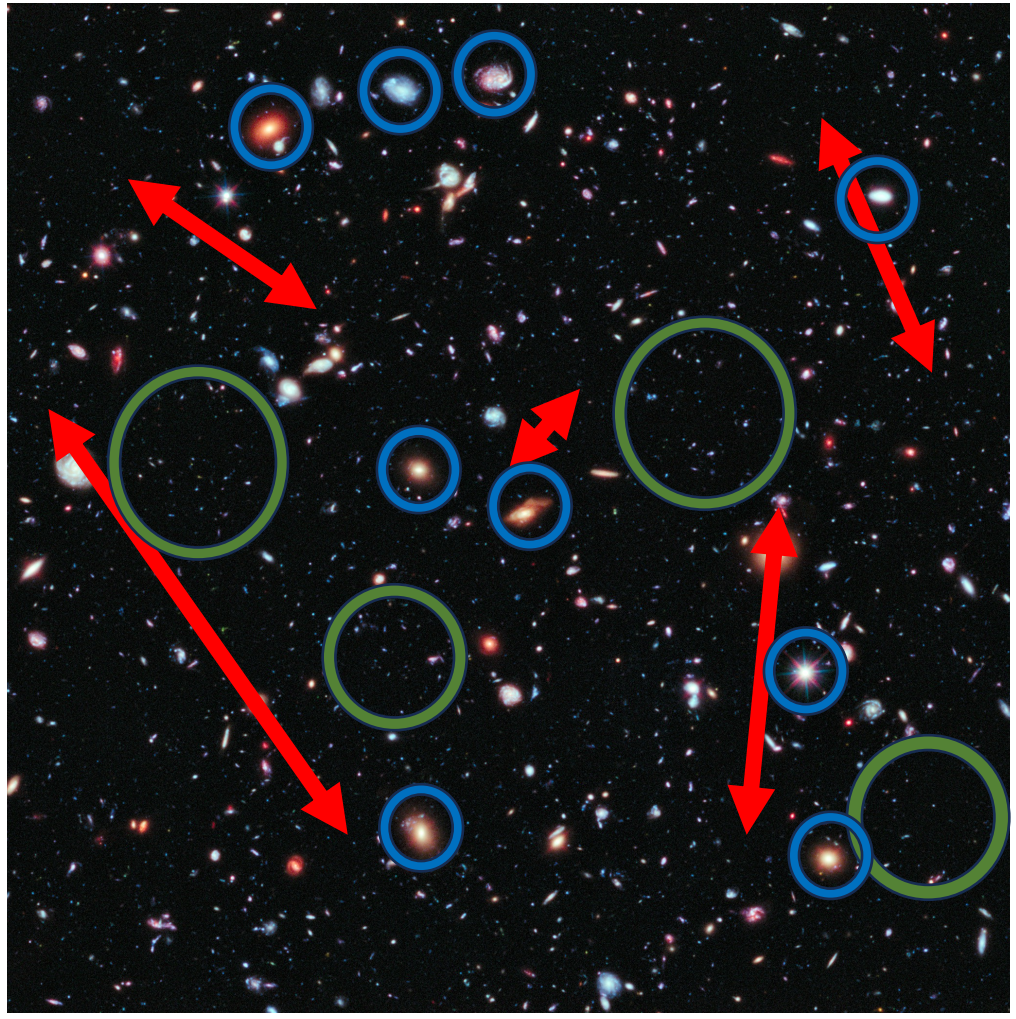
Halo Mass Function

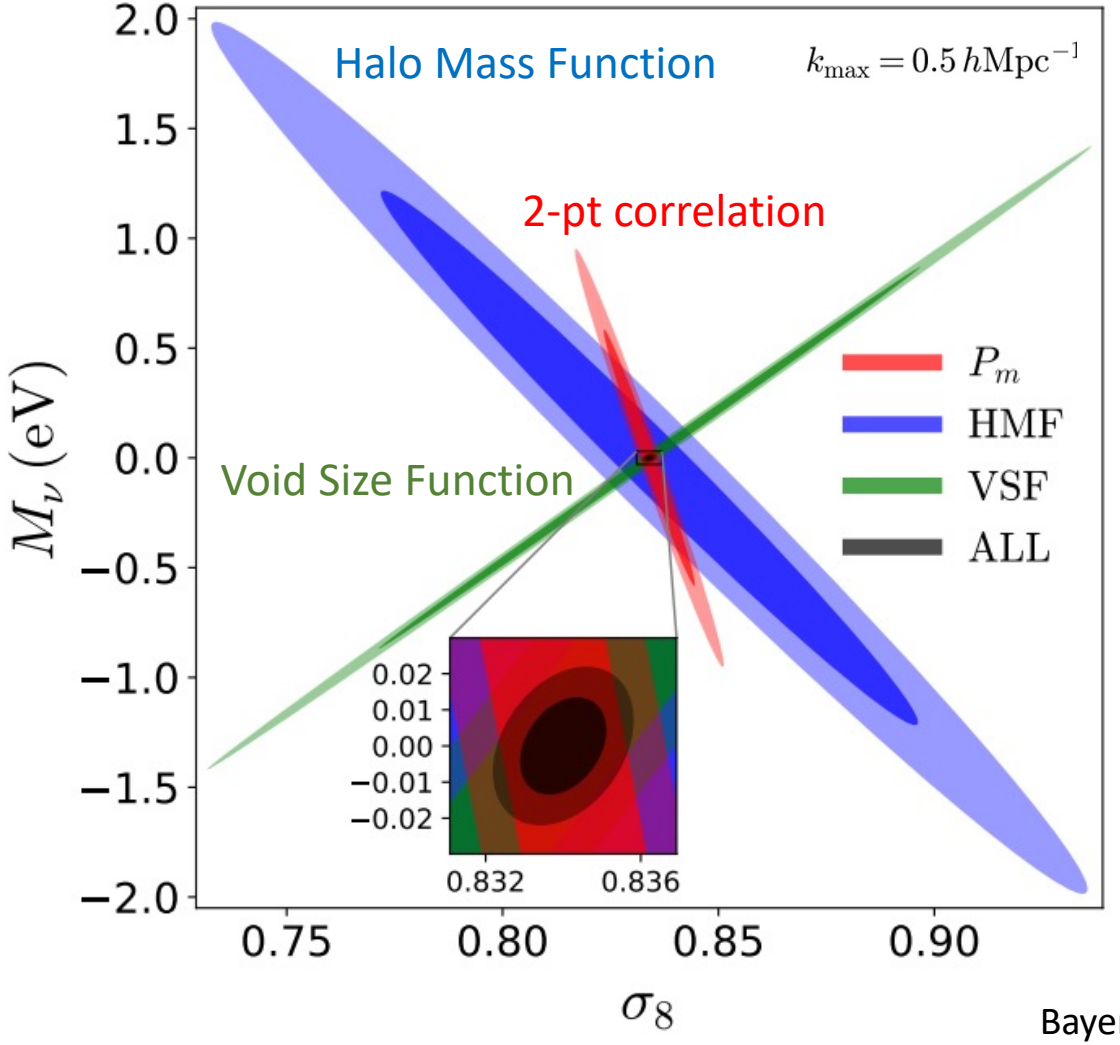
2-pt correlation

Void Size Function

Higher-order statistics

can provide information beyond the 2-pt



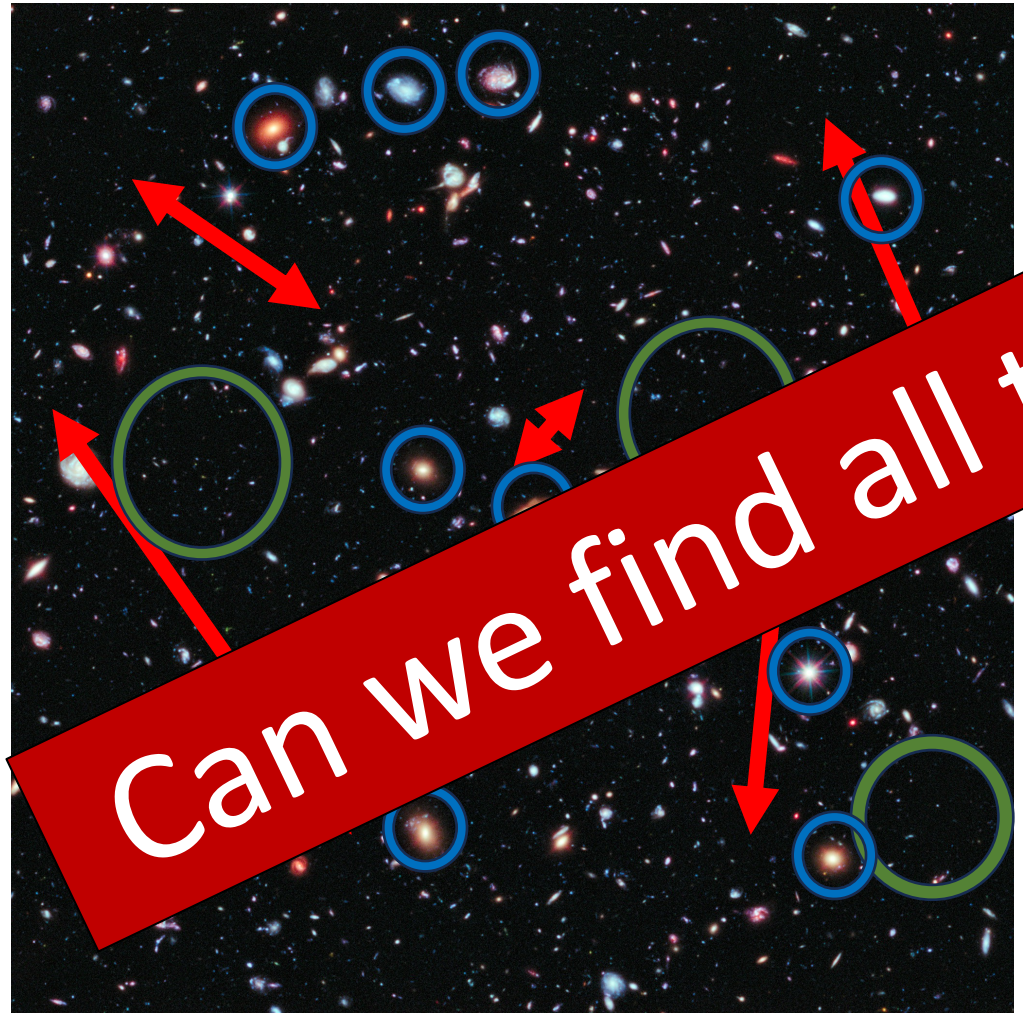


Bayer+ (2021)

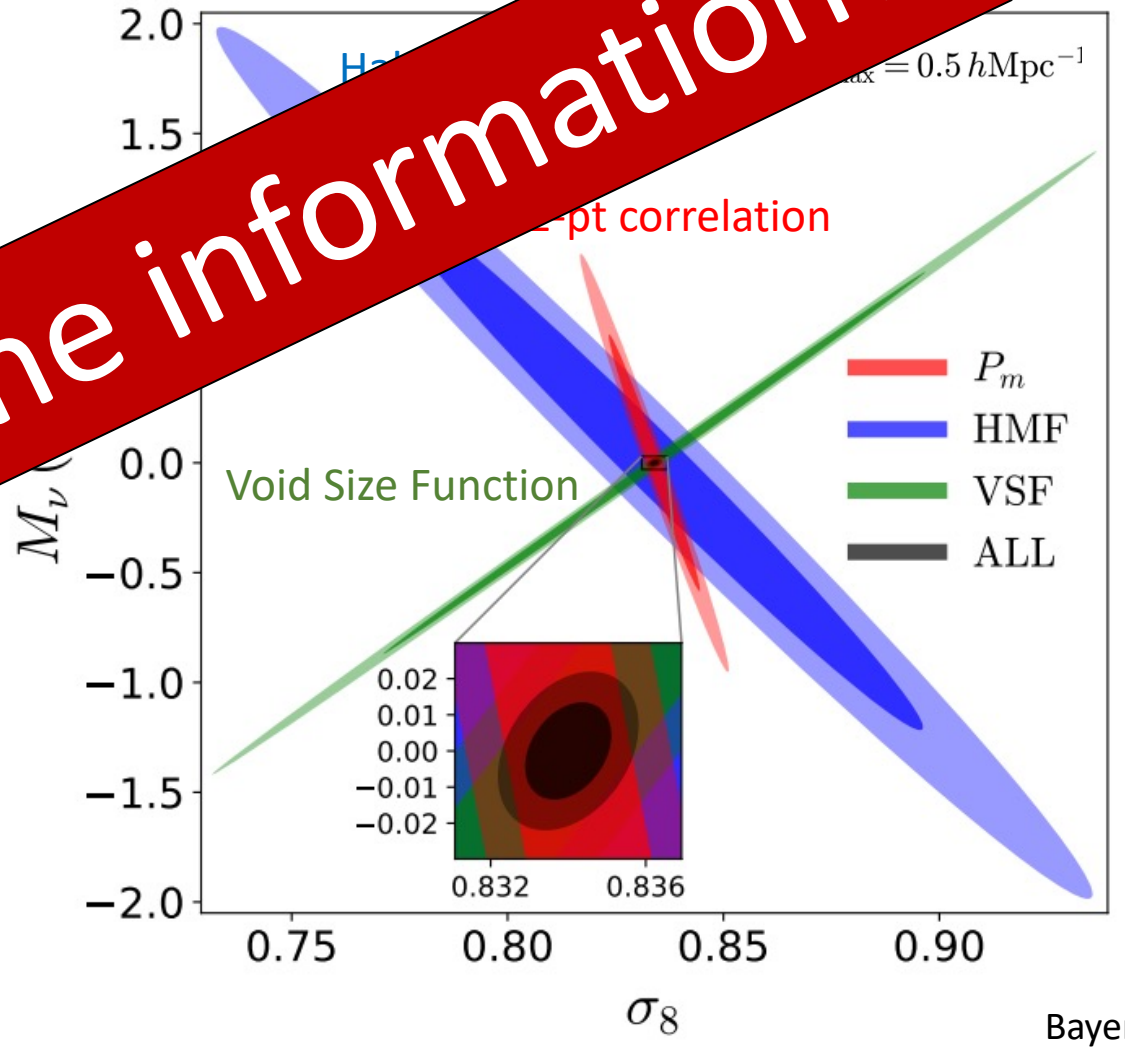
Fake νs? Bayer, Banerjee, Seljak (2022)

Higher-order statistics

can provide information beyond the 2-pt



Can we find all the information?



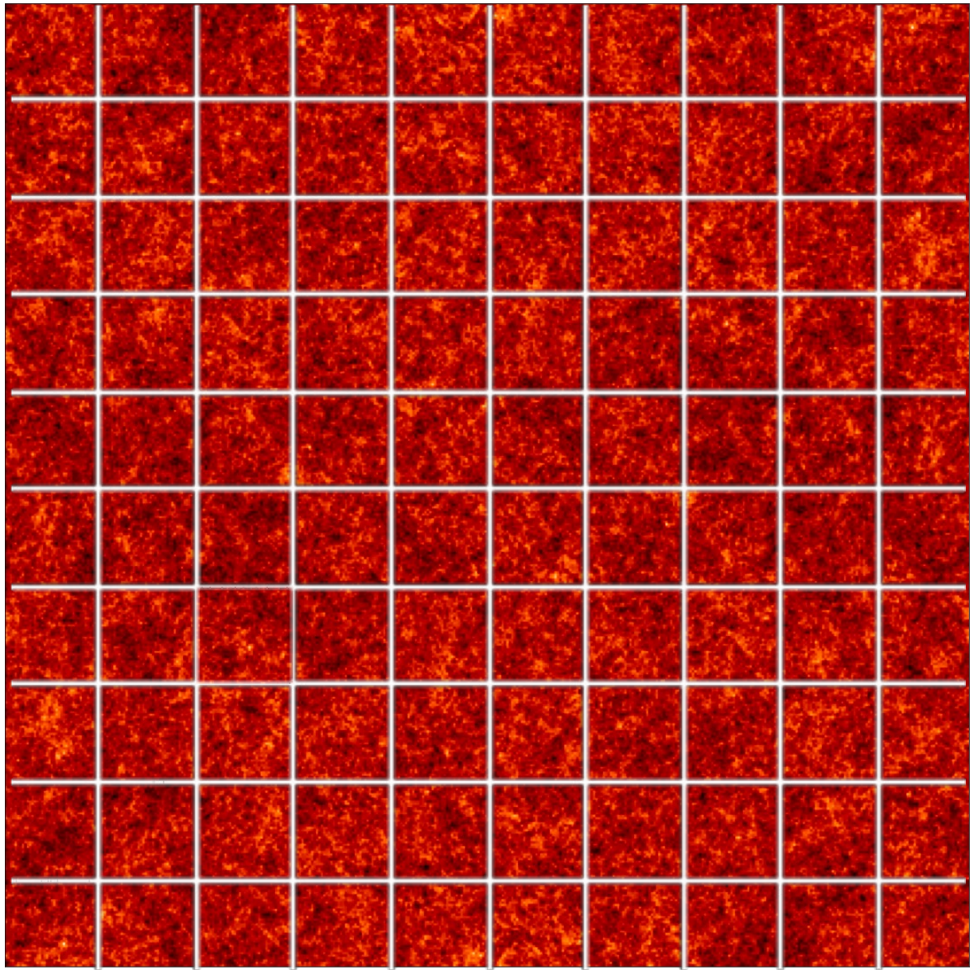
Bayer+ (2021)

Fake νs? Bayer, Banerjee, Seljak (2022)

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

Forward modeling

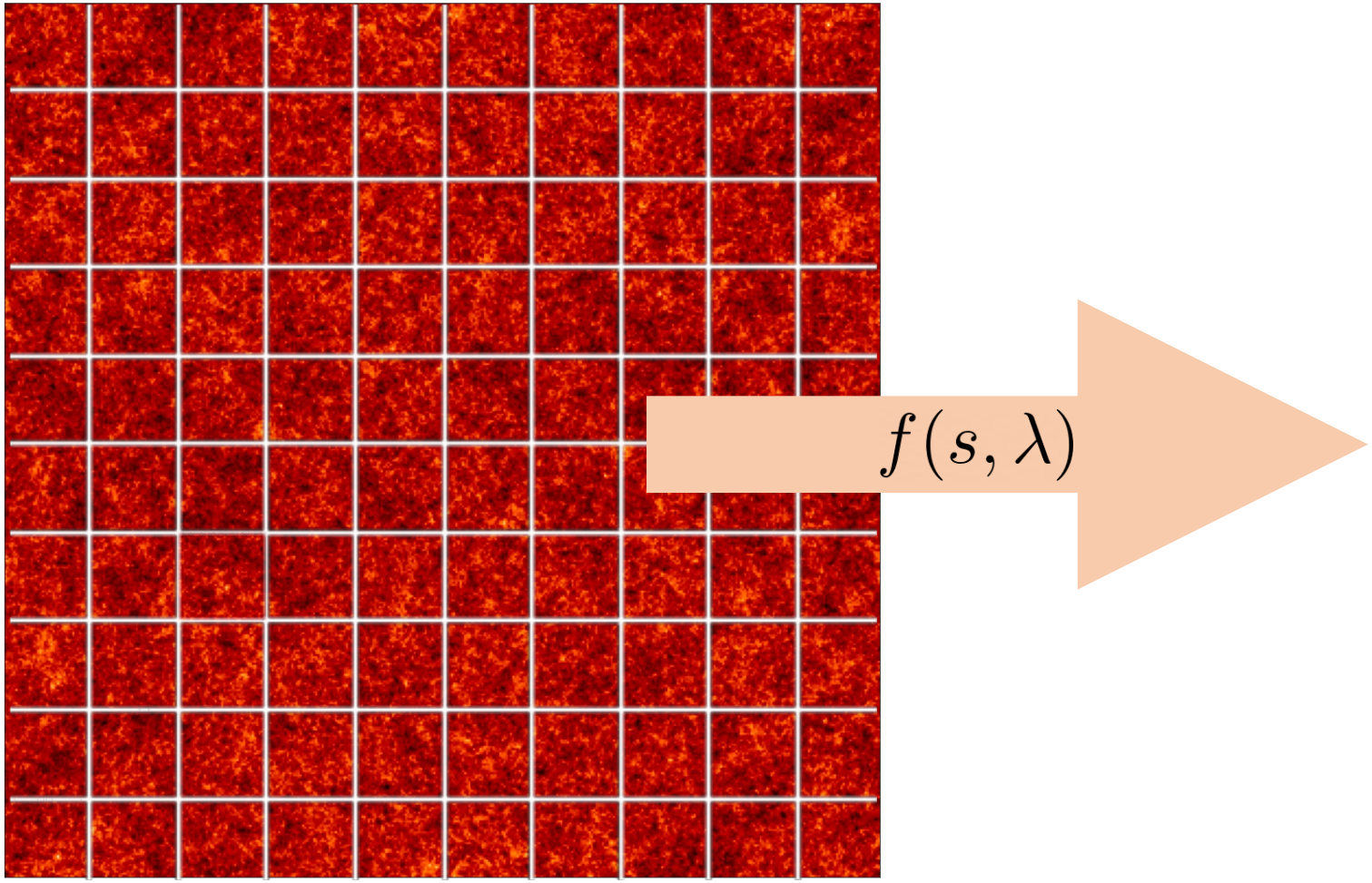
INITIAL s



Kitaura & Ensslin (2007), Jasche & Wandelt (2012), Jasche & Lavaux (2017), Seljak et al. (2017), Schmidt et al. (2020), …

Forward modeling

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

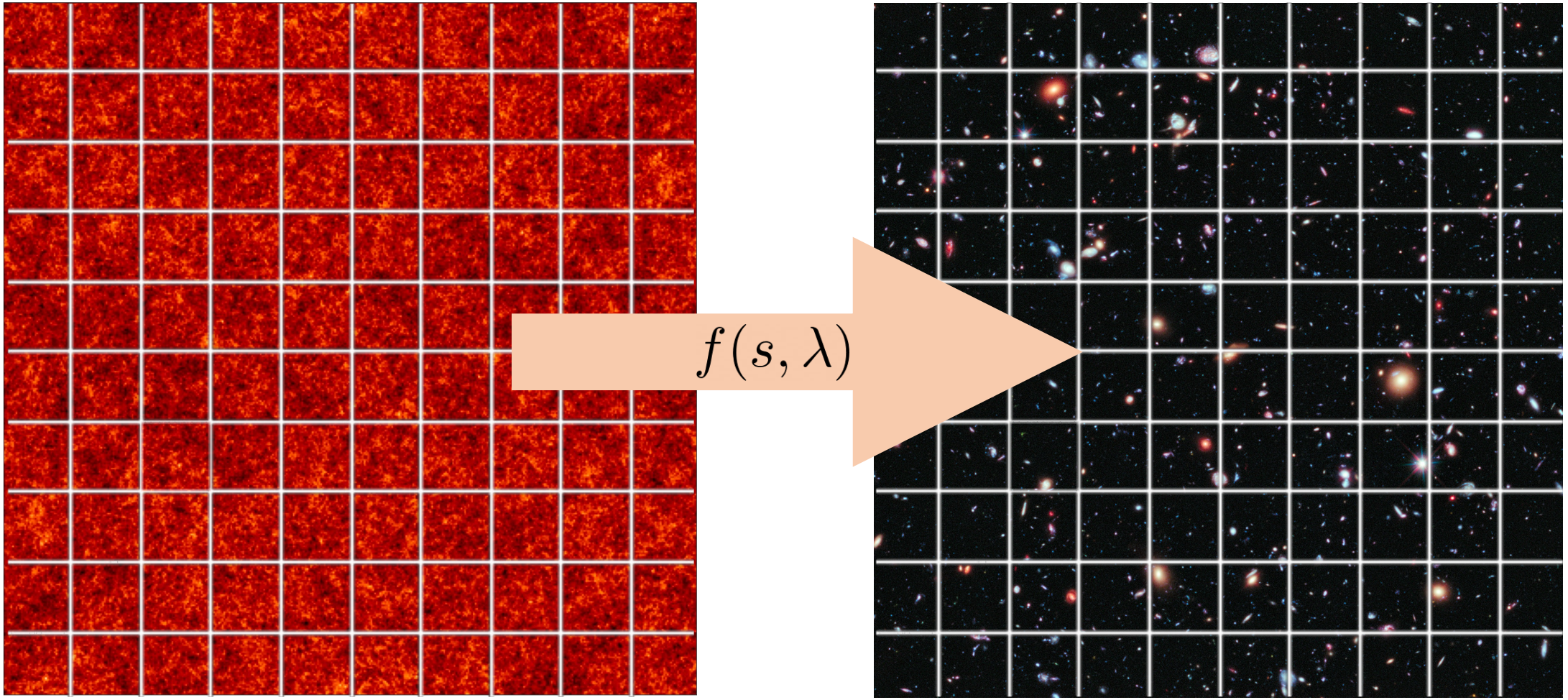


$f(s, \lambda)$

Kitaura & Ensslin (2007), Jasche & Wandelt (2012), Jasche & Lavaux (2017), Seljak et al. (2017), Schmidt et al. (2020), …

