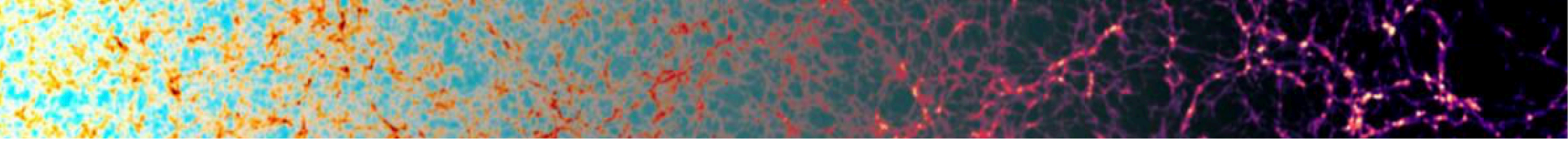


Learning to Optimize Cosmic Initial Conditions with Non-Differentiable Structure Formation Models

Doeser et al. 2025
arXiv: 2502.13243

Ludvig Doeser,
European AI for Fundamental Physics Conference 2025 (Cagliari, Sardinia, Italy)
Simulations & Generative Modelling

Oskar Klein centre

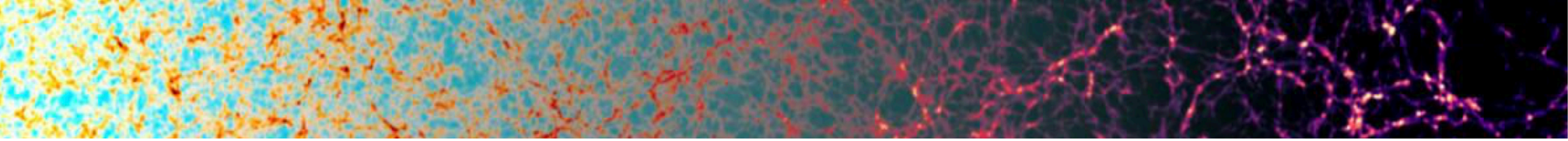
Universitet Stockholms

Swedish Research Council

Aquila

Learning the Universe Collaboration

Simons Foundation



Learning to Optimize Cosmic Initial Conditions with Non-Differentiable Structure Formation Models

Needed to model next-generation data!

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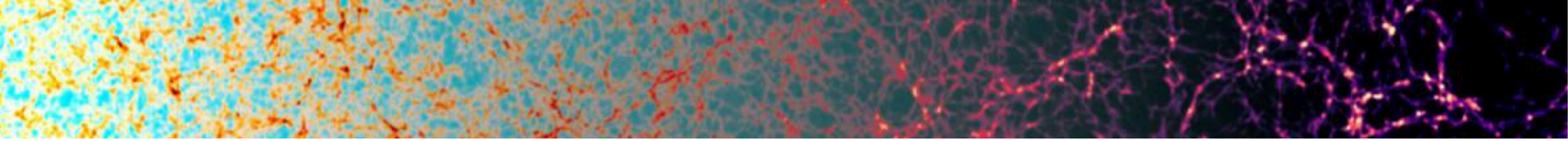

Rigorous test of cosmology!

Learning to Optimize Cosmic Initial Conditions with Non-Differentiable Structure Formation Models

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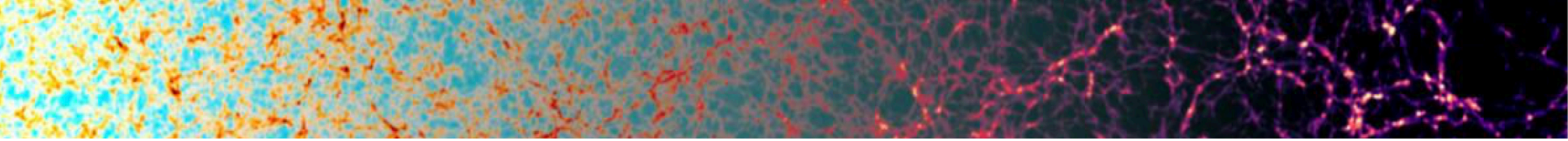

Leveraging neural networks **Rigorous test of cosmology!**

Learning to Optimize Cosmic Initial Conditions with Non-Differentiable Structure Formation Models

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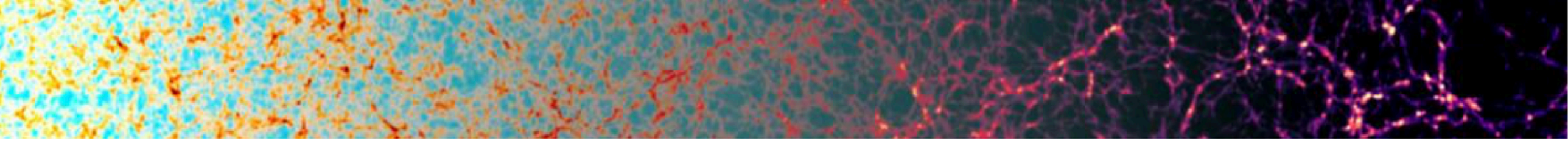
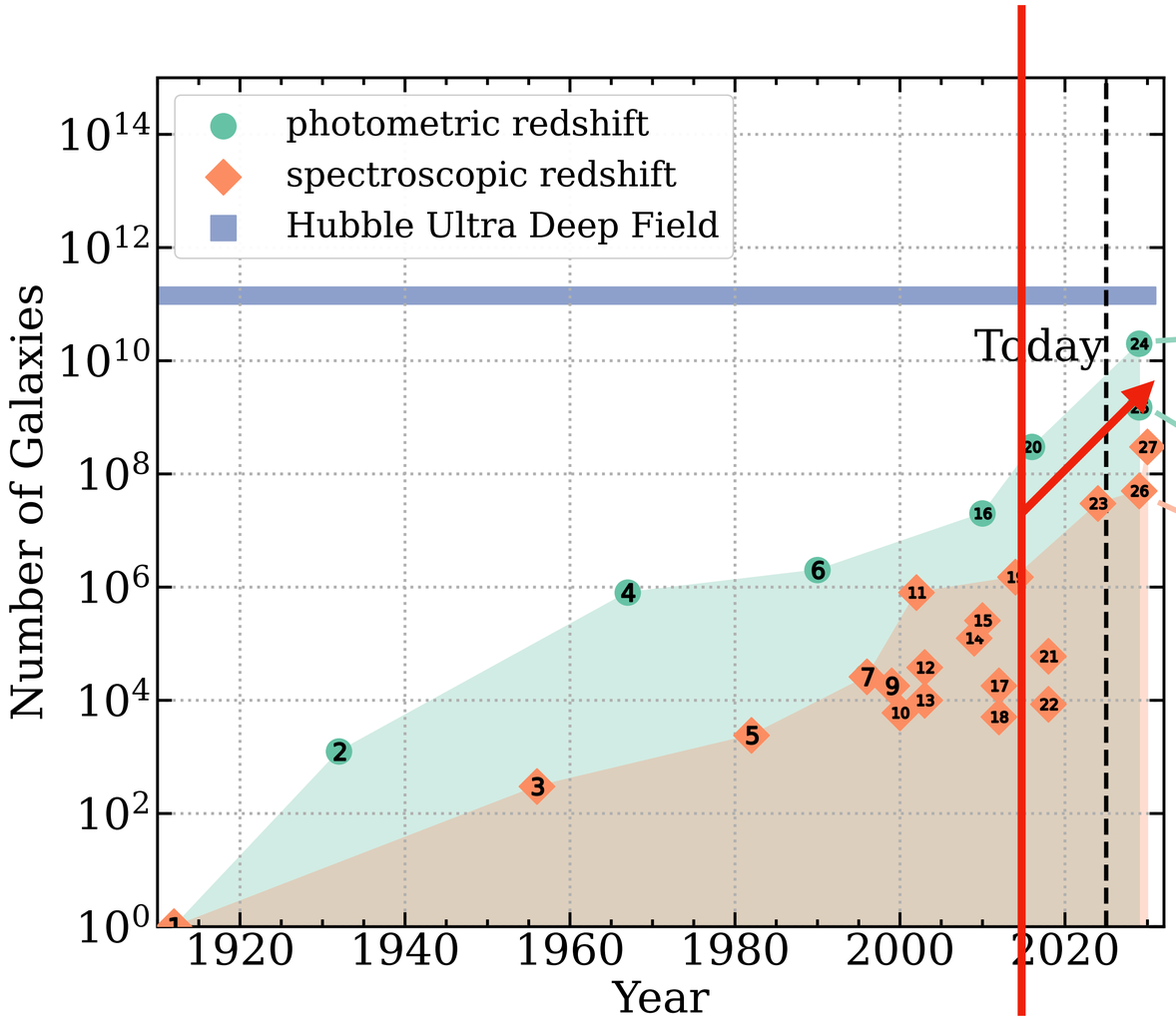


Learning to Optimize Cosmic Initial Conditions with Non-Differentiable Structure Formation Models

1 Needed to model next-generation data!

Cosmology is becoming an increasingly data-driven science



1	Slipher
2	Shapley-Ames Catalog
3	Humason
4	Shane-Wirtanen Counts
5	CfA
6	APM
7	LCRS
8	Las Campanas Redshift Survey
9	CfA2
10	CNOC2
11	SDSS
12	DEEP2
13	MGC
14	6dFGS
15	GAMA
16	WISE
17	AGES
18	ACES
19	BOSS
20	DES
21	DE
22	DE
23	DE
24	LSS
25	Euc
26	Euc
27	SPH

