



21st International Workshop on Advanced  
Computing and Analysis Techniques in Physics  
Research

# From Galaxy Clusters to Cosmic Evolution with Simulation-Based Inference

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# Galaxy Clusters

**Largest known gravitationally-bound structures in the Universe**

Mass range  $10^{14} - 10^{15} M_{\odot}$

Contains hundreds to thousands of galaxies



Galaxy Cluster SMACS 0723

Credit: James Webb Space Telescope

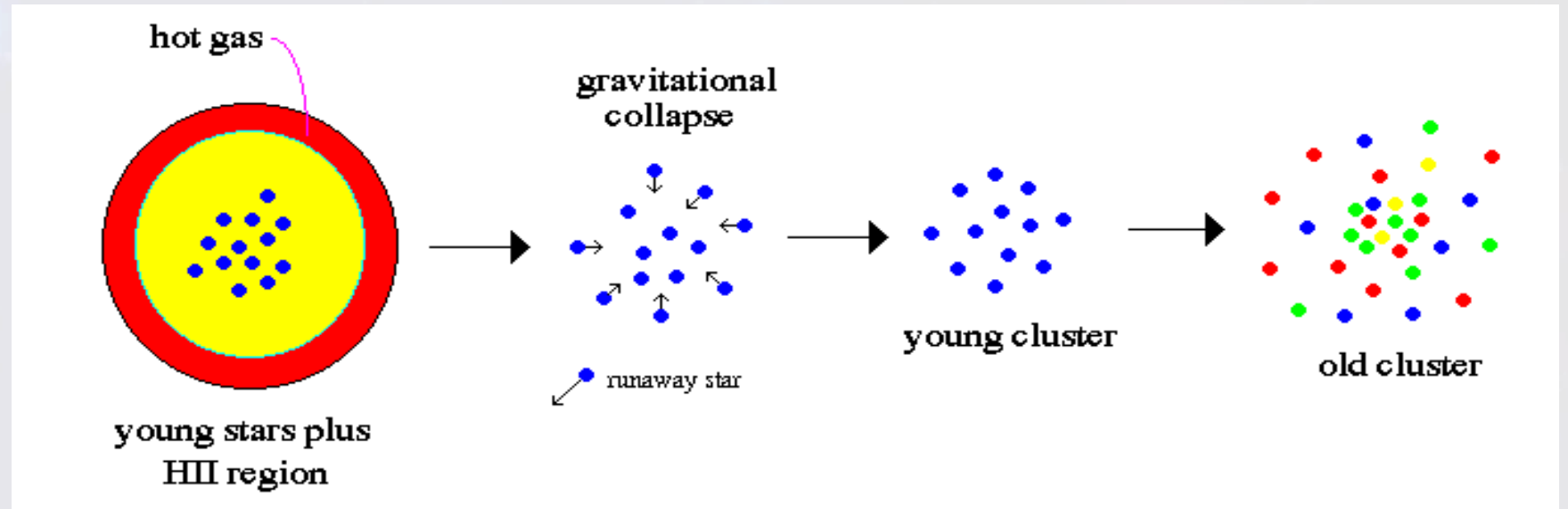