Forward modeling

INITIAL s $\lambda = \{\sigma_8, \Omega_m, ...\}$ FINAL



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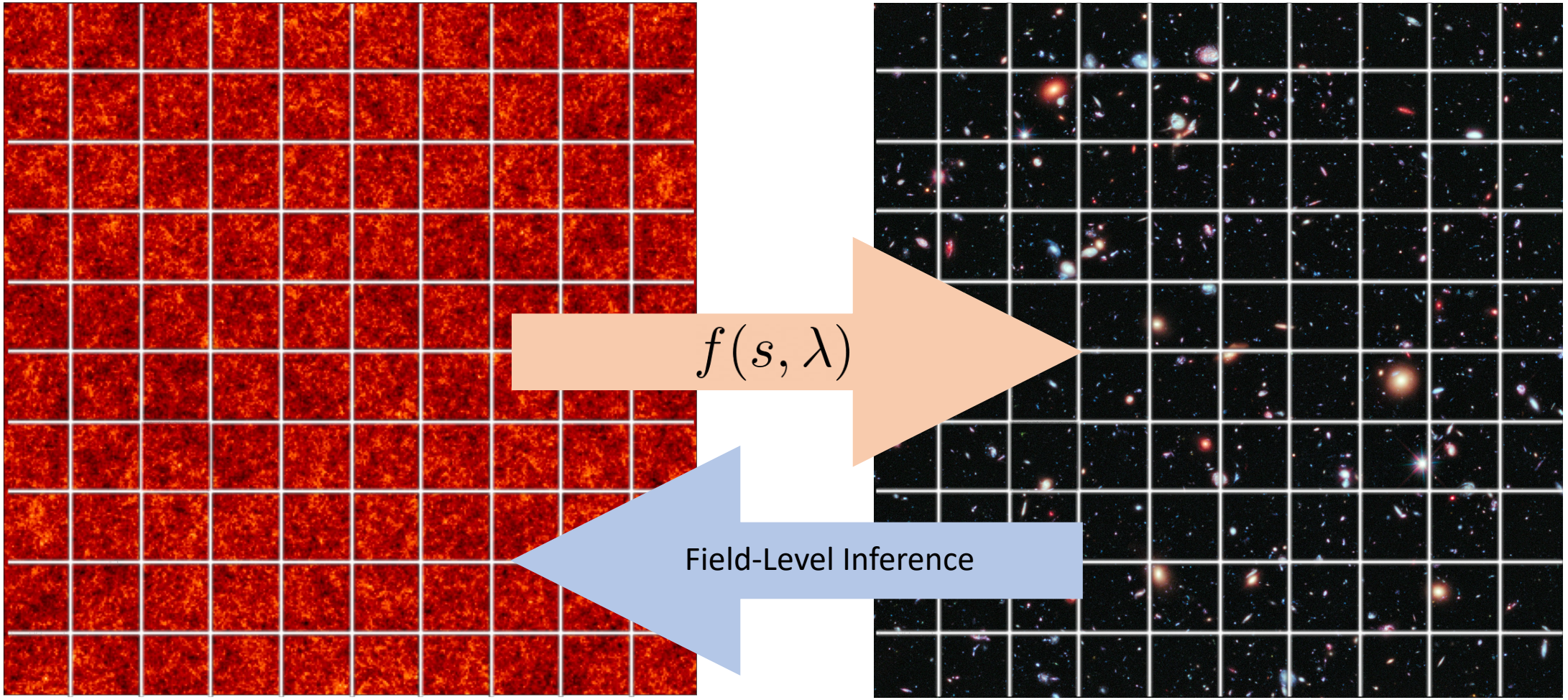

Kitaura & Ensslin (2007), Jasche & Wandelt (2012), Jasche & Lavaux (2017), Seljak et al. (2017), Schmidt et al. (2020), …

Field-Level Inference

Given field data d and forward model f infer

initial modes s and cosmological parameters λ

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

posterior likelihood prior

Field-Level Inference

Given field data d and forward model f infer

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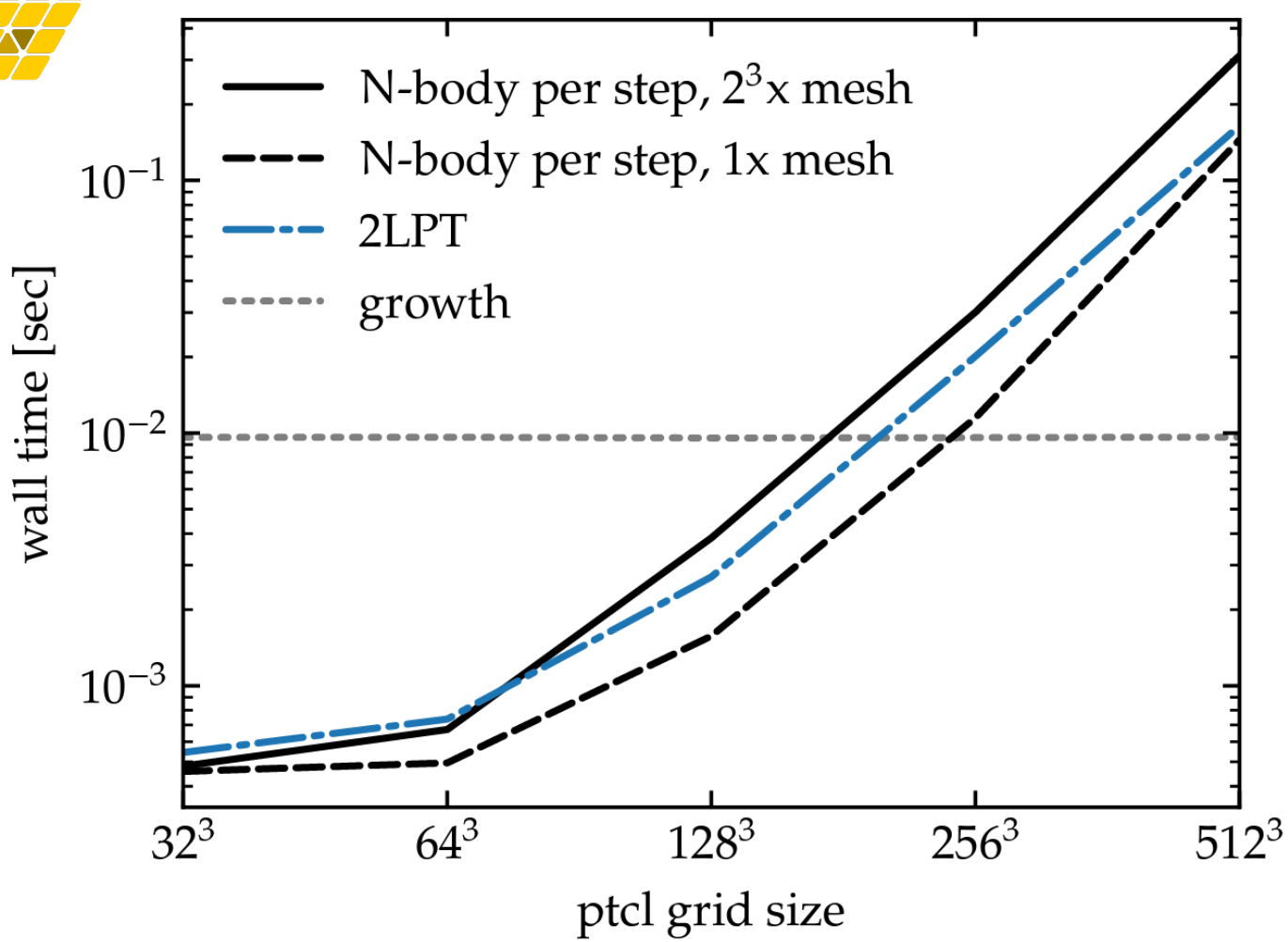
posterior | likelihood | prior

CHALLENGE: Multimillion dimensional parameter space!

1. Need fast forward model

2. Need differentiable forward model

3. Need fast sampler



1. Fast forward model ✅

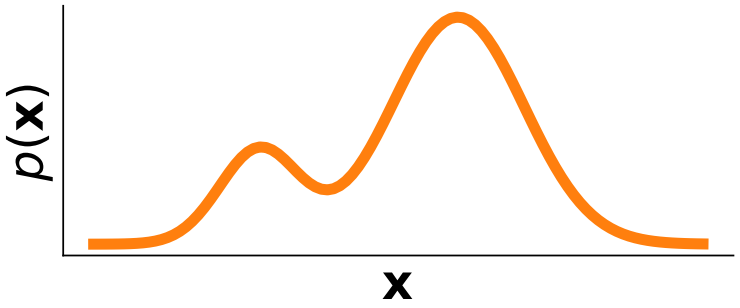
2. Differentiable forward model ✅

3. Need fast sampler

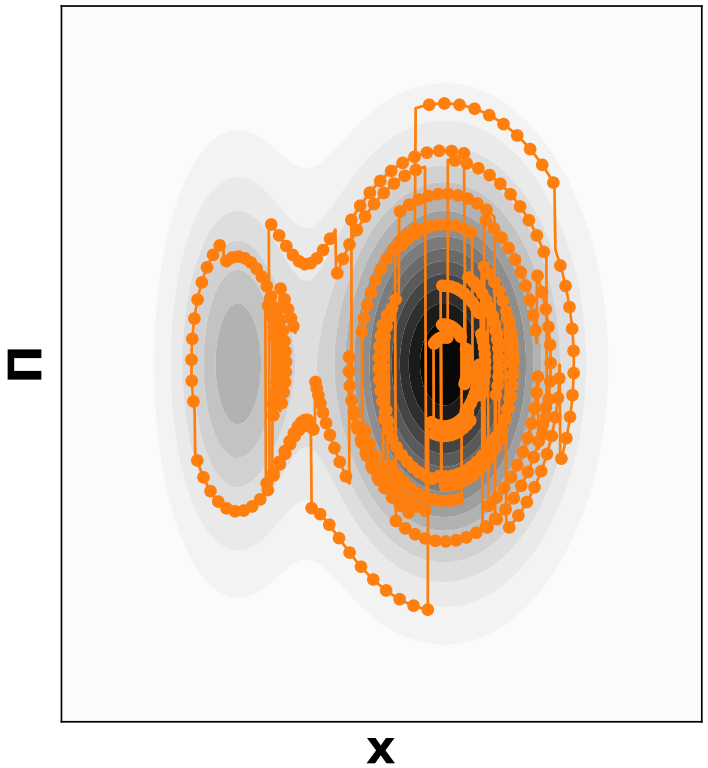
Li+2022

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

Canonical HMC

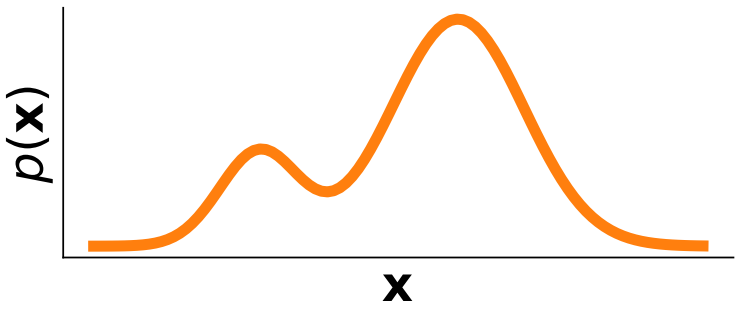


$$p(\mathbf{x}, \mathbf{\Pi}) \propto e^{-H(\mathbf{x}, \mathbf{\Pi})}$$

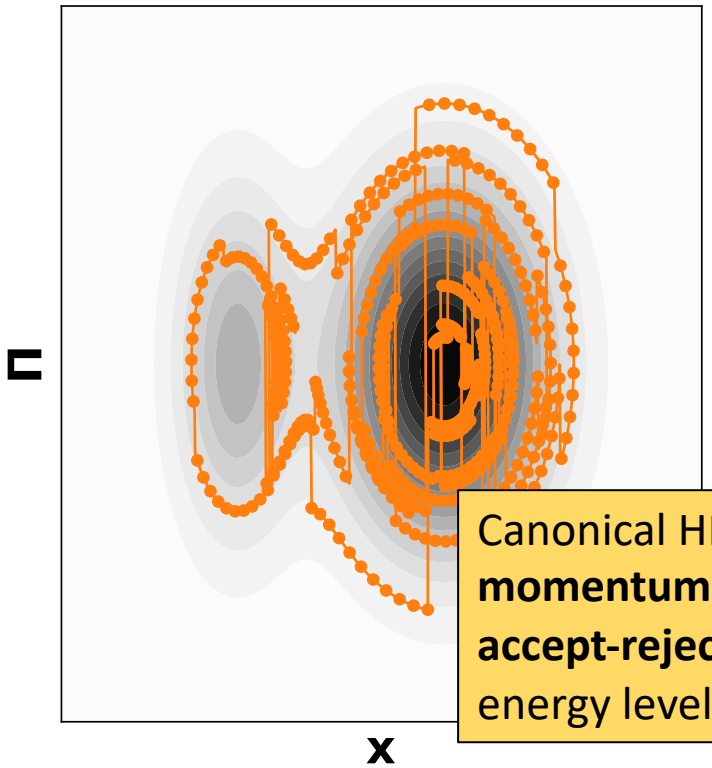


Robnik+2022

Canonical HMC



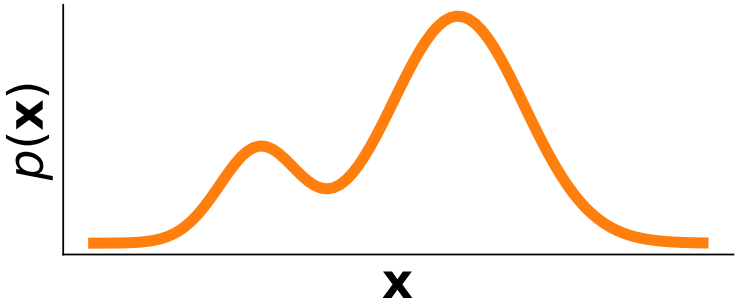
$$p(\mathbf{x}, \mathbf{\Pi}) \propto e^{-H(\mathbf{x}, \mathbf{\Pi})}$$



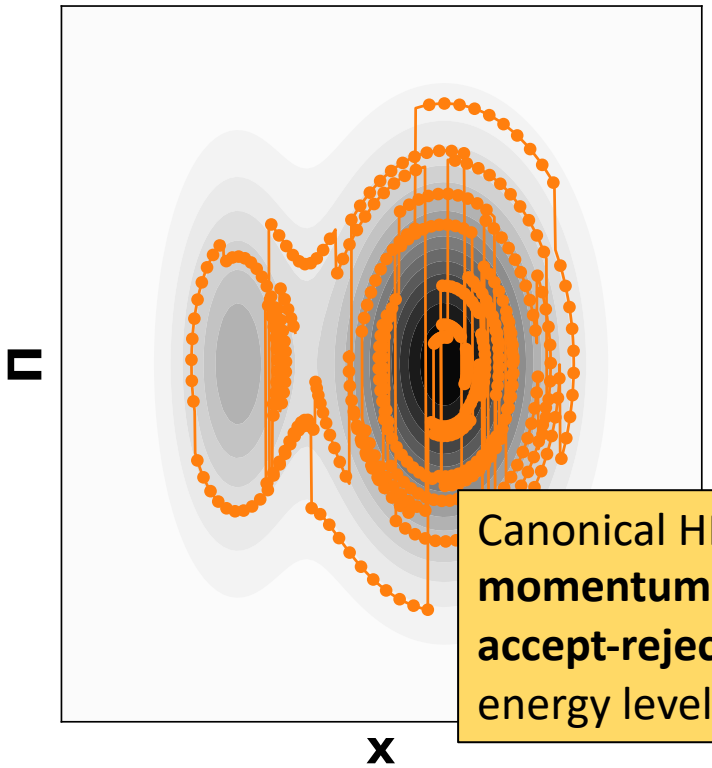
Canonical HMC requires **momentum resampling** and **accept-reject step** to change energy levels and converge

Robnik+2022

Canonical HMC

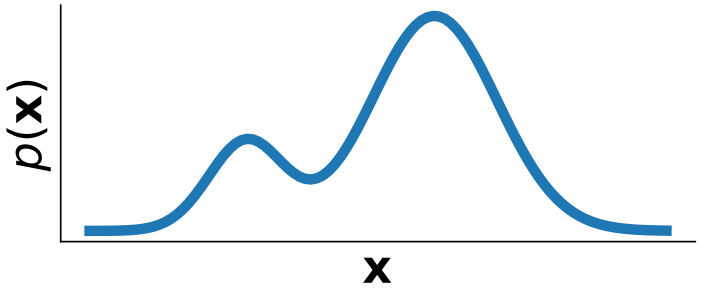


$$p(\mathbf{x}, \boldsymbol{\Pi}) \propto e^{-H(\mathbf{x}, \boldsymbol{\Pi})}$$

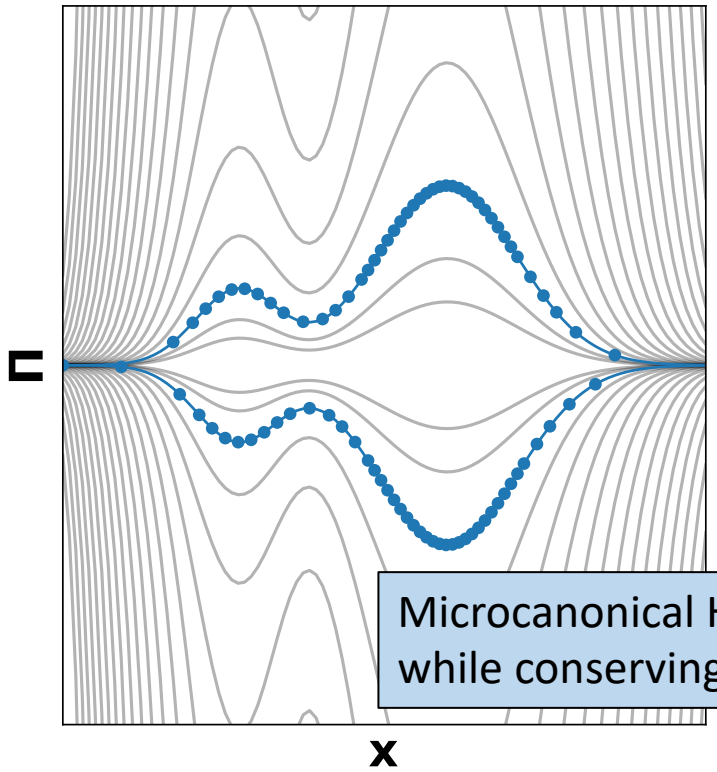


Canonical HMC requires **momentum resampling** and **accept-reject step** to change energy levels and converge

Microcanonical HMC



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



Microcanonical HMC converges while conserving energy

Robnik+2022

Microcanonical Hamiltonian Monte Carlo

$$dz = udt$$

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

MCHMC

Robnik+2022

Microcanonical Langevin Monte Carlo

$$dz = u dt$$

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

MCHMC **MCLMC**

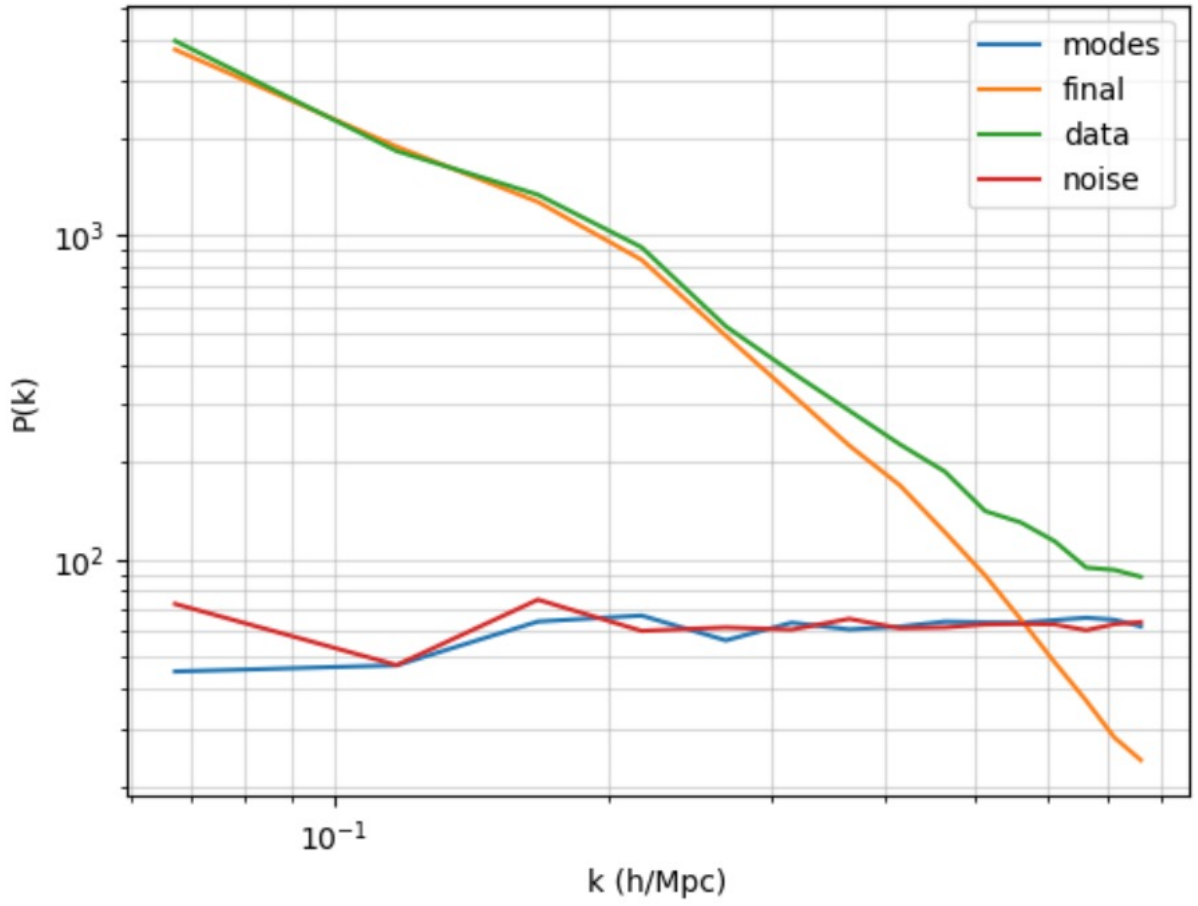
Improve ergodicity by including Langevin-like stochastic term