Analysis of galaxy clustering at field-level is here

Large Synoptic Survey Telescope

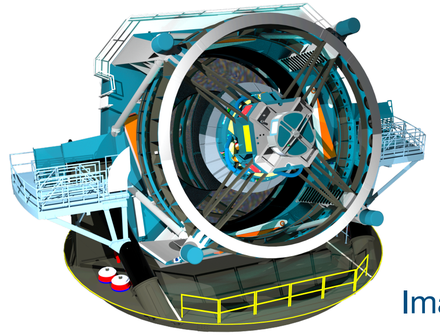


Image credit: LSST

Euclid Spacecraft

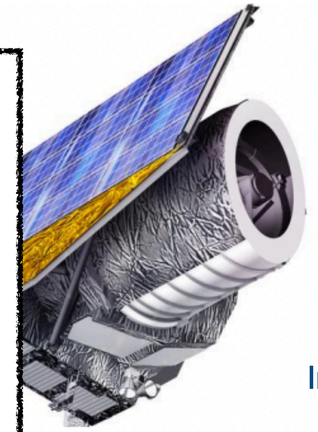


Image credit: ESA

Data challenges:
10^5 to 10^9 galaxies

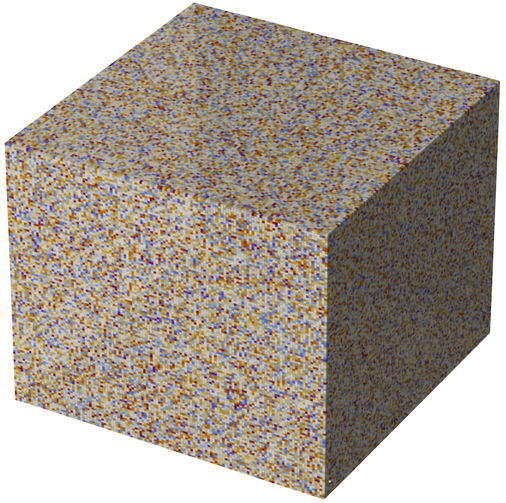
Small-scales
Large volumes

Field-level analysis for optimal information extraction

- To truly test cosmology, we must **fit our state-of-the-art models to their limits** and look where they fail
- In particular at smaller non-linear scales where most information lies

Current analysis of galaxy clustering:

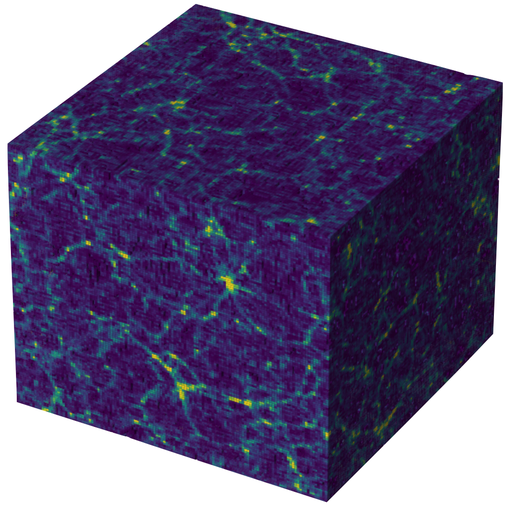
Initial conditions



Approximate model

N-body simulation
non-differentiable

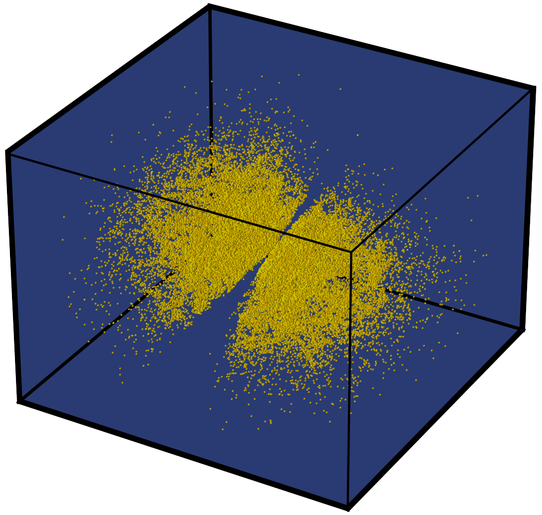
Dark-matter density



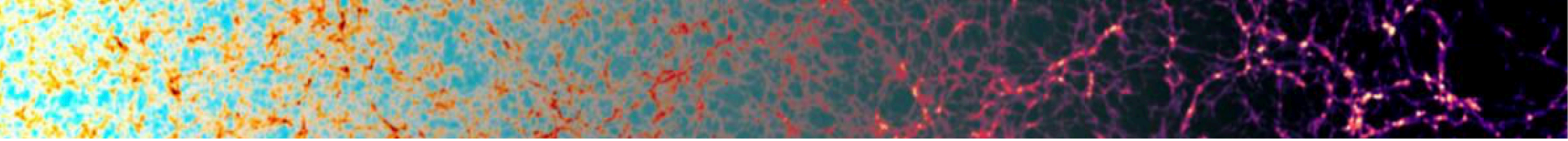
Approximate galaxy bias

Halo finder, HOD, hydrodynamics etc
non-differentiable

Haloes/Galaxies



Improvements:



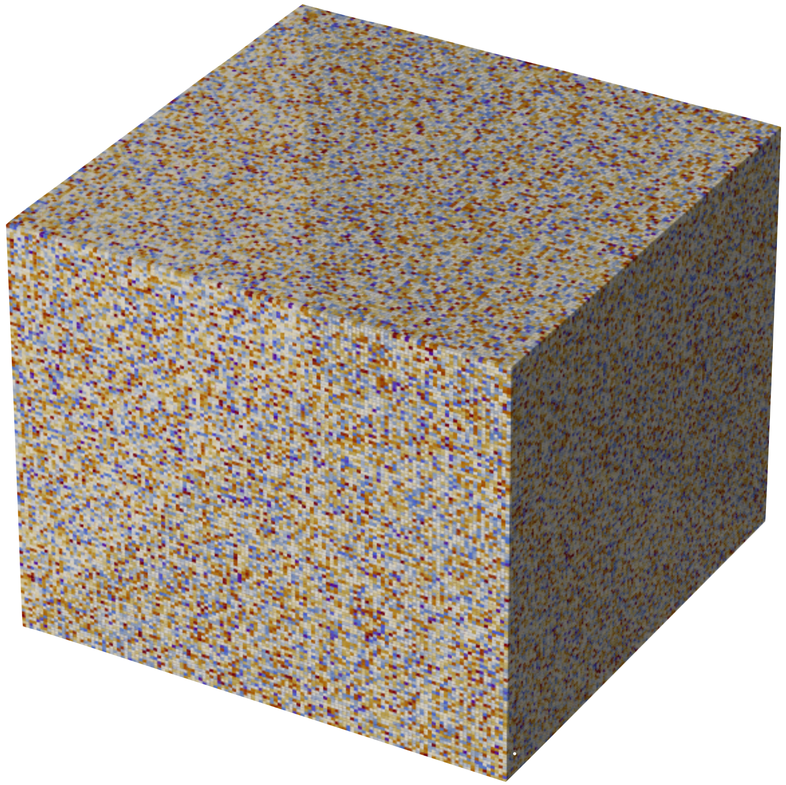
Learning to Optimize Cosmic Initial Conditions with Non-Differentiable Structure Formation Models

1 Needed to model next-generation data!

2 Rigorous test of cosmology!

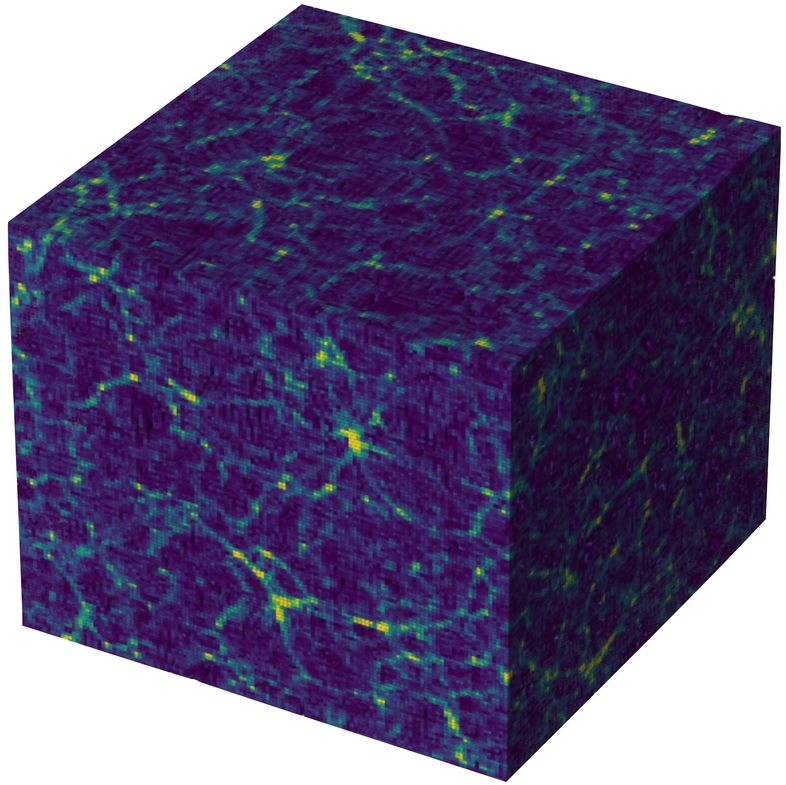
The seeds from which all observable structures originate