# Cosmological Parameters

Parameters:  $\Omega_m$  &  $\sigma_8$

## Galaxy Cluster Formation and Evolution

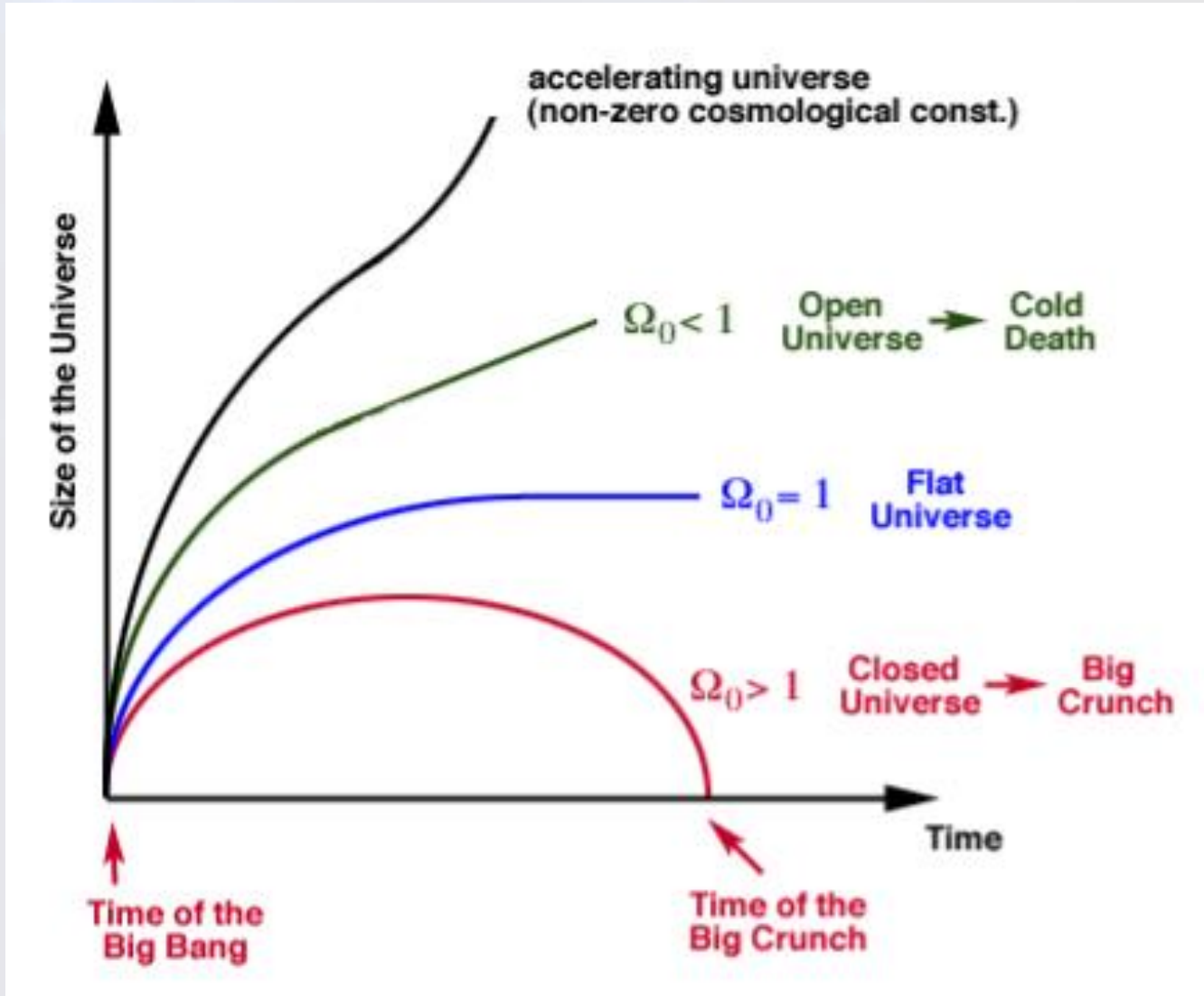


Credit: James Webb  
Space Telescope



Credit: abyss.uoregon.edu

# Cosmological Parameters



Parameter:  $H_0$

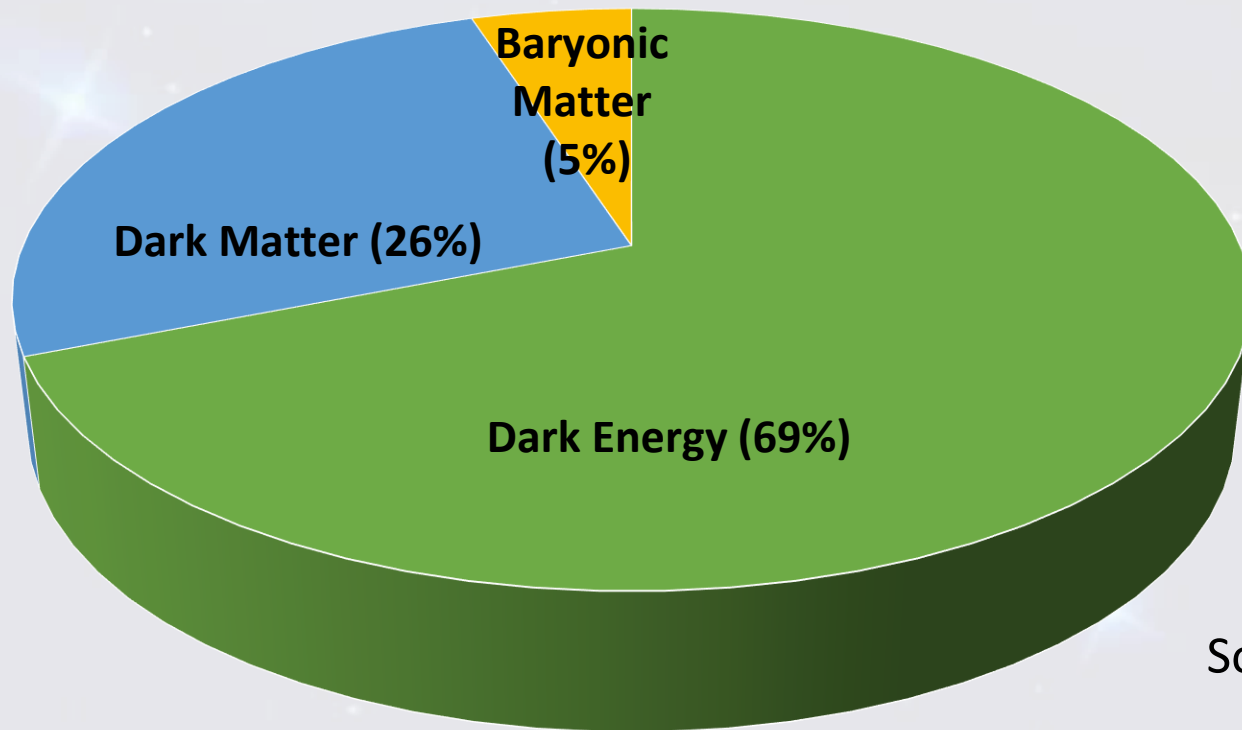
Ultimate Fate of the Universe

$\rightarrow \Omega_0 = \Omega / \Omega_c$

Credit: <https://astro.umass.edu>

# Mass-Energy Distribution of the Universe

We know about only  
5% of the Universe!