Robnik+2022

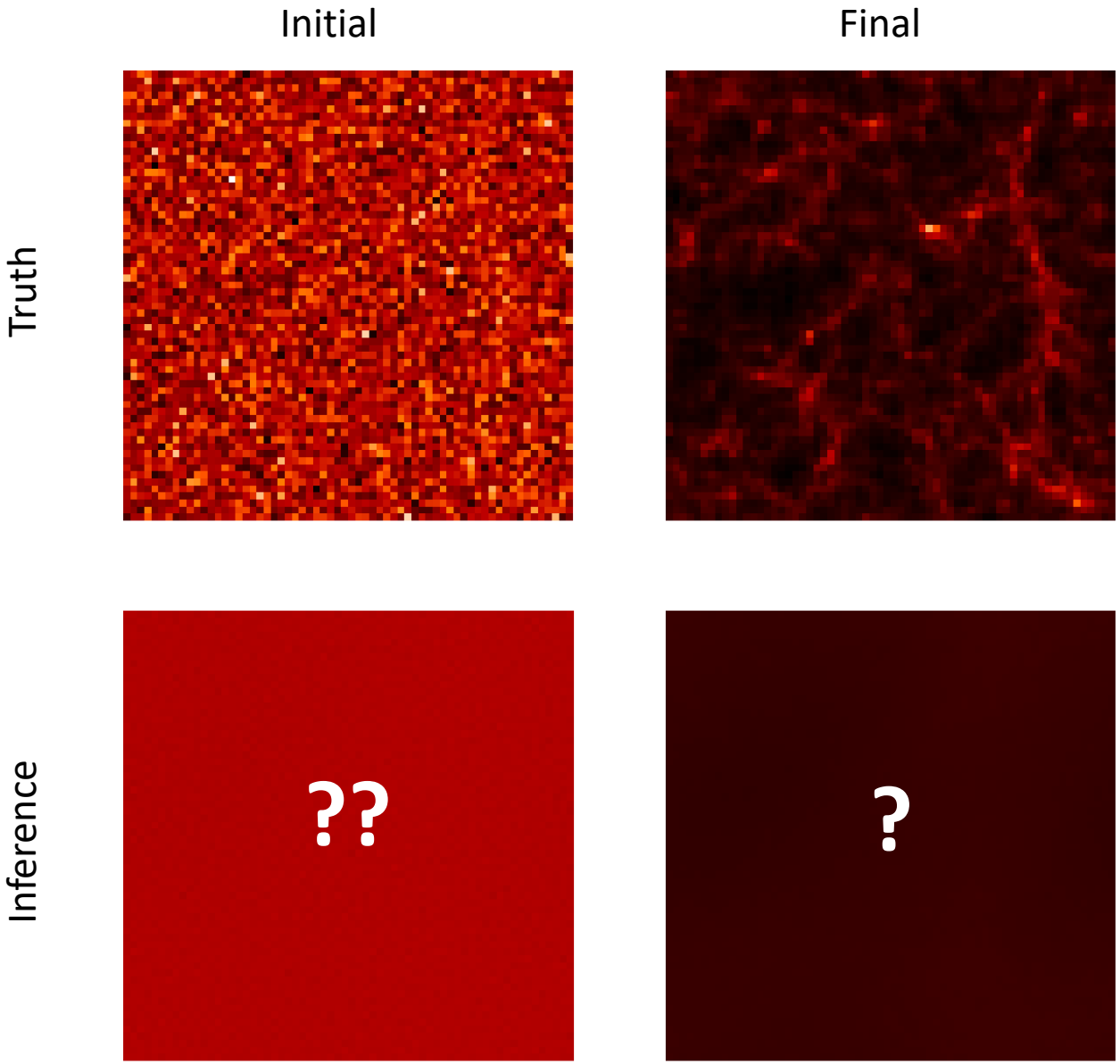
Cosmological Field-Level Inference *with* Microcanonical Langevin Monte Carlo

Experiments

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



Bayer, Seljak, Modi (2023)



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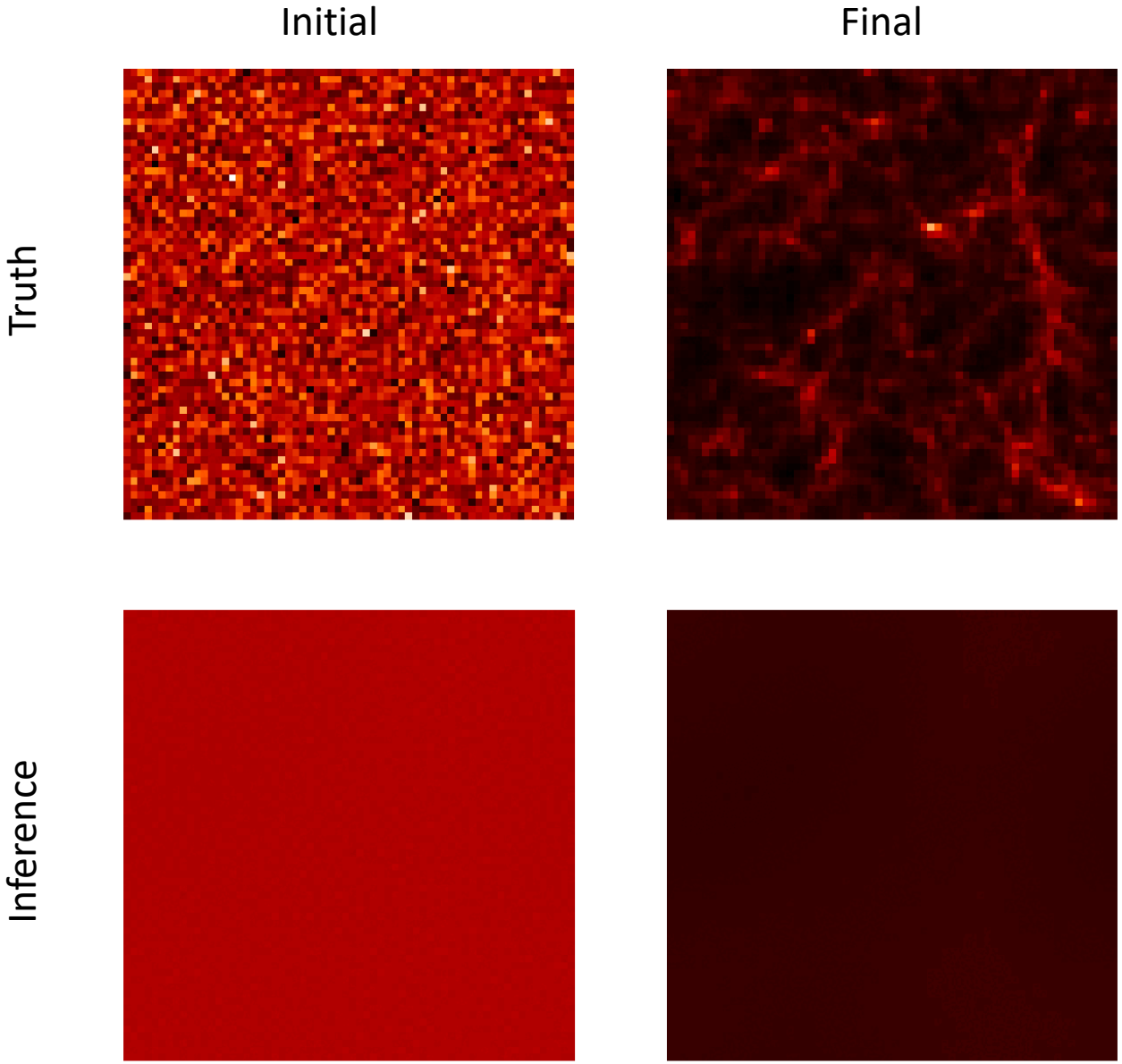

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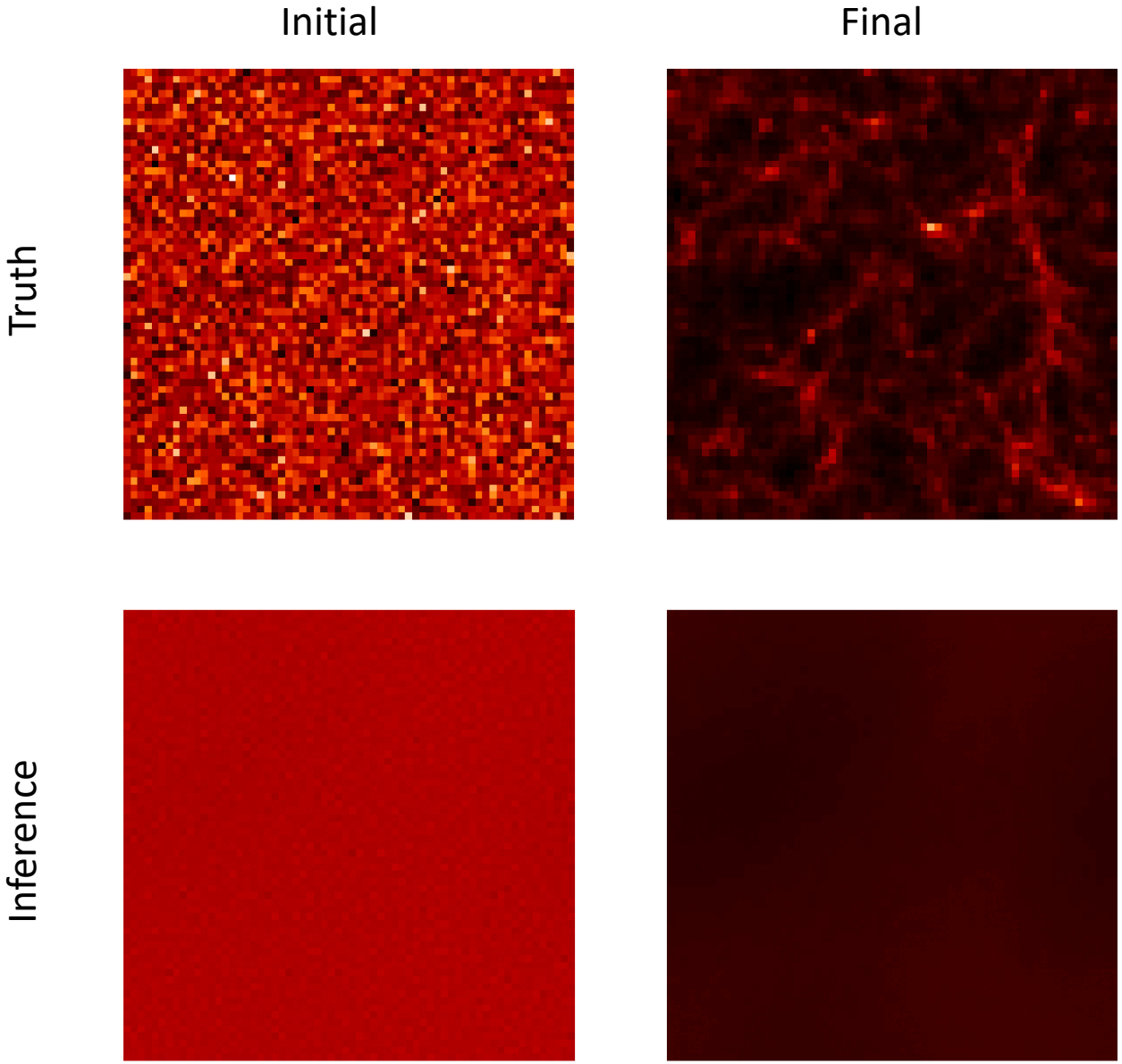

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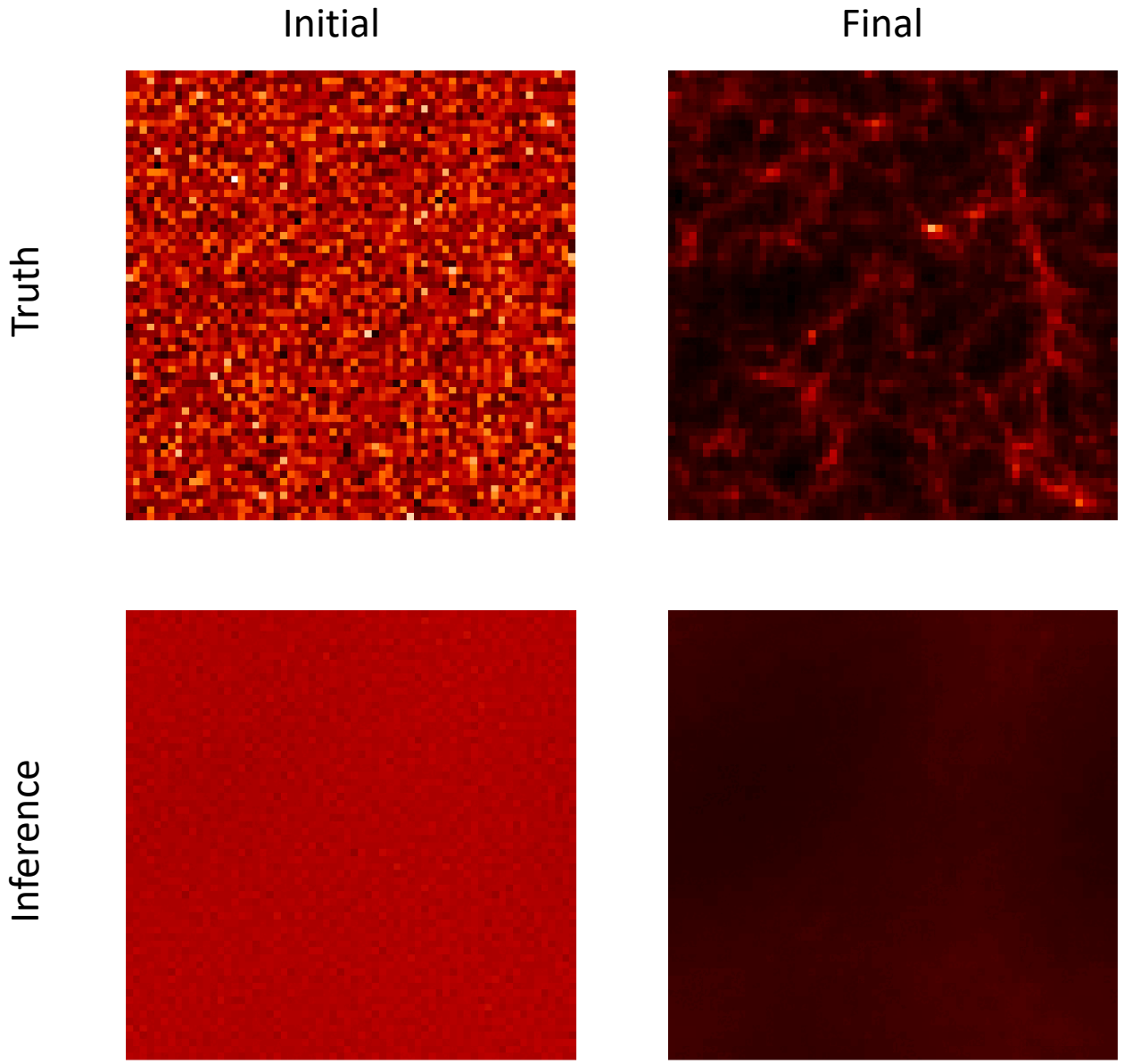

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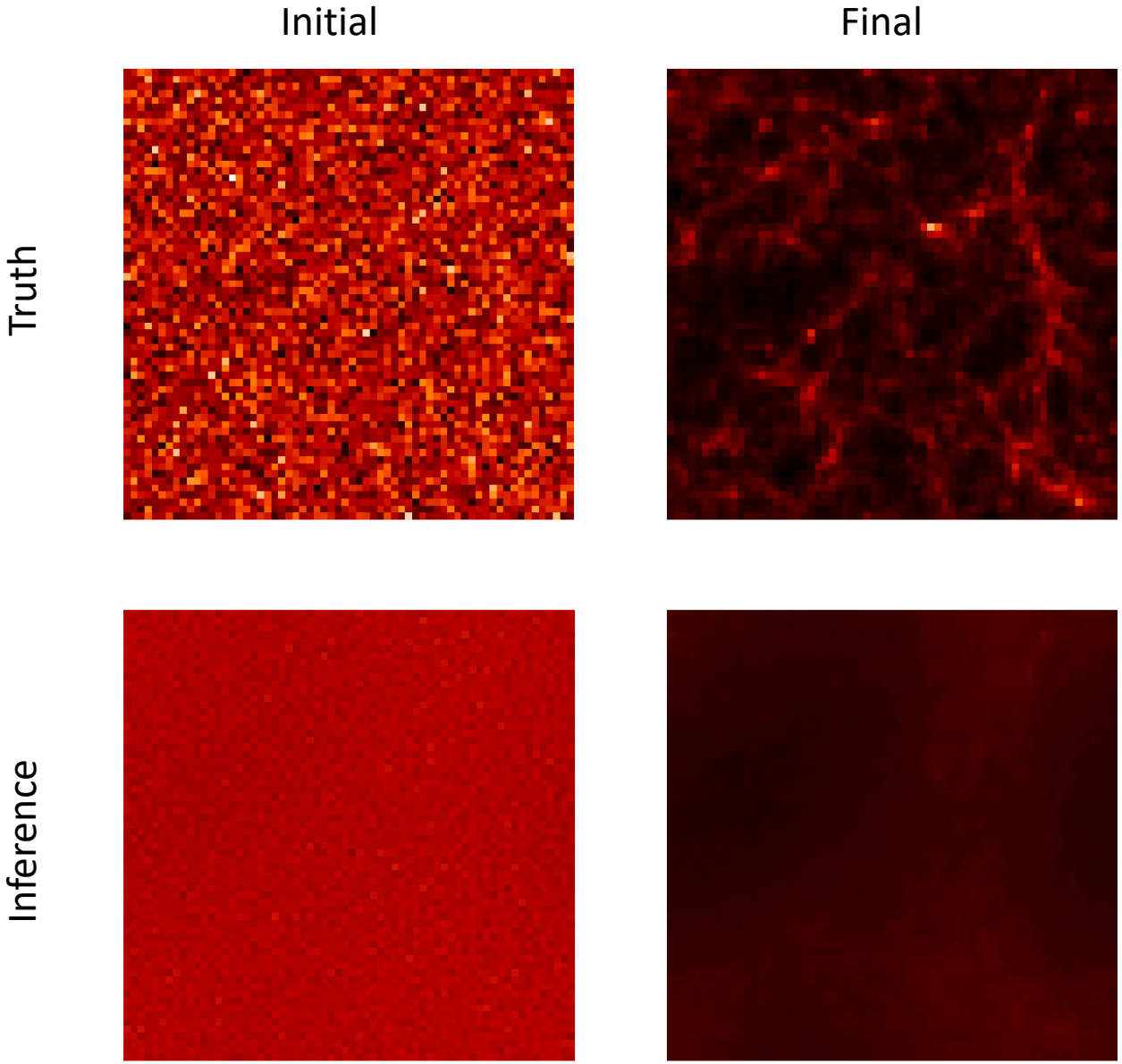

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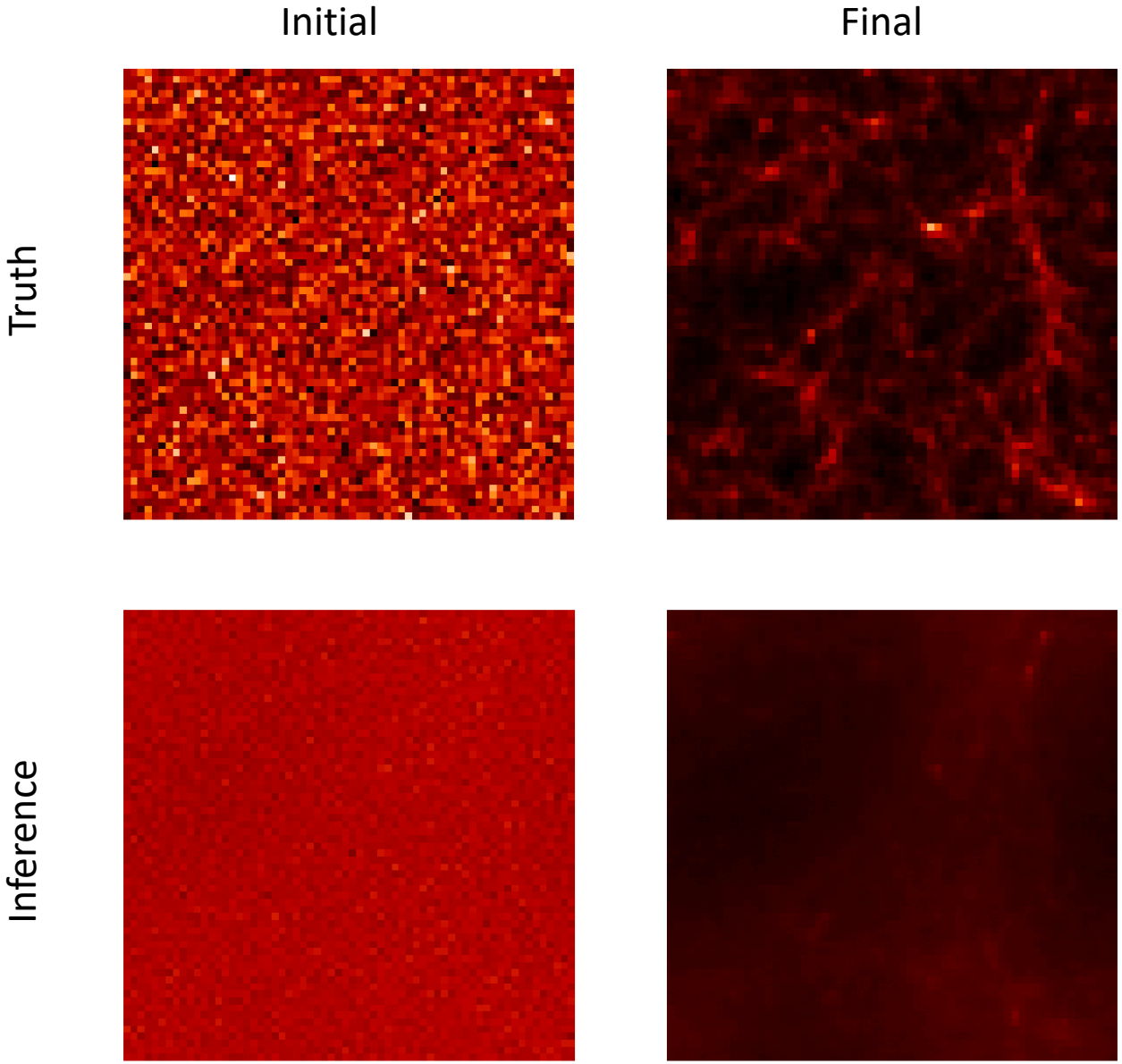

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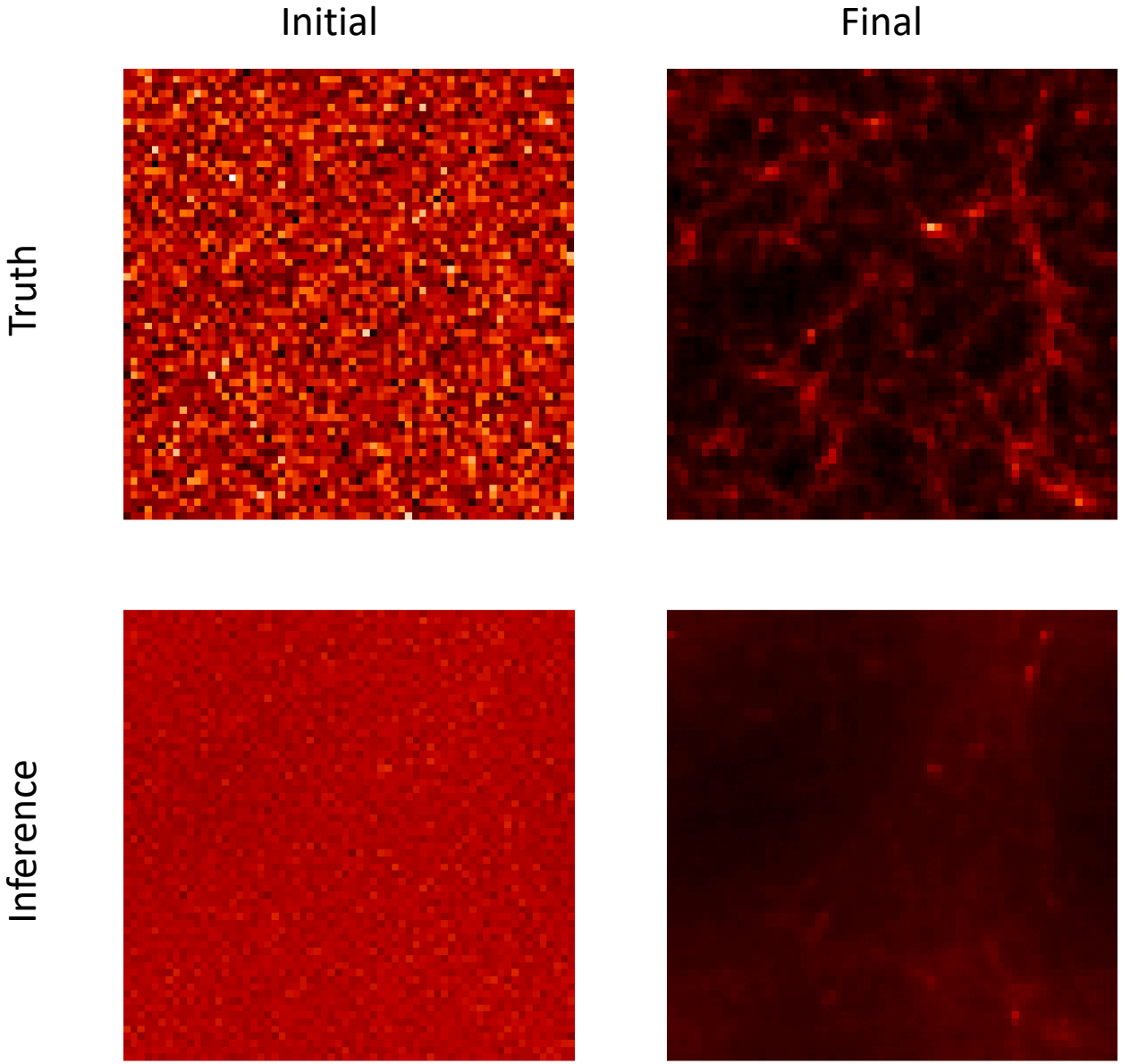