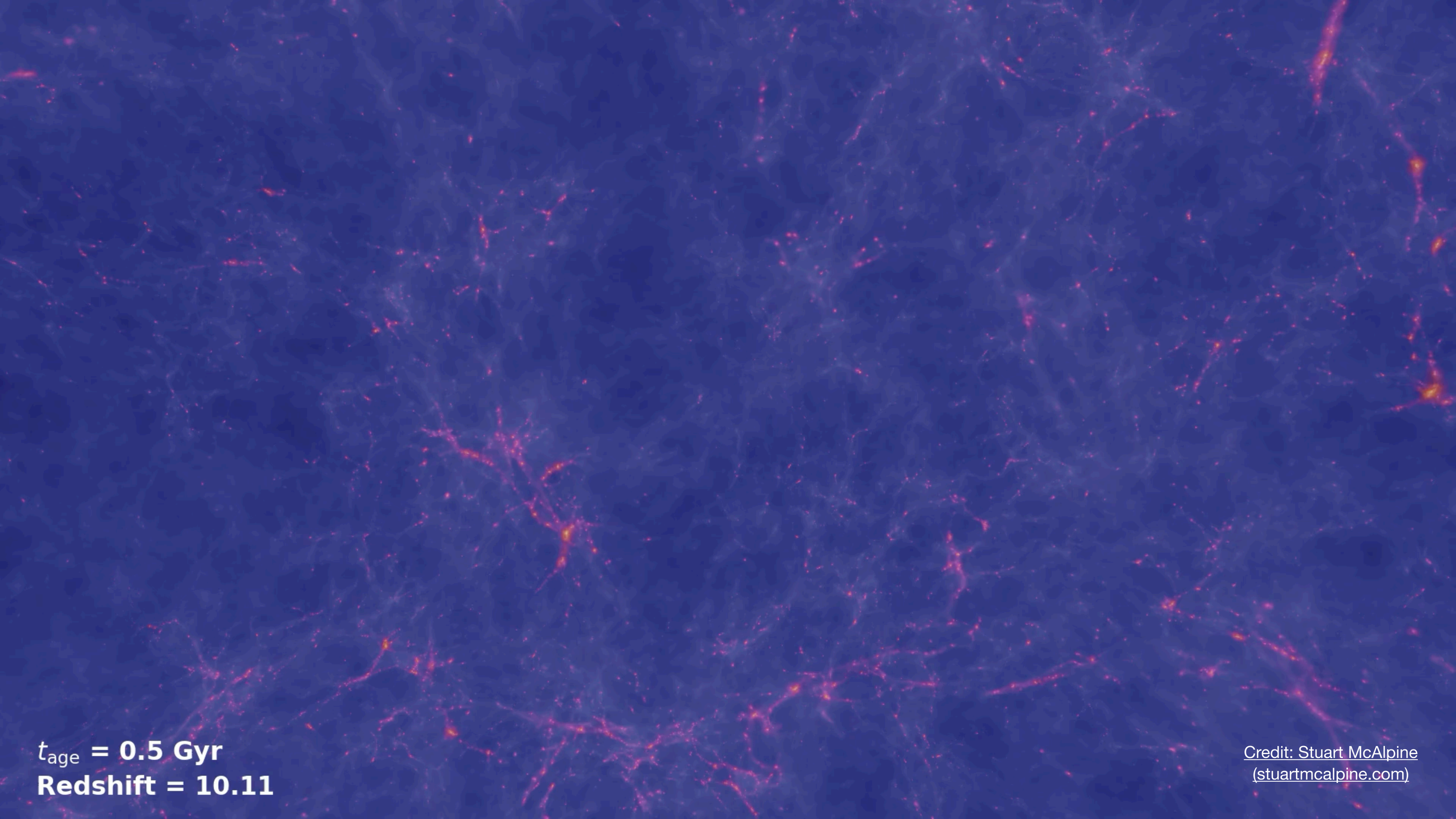
Cosmic initial conditions =
Gaussian field encoding the density perturbations in Early Universe



13.8 billion years

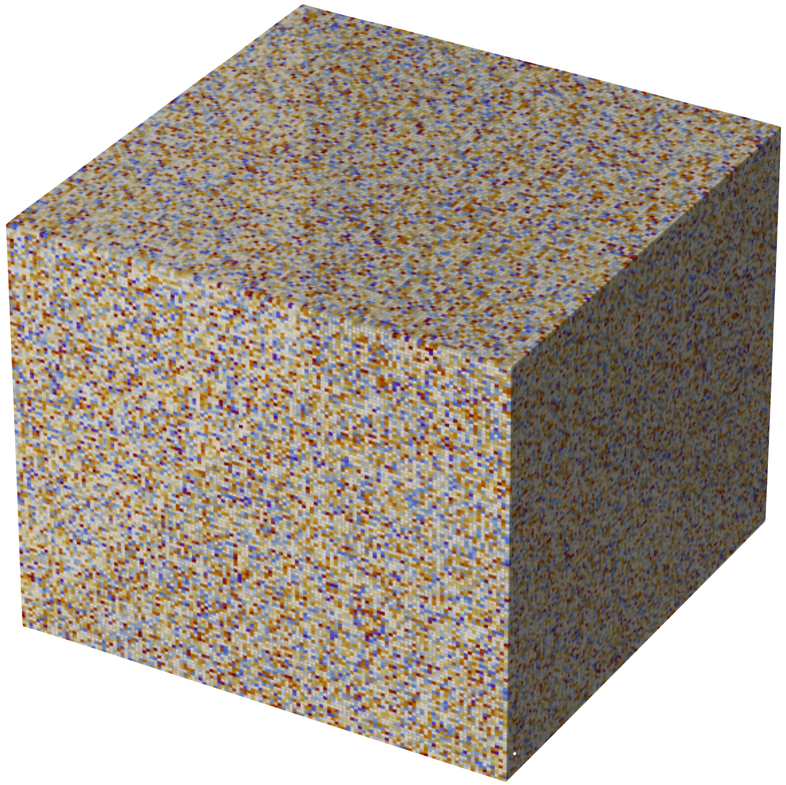
Large-scale structure of galaxies of the Universe today




t_{age} = 0.5 Gyr
Redshift = 10.11
Credit: Stuart McAlpine
(stuartmcalpine.com)

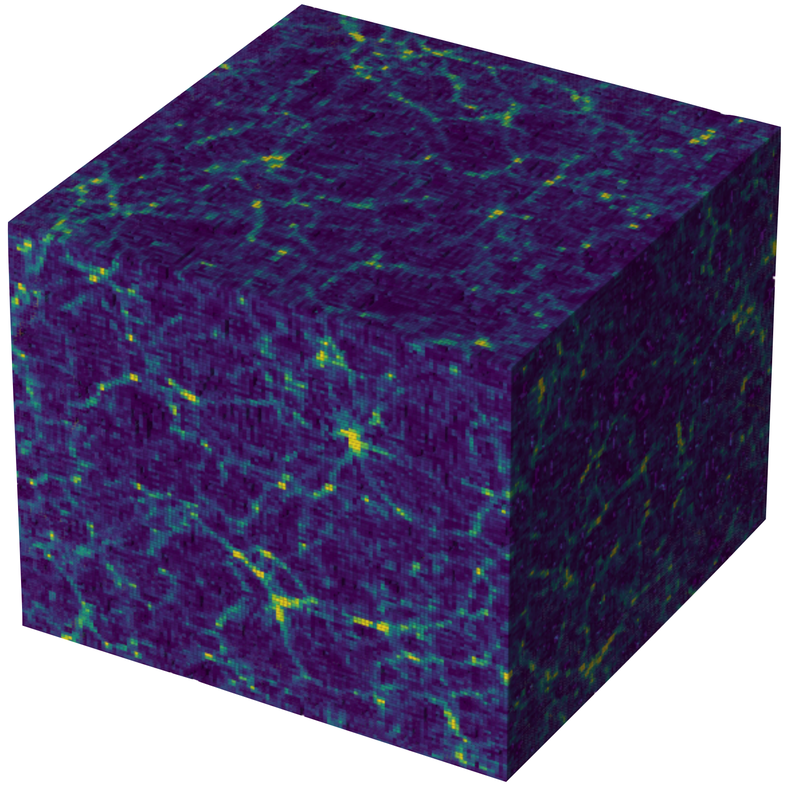
The seeds from which all observable structures originate

Cosmic initial conditions



13.8 billion years

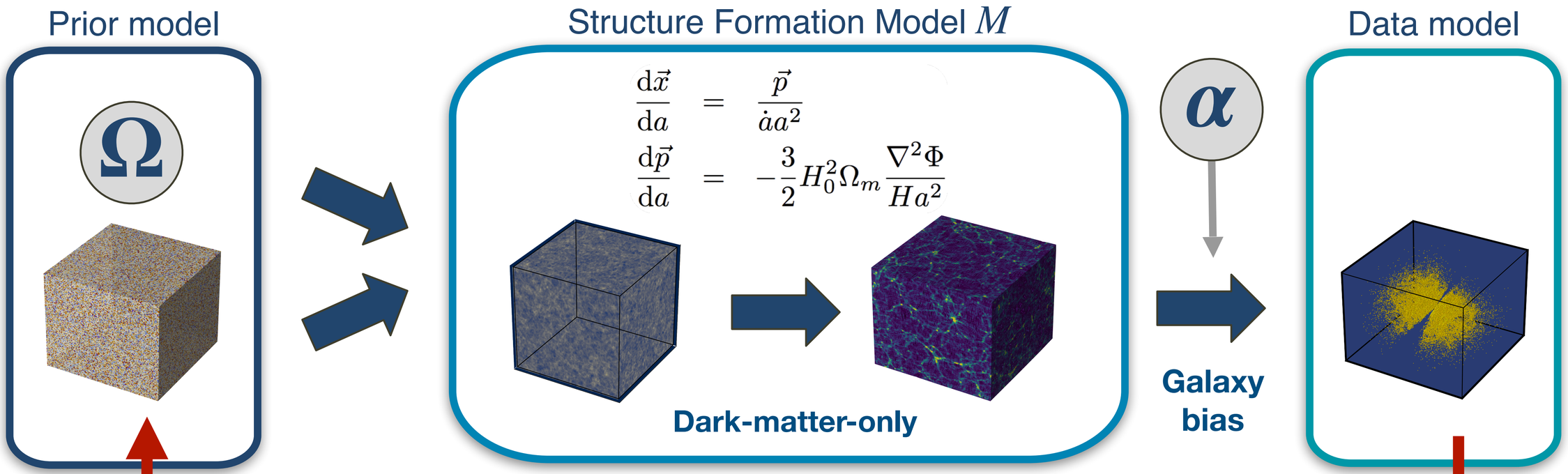
Large-scale structure



Field-level analysis: Making use of numerical simulations

Given a model M and cosmo. params $\boldsymbol{\Omega}$, find initial conditions $\boldsymbol{x}$ that evolve into the observed 3D galaxy dist.

