CONVERGENCE MAPS WITH DENOISING DIFFUSION PROBABILISTIC MODELS

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Denoising Diffusion Probabilistic Models

A New Era of Image Generation

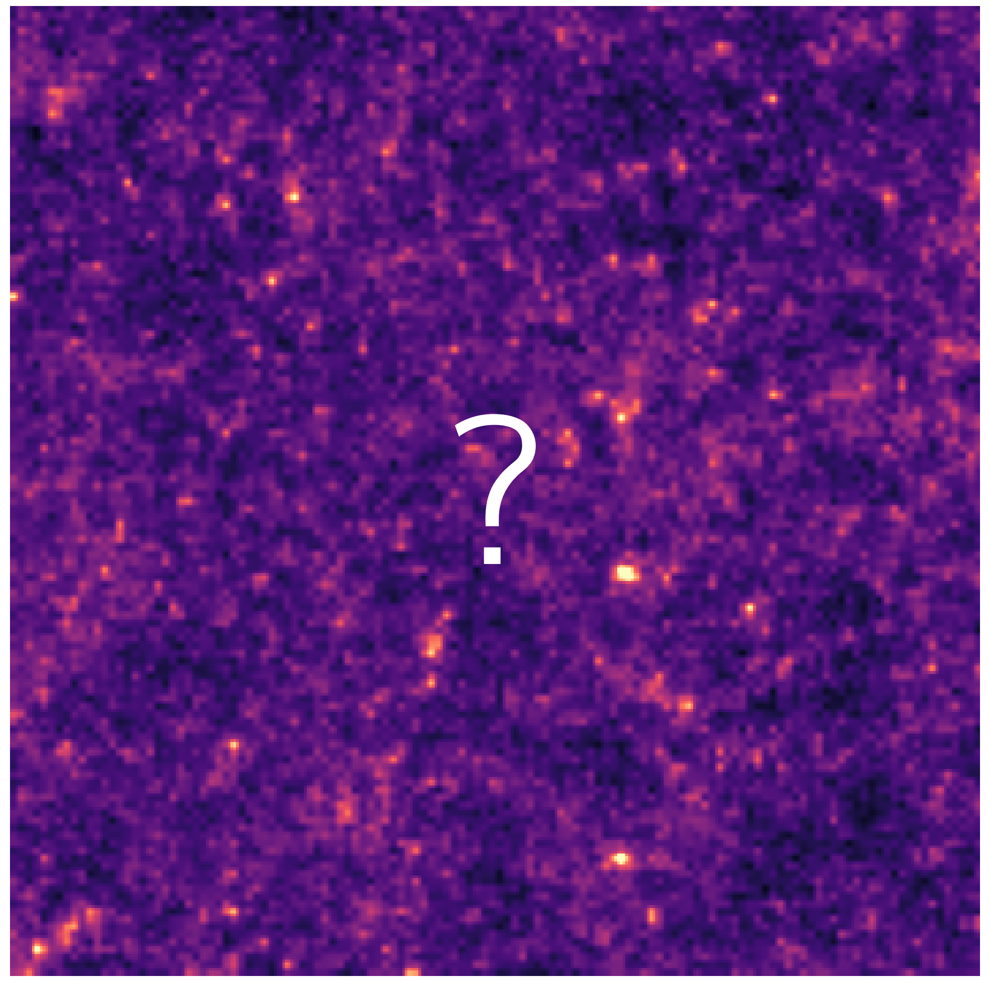
Corgis

Dall-E 2

Midjourney

Stable Diffusion

Convergence Maps



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1. Denoising Diffusion Probabilistic Models (DDPM)
2. Conditional Wasserstein Generative Adversarial Networks (CWGAN) (Perraudin et al. 2020)
3. Training Data
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5. Discussion on Hyper-parameters and Sampling Methods
6. DDPM vs. CWGAN
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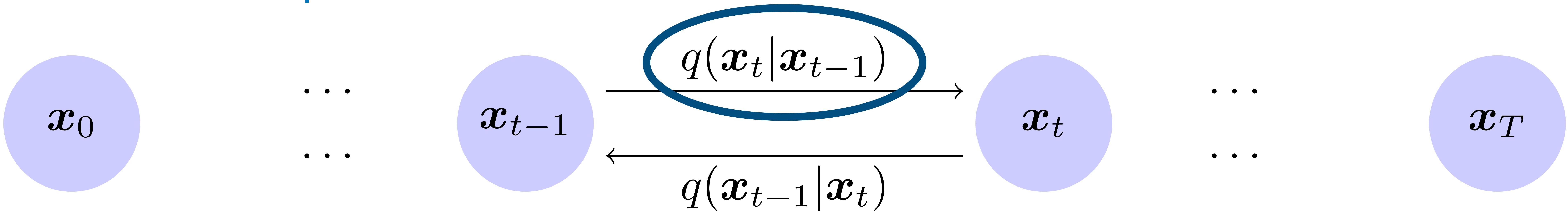
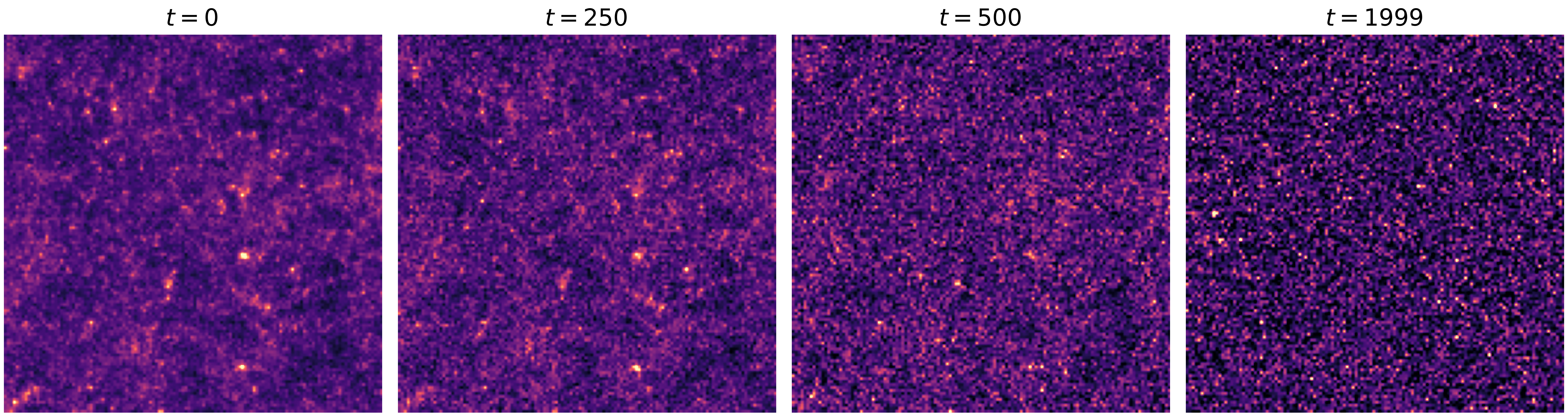
Denoising Diffusion Probabilistic Models

Forward diffusion process



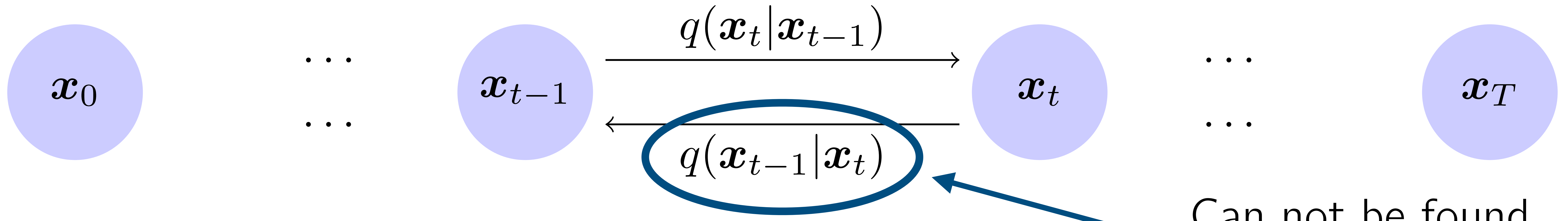
Conditional probability: $q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{1-\beta_t}\boldsymbol{x}_{t-1}, \beta_t)\,,$ $\qquad \boldsymbol{x}_t = \sqrt{1-\beta_t}\boldsymbol{x}_{t-1} + \sqrt{\beta_t}\boldsymbol{\epsilon}_{t-1}$



(Ho, Jain, and Abbeel 2020)

Denoising Diffusion Probabilistic Models

Reverse diffusion process



Can not be found analytically

Need an approximate model:

$$q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) \approx p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) = \mathcal{N}(\boldsymbol{x}_{t-1}; \mu_\theta(\boldsymbol{x}_t, t), \beta_\theta(\boldsymbol{x}_t, t))$$

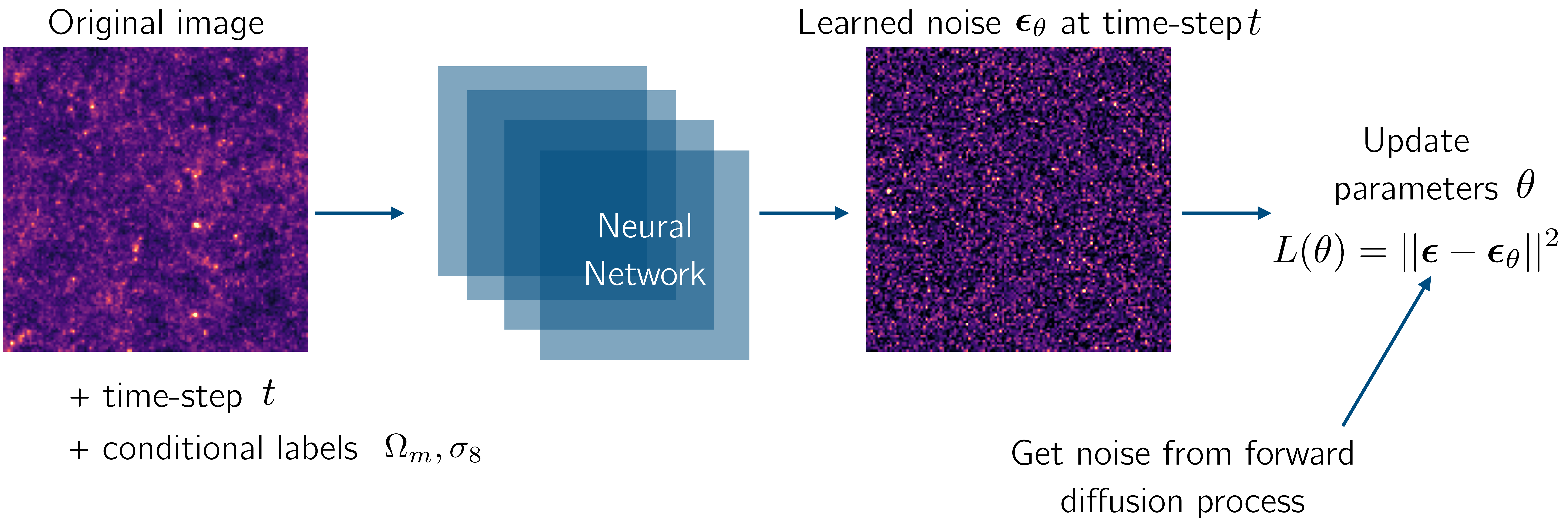
$$\mu_\theta(\boldsymbol{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\boldsymbol{x}_t, t)\right)$$

Only need to learn noise term $\longrightarrow$ $\boxed{L(\theta) = \mathbb{E}_{t,\mathbf{x}_0,\epsilon}\left[||\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)||^2\right]}$

(Ho, Jain, and Abbeel 2020)