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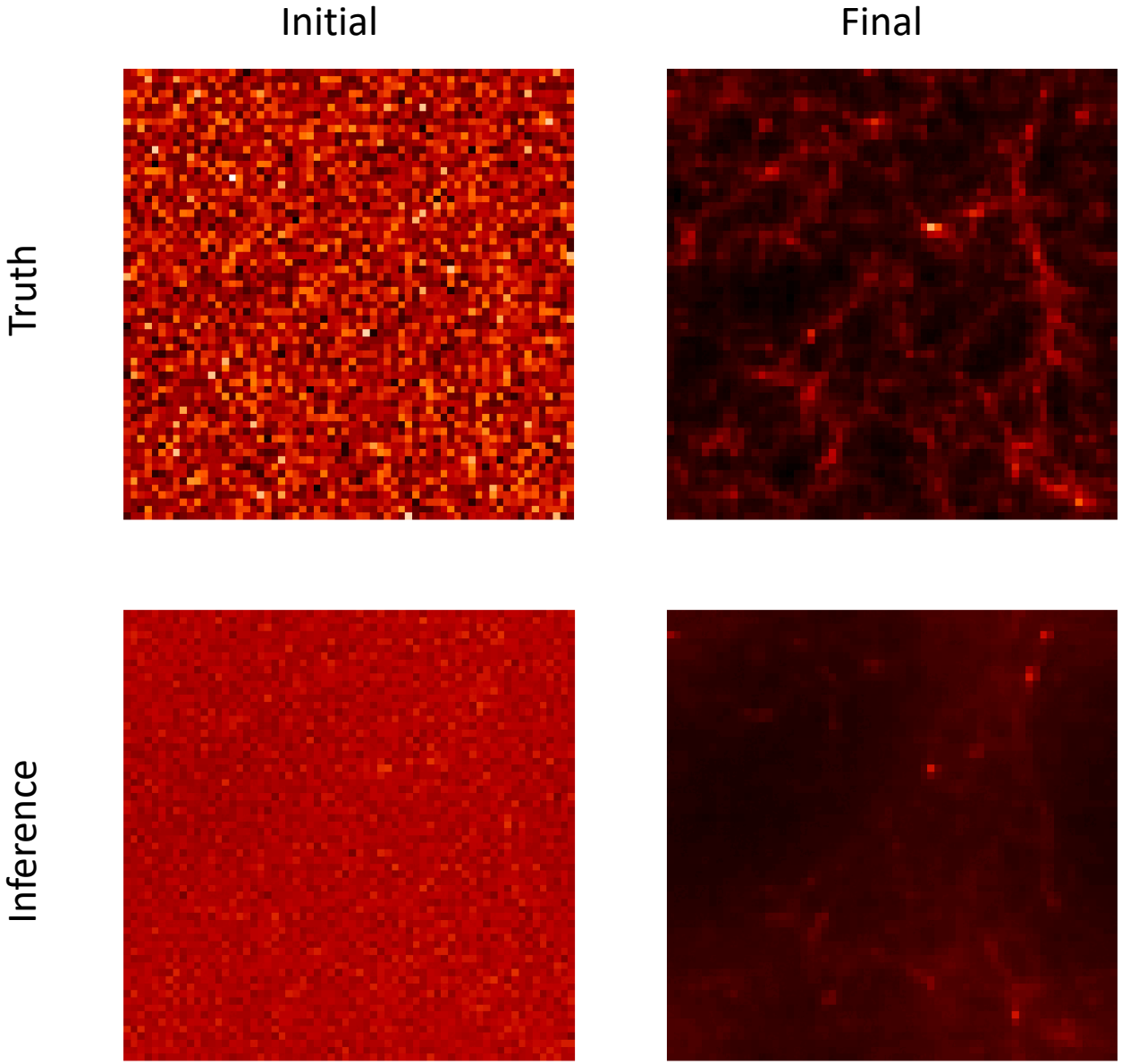

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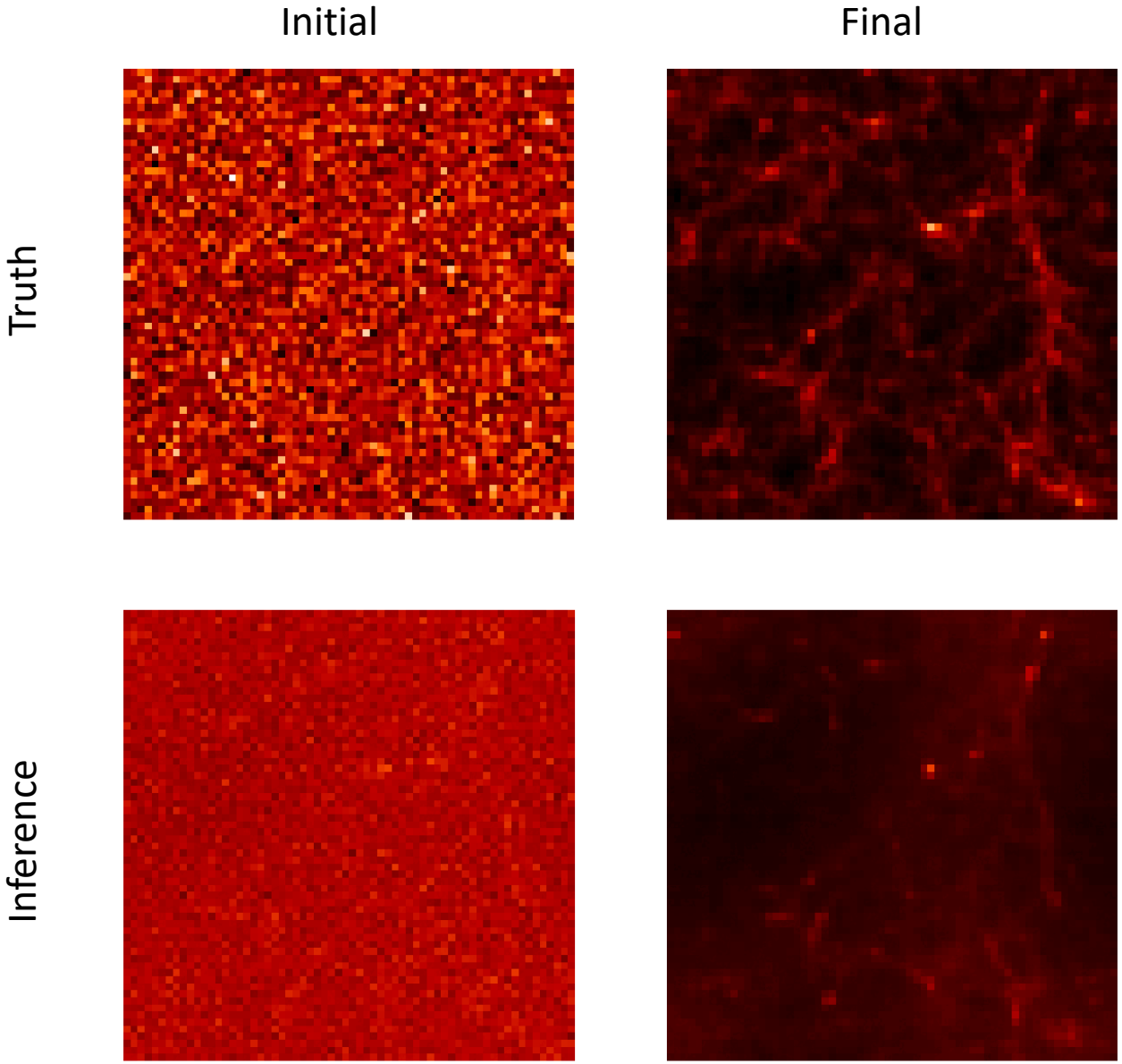

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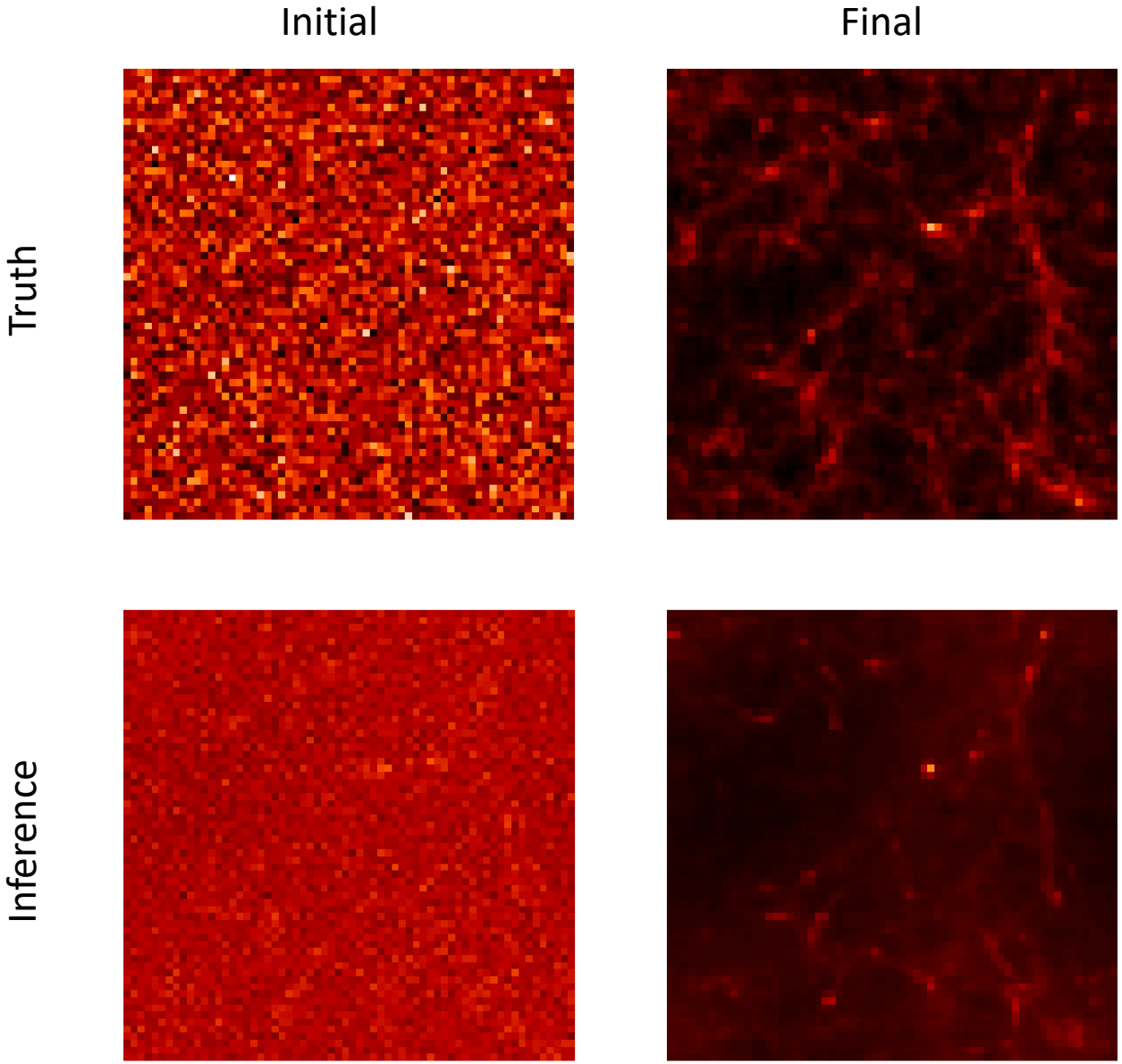

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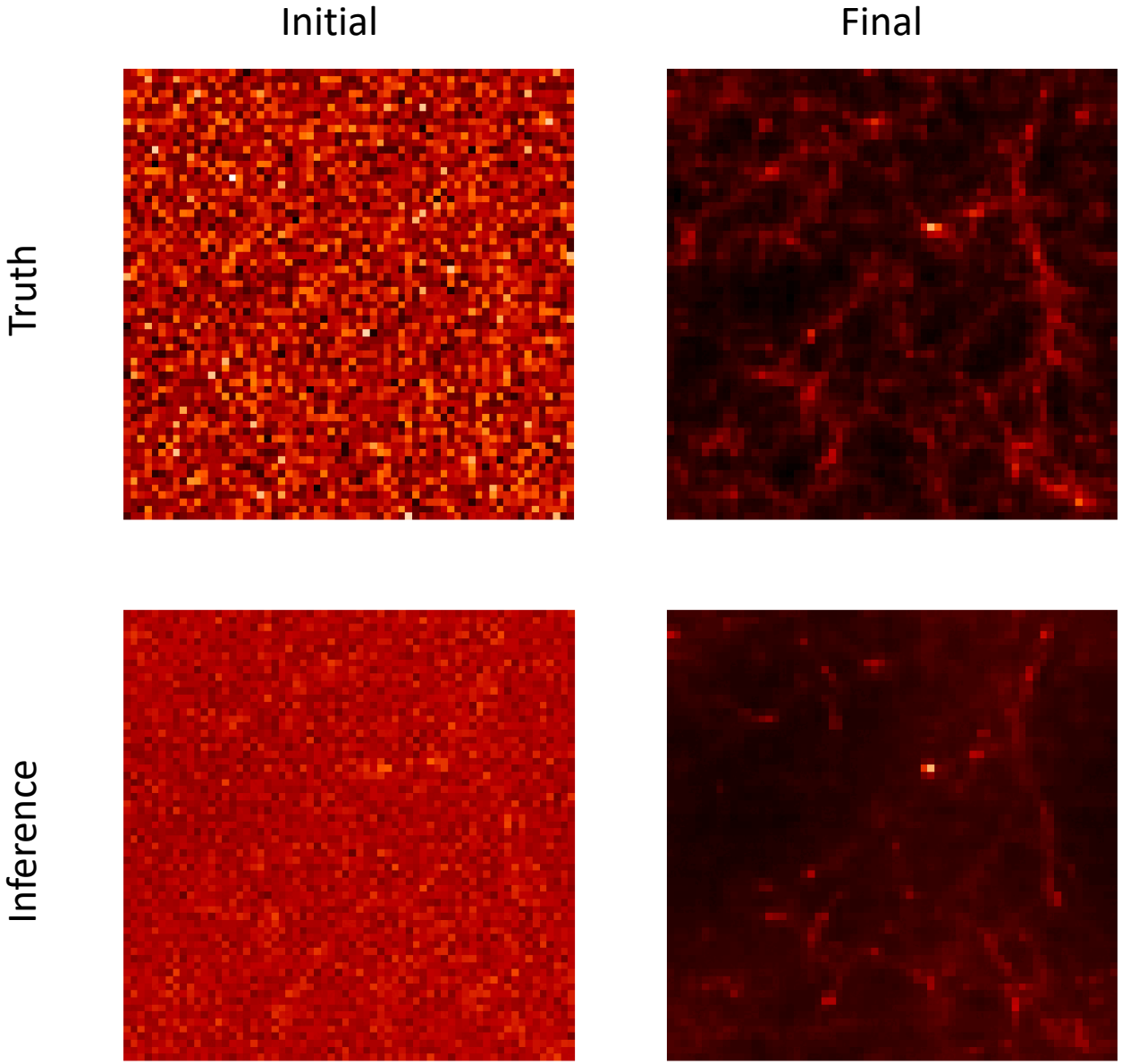

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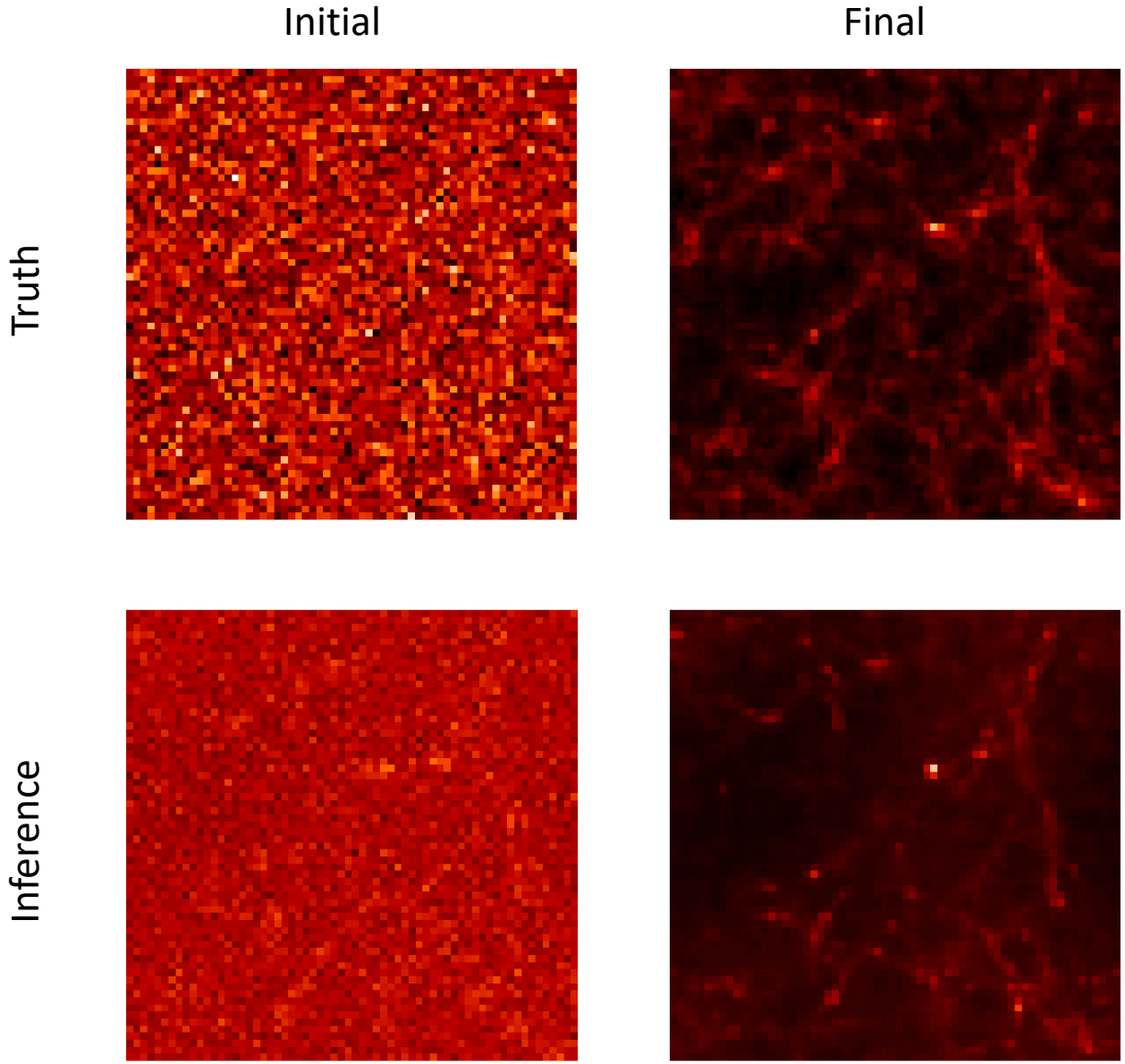

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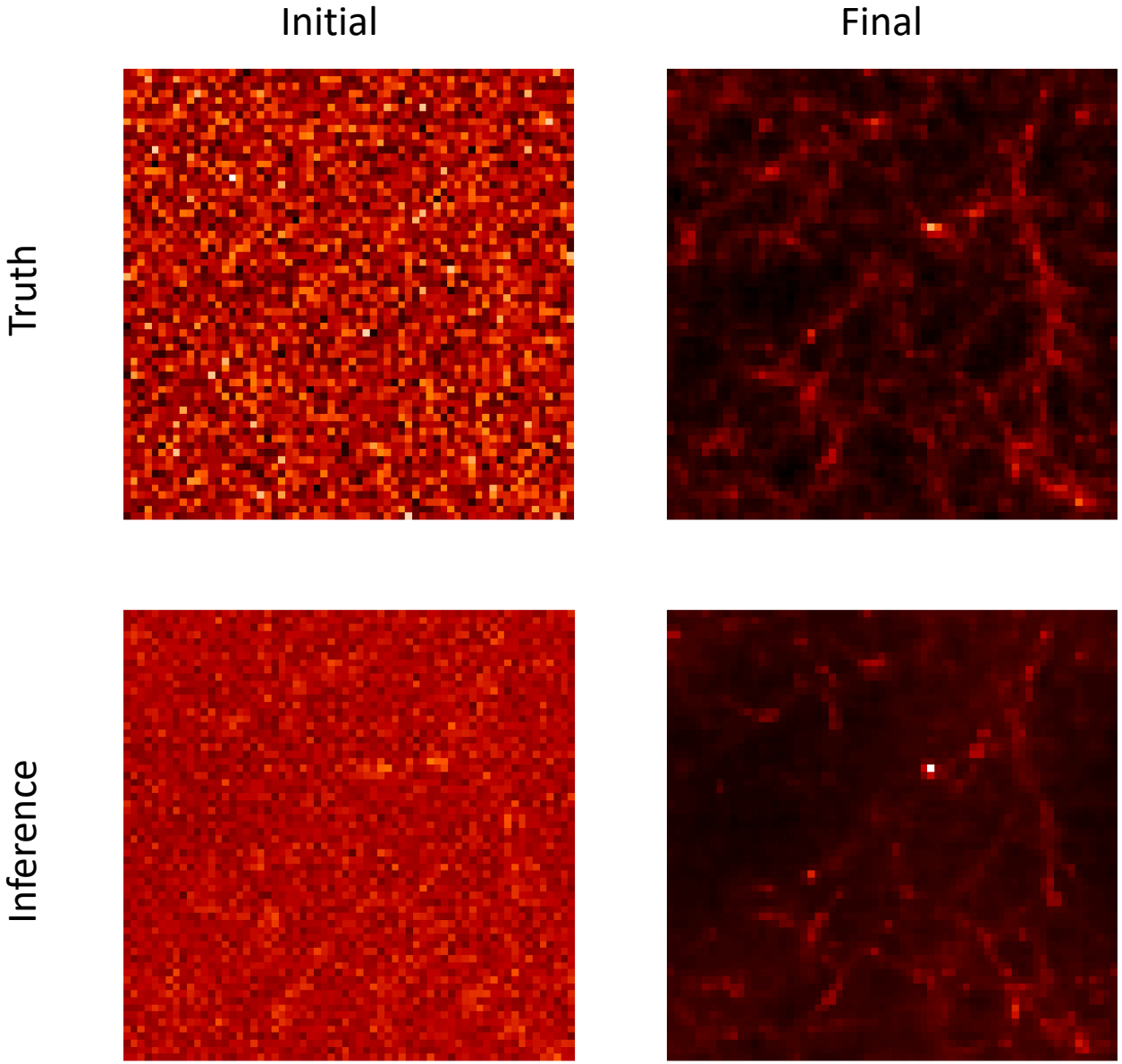