BORG (*Bayesian Origin Reconstruction from Galaxies*) Jasche & Wandelt 2014, J. Jasche, F. Leclercq, B. D. Wandelt 2015, G. Lavaux, J. Jasche, F. Leclercq 2019, G. Lavaux, J. Jasche 2016, Jasche & Lavaux 2019



$128^3 \sim 10^6$ **dim!**

Statistical inference: Update initial conditions to better match the data

Similar to back-propagation in neural networks: need **differentiable** model

Inferring the initial conditions is a rigorous test of cosmology

Initial conditions (ICs) of our Universe → full dynamical formation history of densities and velocities

Enables creating a physics laboratory, a **Digital Twin**

- Simultaneously fit all observed structures and galaxies

Inferring the initial conditions is a rigorous test of cosmology

Initial conditions (ICs) of our Universe → full dynamical formation history

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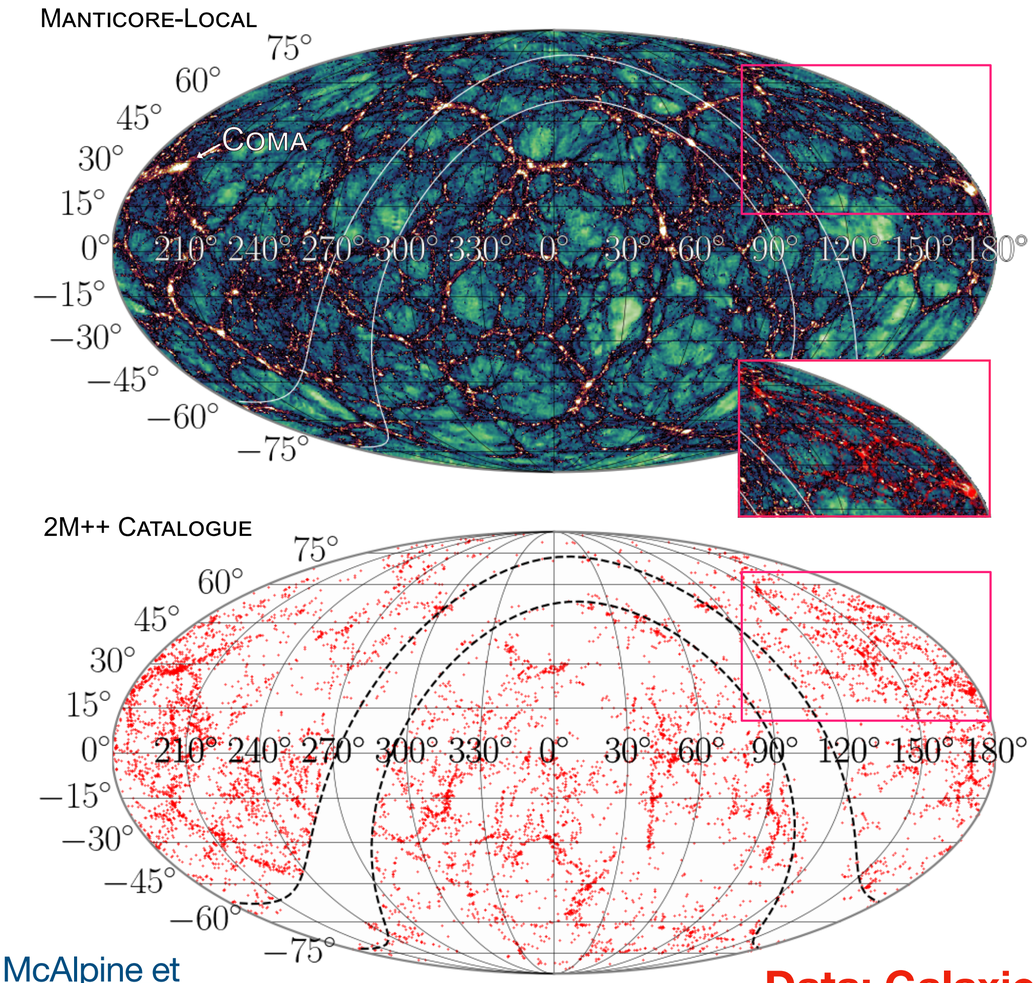
- **Simultaneously fit all observed structures and galaxies**
- Intricate properties of individual clusters
- Rarity of massive clusters
- Velocity reconstructions (e.g. useful for Hubble tension)
- Anomalous superstructures (“Great Wall”, “Giant Arc” etc)
- Formation of and dynamics around our Local Group

Model: simulation from inferred ICs



McAlpine et al. 2025

Data: Galaxies

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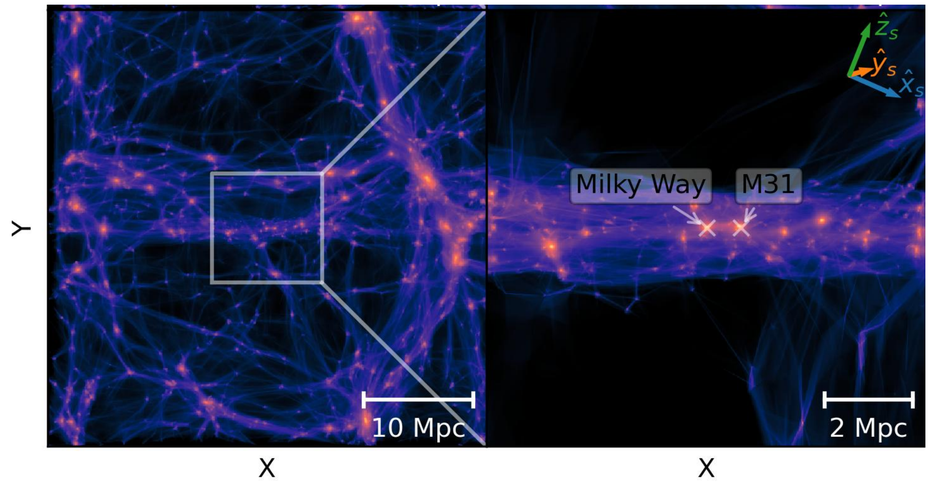
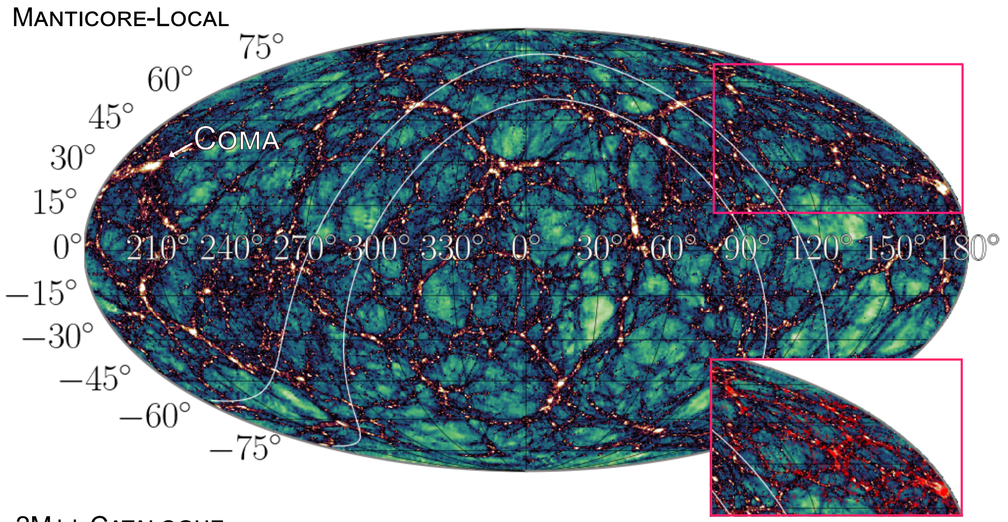
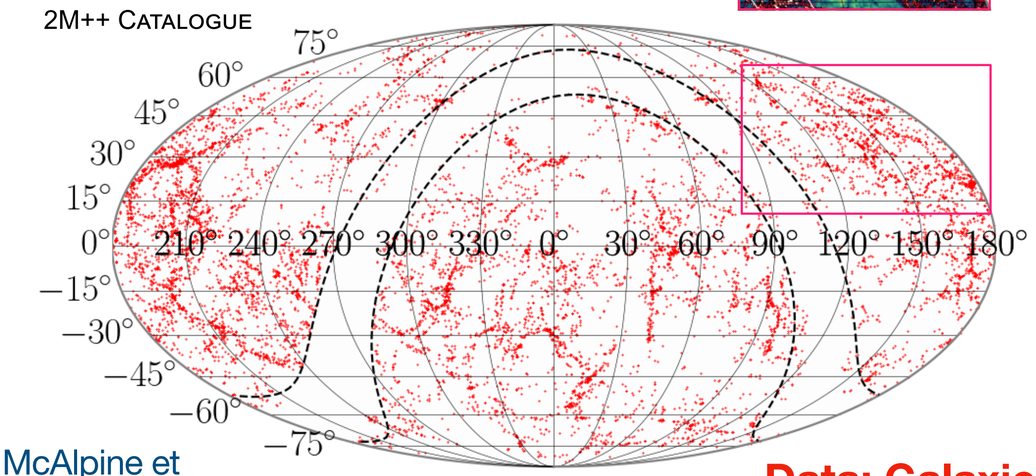