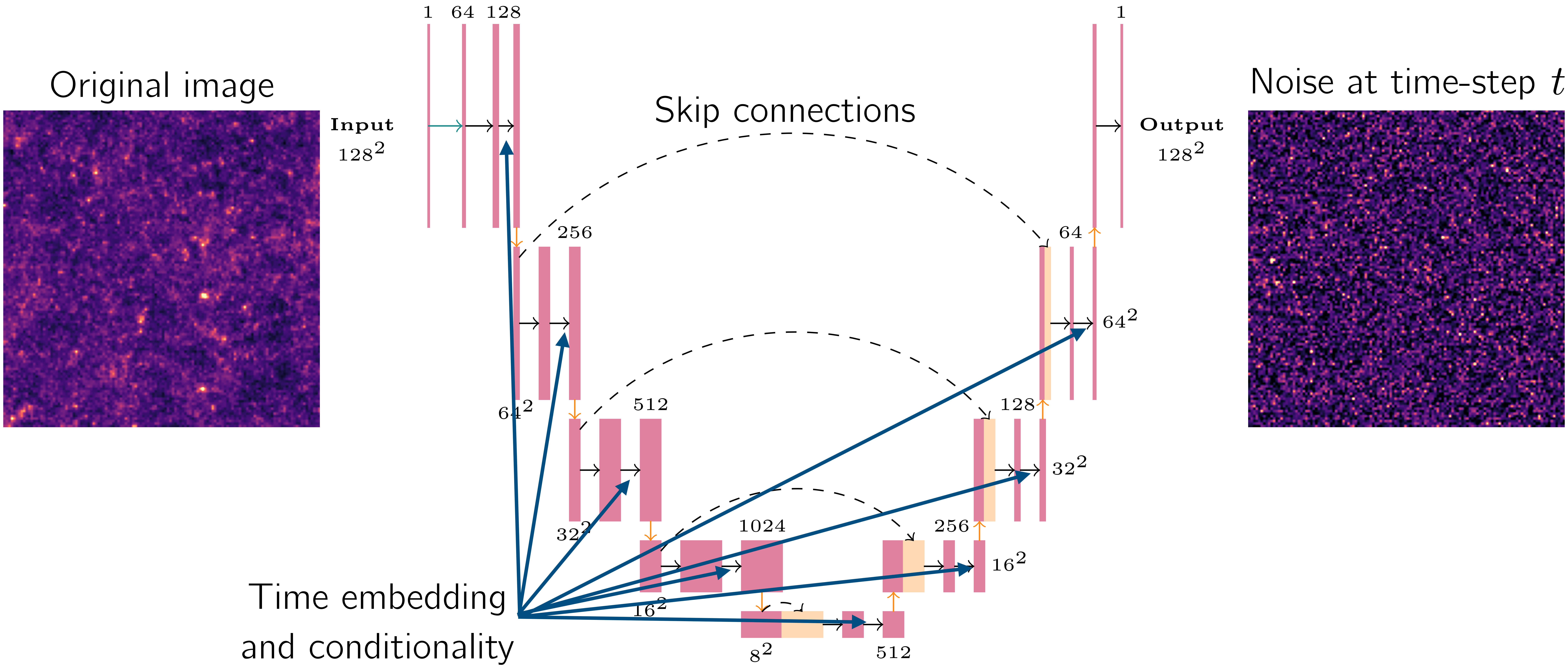
Neural Networks: DDPM

Architecture



Neural Networks: DDPM

UNet



Denoising Diffusion Probabilistic Models

Ancestral sampling

Sampling Algorithm:

Call model

1. Sample noise $\boldsymbol{x}_T \sim \mathcal{N}(0,1)$

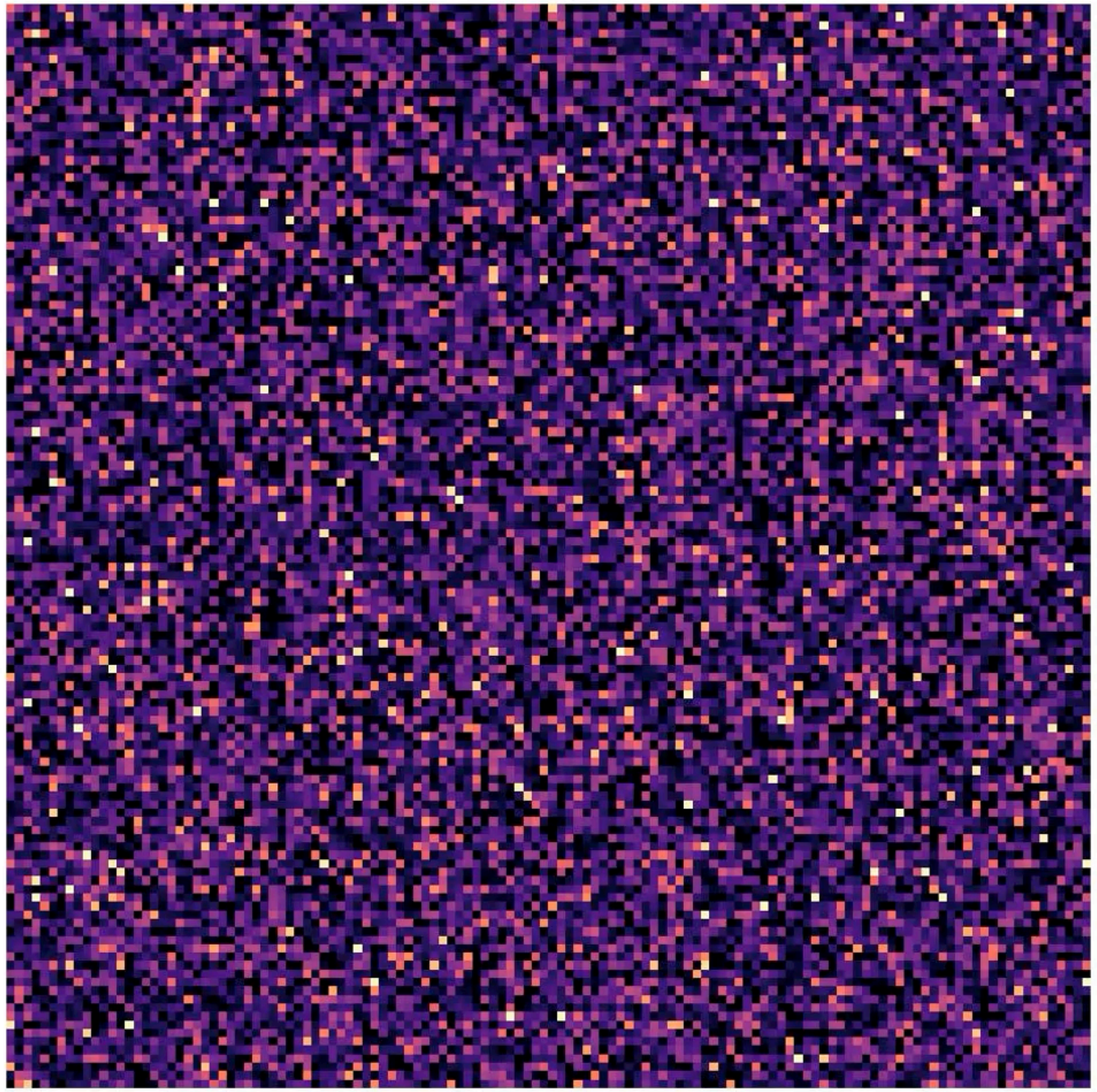
2. for each time-step $t = T, \ldots, 1$ do

$$\boldsymbol{x}_{t-1} = \frac{1}{\sqrt{\bar{\alpha}}}(\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\boldsymbol{x}_t, t))$$

   if $t > 1$ do $\boldsymbol{x}_{t-1} = \boldsymbol{x}_{t-1} + \sqrt{\tilde{\beta}_t}\boldsymbol{z}$ where $\boldsymbol{z} \sim \mathcal{N}(0,1)$

3. Return denoised image $\boldsymbol{x}_0$

$t = 1995$



(Ho, Jain, and Abbeel 2020)

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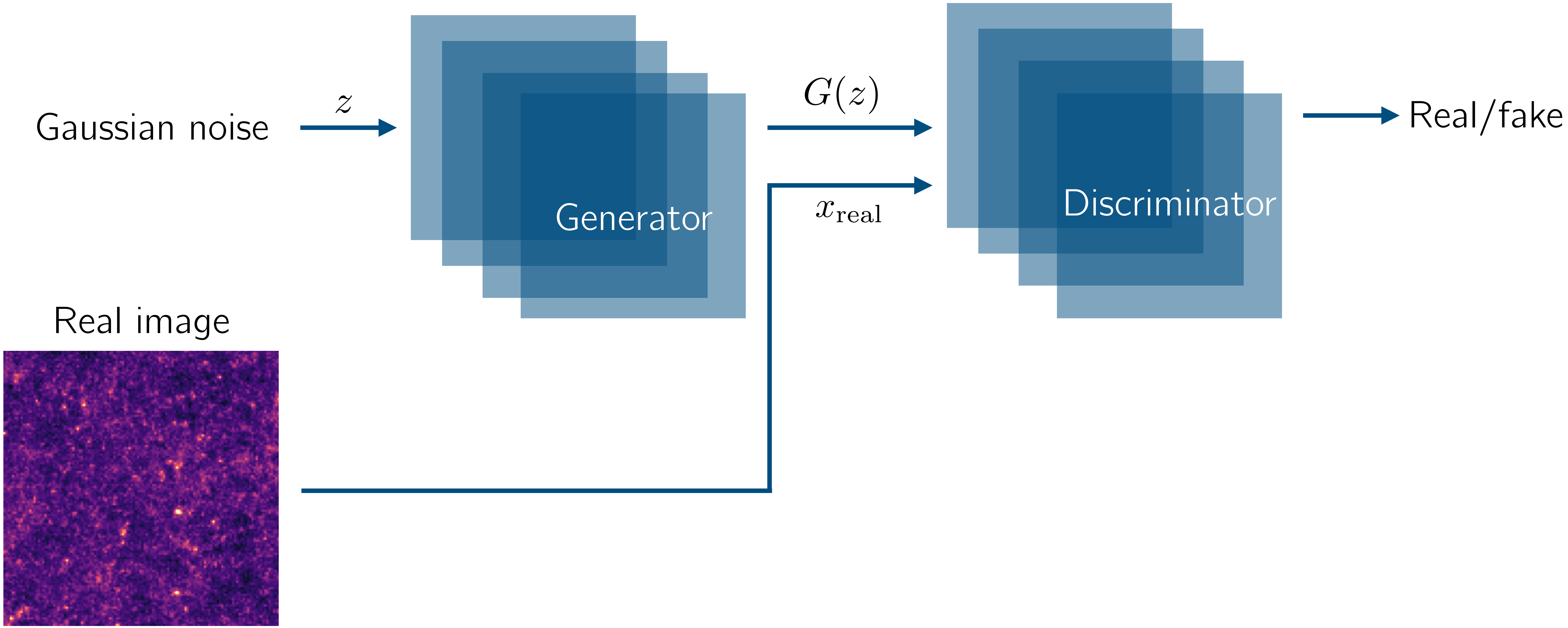
Generative Adversarial Network