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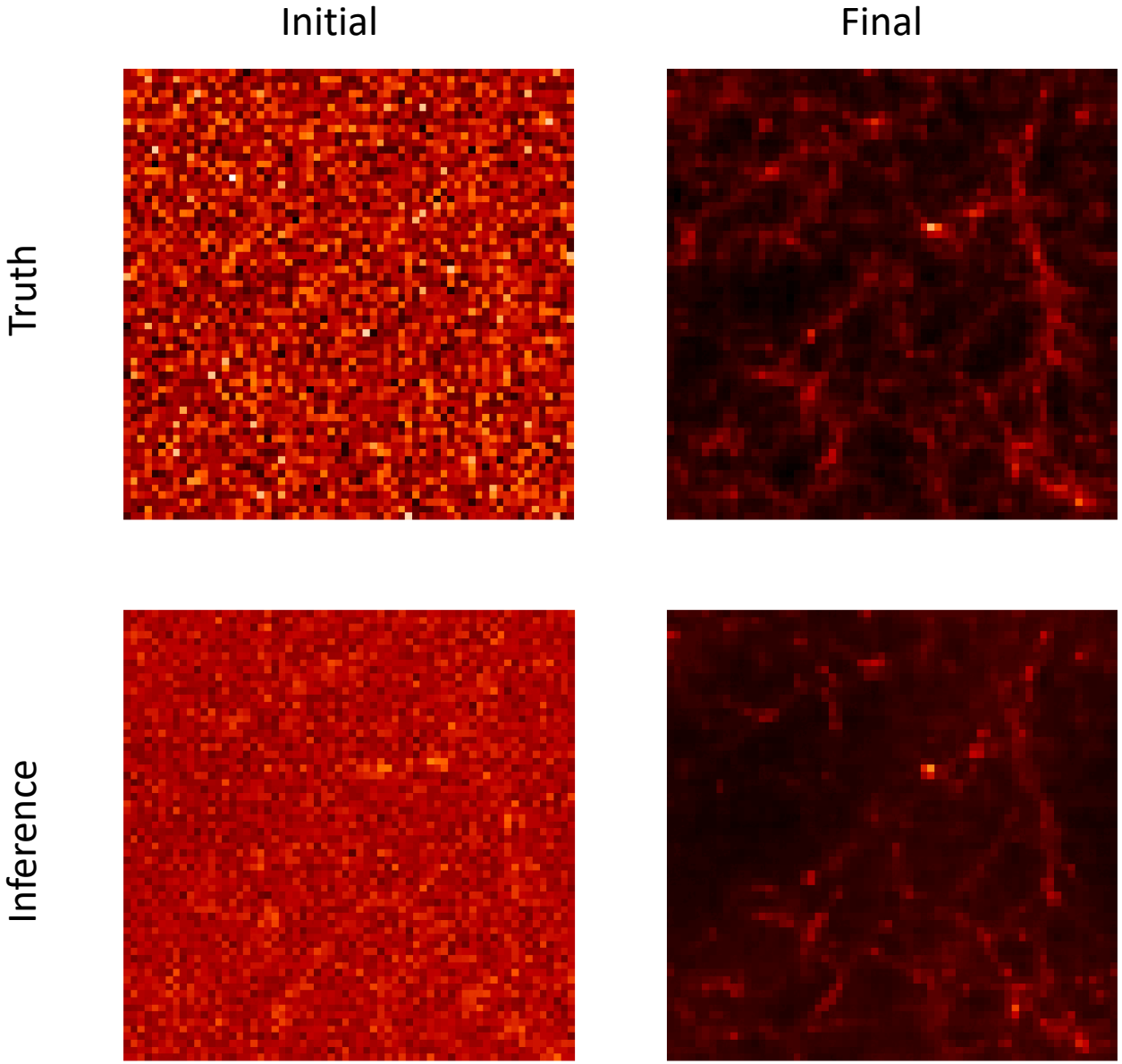

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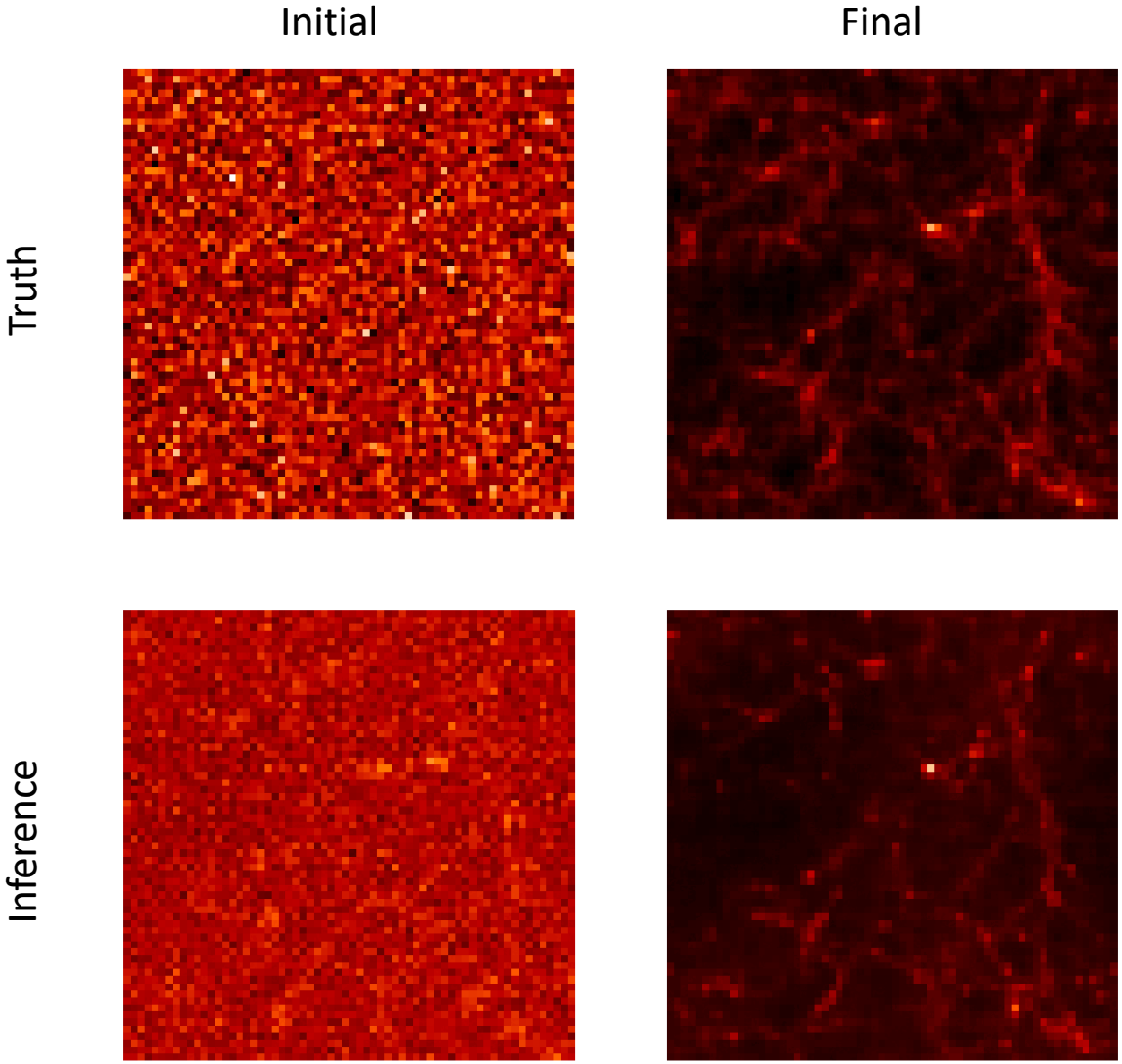

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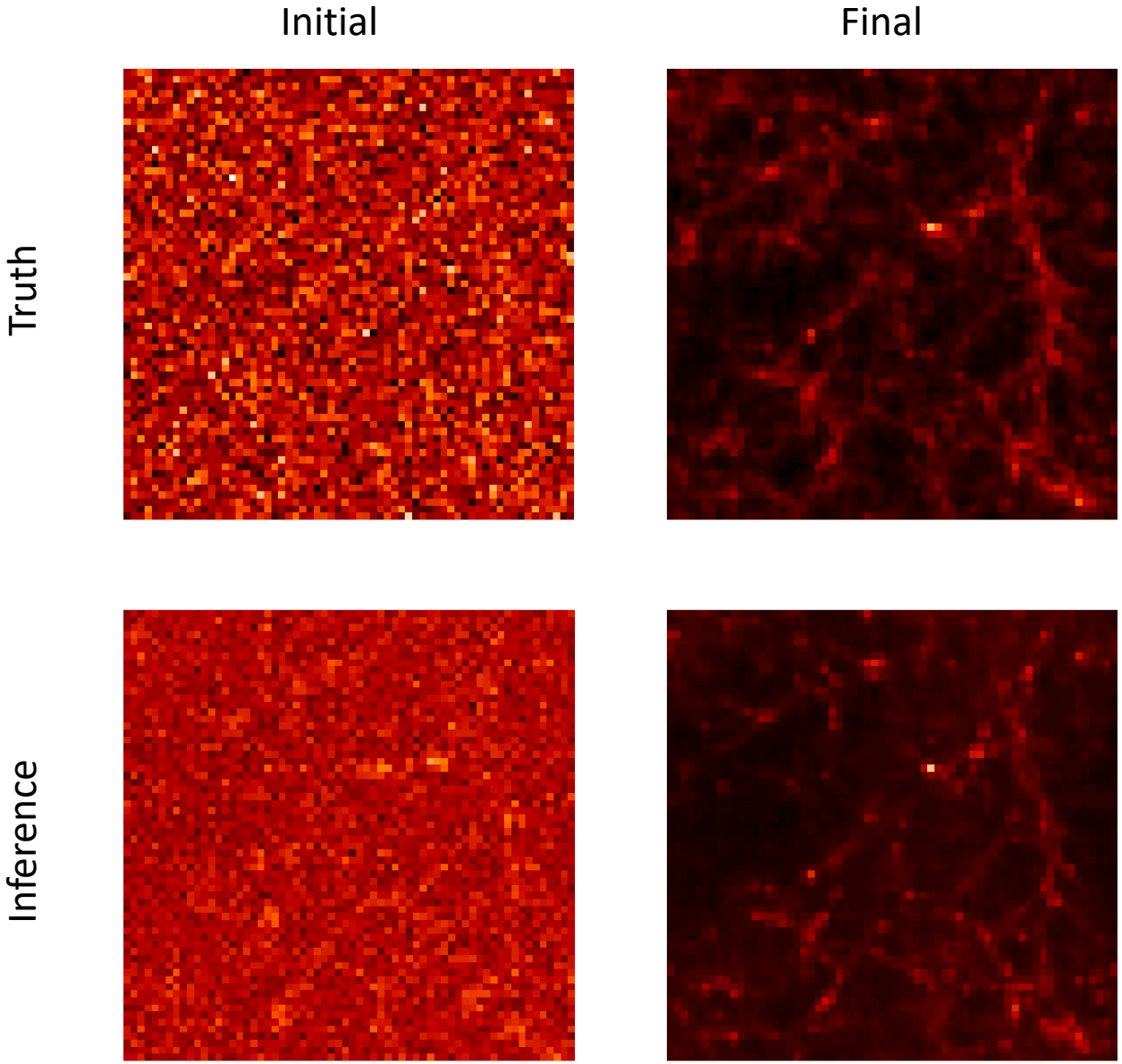

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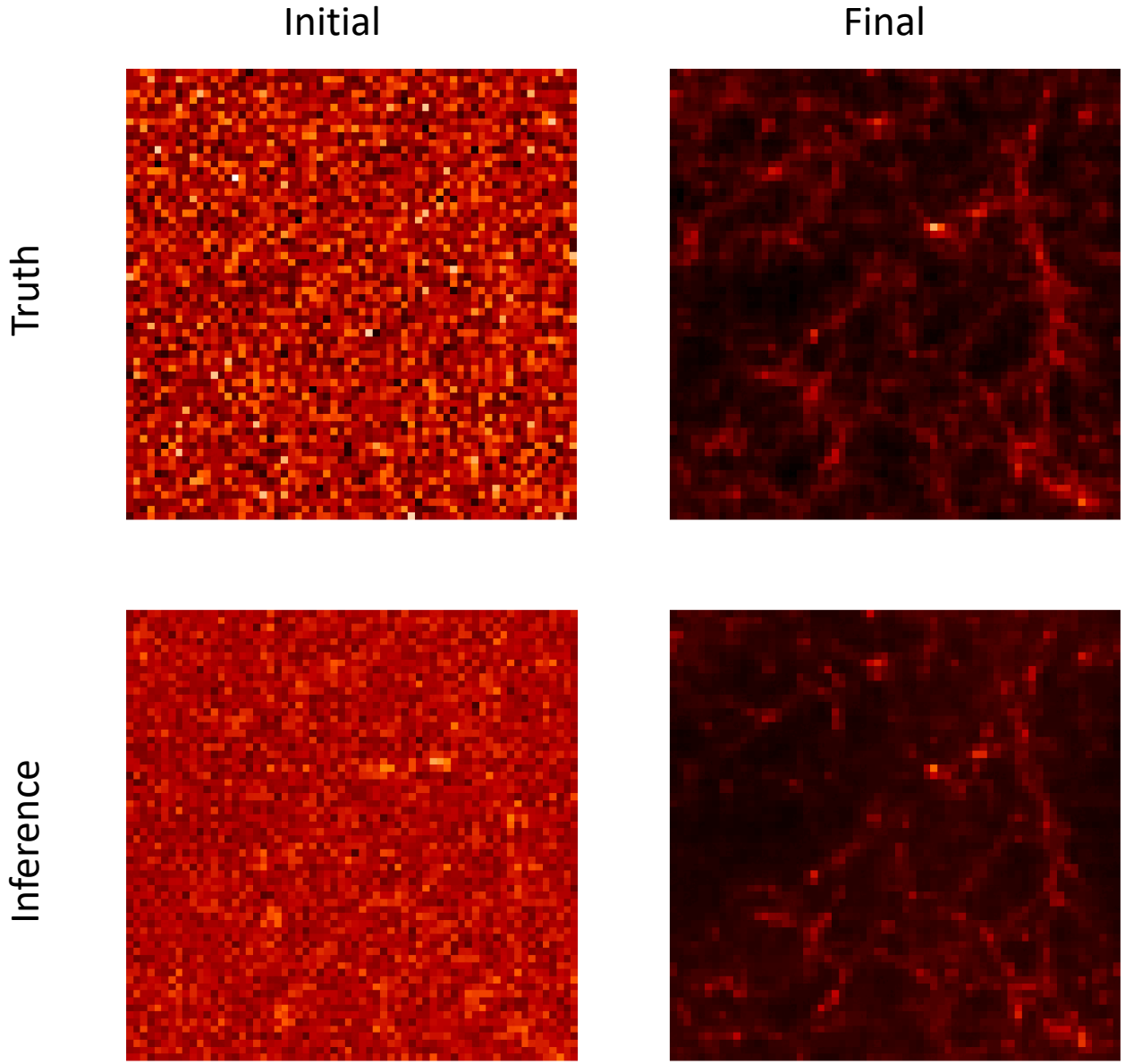

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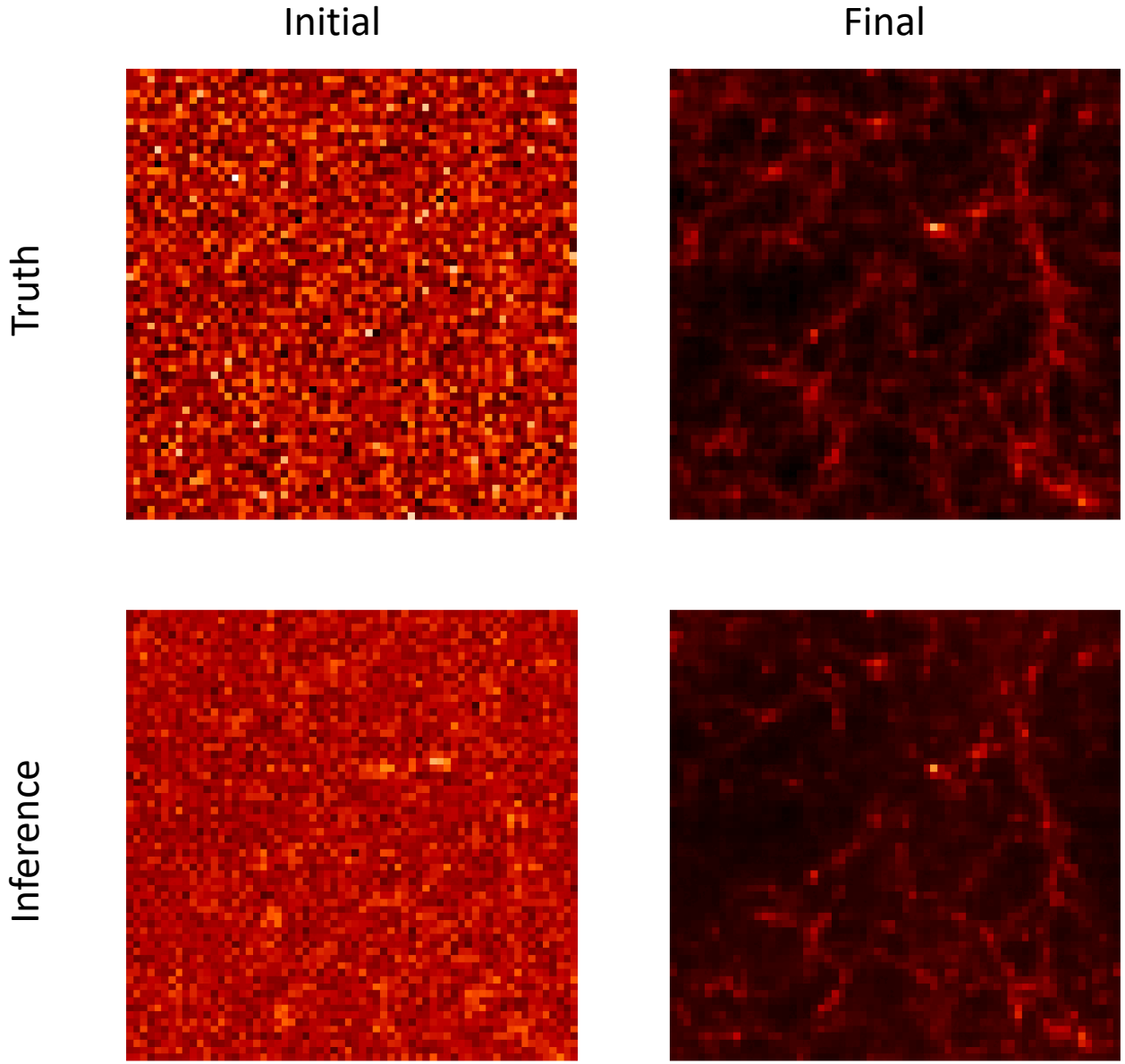

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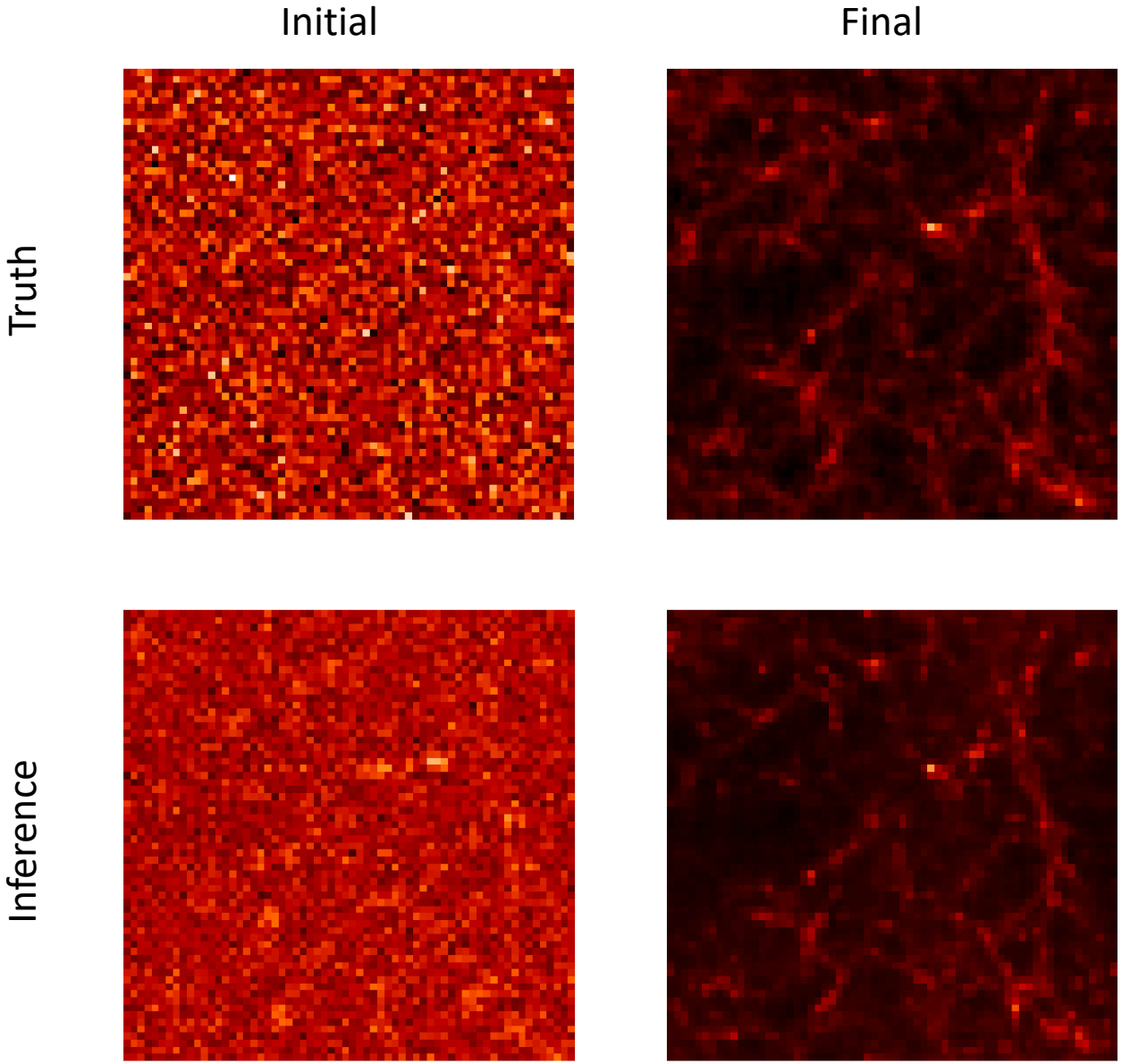