Wempe et al. 2024

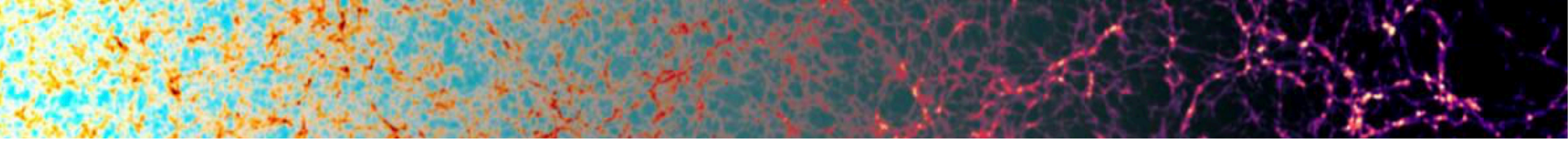
Model: simulation from inferred ICs





McAlpine et al. 2025

Data: Galaxies

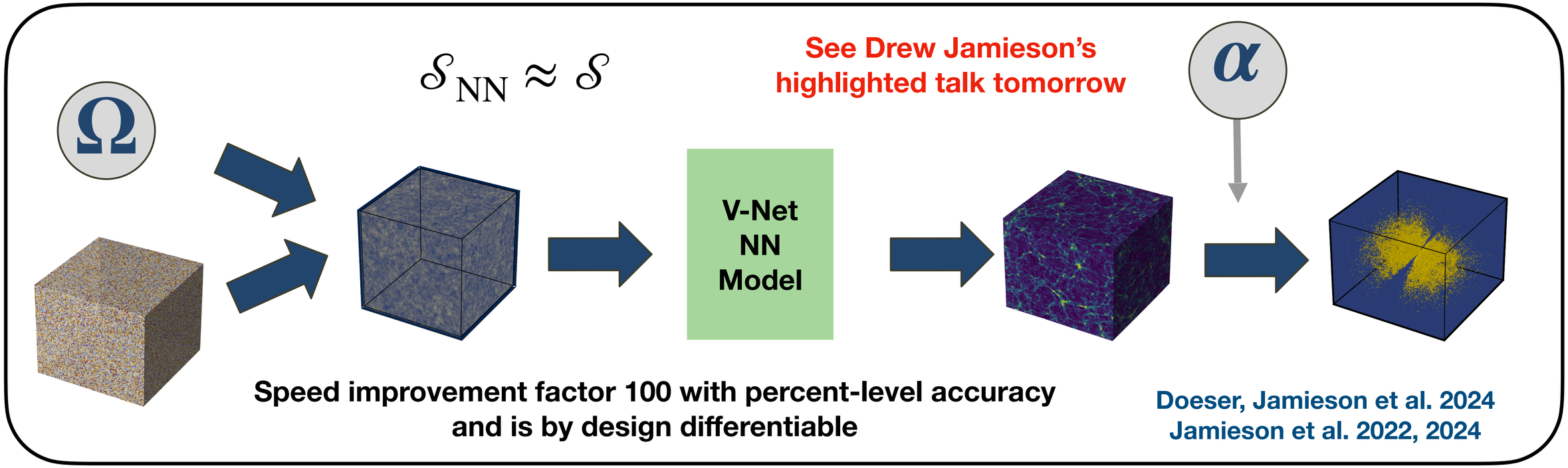


Learning to Optimize Cosmic Initial Conditions with Non-Differentiable Structure Formation Models

1. Rigorous test of cosmology!
2. Needed to model next-generation data!
3. Leveraging neural networks

Using state-of-the-art simulations via Neural networks

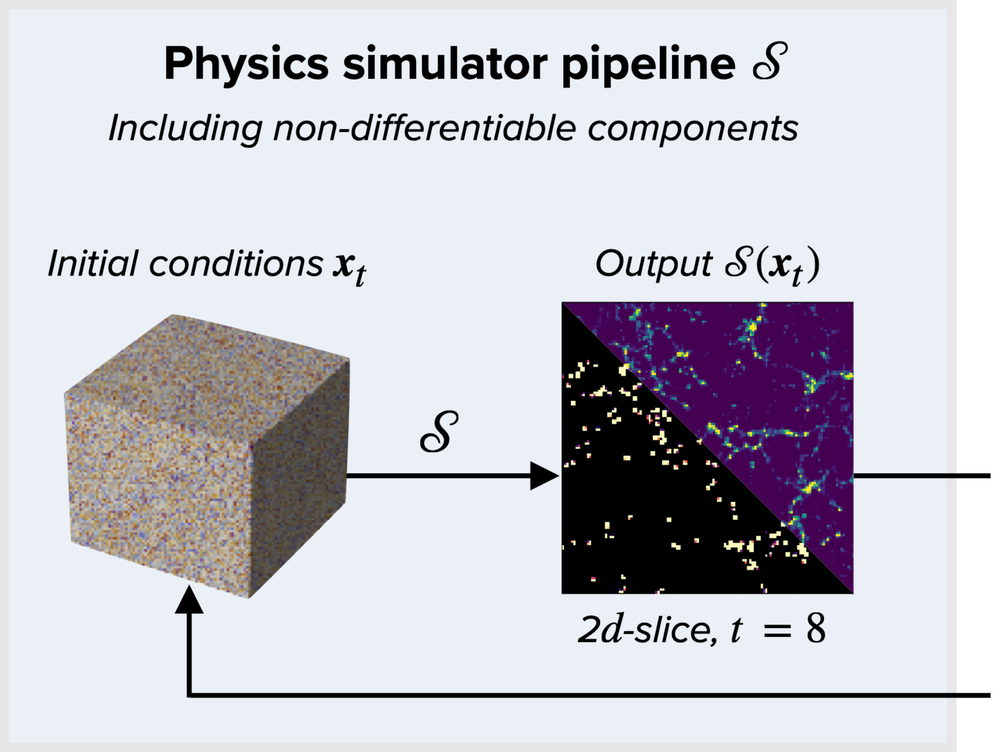
- Neural network can be used either as **(1) predictor (emulator)** or **(2) search engine (optimizer)**
- As **field-level emulator** to speed up **state-of-the-art simulations** $\mathcal{S}$ at non-linear scales



- How to use **state-of-the-art simulations** $\mathcal{S}$ without approximation?

Learning the Universe by Learning to Optimize (**LULO**)

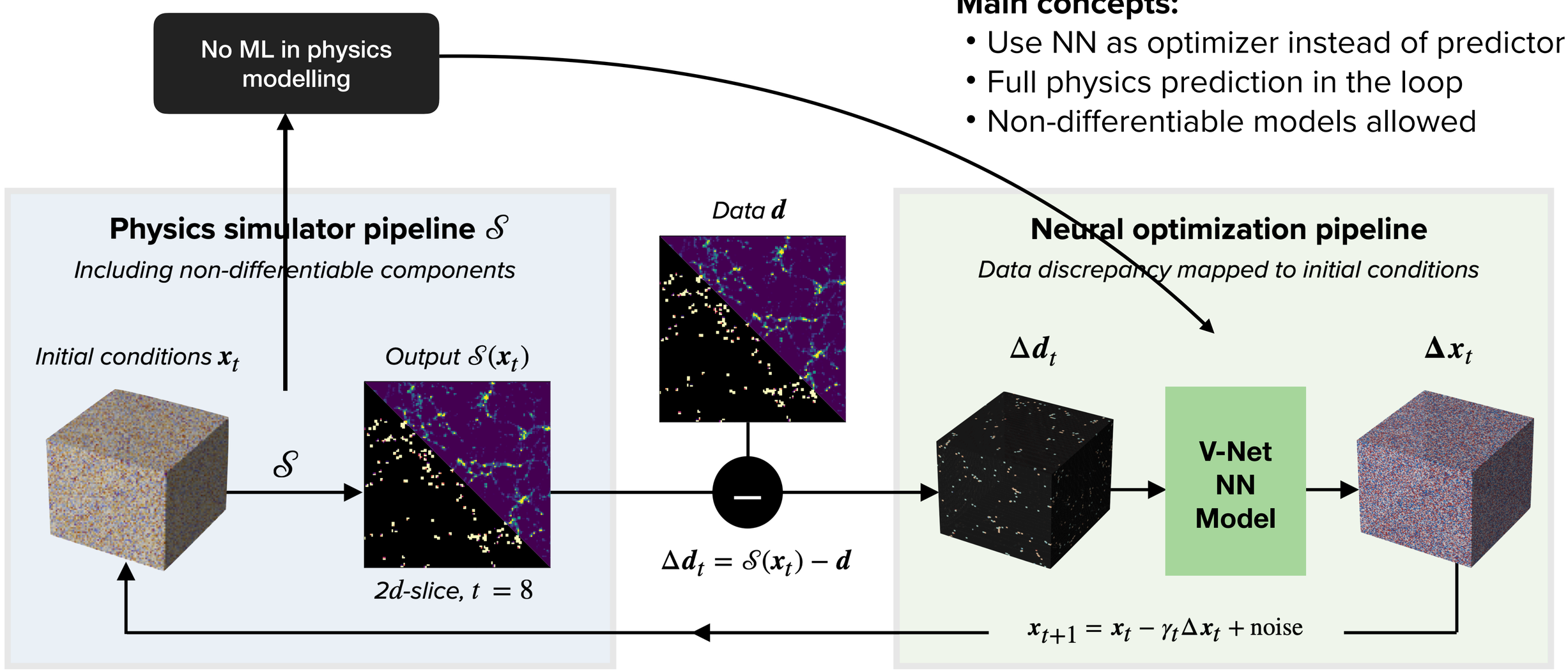
- Use of **neural optimizer:** We speed up the inference/optimization pipeline instead of the simulator!



Learning the Universe by Learning to Optimize (LULO)

Main concepts:

- Use NN as optimizer instead of predictor
- Full physics prediction in the loop
- Non-differentiable models allowed

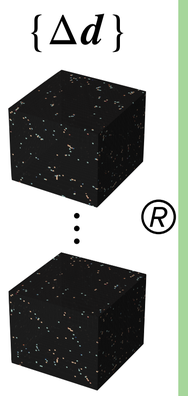


Learning how to map Δd to Δx

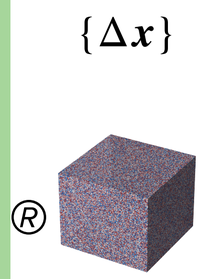
Any data fields can be used!