Source: National Radio Astronomy Observatory

# Inputs and Outputs

## Inputs (Observables)

- Average mass of galaxy clusters
- Total number of galaxy clusters

## Outputs (Parameters)

- Cosmic (Simplified Halo)
- Cosmic and Astrophysical (Cluster)

## Cosmological Parameters

- Baryonic density ( $\Omega_b$ )
- Matter density ( $\Omega_m$ )
- Hubble's constant ( $H_0$ )
- Power law index ( $n_s$ )
- Amplitude fluctuation ( $\sigma_8$ )

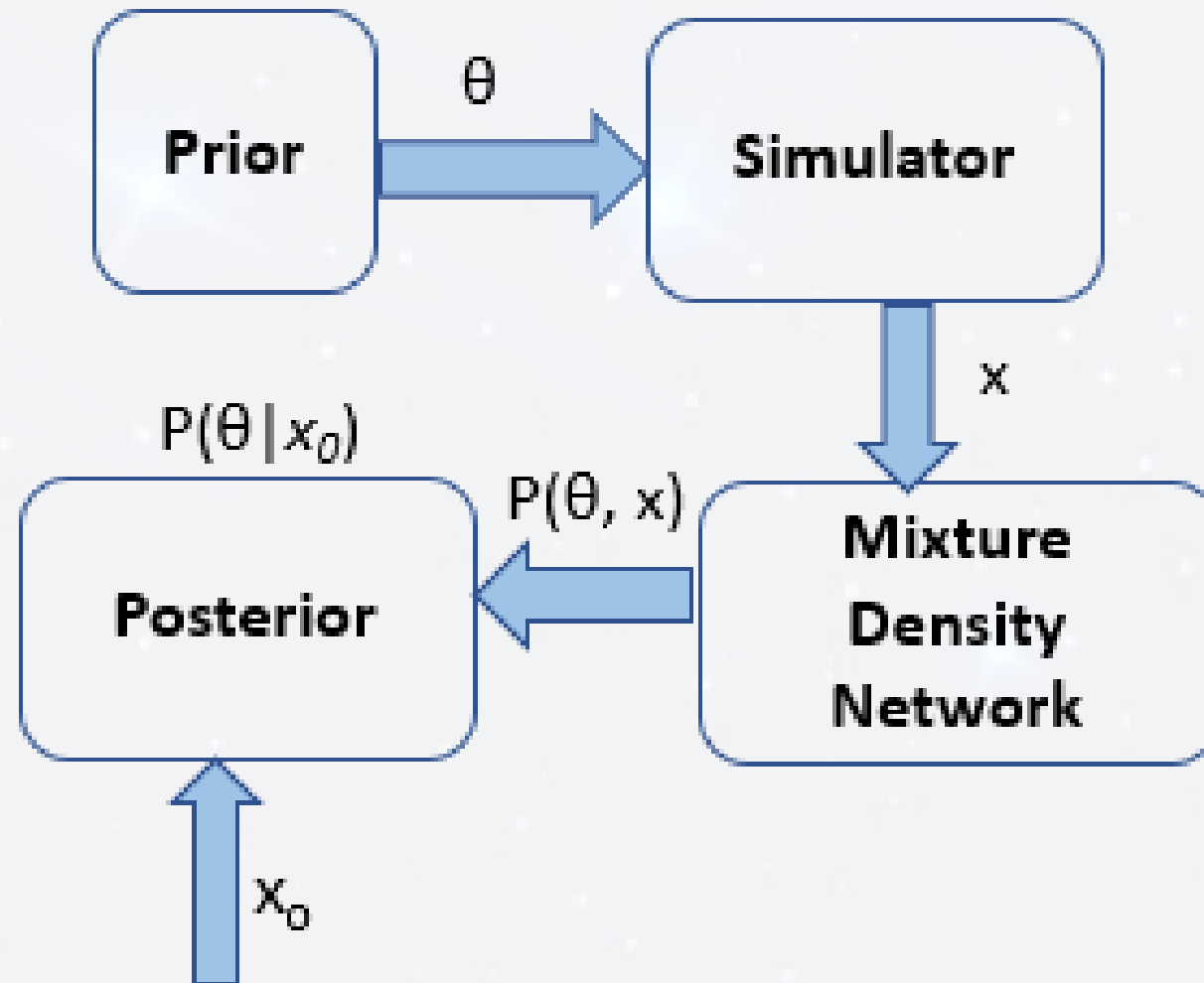
## Astrophysical Parameters

$\ln \lambda = M_A + M_B \ln(M)$ , with scatter  $\sigma$

- $M_A$
- $M_B$
- $\sigma$

(Murata et al. 2017)