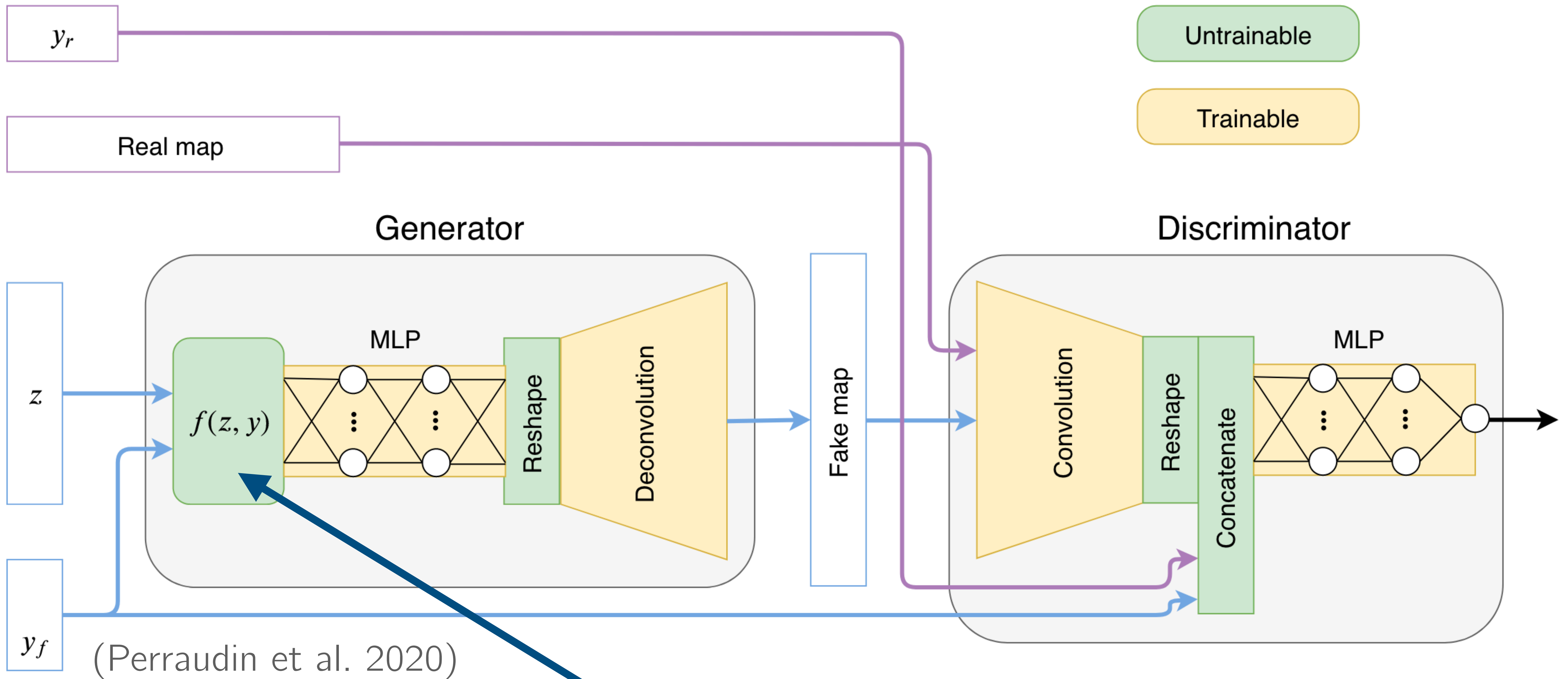
Architecture



Neural Networks: CWGAN

Architecture

Conditioning parameters



(Perraudin et al. 2020)

Loss Function:

Wasserstein loss function to combat mode collapse

Conditioning Function:

$$\hat{z} = f(z, y) = \left(l_0 + \frac{l_1 - l_0}{b - a}(y - a) \right) \frac{z}{\|z\|_2}$$

DDPM vs. CWGAN

Differences

GAN

+ high quality image generation

- hard to train

- mode collapse

+ fast sampling

- requires a lot of training data

DDPM

+ high quality image generation

+ easy training

+ no mode collapse

- slow sampling speed

+ more faithful to data

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Training Data

Convergence maps

N-Body simulations:

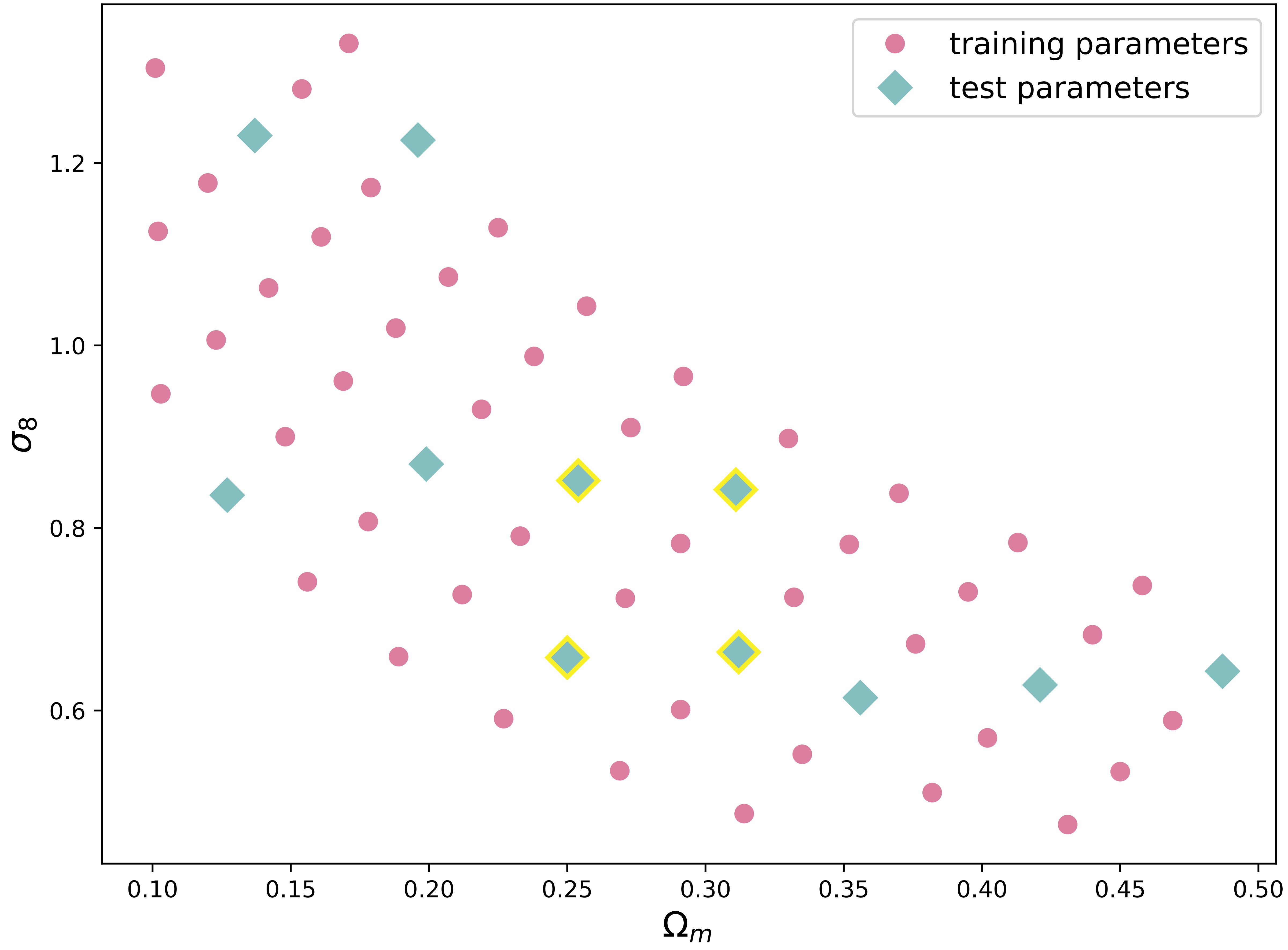
- PKDGrav3
- flat LambdaCDM universe
- 57 cosmologies: $\Omega_m,\ \sigma_8$

Convergence maps:

- 3D particle boxes to 2D convergence maps
- UFalcon

Training data:

- 46 training and 11 test cosmologies



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Results

Best Checkpoint

Preprocessing:

Standardised $\mathcal{N}(0,1)$

Beta scheduler:

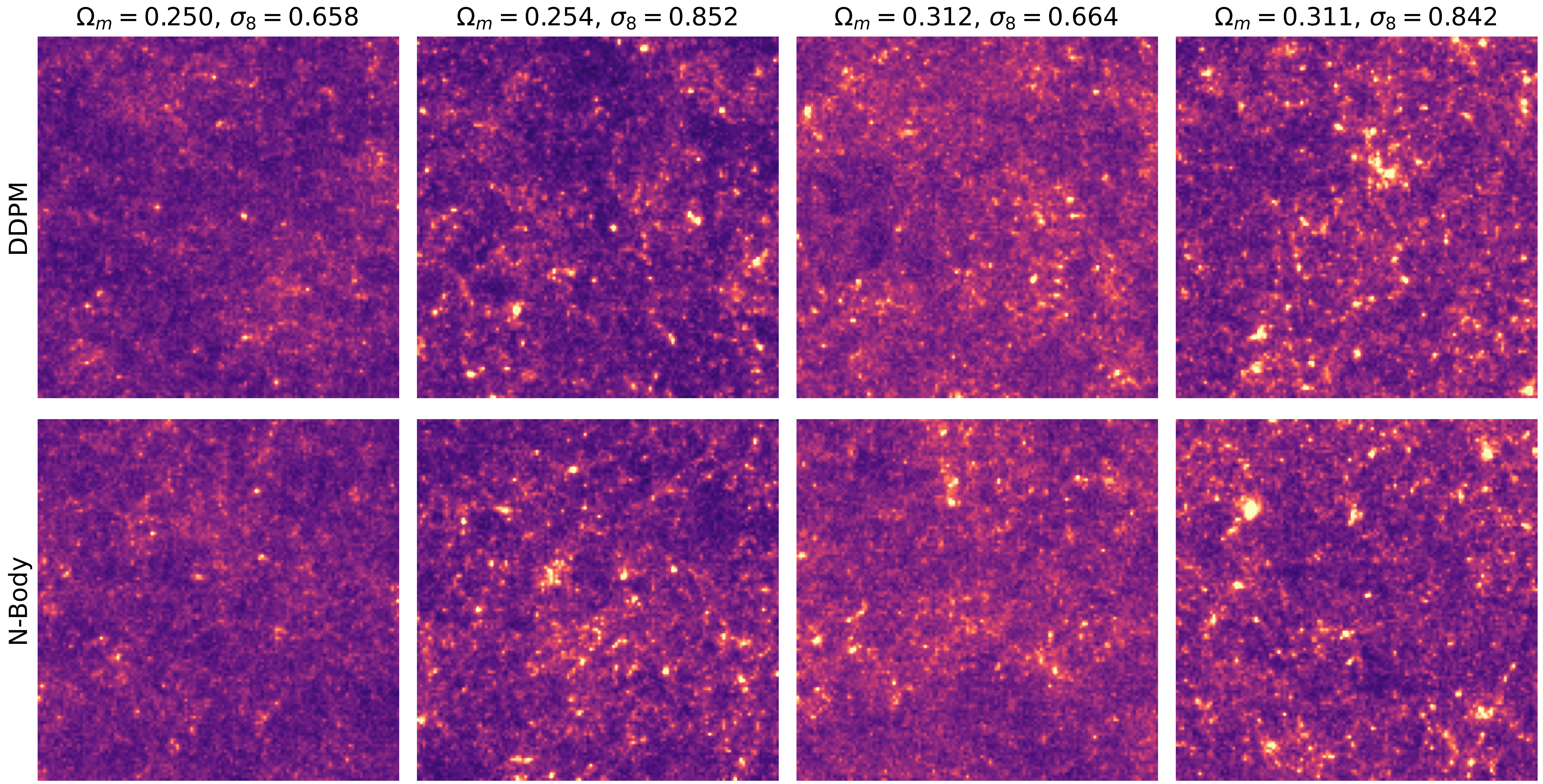
Linear beta scheduler:

$T = 2000,\ \beta_0 = 0.01,\ \beta_T = 0.00005$

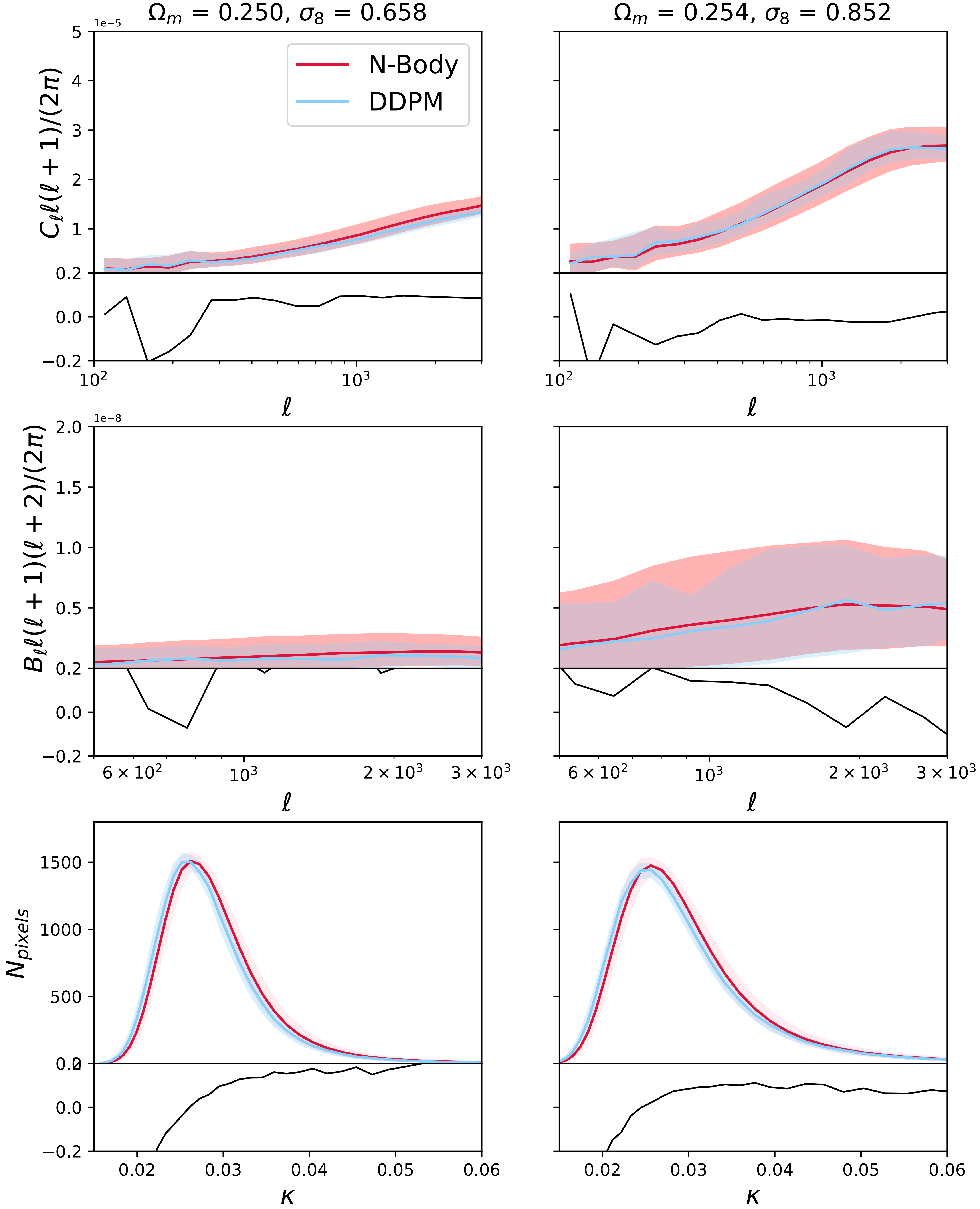
Architecture:

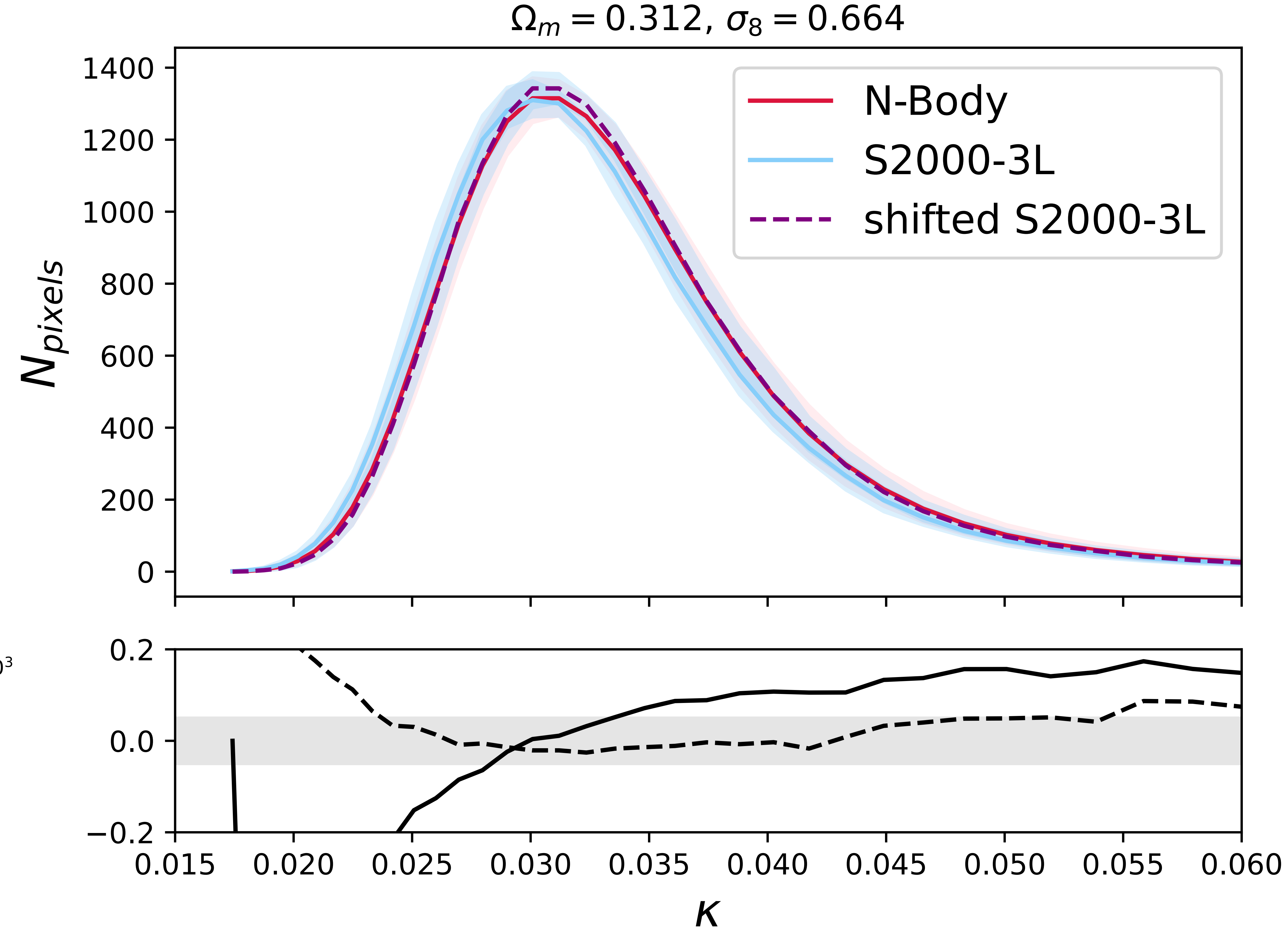
3 UNet layers

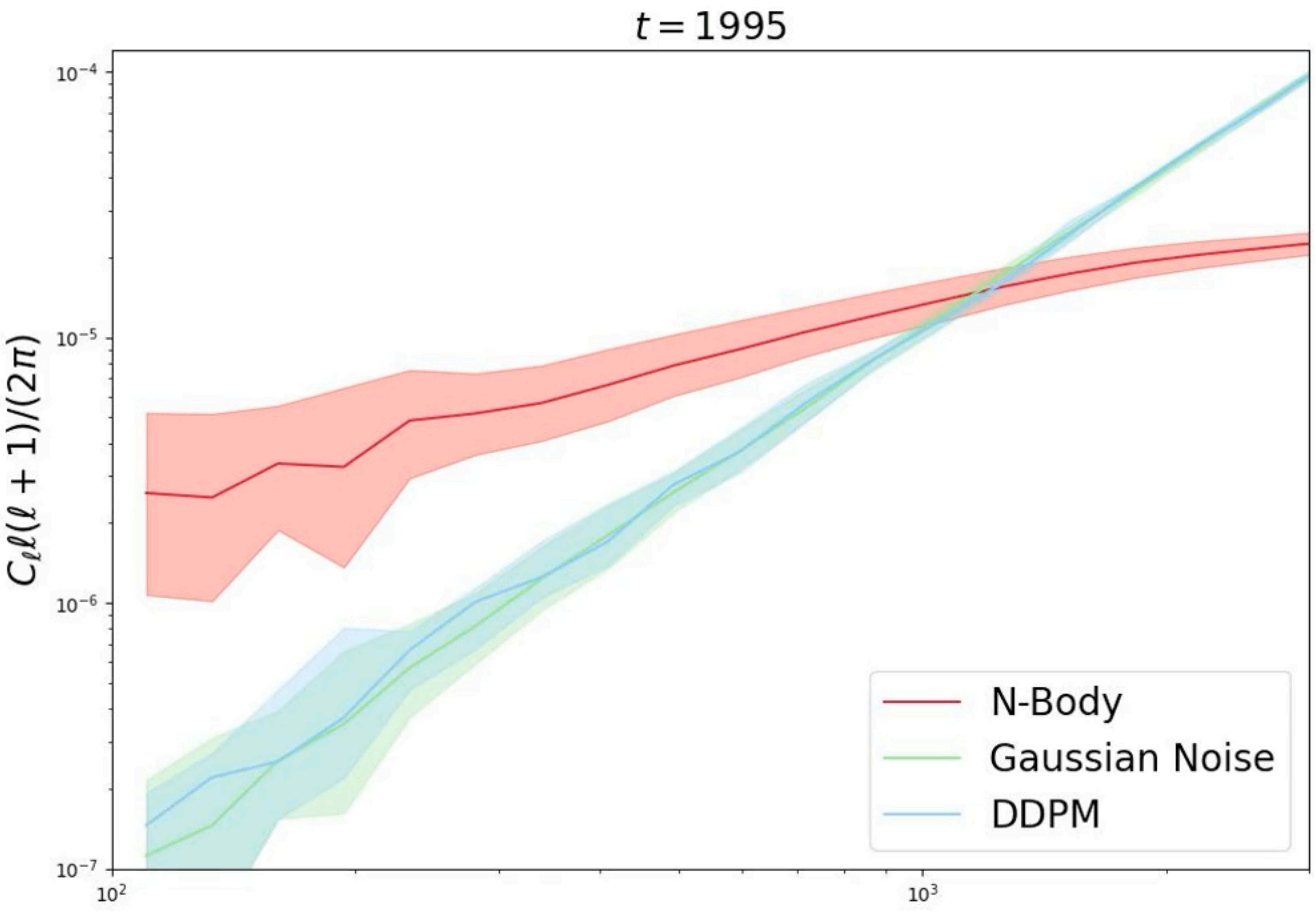
Test cosmologies

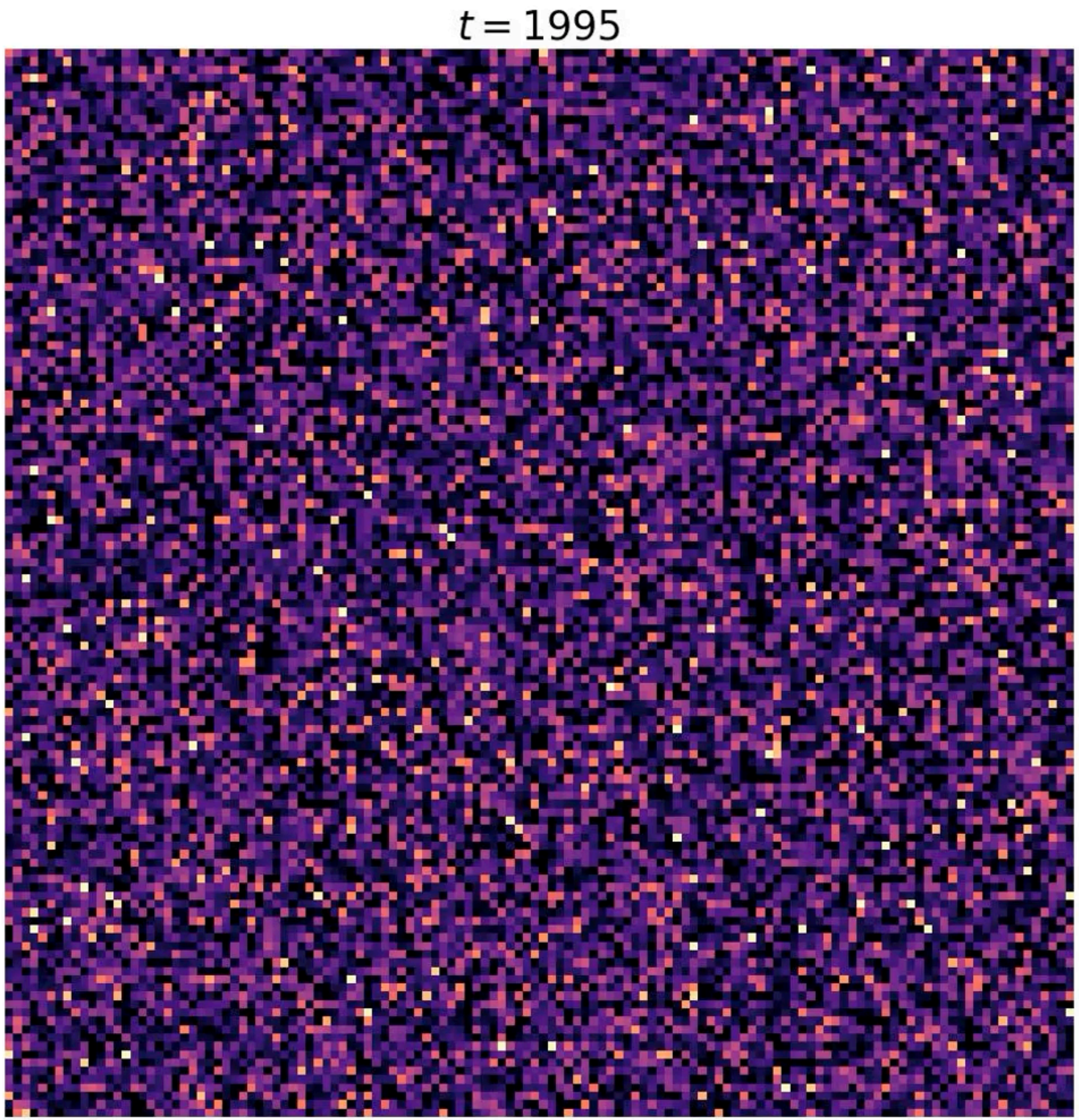


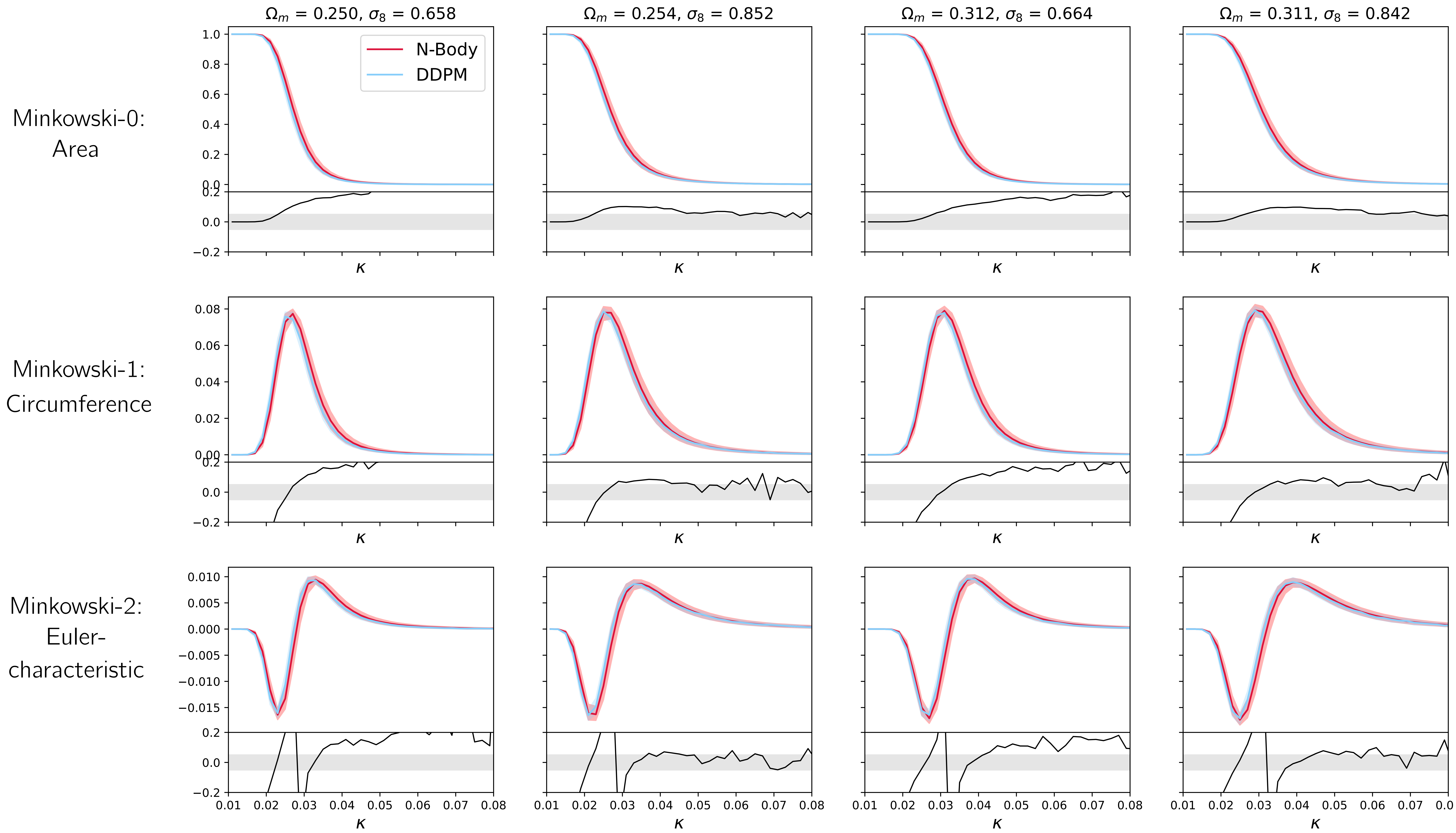
Summary Statistics



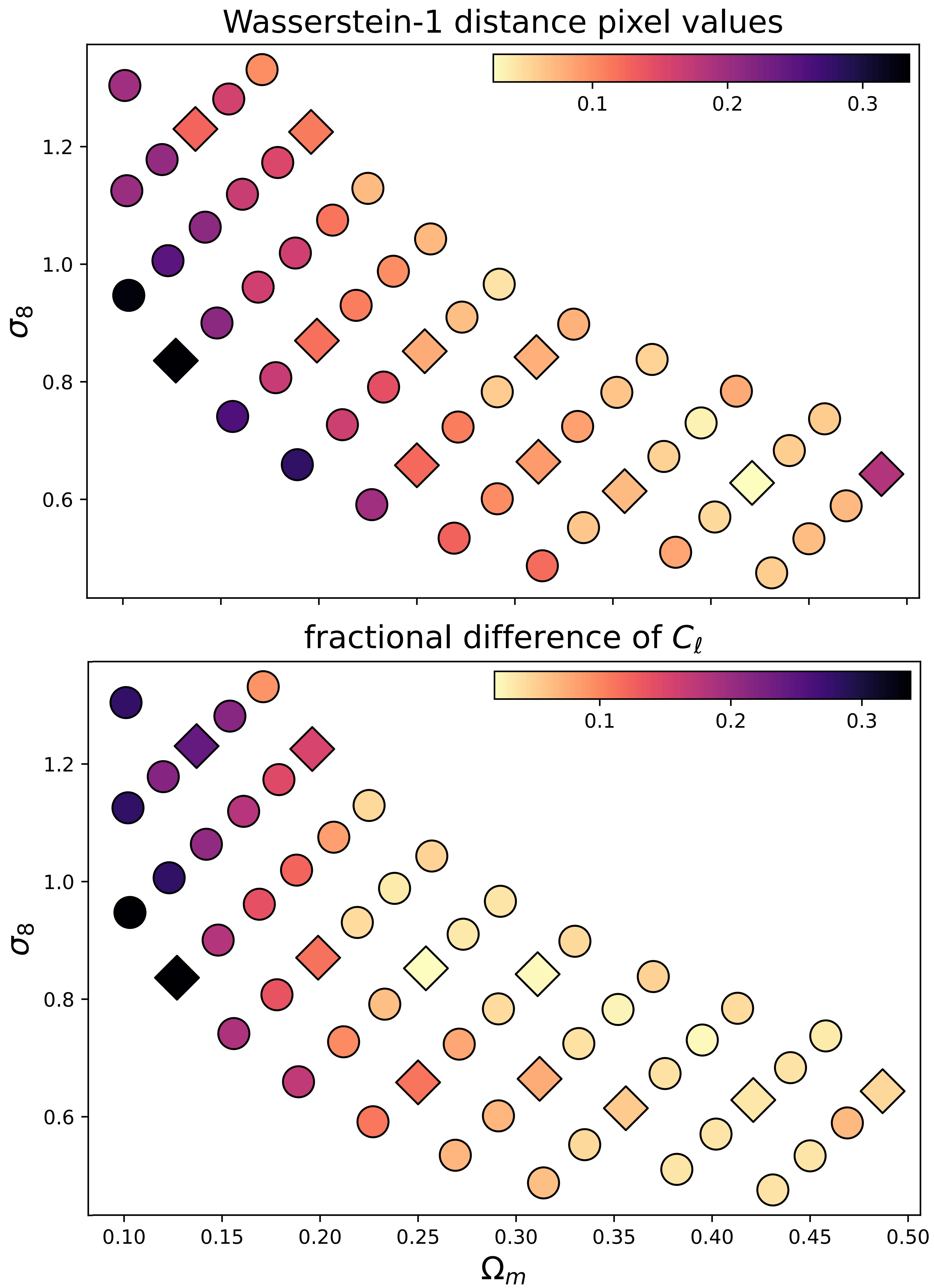


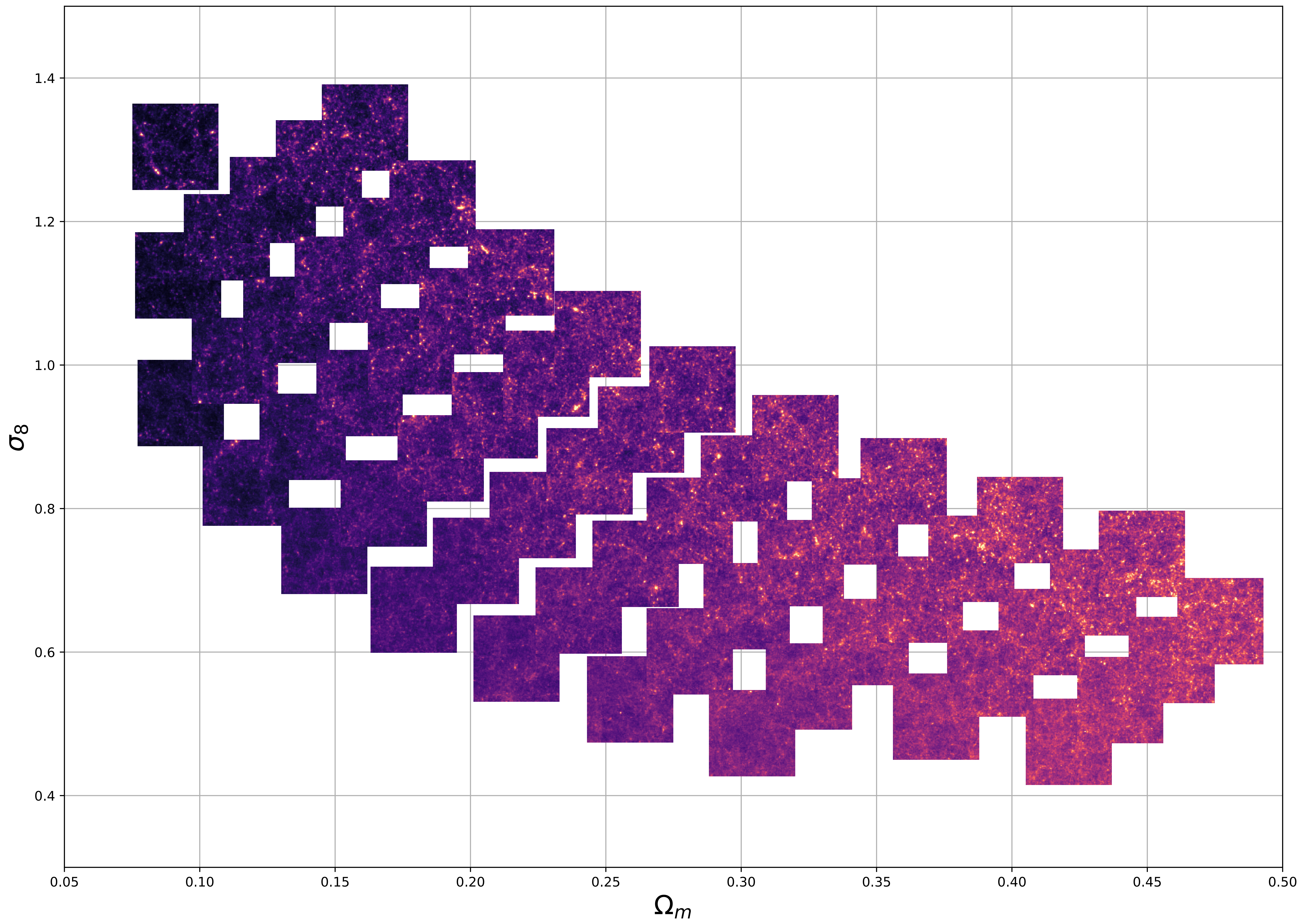

$t = 1995$
10^{-4}
10^{-5}
10^{-6}
10^{-7}
$C_\ell \ell(\ell+1)/(2\pi)$
10^2
10^3
N-Body
Gaussian Noise
DDPM