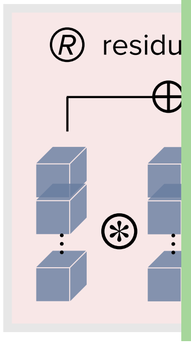
This work:

(1) Halo field
(2) Mass-weighted halo field



V-Net NN Model





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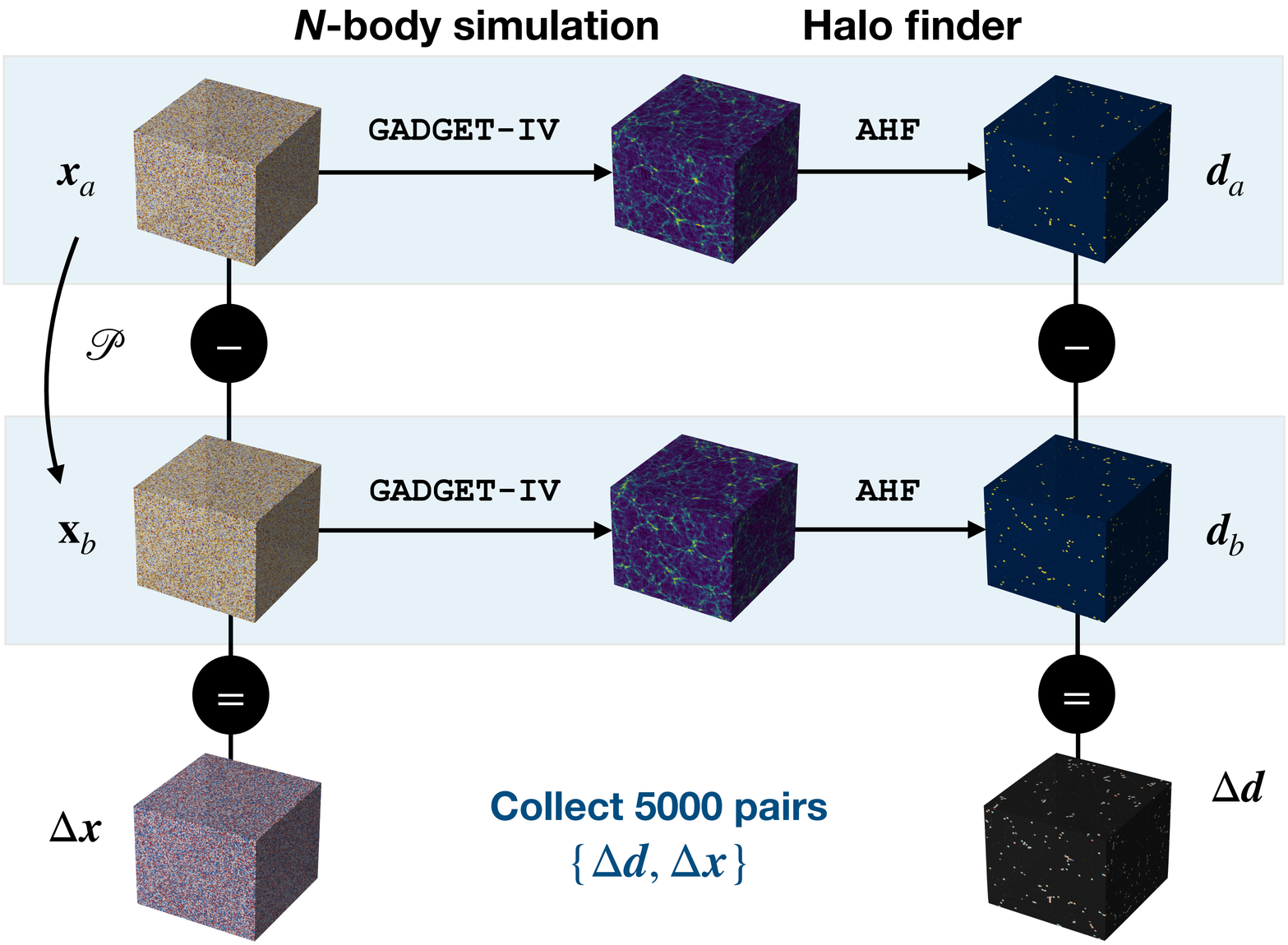
Cosine similarity loss

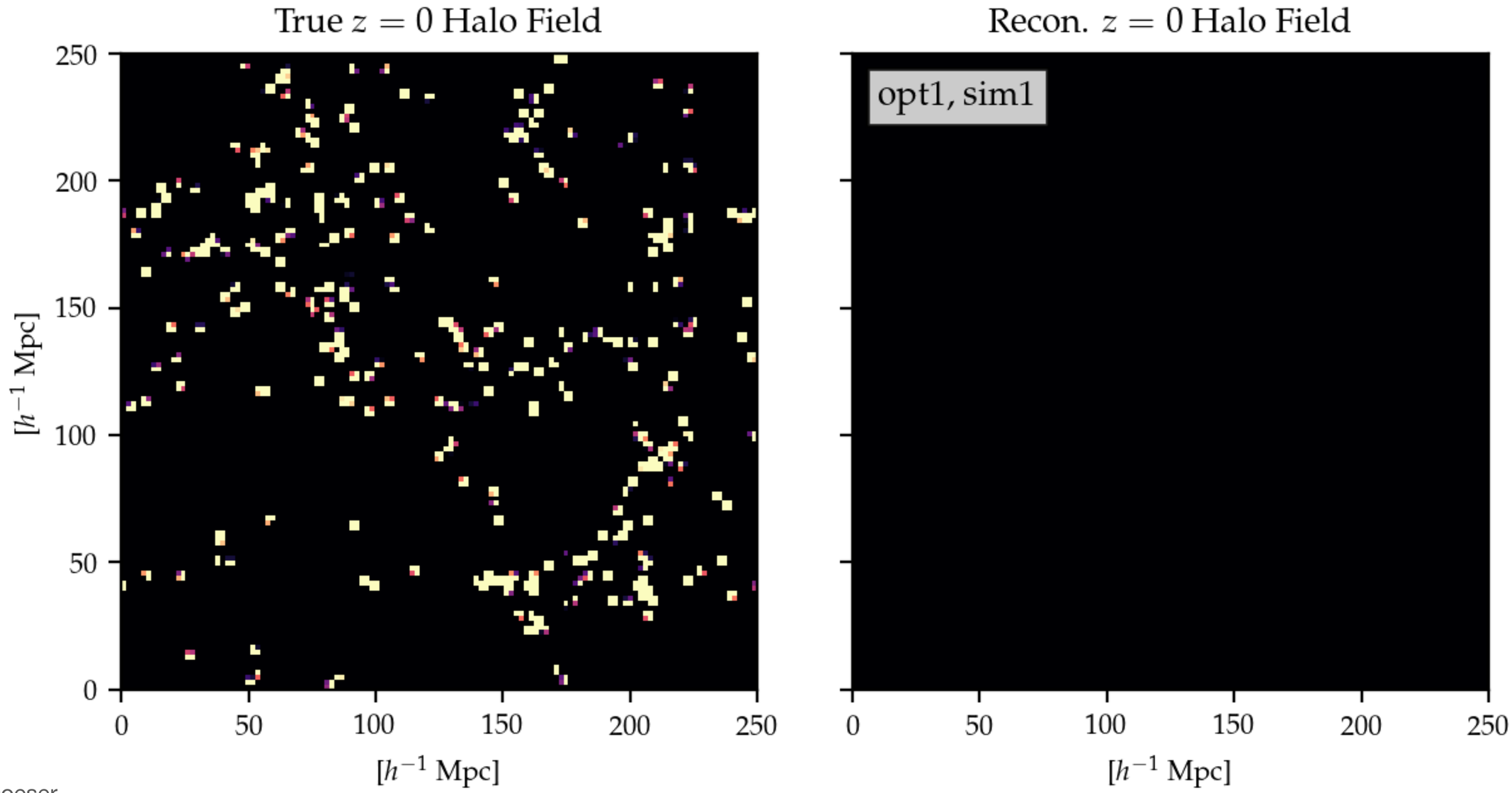
$$L = 1 - \frac{\Delta \boldsymbol{x}_{\text{true}}^{\top} \Delta \boldsymbol{x}_{\text{pred}}}{||\Delta \boldsymbol{x}_{\text{true}}|| \, ||\Delta \boldsymbol{x}_{\text{pred}}||}$$

Generating training data to map Δd to Δx

Ensures a perturbed initial conditions field with same mean and variance



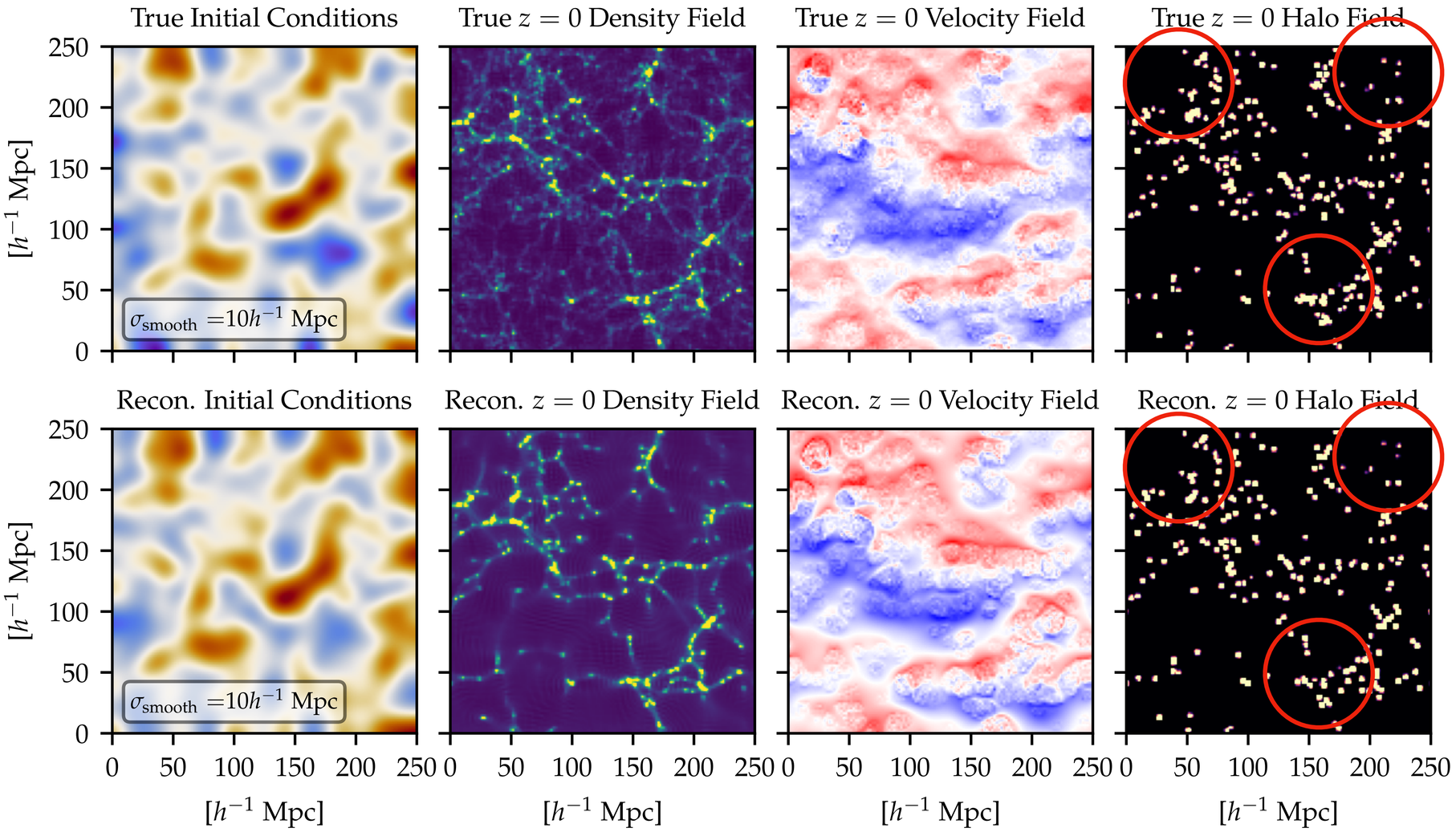
Reconstructing the initial conditions with **LULO**