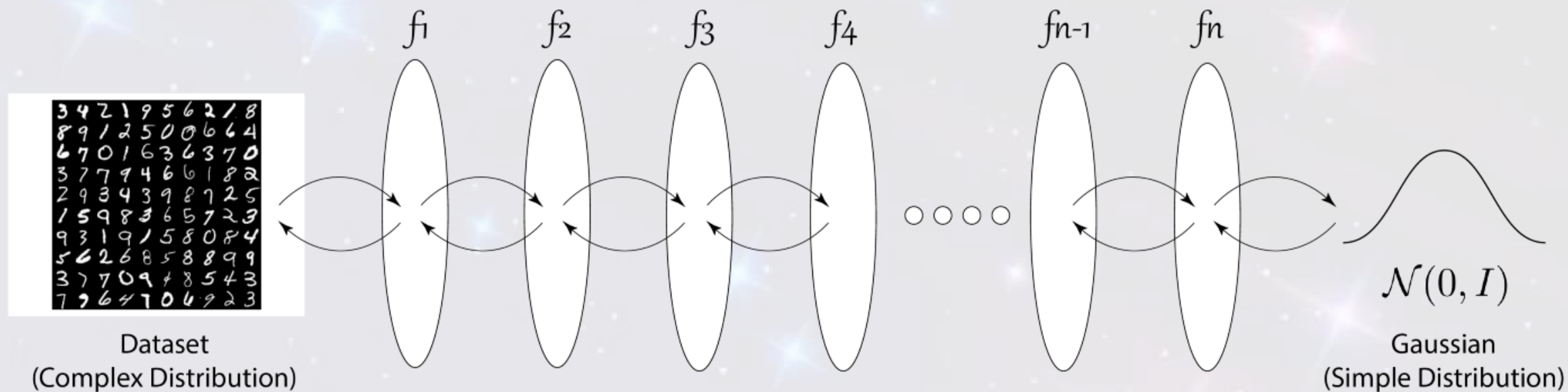
# Simulation-based Inference (SBI)



Working principle of SBI method

# Normalizing Flow-based SBI

- ✓ Consists of a series of simple invertible functions
- ✓ Used for complex data representation





# Markov Chain Monte Carlo (MCMC)

Used to:

draw samples from high-dimensional pdf

Disadvantages:

explicit likelihood dependence  
dependent chains

Sampling Strategies:

Metropolis-Hastings  
Gibbs Sampling

# SBI vs MCMC

## SBI

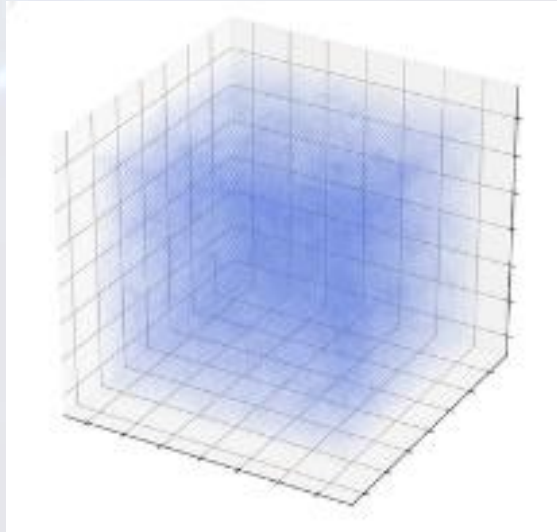
- Easy to incorporate complex physical models
- Precomputes mock observables for training
- Convenient speed

## MCMC

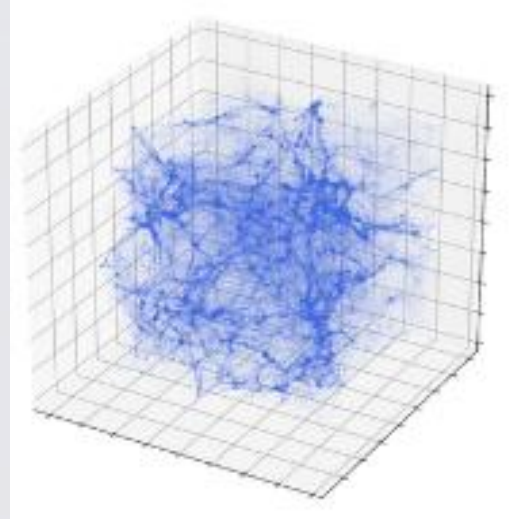
- Difficult to include complex phenomena
- Calculates likelihood during runtime
- Much slower

# Dataset 1: Quijote Simulations

N-body simulations: Large Scale Structure Formation



Early Universe



Late Universe

Credit: TensorFlow Blog

Villaescusa-Navarro, F., et al. "The Quijote Simulations," *arXiv:1909.05273* (2019).