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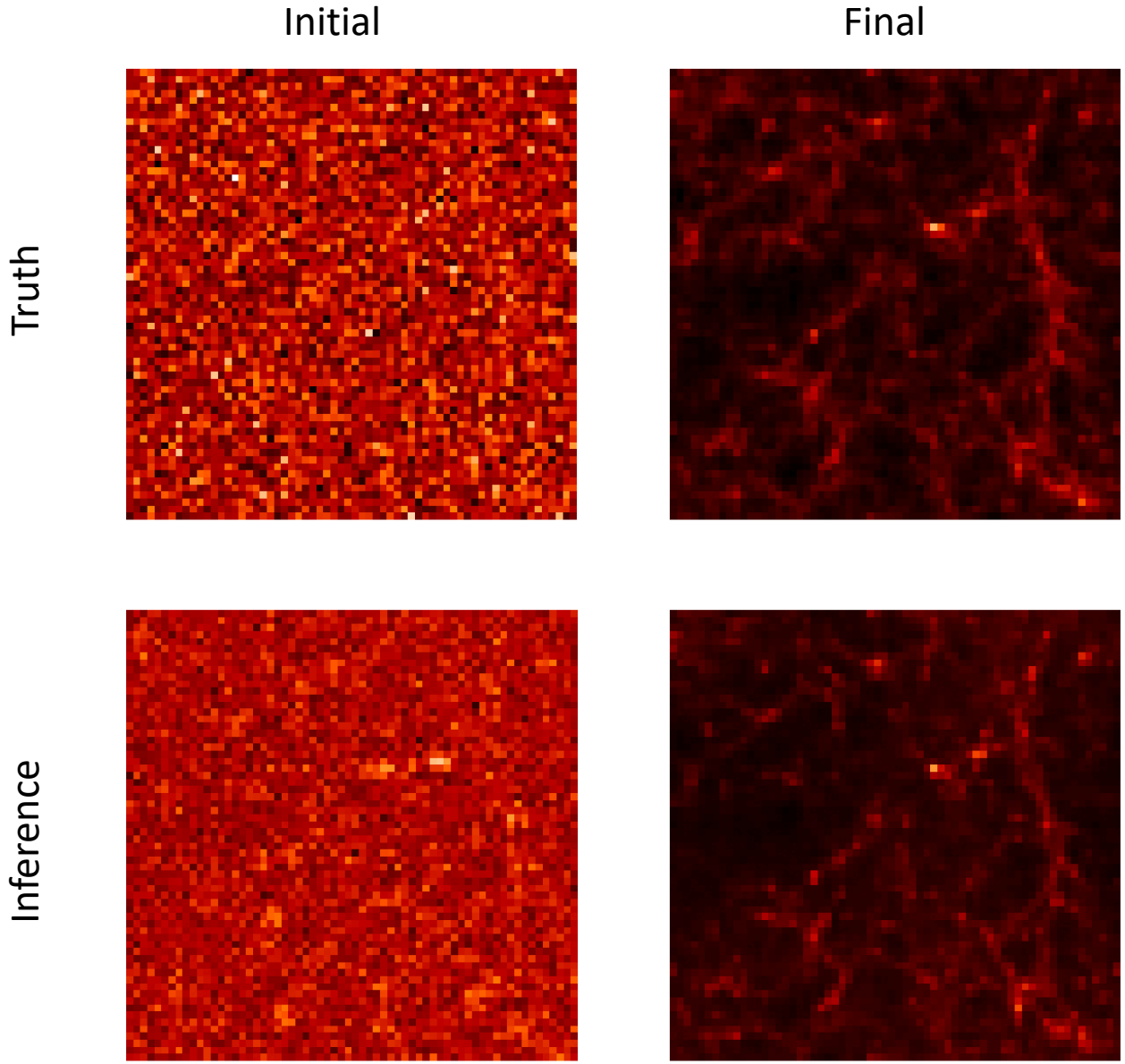

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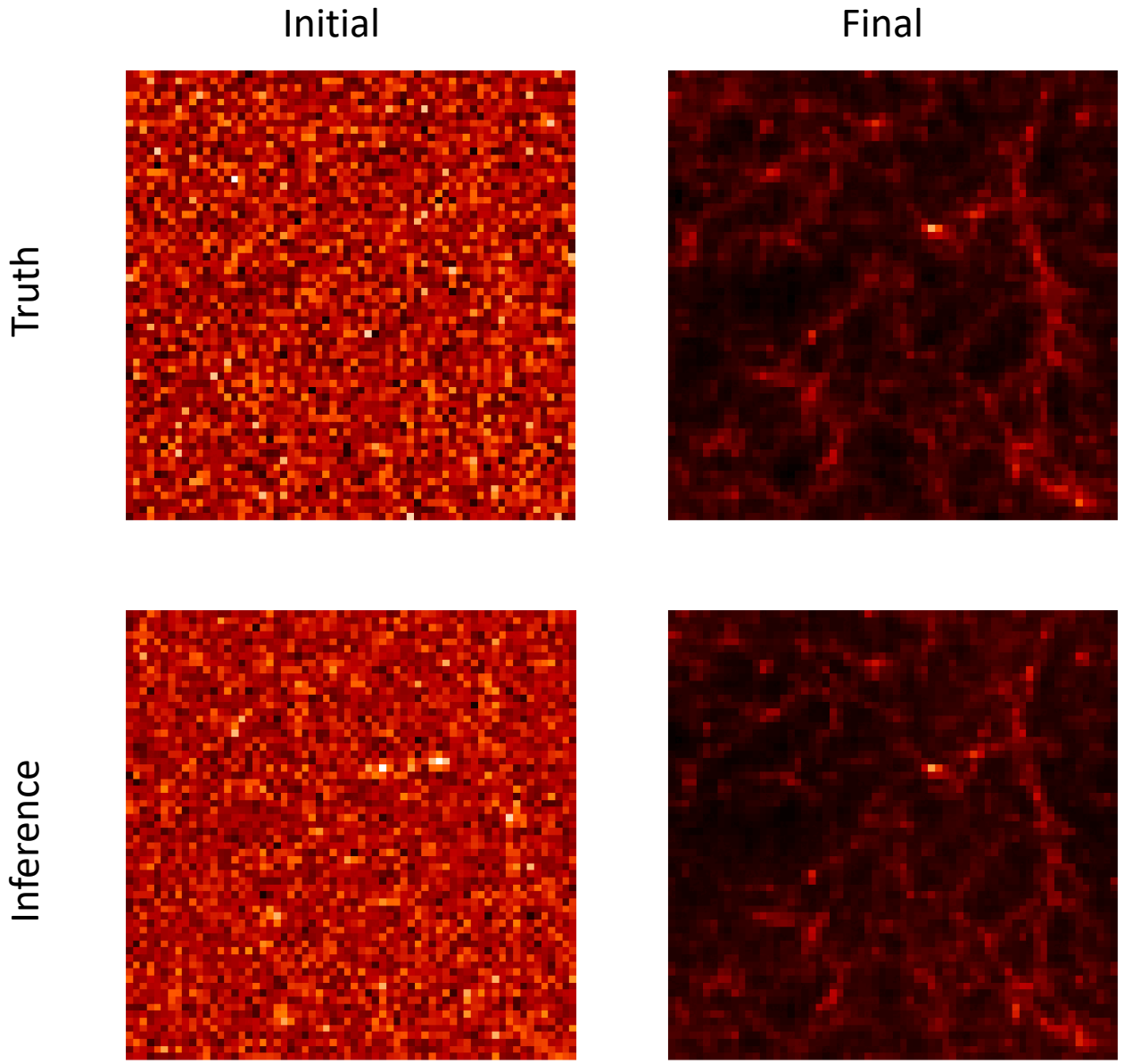

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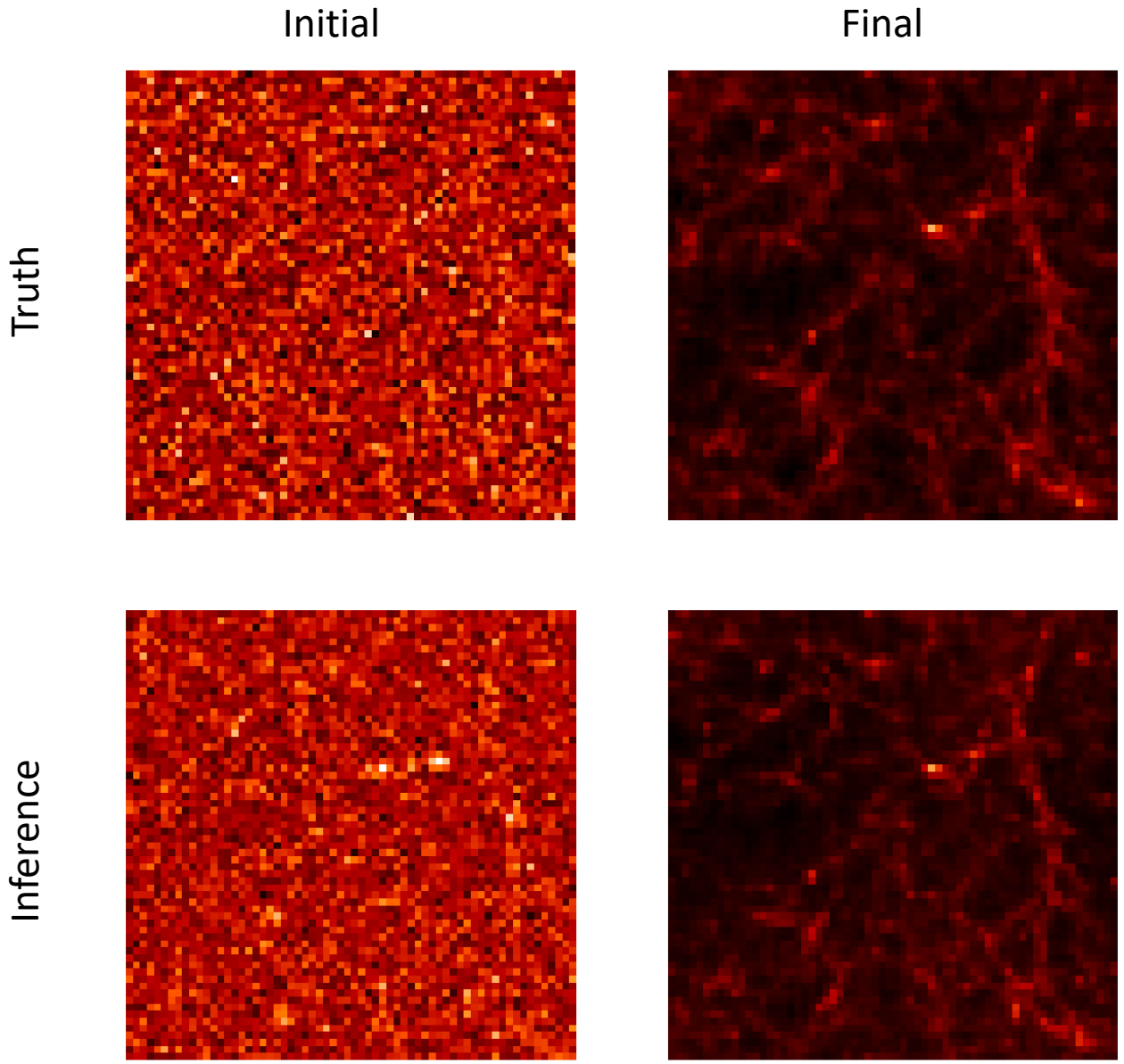

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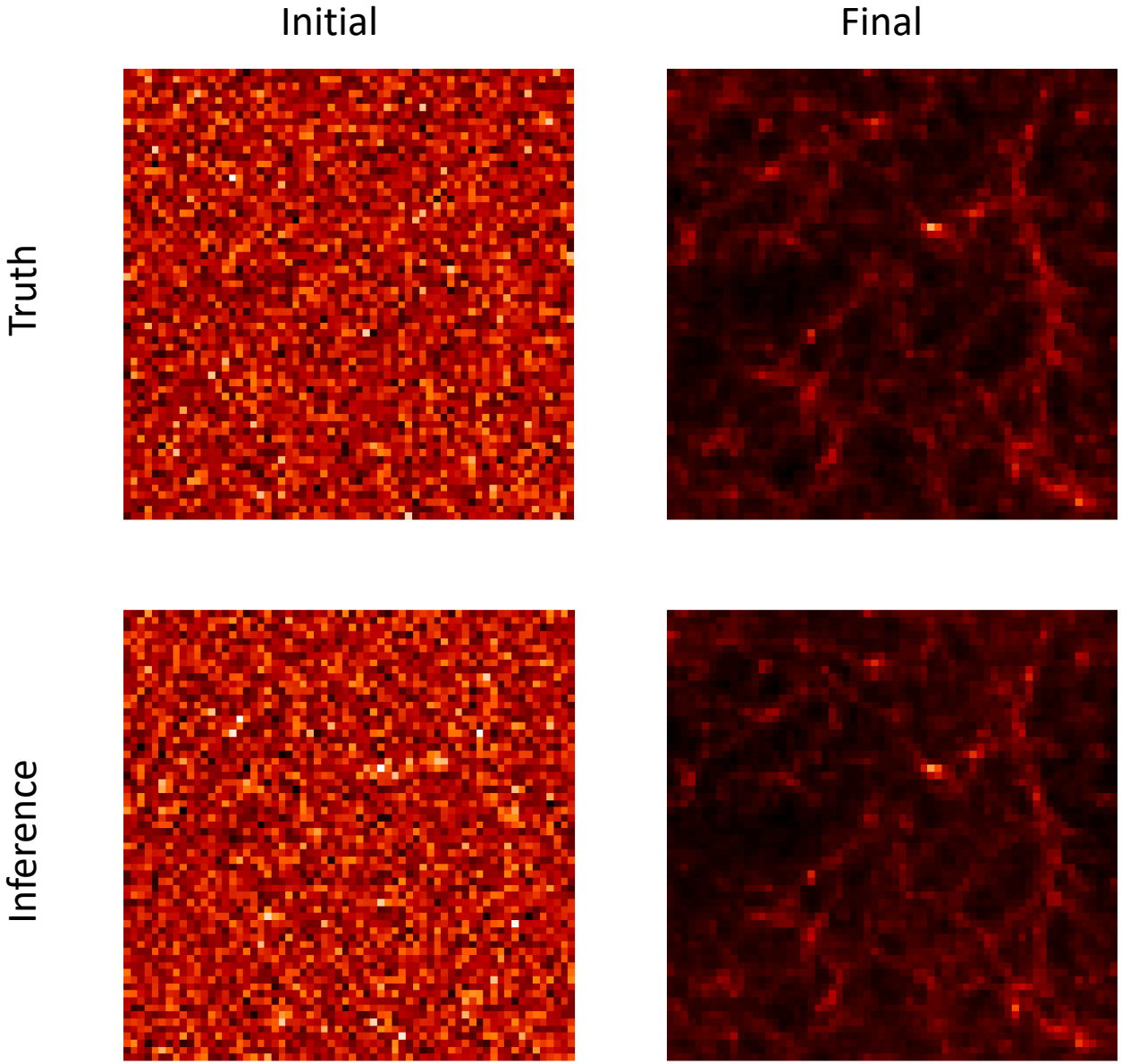
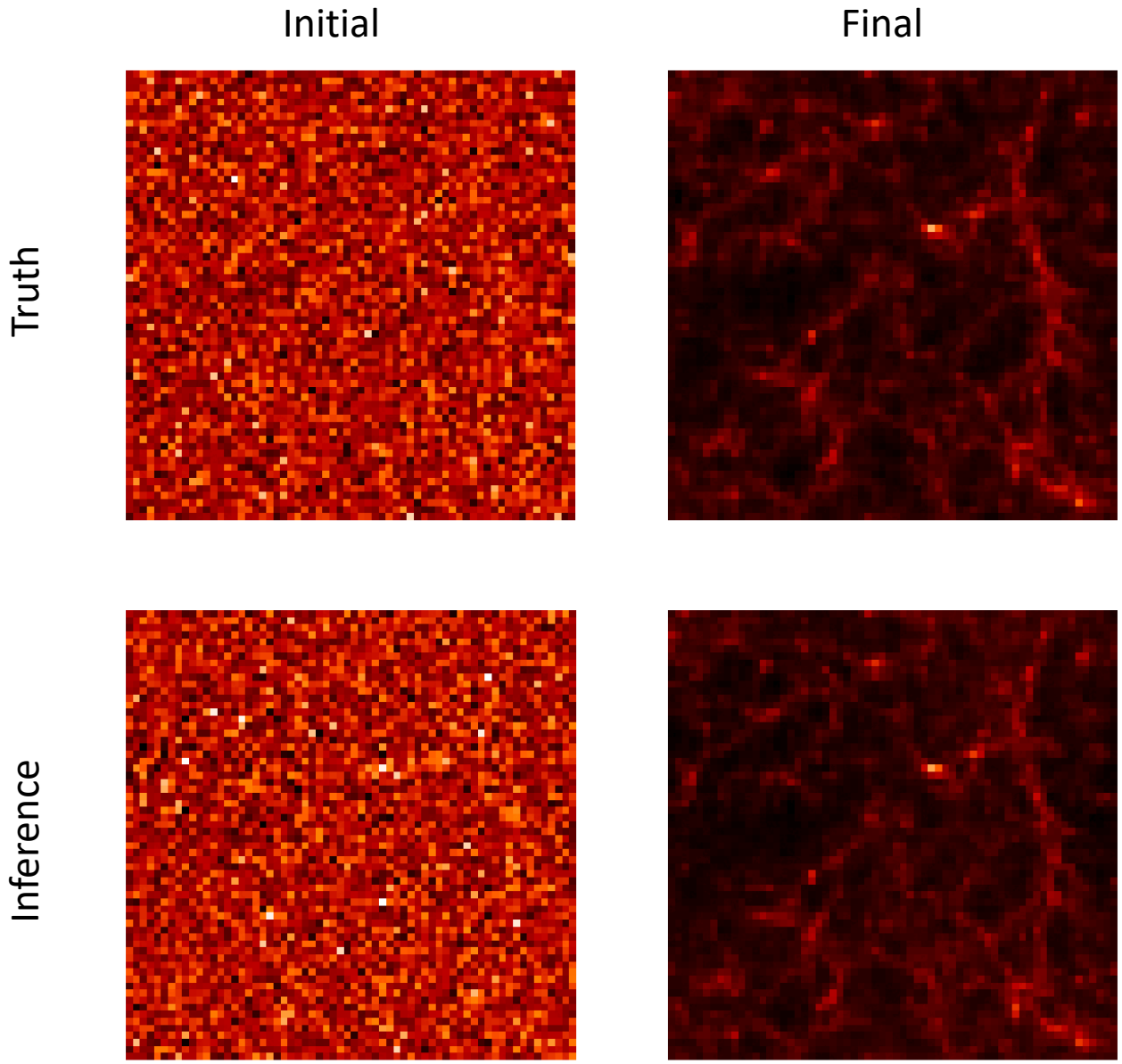
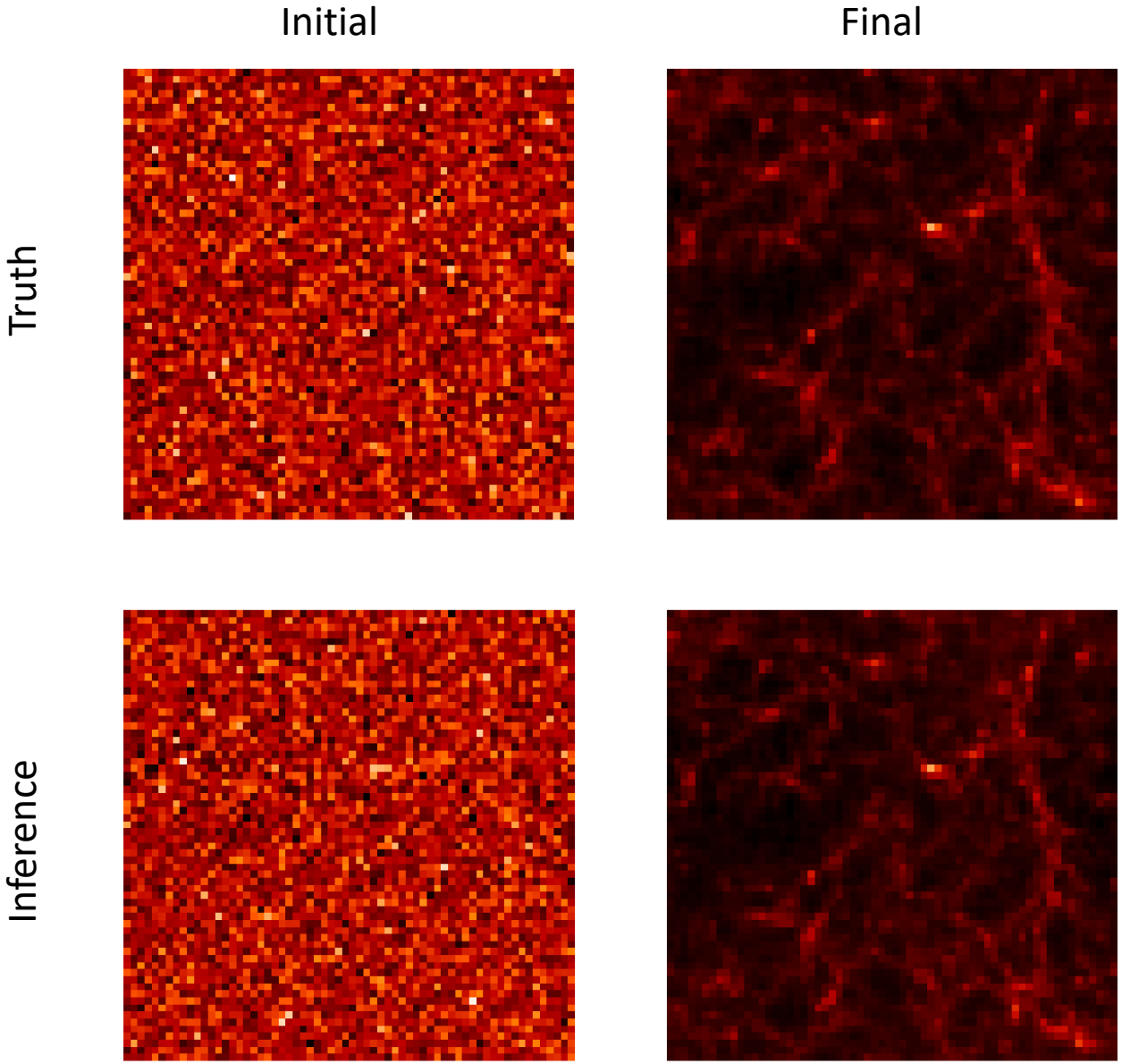


Bayer, Seljak, Modi (2023)



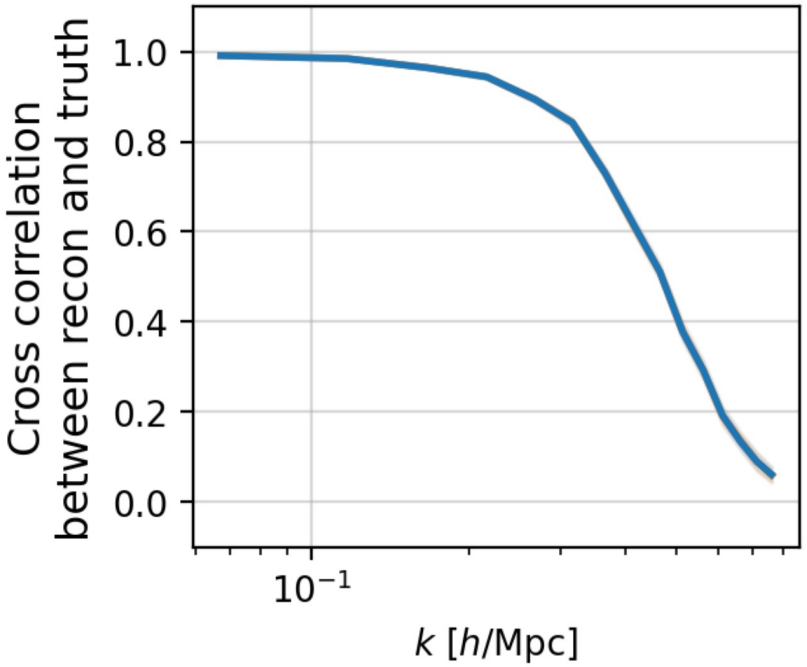
Bayer, Seljak, Modi (2023)