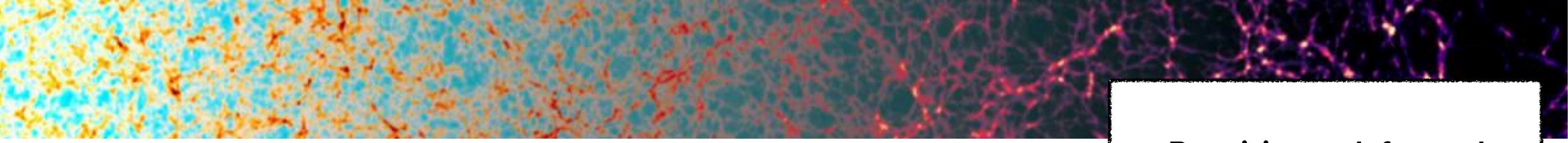


Reconstruction after 22 opt steps (96 simulations)

True fields:

Reconstructed fields:





Summary & Conclusions

Next-generation galaxy clustering surveys are here

- Capability to analyse data at non-linear scales will limit knowledge gains

Inference technology

- Field-level inference of initial conditions offers information optimality
- Complete characterisation of cosmic structure without compression
  - 1) Non-linear model of structure formation, 2) Entire model and inference at the field-level
- Rigorous test of the cosmological model

Accelerating cosmological inference with deep learning

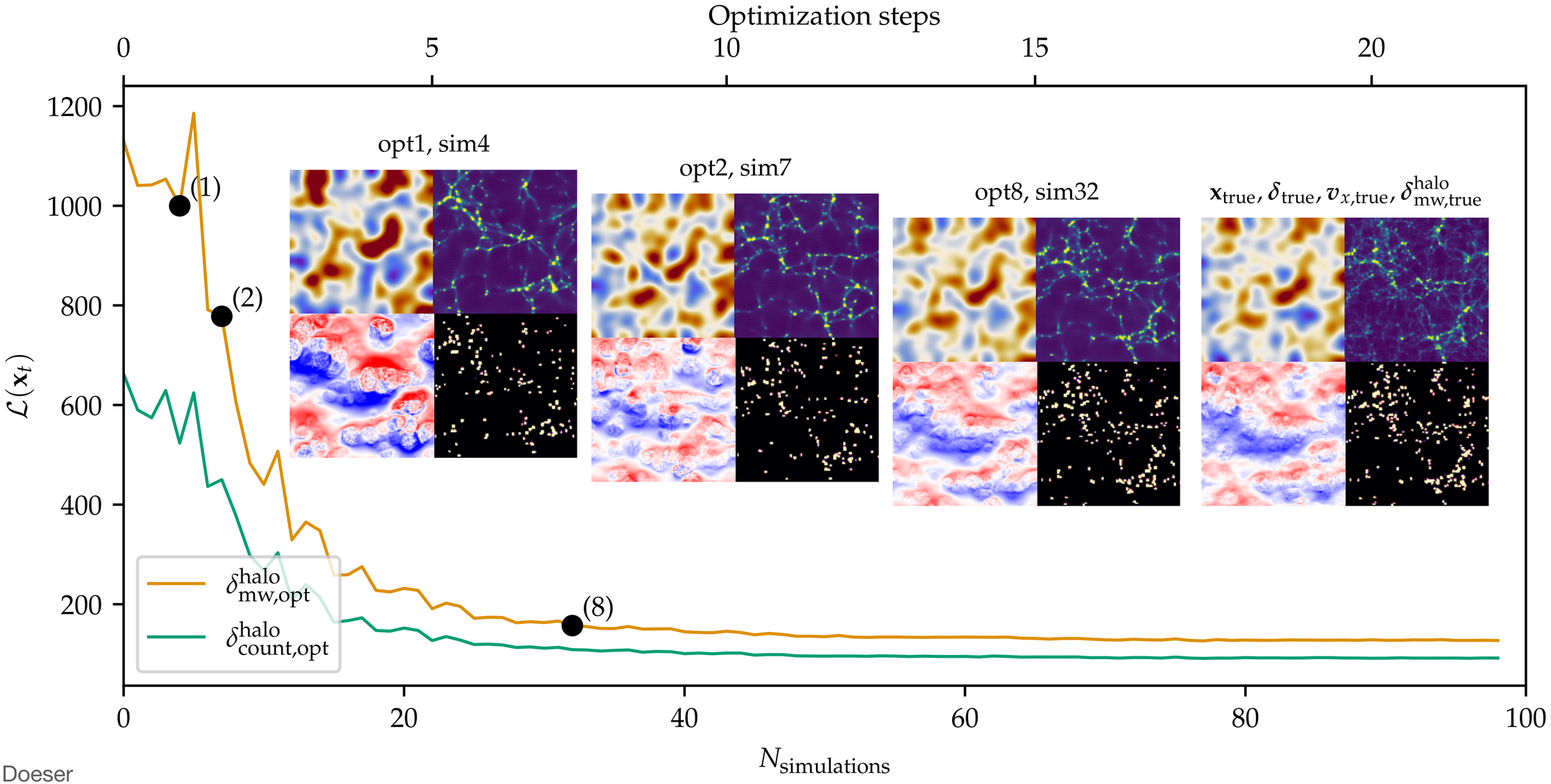
- **Neural model**: increasing efficiency of non-linear simulators of structure formation
- **Neural optimizer:** providing a gradient-free framework to incorporate non-differentiable simulators

Promising path forward towards analyzing current-generation galaxy surveys at non-linear scales