## Characteristics:

- 44,100 full N-body simulations
- Snapshots at multiple redshifts

## Purpose:

- Constrain cosmological models
- Provide statistics to train ML algorithms

# Dataset 1: Quijote Simulations

**Training Set:**  
**Latin Hypercube Simulations**  
**(Variable Cosmology)**

$$\Omega_m : [0.1 - 0.5]$$

$$\Omega_b : [0.03 - 0.07]$$

$$h : [0.5 - 0.9]$$

$$n_s : [0.8 - 1.2]$$

$$\sigma_8 : [0.6 - 1.0]$$

**Test Set:**  
**Fiducial Planck Cosmology**  
**(Fixed Cosmology)**

$$\Omega_m : 0.318$$

$$\Omega_b : 0.049$$

$$h : 0.671$$

$$n_s : 0.962$$

$$\sigma_8 : 0.834$$

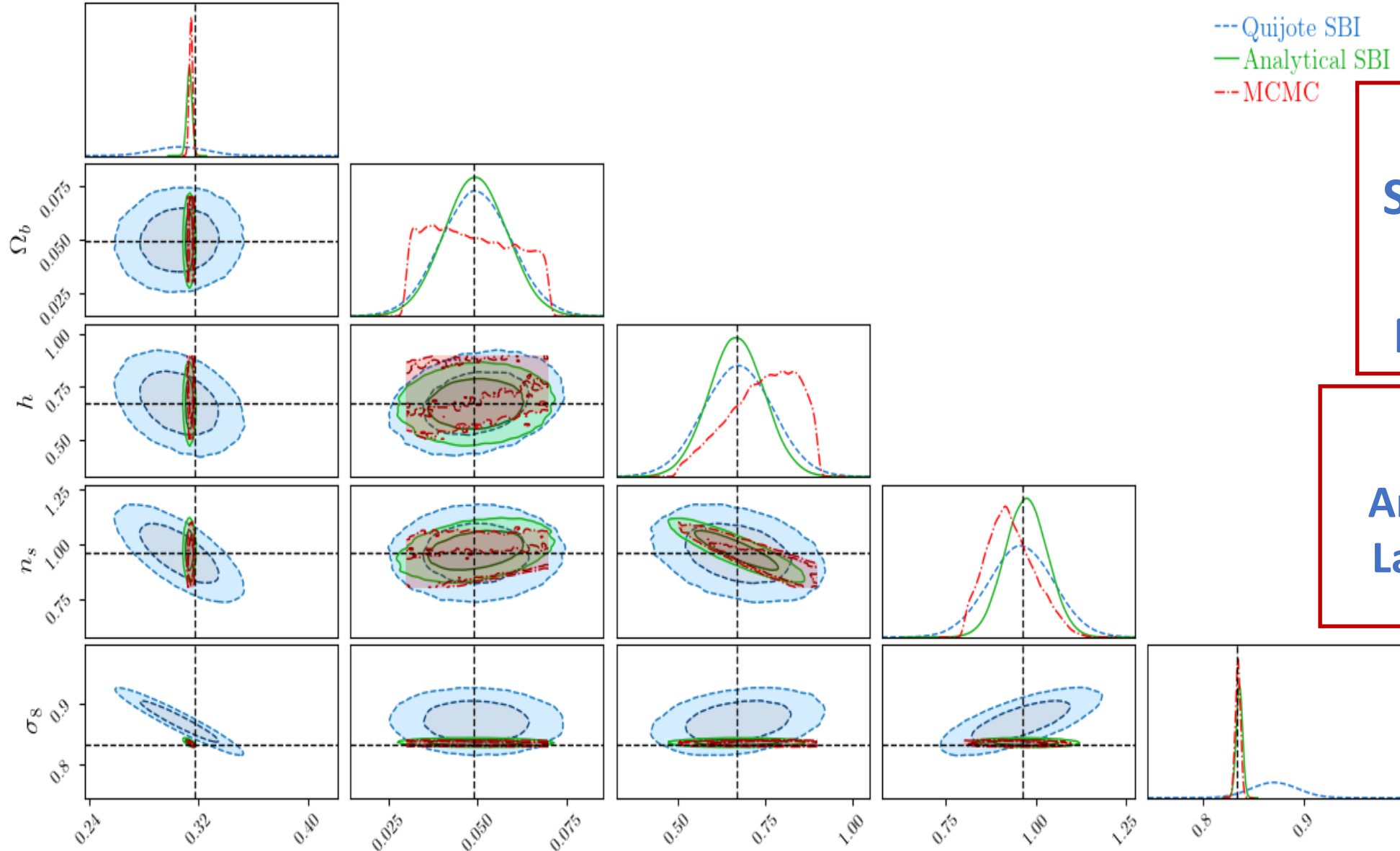
# Dataset 2: Analytical Simulations

Analytical simulations are generated by **CosmoSIS**:

$$\mathbf{N} = v \int n(m, z = 0) | \Omega_m, \sigma_8$$
$$\mathbf{M} = v \int n(m, z = 0) | \Omega_m, \sigma_8 * m$$

- N and M are the mock observables used for training
- n is the cluster density function (depends on the model)