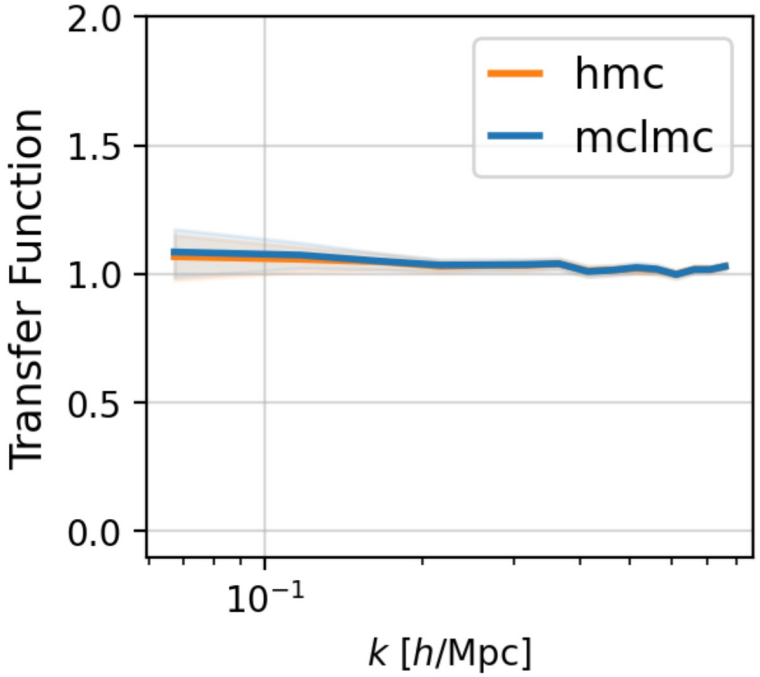


Bayer, Seljak, Modi (2023)

Samples of Initial Modes

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





Bayer, Seljak, Modi (2023)

Samples of Initial Modes

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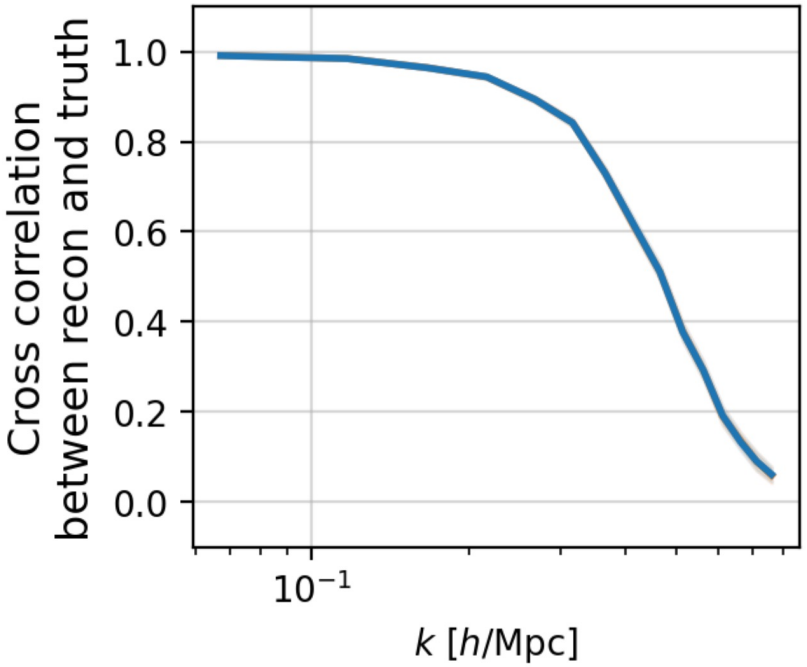
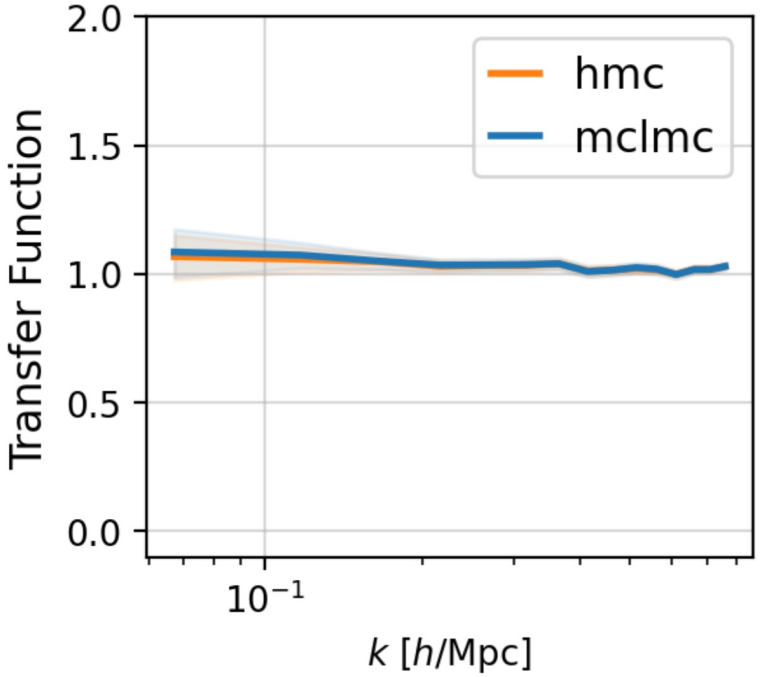
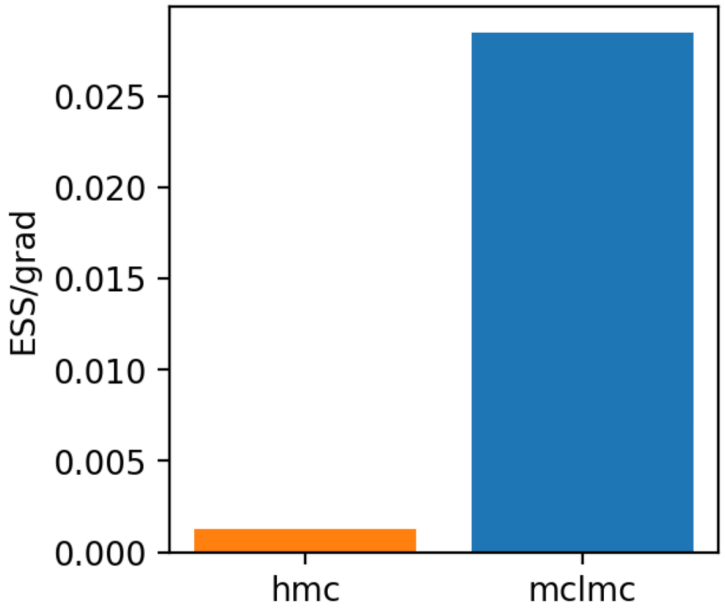




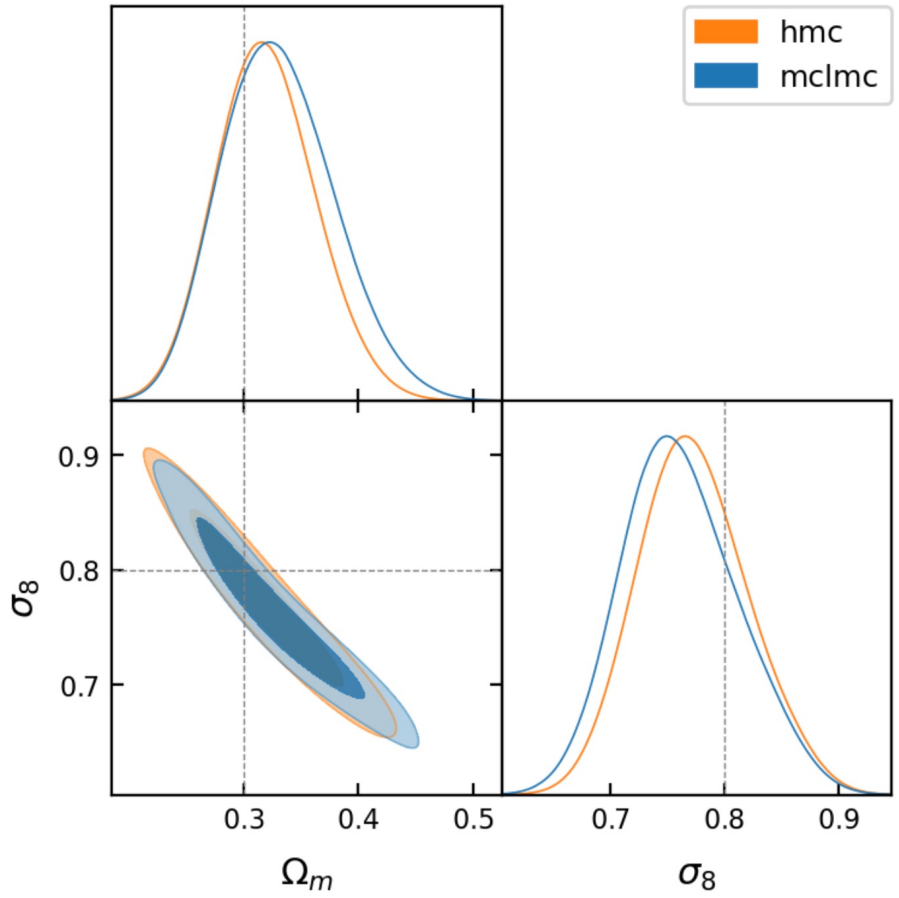


MCLMC is 22 times faster!

Bayer, Seljak, Modi (2023)

Samples of Cosmological Parameters

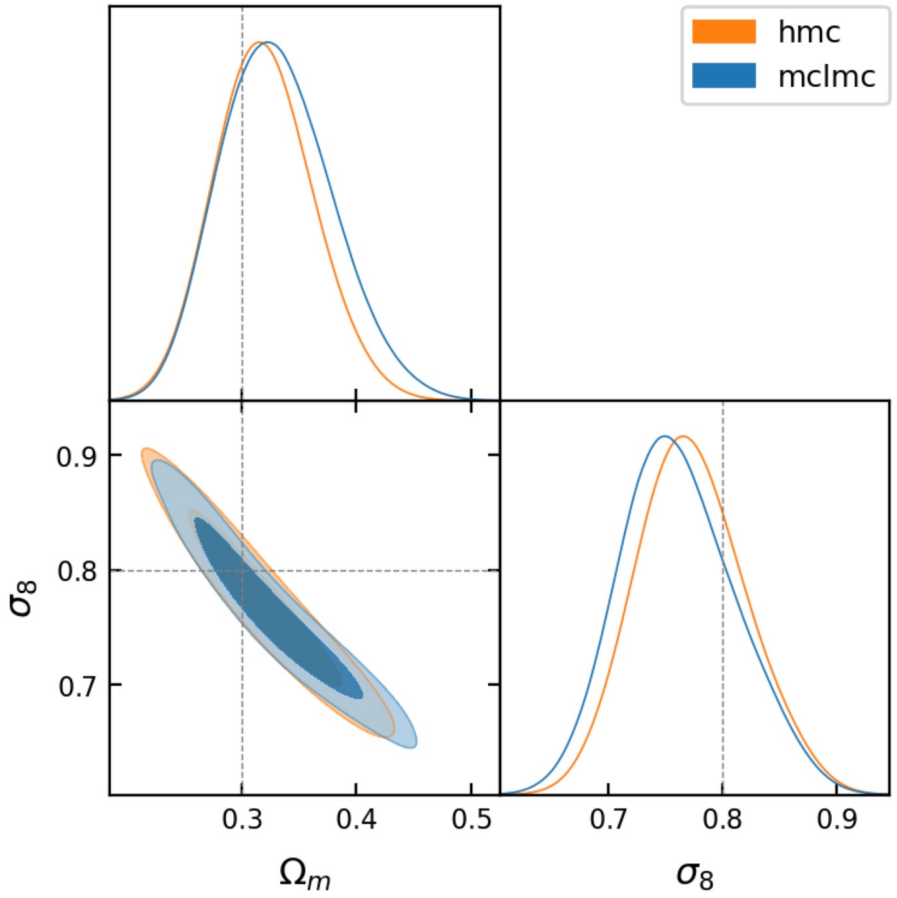
$d = 32^3 + 2 = 32{,}770$

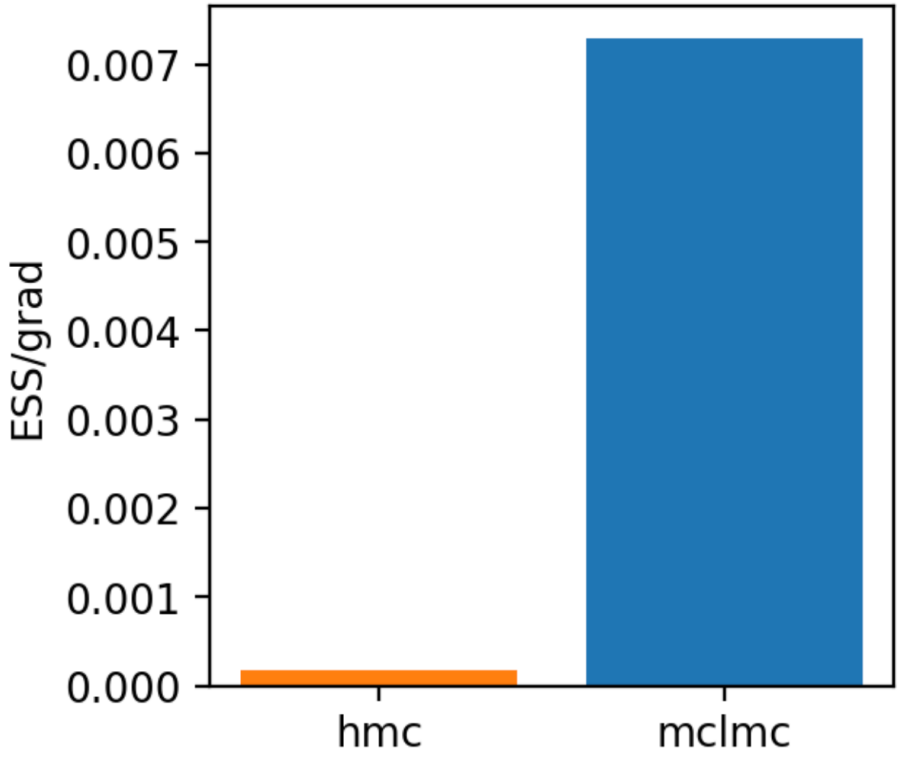


Bayer, Seljak, Modi (2023)

Samples of Cosmological Parameters

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

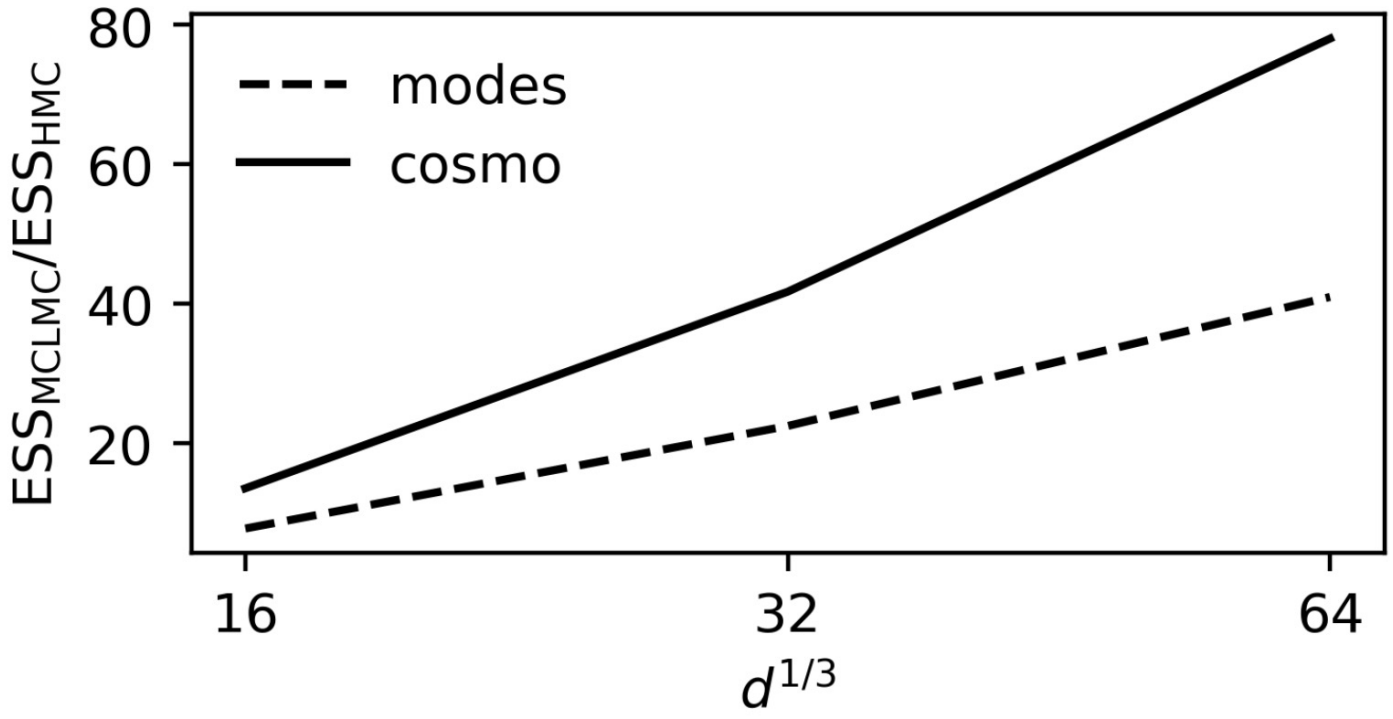




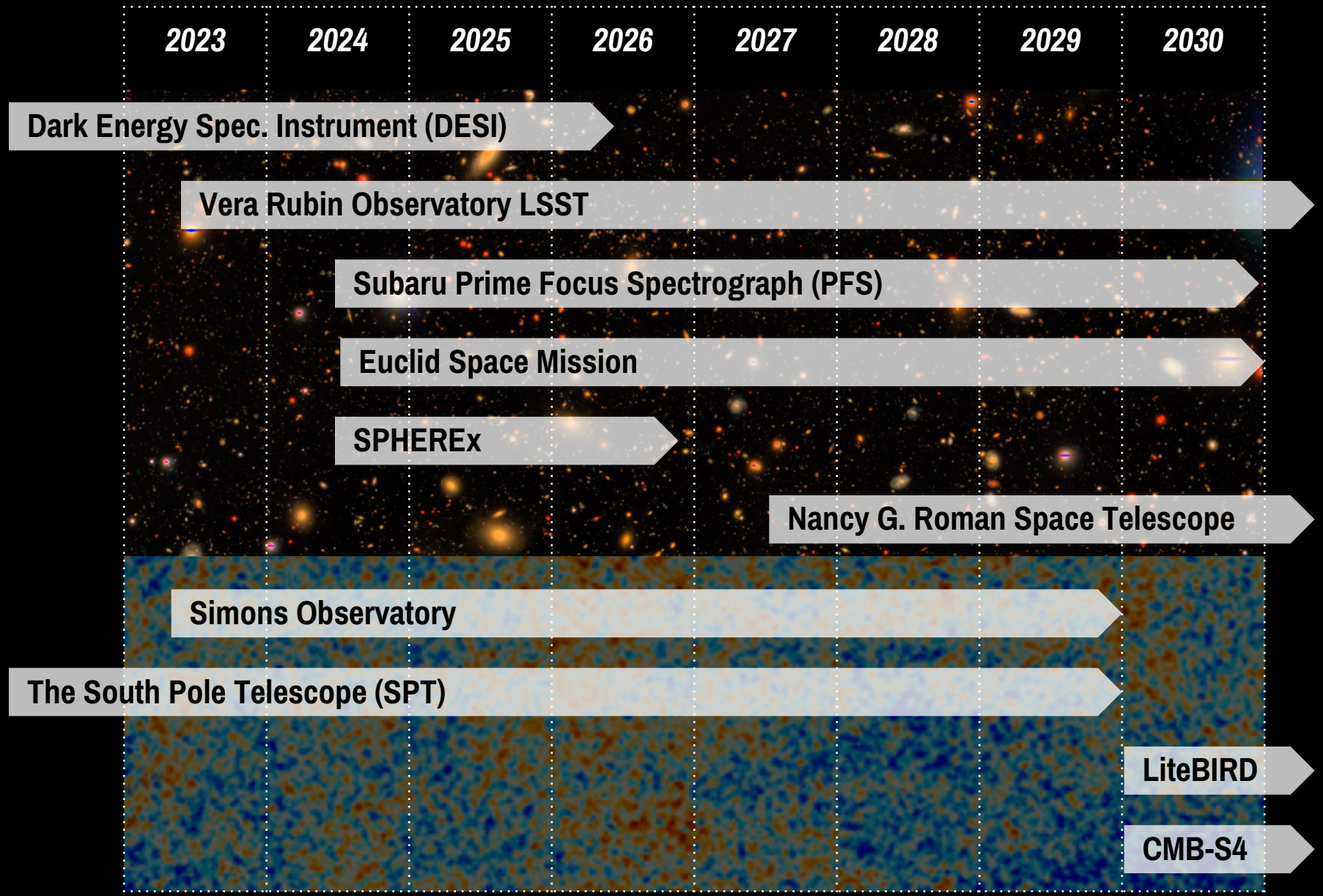
MCLMC is 42 times faster!