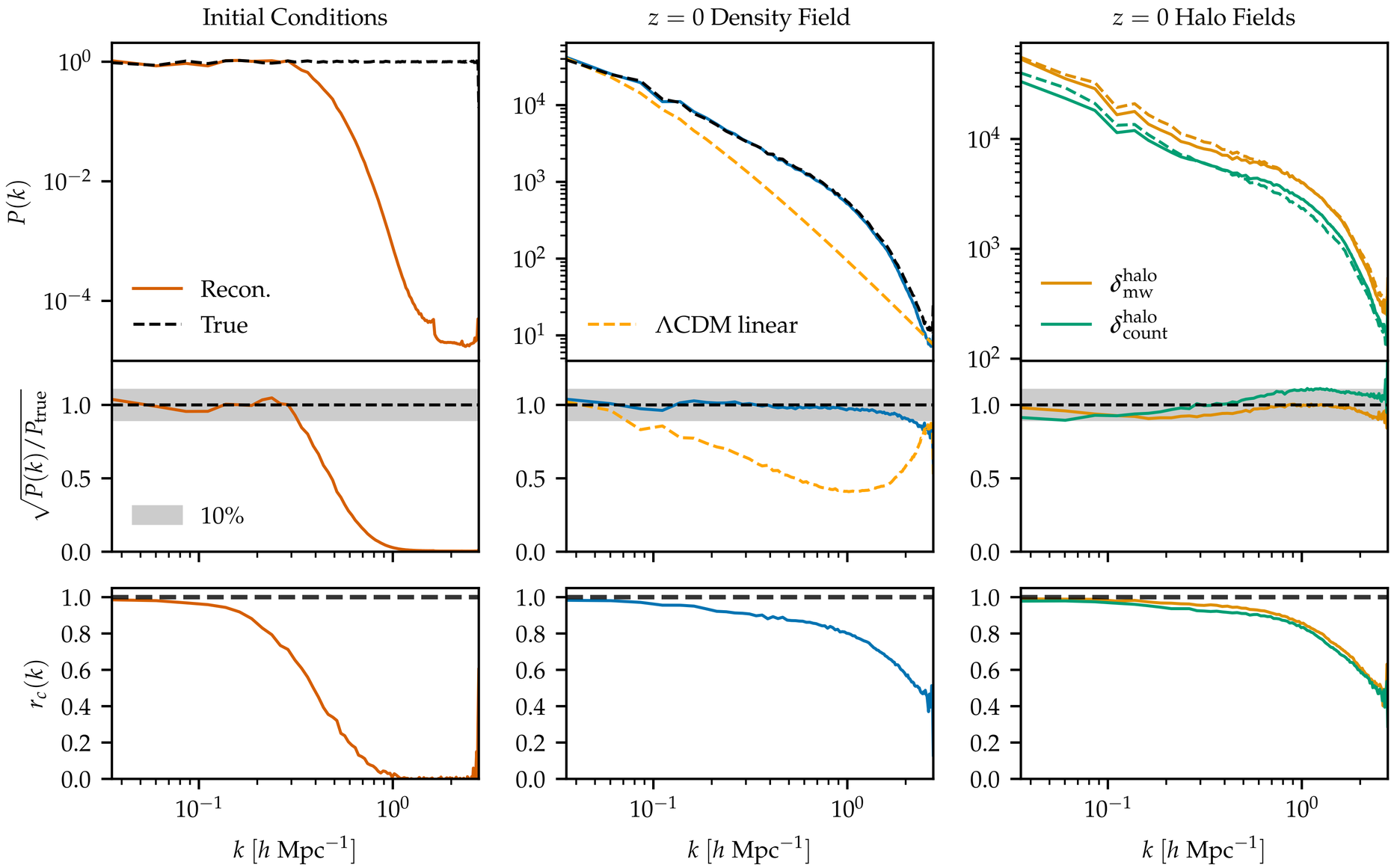
arXiv: 2312.09271

arXiv: 2502.13243

Monitoring the decreasing data discrepancy



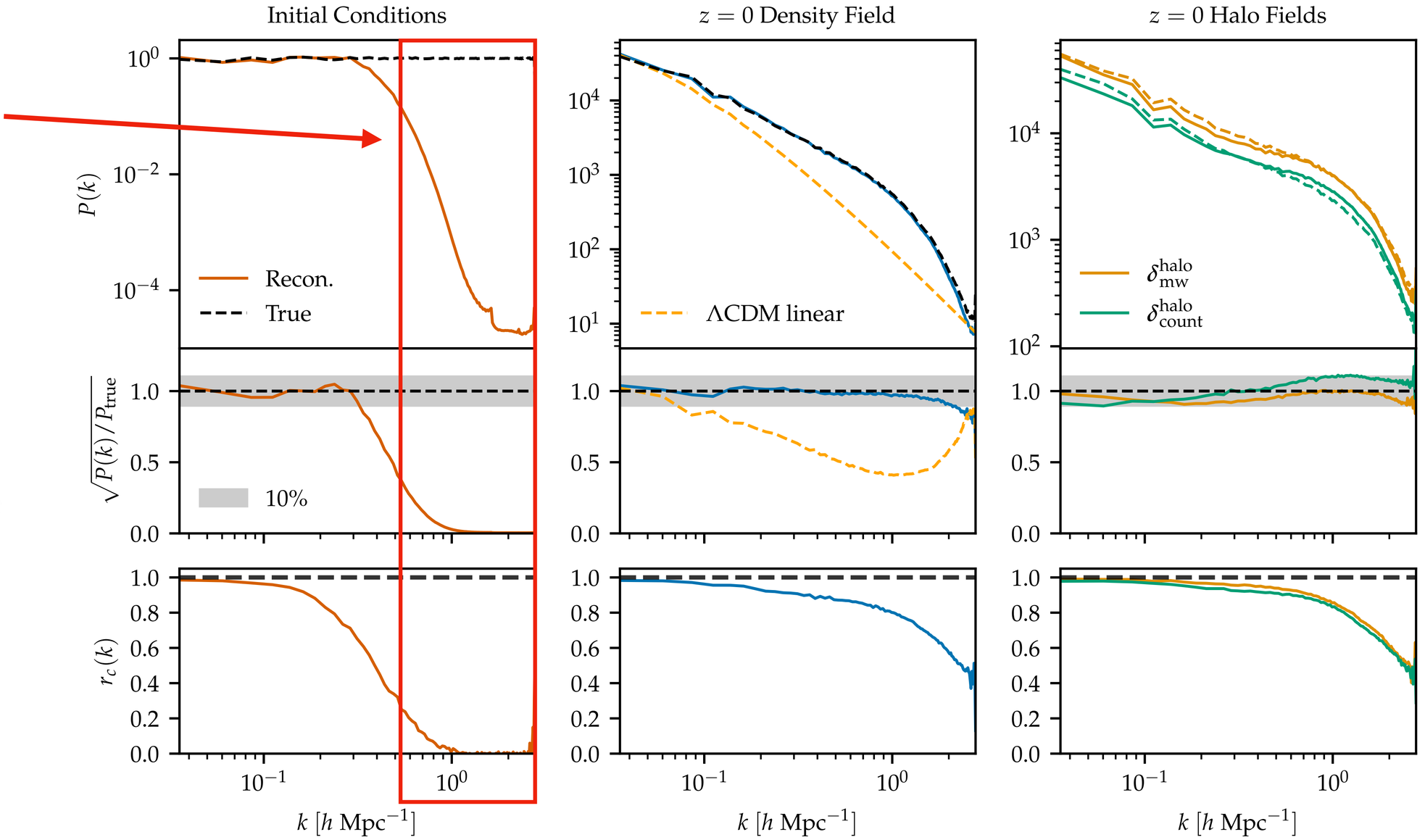
Reconstruction of initial conditions



Reconstruction of initial conditions

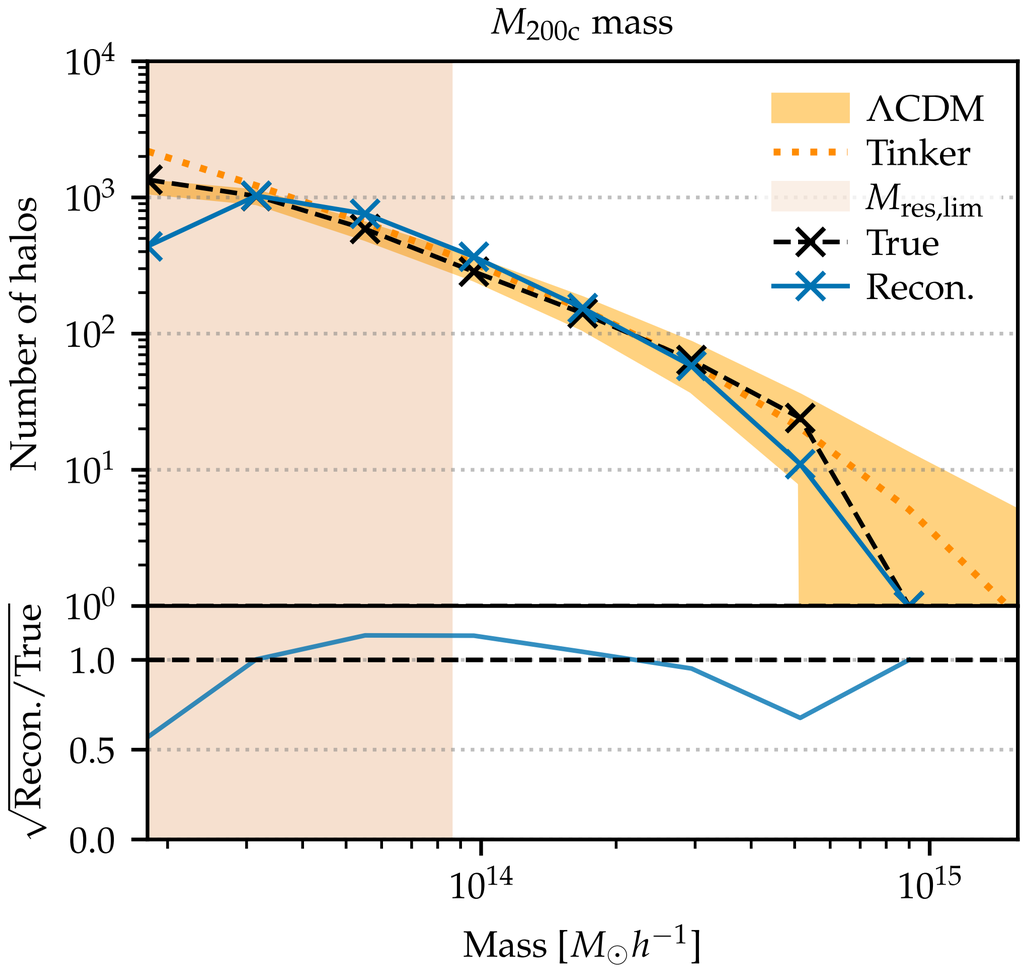
These scales collapse below data resolution

- Non-linear modelling required to explain linear regions in the initial conditions

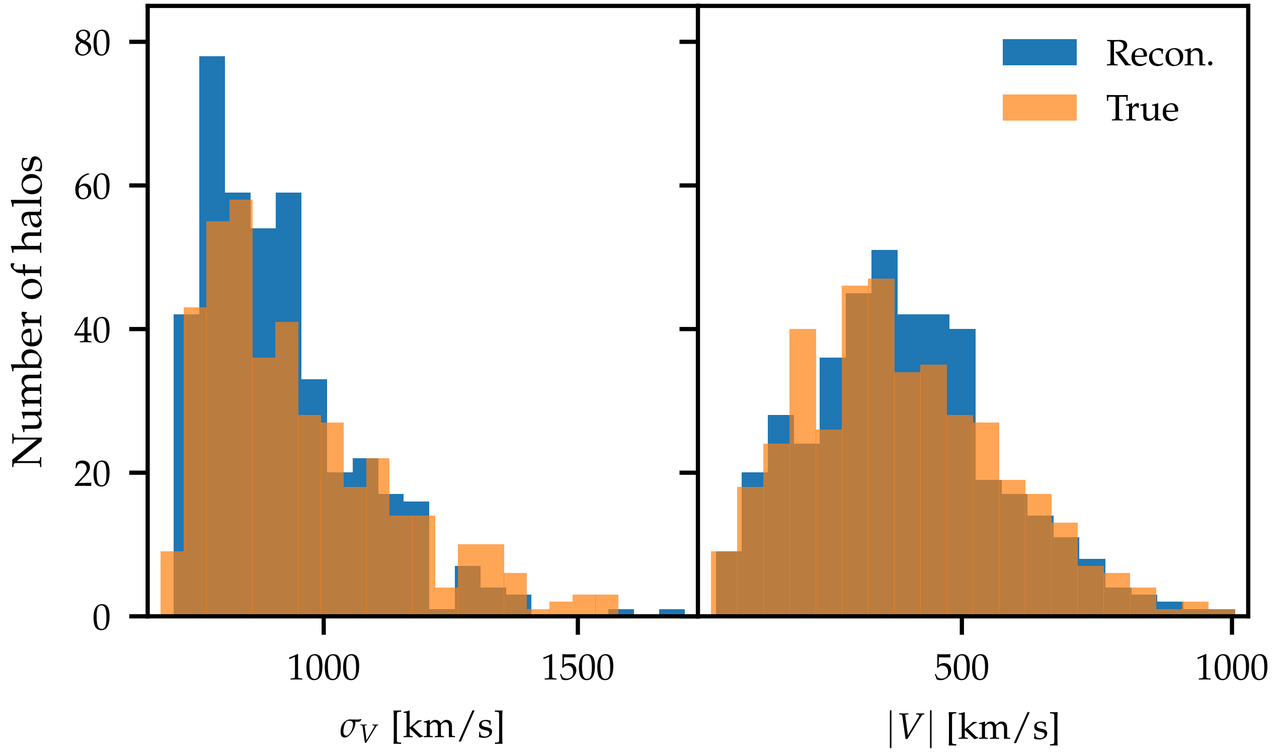


Reconstructed halos

Halo mass function



Derived properties: halo velocities



Generalizability to any initial conditions (here 10 recon.)