$t = 1995$



Ω_m = 0.250, σ_8 = 0.658
Ω_m = 0.254, σ_8 = 0.852
Ω_m = 0.312, σ_8 = 0.664
Ω_m = 0.311, σ_8 = 0.842
N-Body
DDPM
Minkowski-0: Area
Minkowski-1: Circumference
Minkowski-2: Euler-characteristic
κ


Wasserstein-1 distance pixel values
0.1
0.2
0.3
1.2
1.0
0.8
0.6
σ_8
fractional difference of C_ℓ
0.1
0.2
0.3
1.2
1.0
0.8
0.6
σ_8
0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50
Ω_m


1.4
1.2
1.0
0.8
0.6
0.4
σ_8
0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50
Ω_m

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Hyper-parameters

Preprocessing, beta-scheduler, architecture

Preprocessing:

Standardised $\mathcal{N}(0,1)$

Scaled $\in [-1,1]$

Beta scheduler:

Linear beta scheduler:

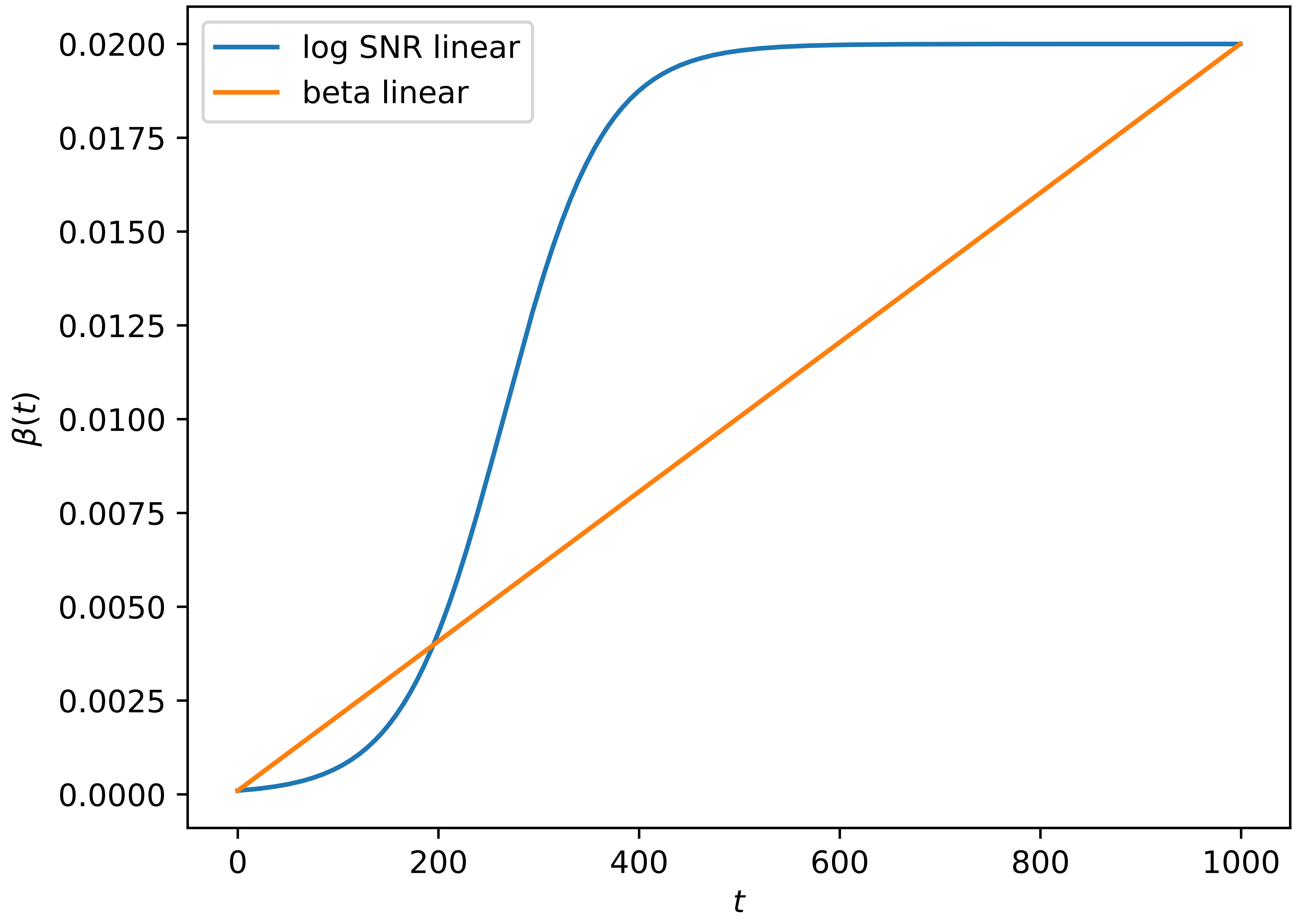
$$T = 1000,\ \beta_0 = 0.02,\ \beta_T = 0.0001$$

$$T = 2000,\ \beta_0 = 0.01,\ \beta_T = 0.00005$$

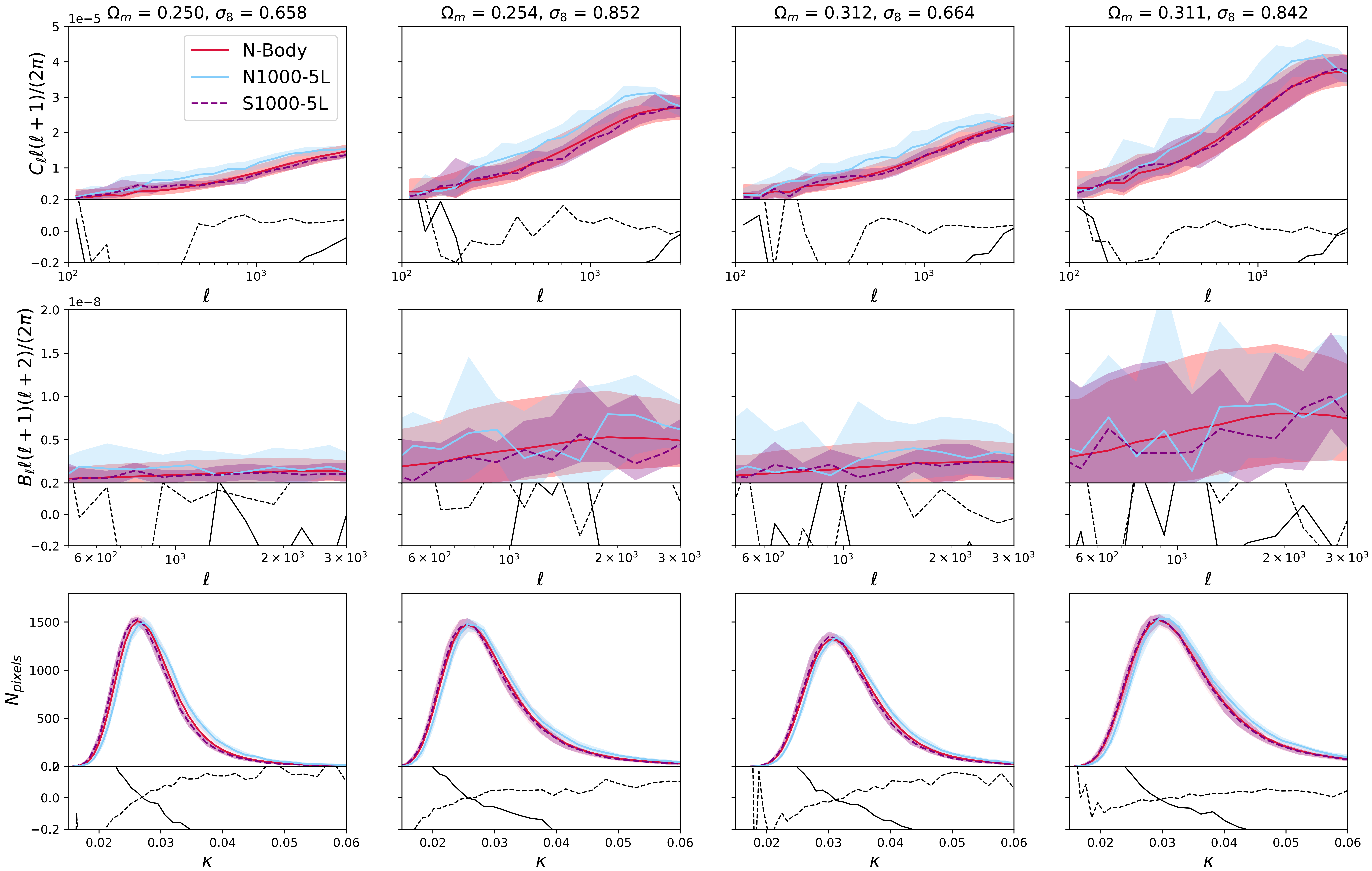
Signal-to-noise scheduler

Architecture:

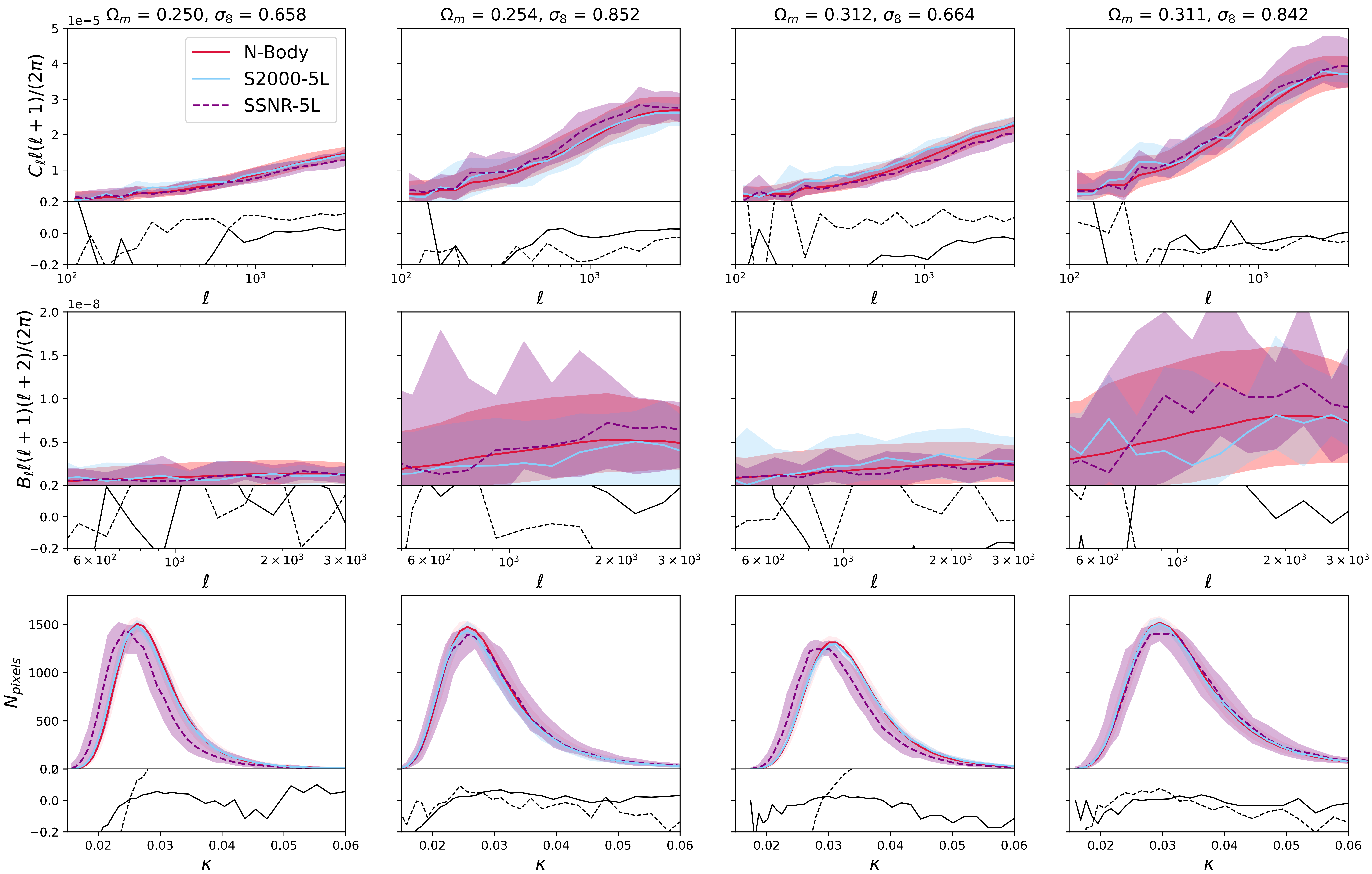
5, 4 and 3 UNet layers



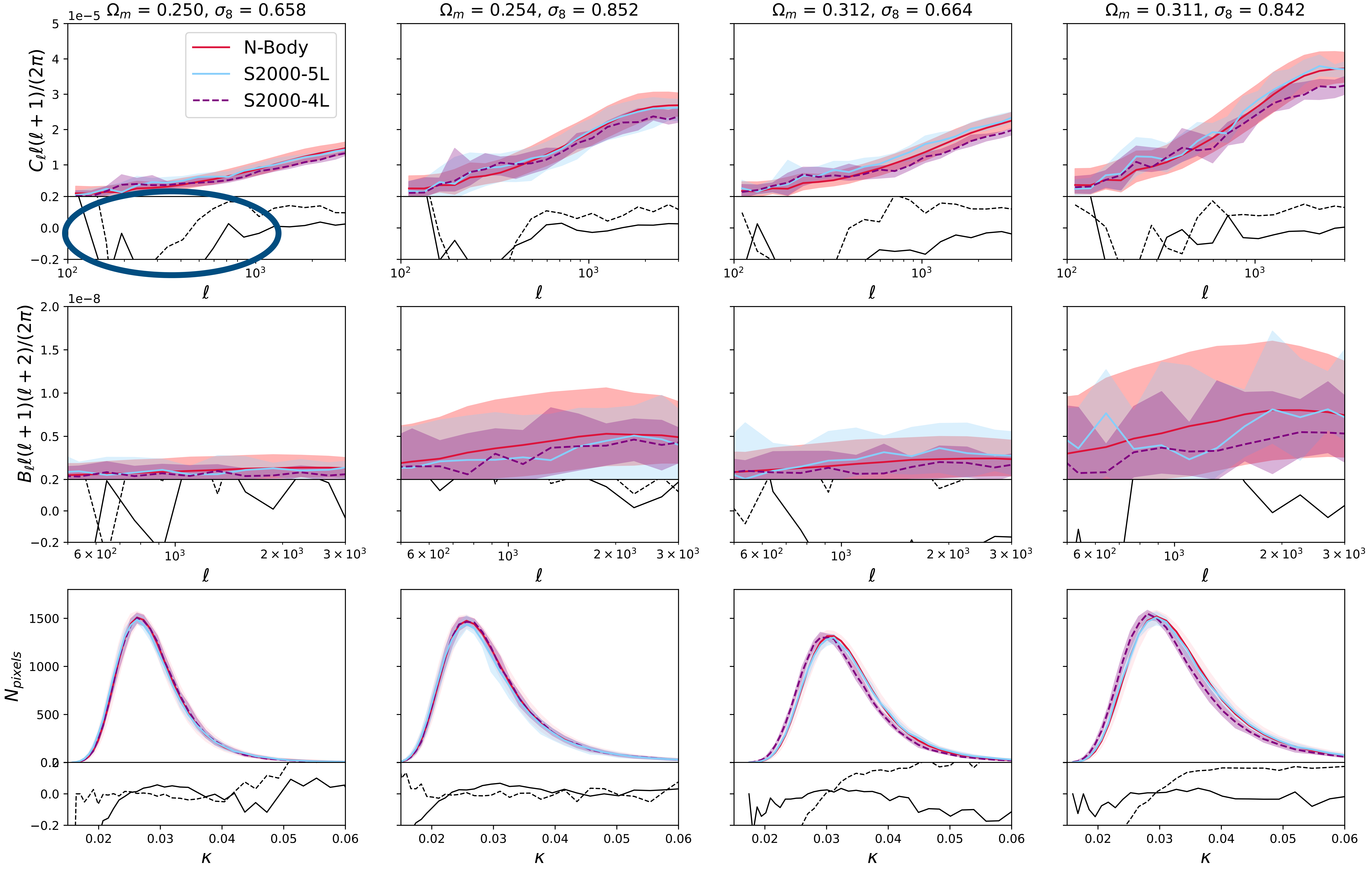
Preprocessing



Beta-Scheduler



Architecture



Results

Sampling methods

Reverse-Time SDE Sampling:

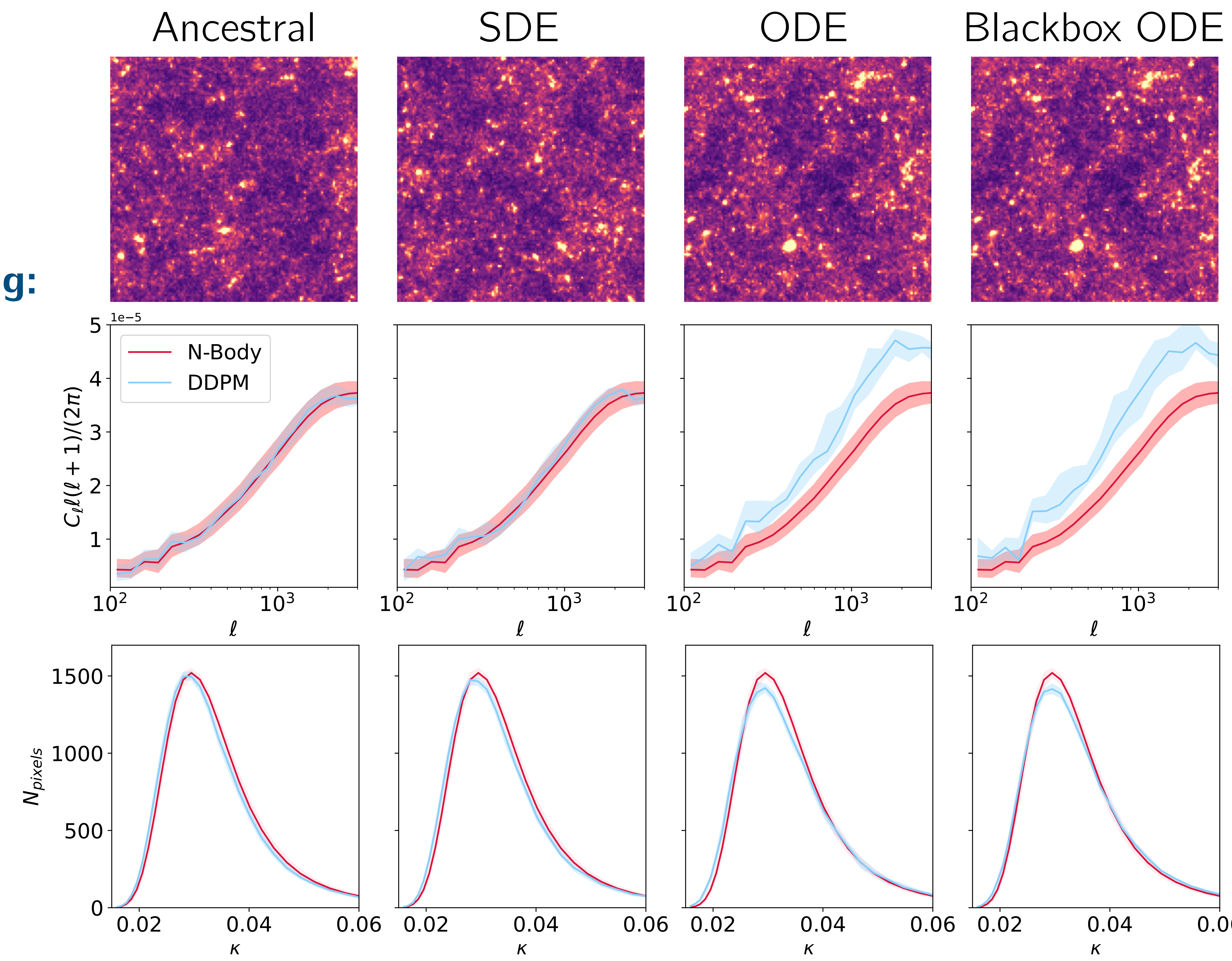
(Y. Song et al. 2021)

Iteratively solve discretised RT-SDE at each time-step

ODE Sampling:

(Y. Song et al. 2021)

Iteratively solve discretised ODE or use blackbox solver (Runge-Kutta of order 5)