Bayer, Seljak, Modi (2023)

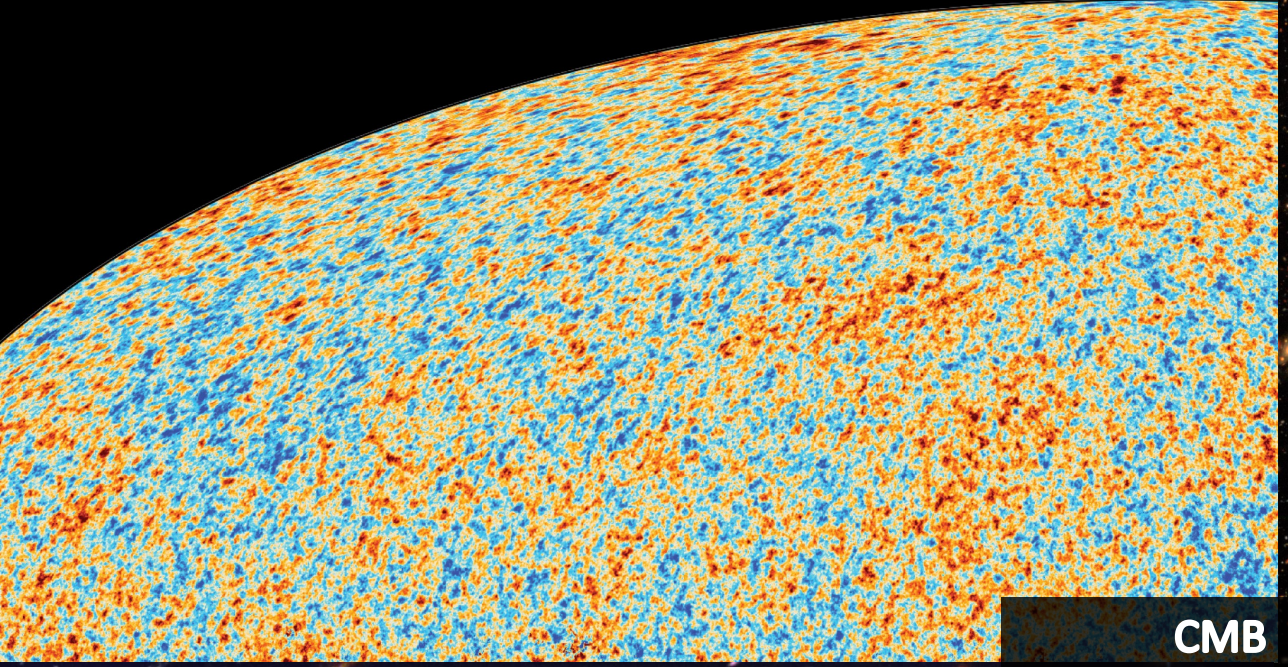
Dependence on dimensionality



Bayer, Seljak, Modi (2023)

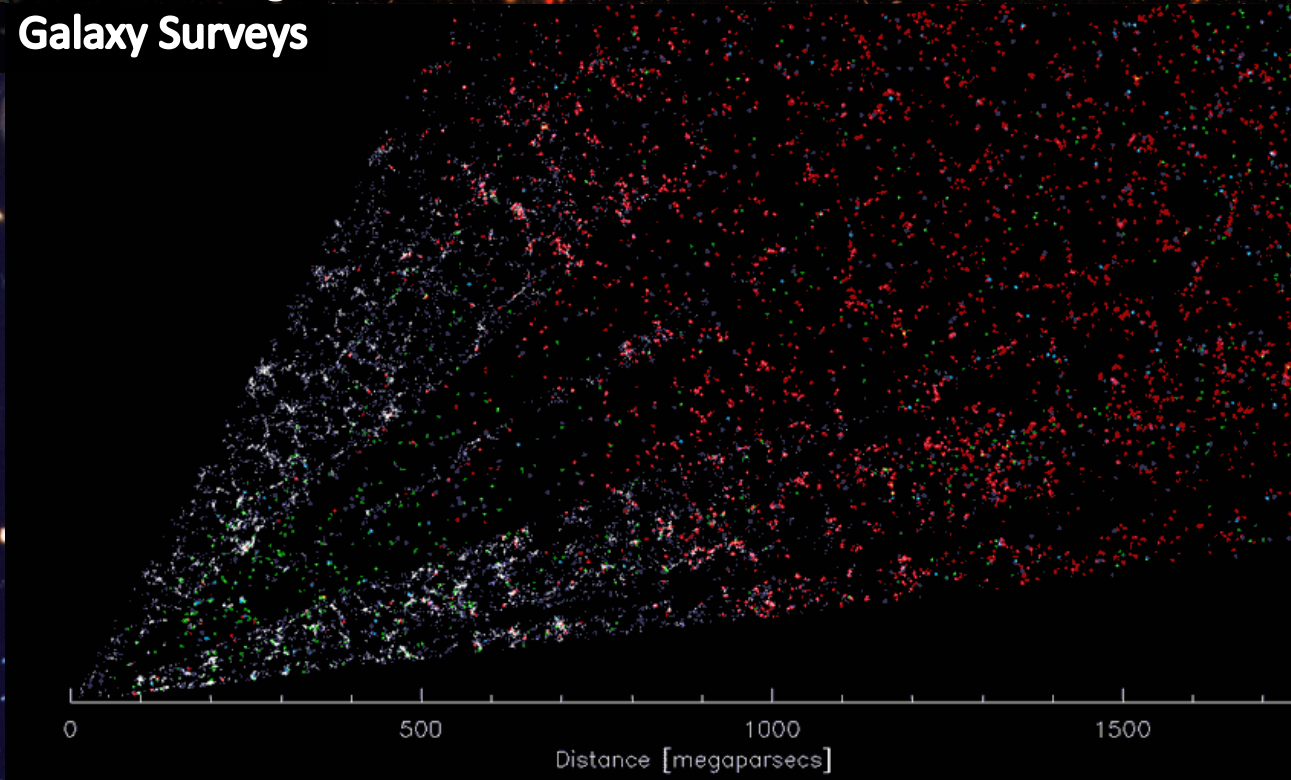

2023
2024
2025
2026
2027
2028
2029
2030
Dark Energy Spec. Instrument (DESI)
Vera Rubin Observatory LSST
Subaru Prime Focus Spectrograph (PFS)
Euclid Space Mission
SPHEREx
Nancy G. Roman Space Telescope
Simons Observatory
The South Pole Telescope (SPT)
LiteBIRD
CMB-S4

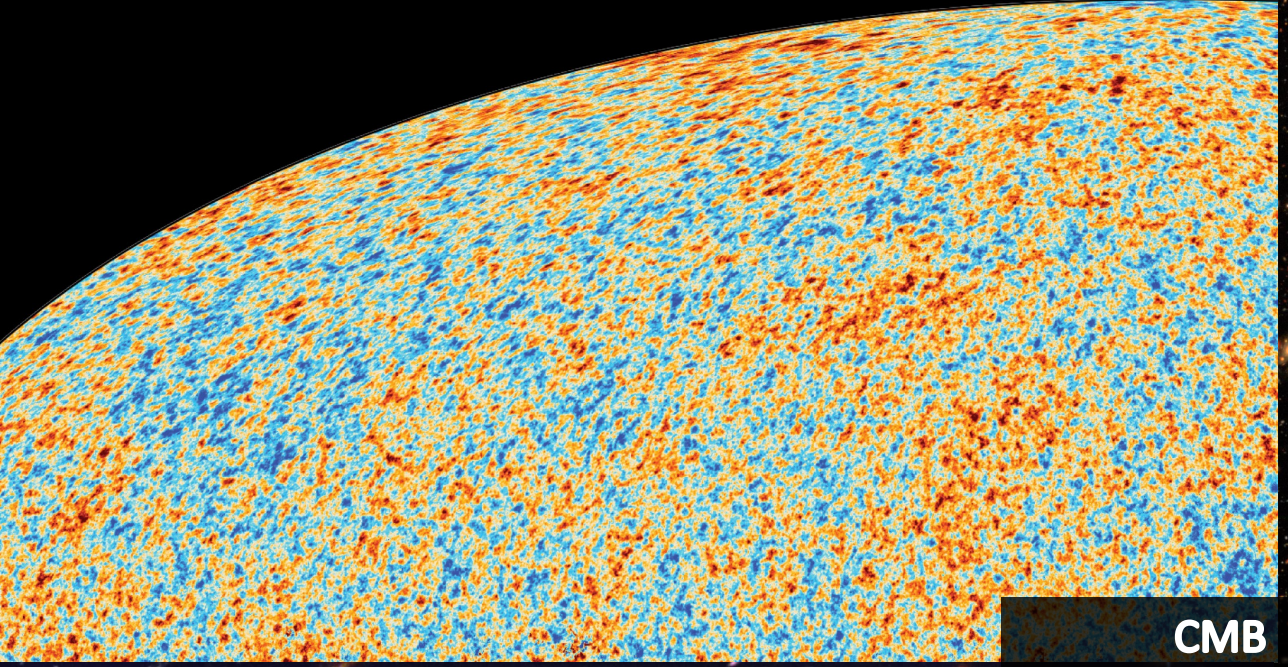
$$d \sim 512^3$$



CMB Weak Lensing

Lyman alpha Galaxy Surveys





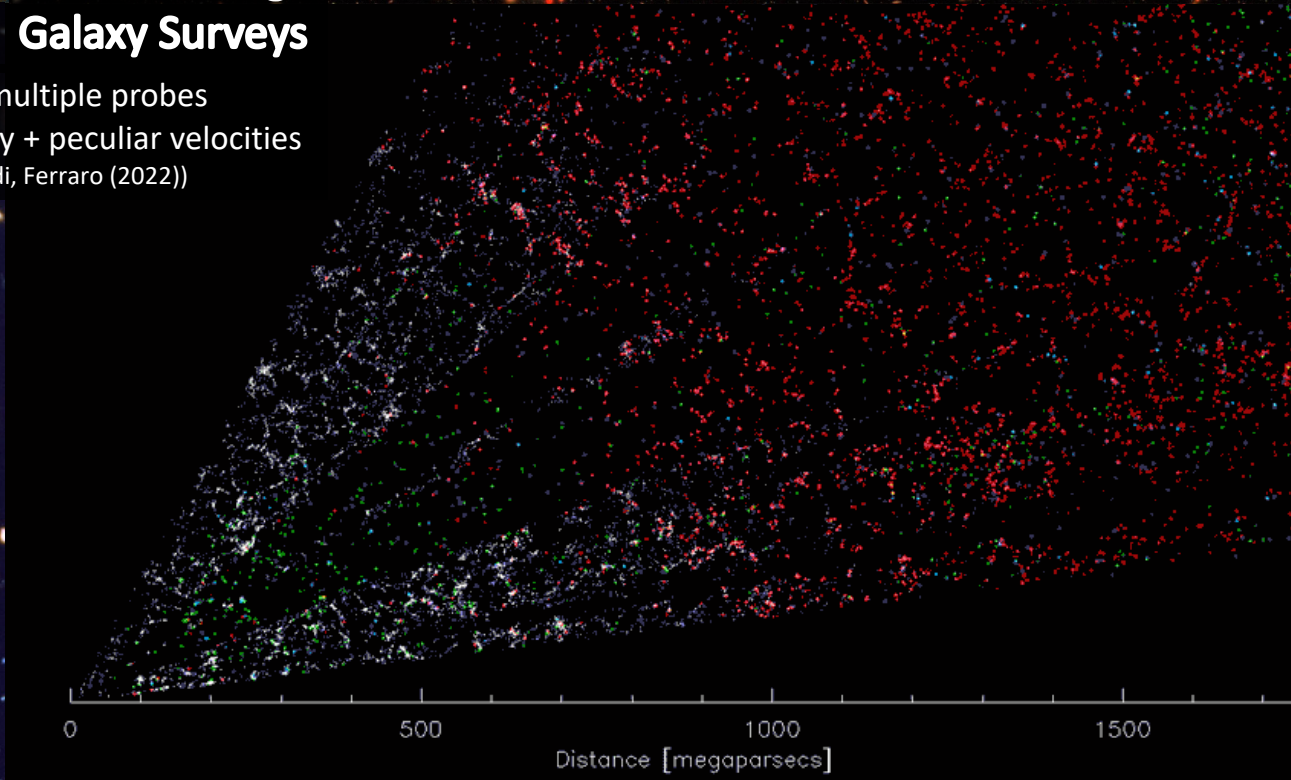
CMB **Weak Lensing**

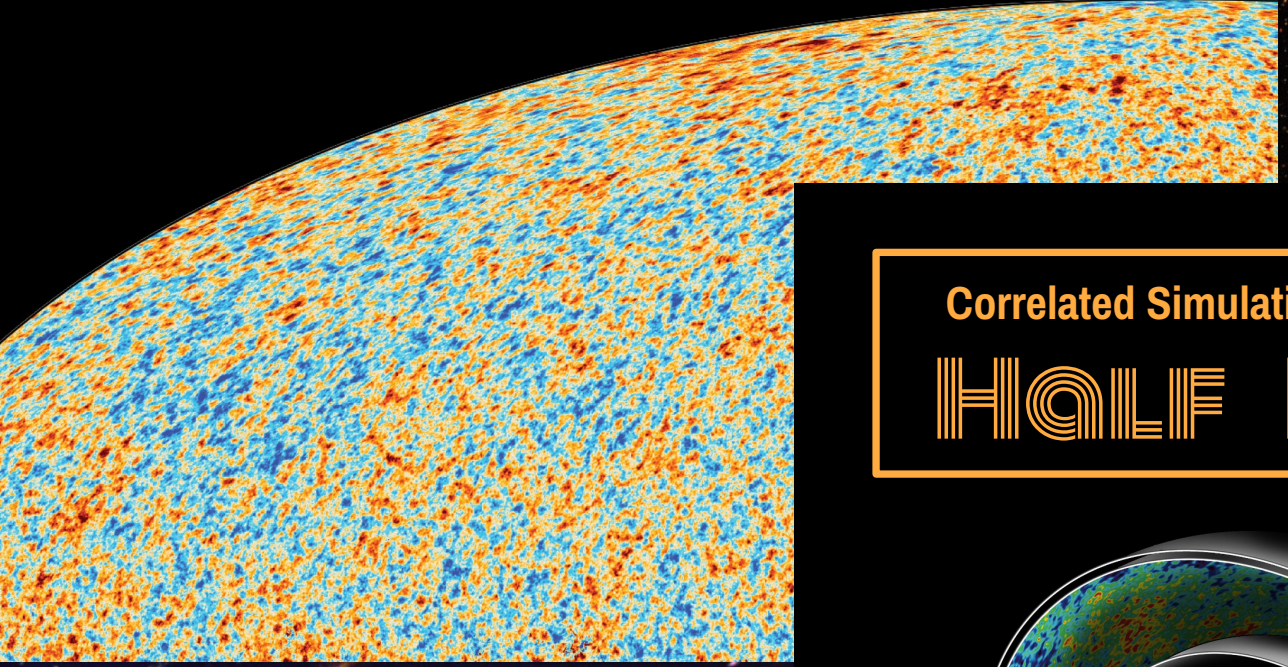
Lyman alpha **Galaxy Surveys**

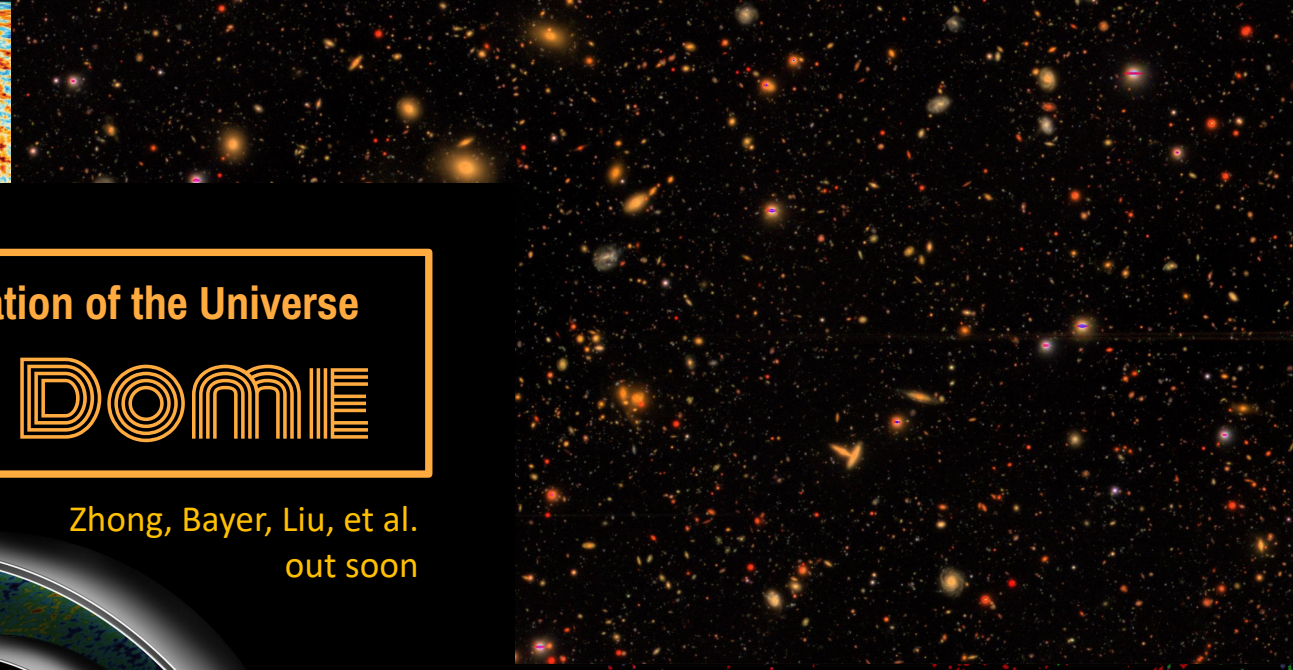
Combine multiple probes

e.g. galaxy density + peculiar velocities

(Bayer, Modi, Ferraro (2022))



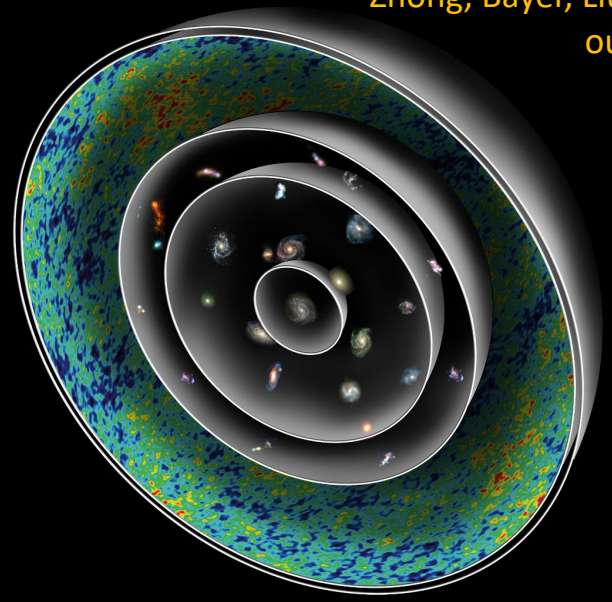


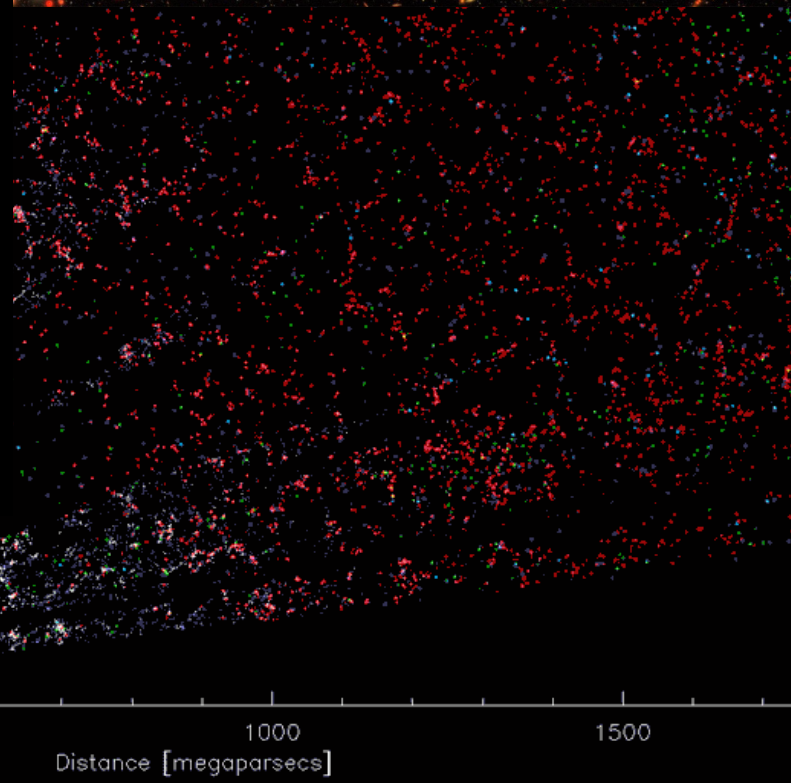


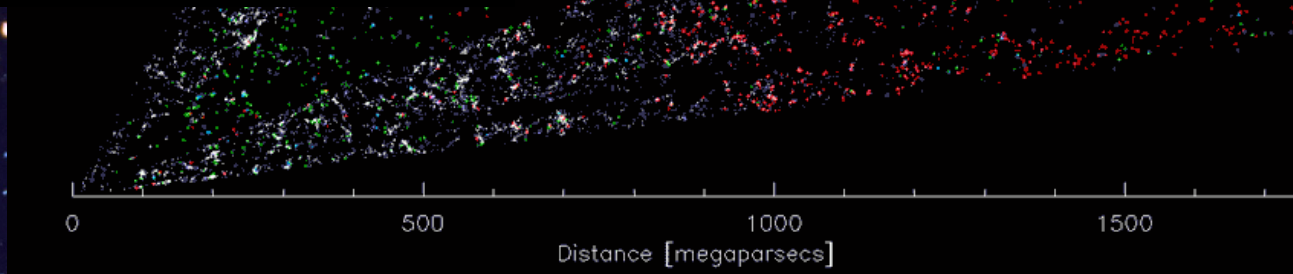
Correlated Simulation of the Universe

Half Dome

Zhong, Bayer, Liu, et al.
out soon



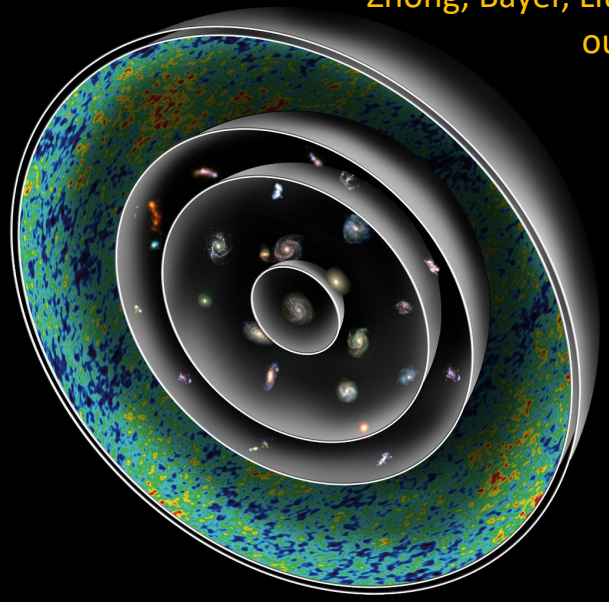




Correlated Simulation of the Universe

HALF DOME

Zhong, Bayer, Liu, et al.
out soon



Thank you!

Adrian Bayer

http://adrianbayer.github.io

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 no-gradient 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 the the marginal of $p(z, \Pi)$ over Π converges to the target distribution,

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

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,

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

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

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

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

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

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,

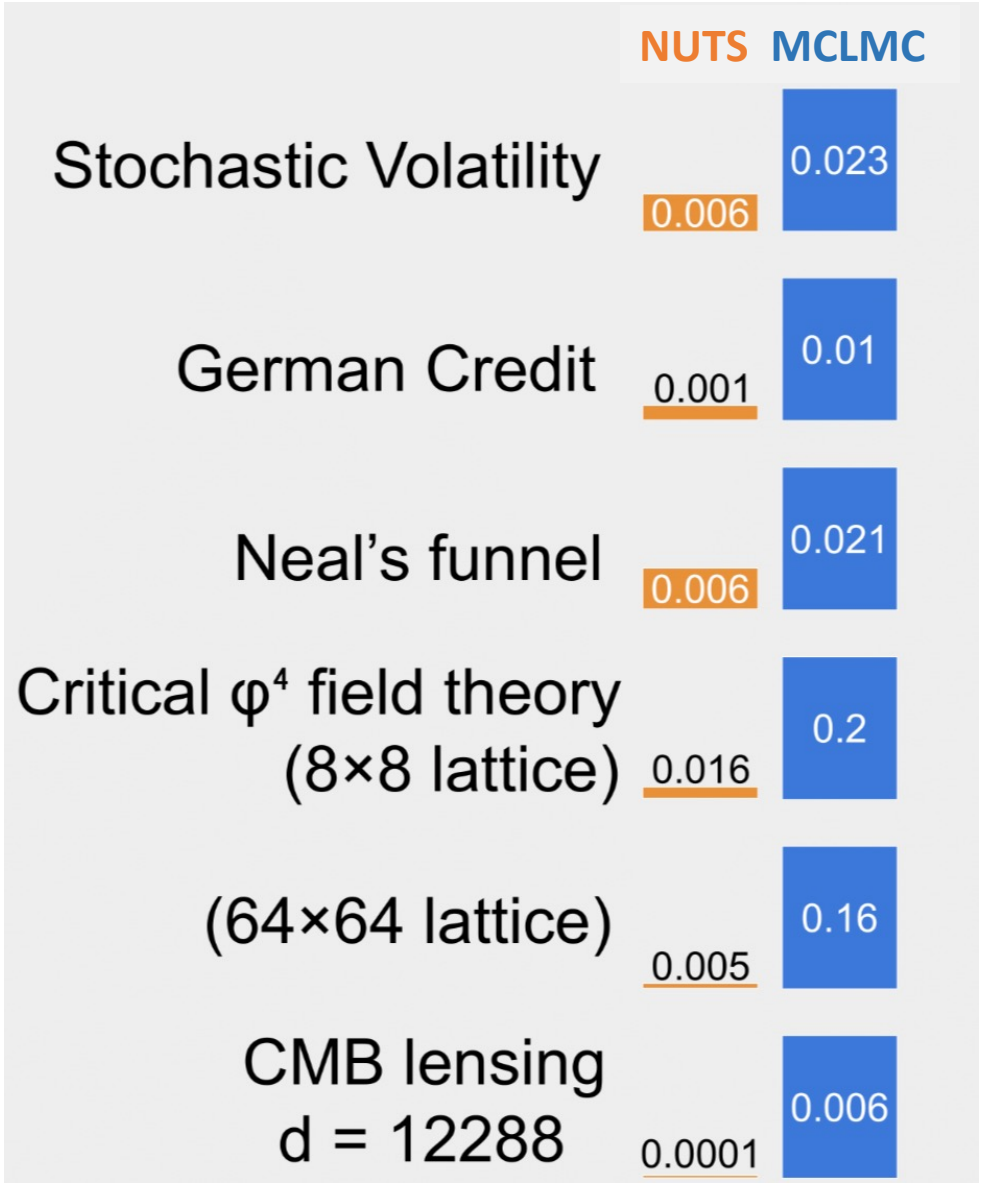
$$dz = u dt, \tag{6}$$

$$du = P(u) \left[f(z) dt + \eta dW \right], \tag{7}$$

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!