# Results [Posterior Distribution]

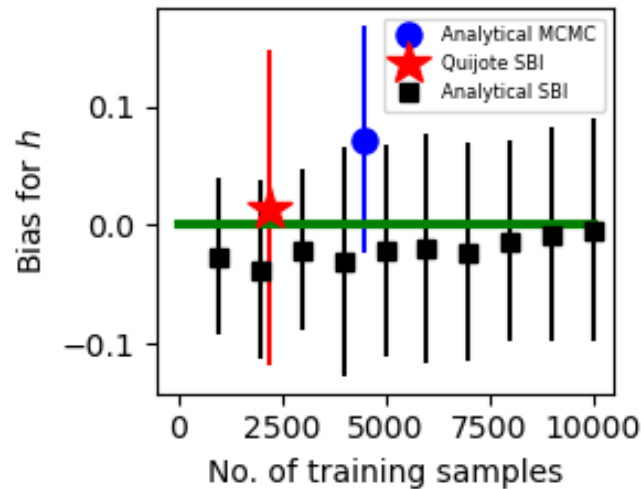
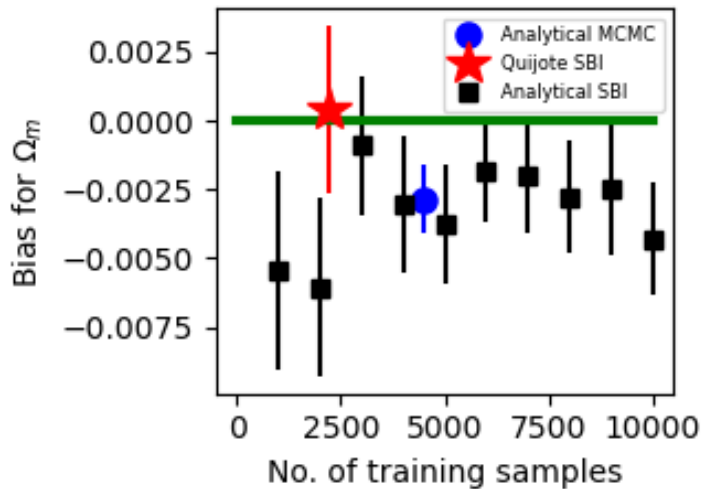
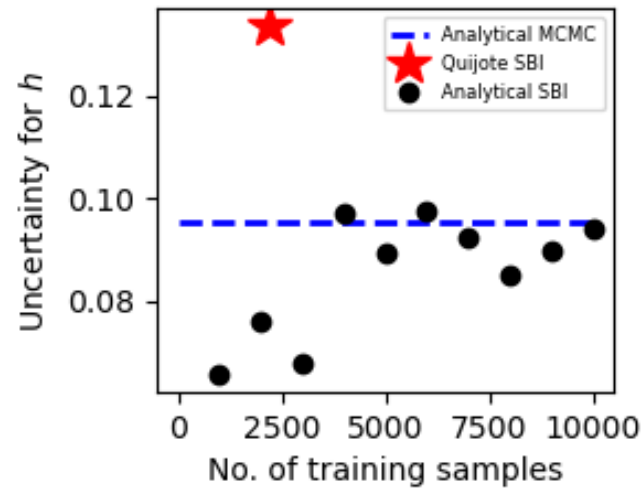
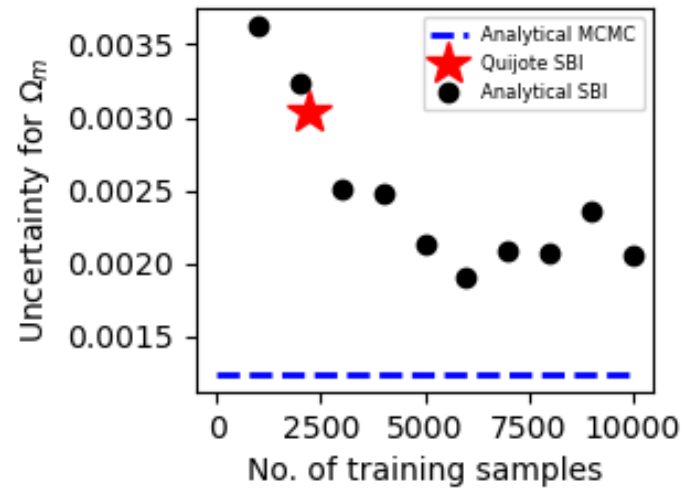


--- Quijote SBI  
— Analytical SBI  
--- MCMC

**Truth**  
**SBI within 2 $\sigma$**   
**Bias**  
**MCMC > SBI**

**Uncertainty**  
**Analytical  $\approx$  MCMC**  
**Largest for Quijote**

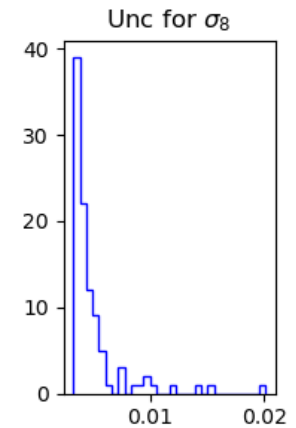
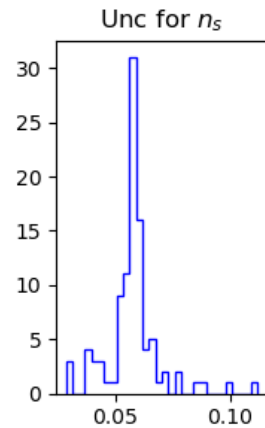
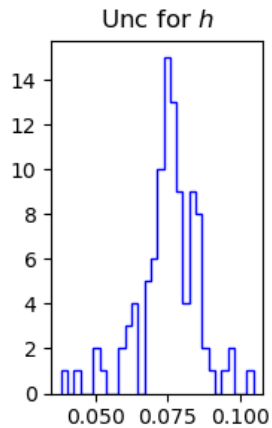
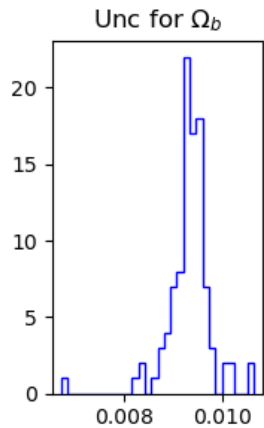
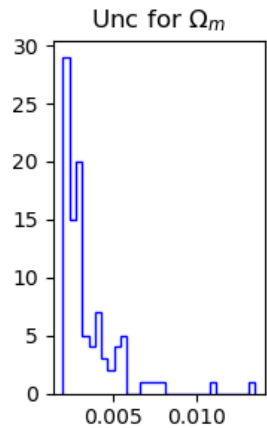
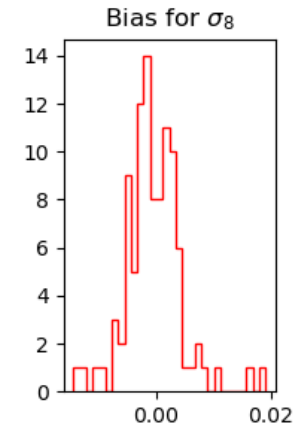
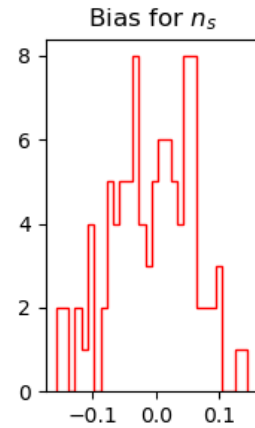
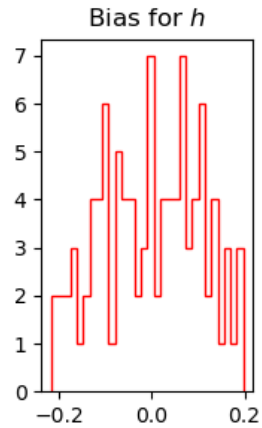
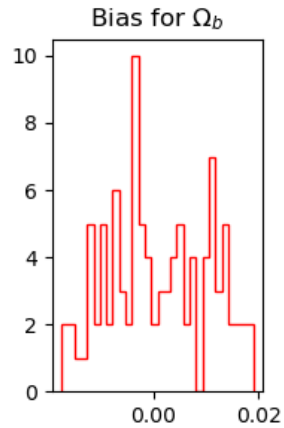
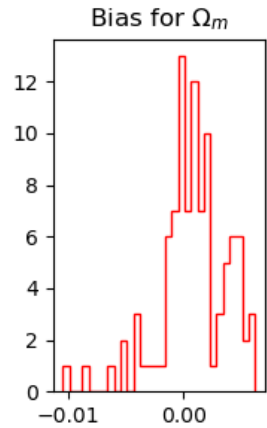
# Results [Training Sample Size]