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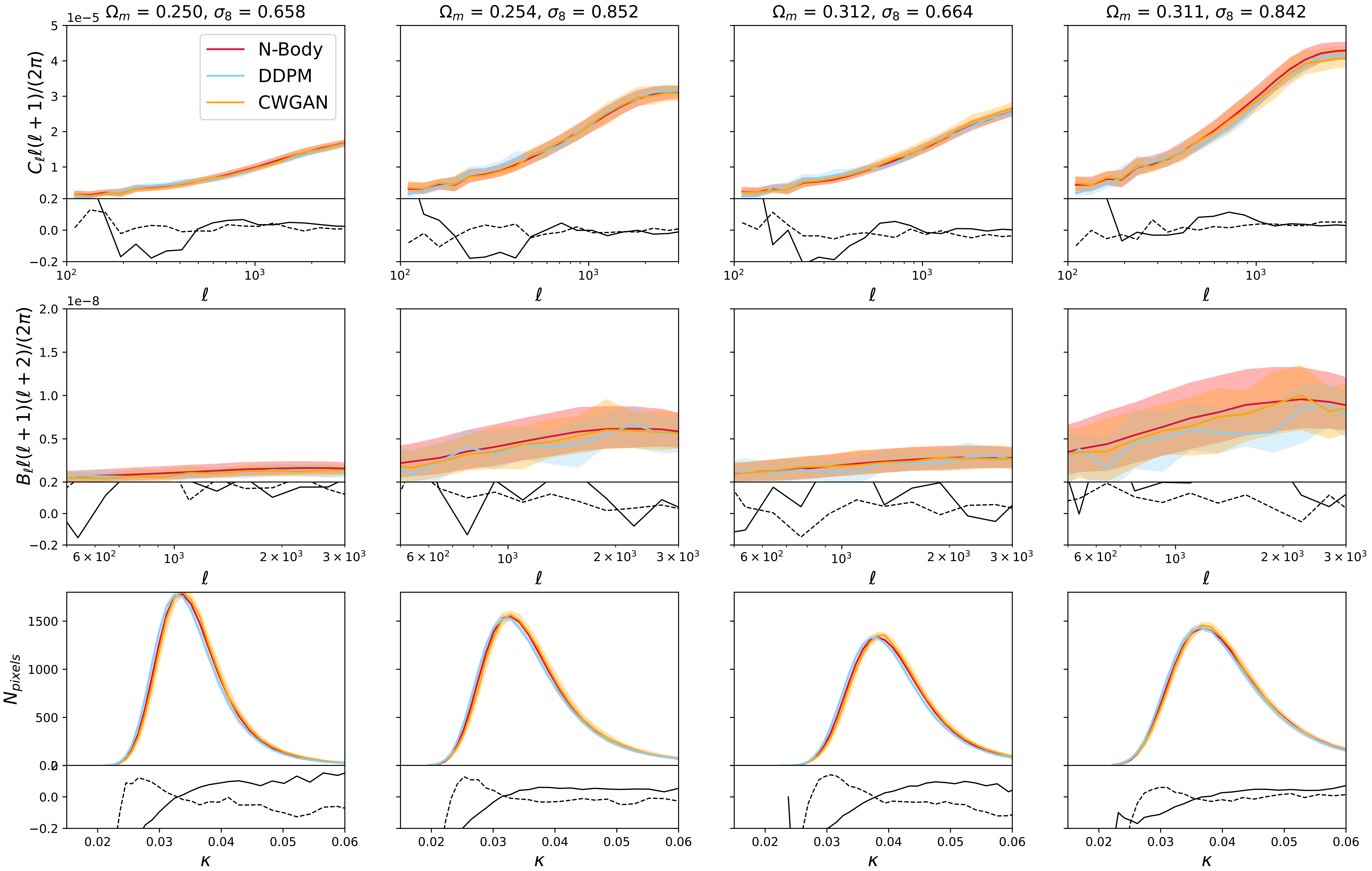
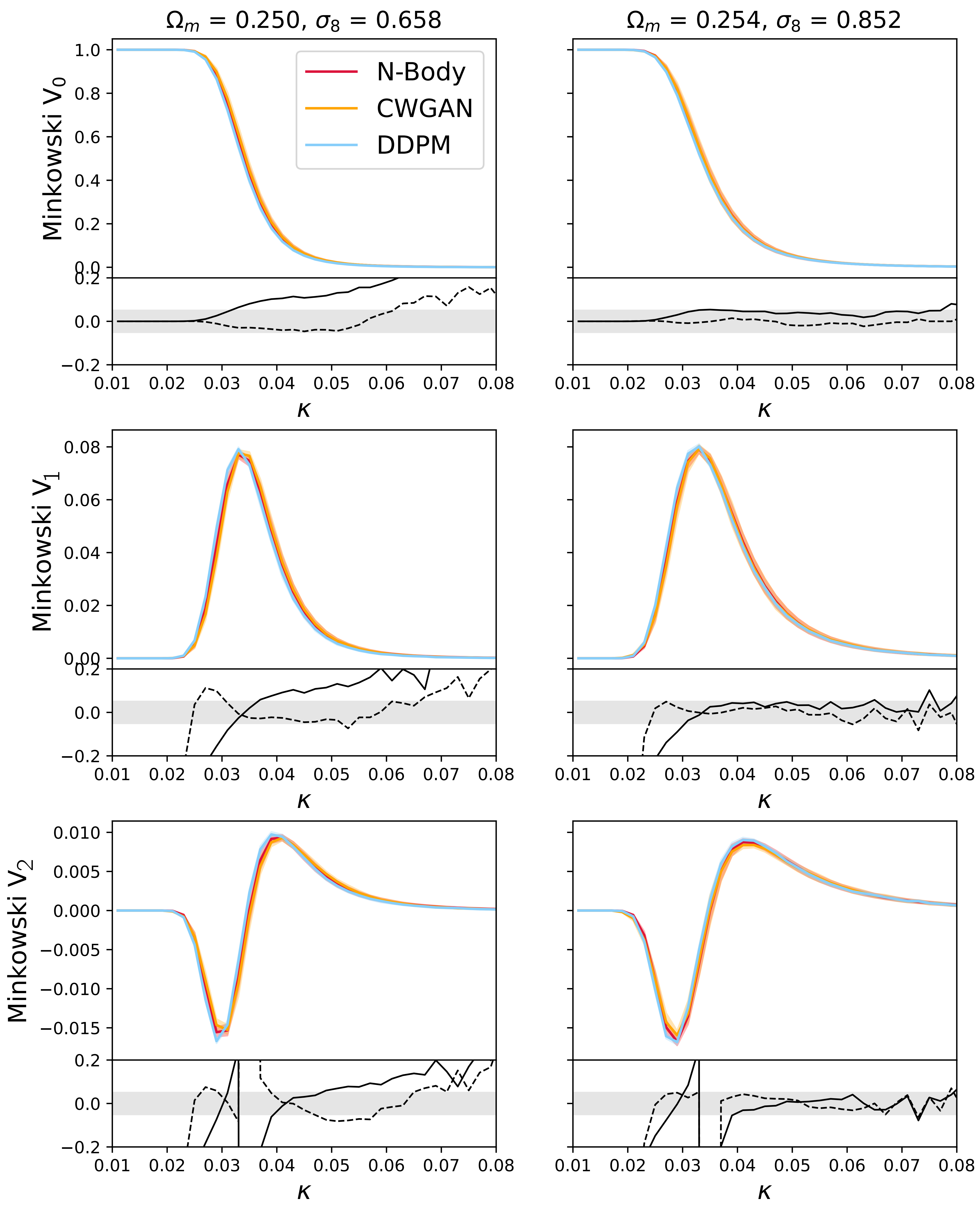
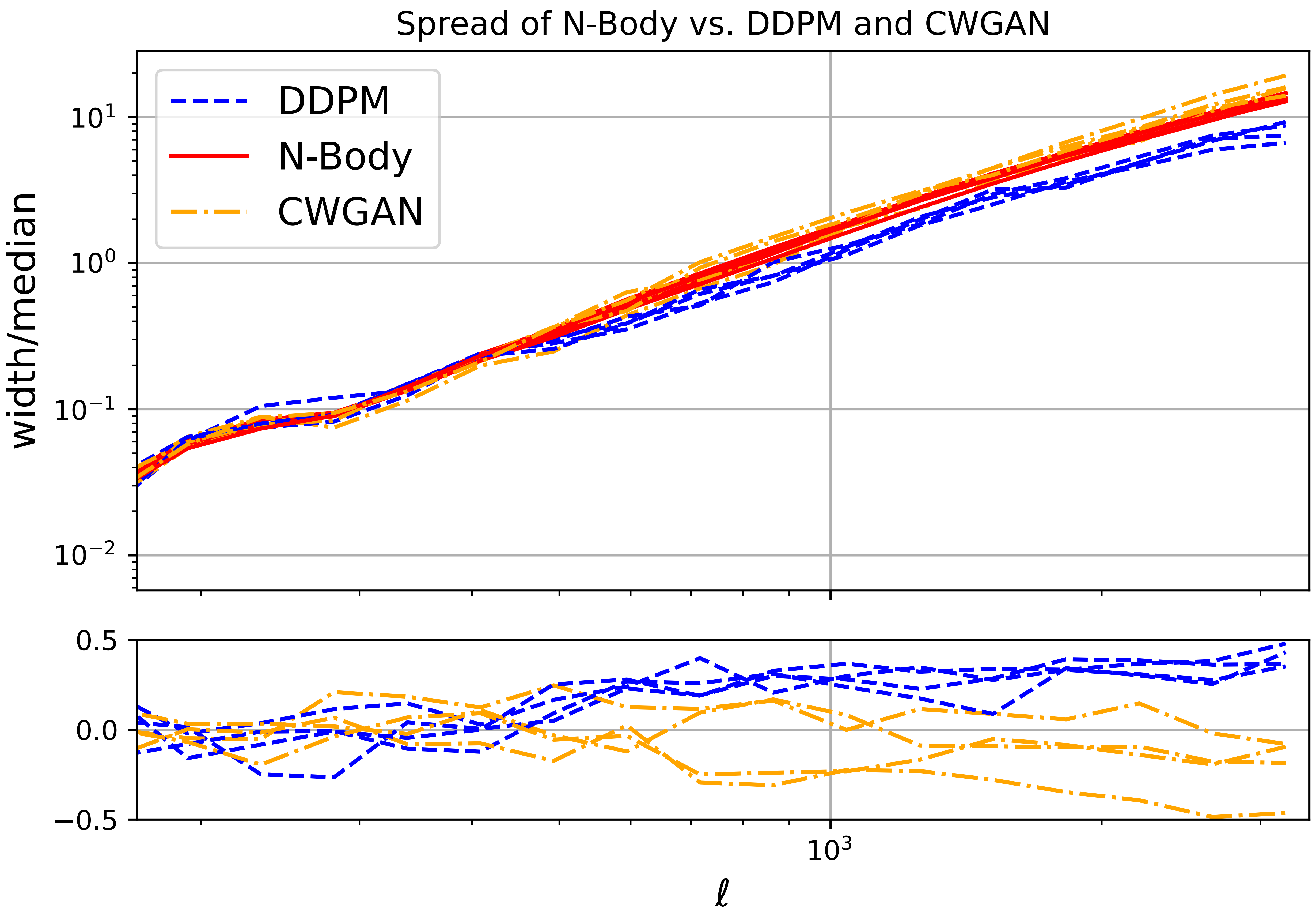




Ω_m = 0.250, σ_8 = 0.658
Ω_m = 0.254, σ_8 = 0.852
N-Body
CWGAN
DDPM
Minkowski V_0
Minkowski V_1
Minkowski V_2
κ



Spread of N-Body vs. DDPM and CWGAN
DDPM
N-Body
CWGAN
width/median
ℓ

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Conclusion

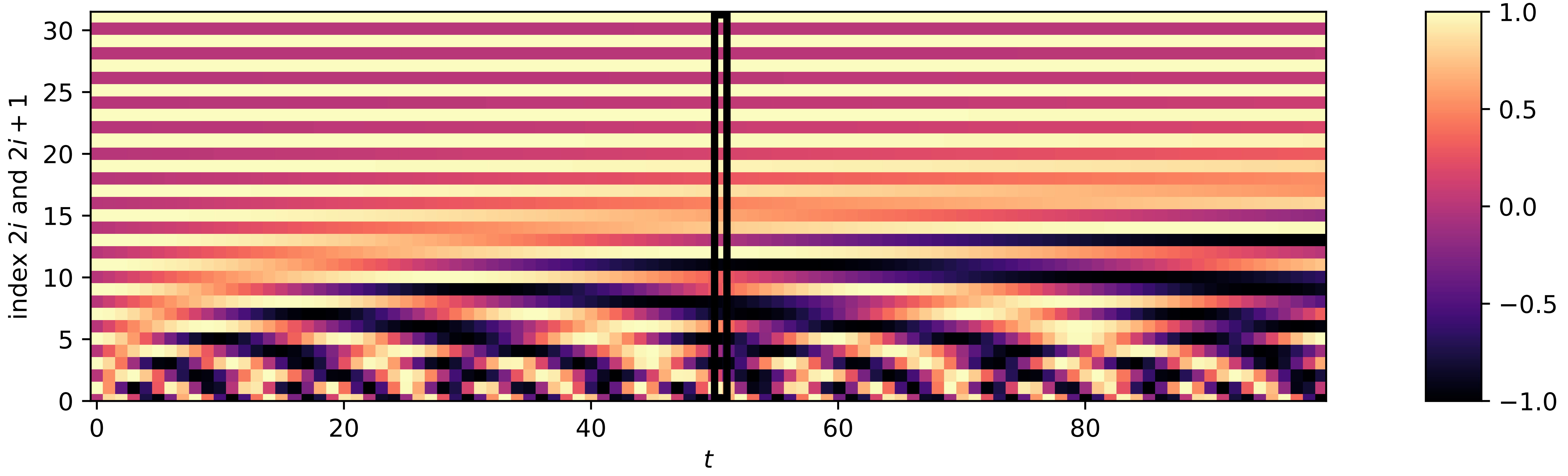
- Successfully trained a conditional DDPM to generate dark matter convergence maps
  - Linear beta scheduler, 2000 time-steps, 3 layer UNet, standardised data and ancestral sampling yield best results
  - Best results for higher matter density values
  - Large scale structure can be improved
- Slightly outperformed by CWGAN
  - With more time to fine-tune the DDPM could surpass the CWGAN

Neural Networks: DDPM

Sinusoidal position embedding

$$PE(\mathrm{t}, 2i) = \sin\left(\frac{\mathrm{t}}{n^{2i/d}}\right)$$

$$PE(\mathrm{t}, 2i+1) = \cos\left(\frac{\mathrm{t}}{n^{2i/d}}\right)$$



→ Encode each time-step onto a unique sinusoidal wave

→ Network learns relative position of one time-step to another