Sample size  $\uparrow$ ,  
Unc  $\downarrow$  for  $\Omega_m$   
No trend for  $h$

Sample size  $\uparrow$ ,  
Bias  $\downarrow$  for  $\Omega_m$   
Constant bias for  $h$

# Results [Analytical Simulations]

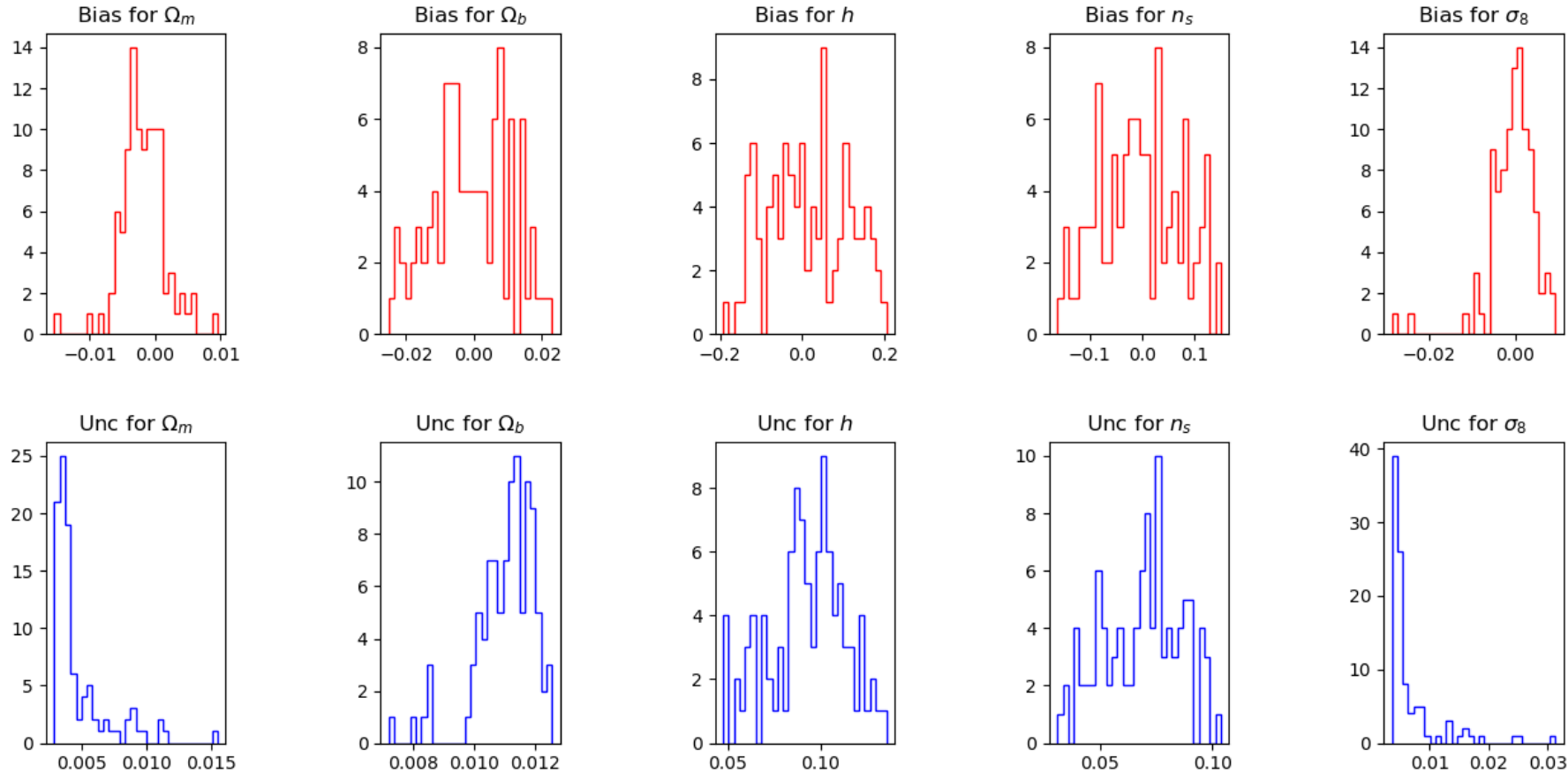


**Bias**  
Single peak  
around zero for  
 $\Omega_b$  and  $\sigma_8$

**Uncertainty**  
Smallest  
for  $\Omega_m$  and  $\sigma_8$



# Results [Quijote Simulations]



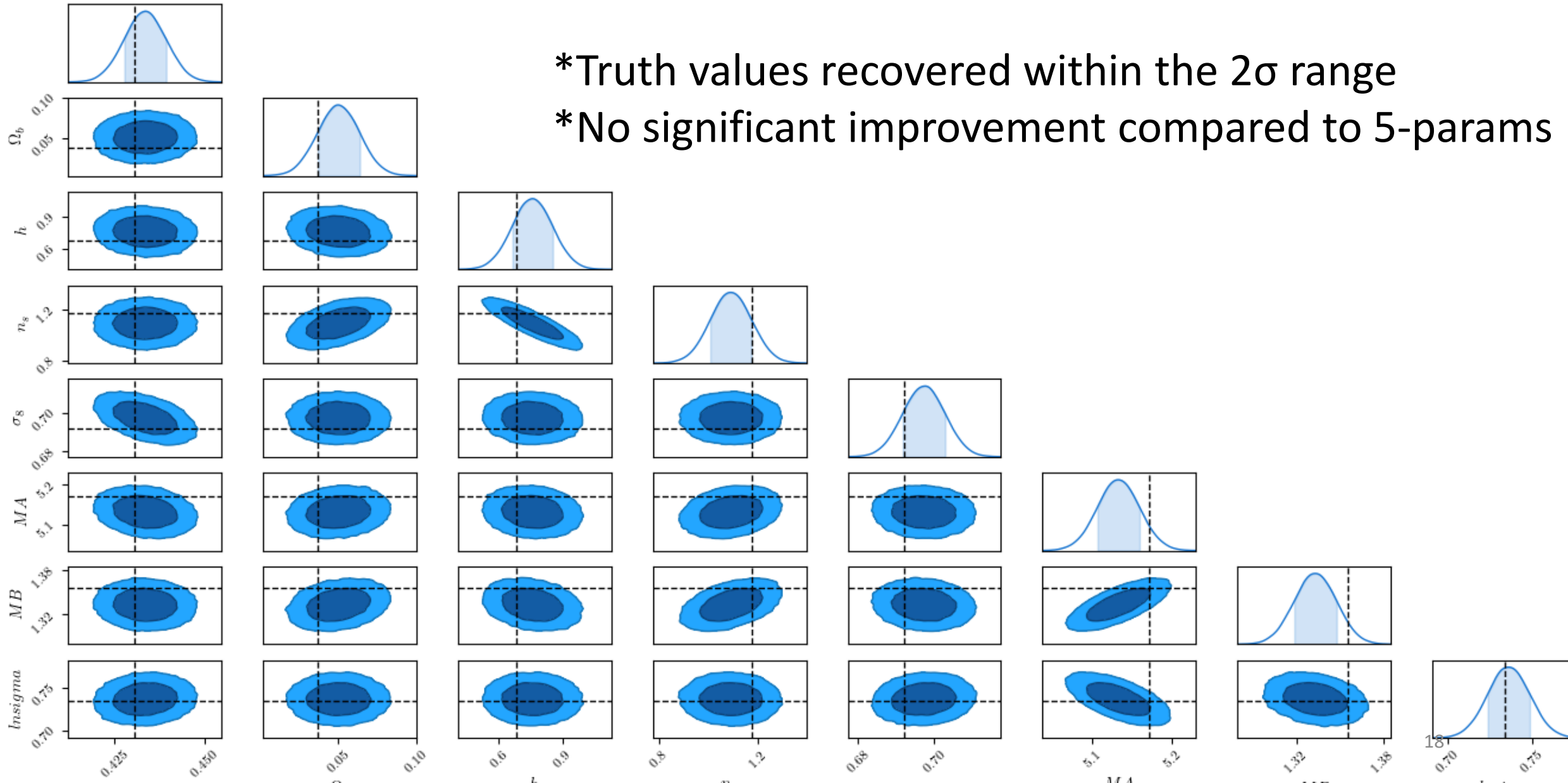
**Bias**  
Dominant peak  
around zero for  
 $\Omega_m, h$  &  $\sigma_8$

**Uncertainty**  
Smallest for  
 $\Omega_m$  &  $\sigma_8$

# Results [Cosmological & Astrophysical]

\*Truth values recovered within the  $2\sigma$  range

\*No significant improvement compared to 5-params



# Conclusions

## Simulation-based Inference (SBI)

- Comparable performance to state-of-the-art-method
  - Satisfying results for the simulated Universe
- Promising tool for large-scale (real) cosmic surveys
  - Answer fundamental cosmological questions

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