Conditional Normalizing Flow for Lattice Field Theory

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INTRODUCTION

Quantum Field Theory describes physical world at the smallest scales.

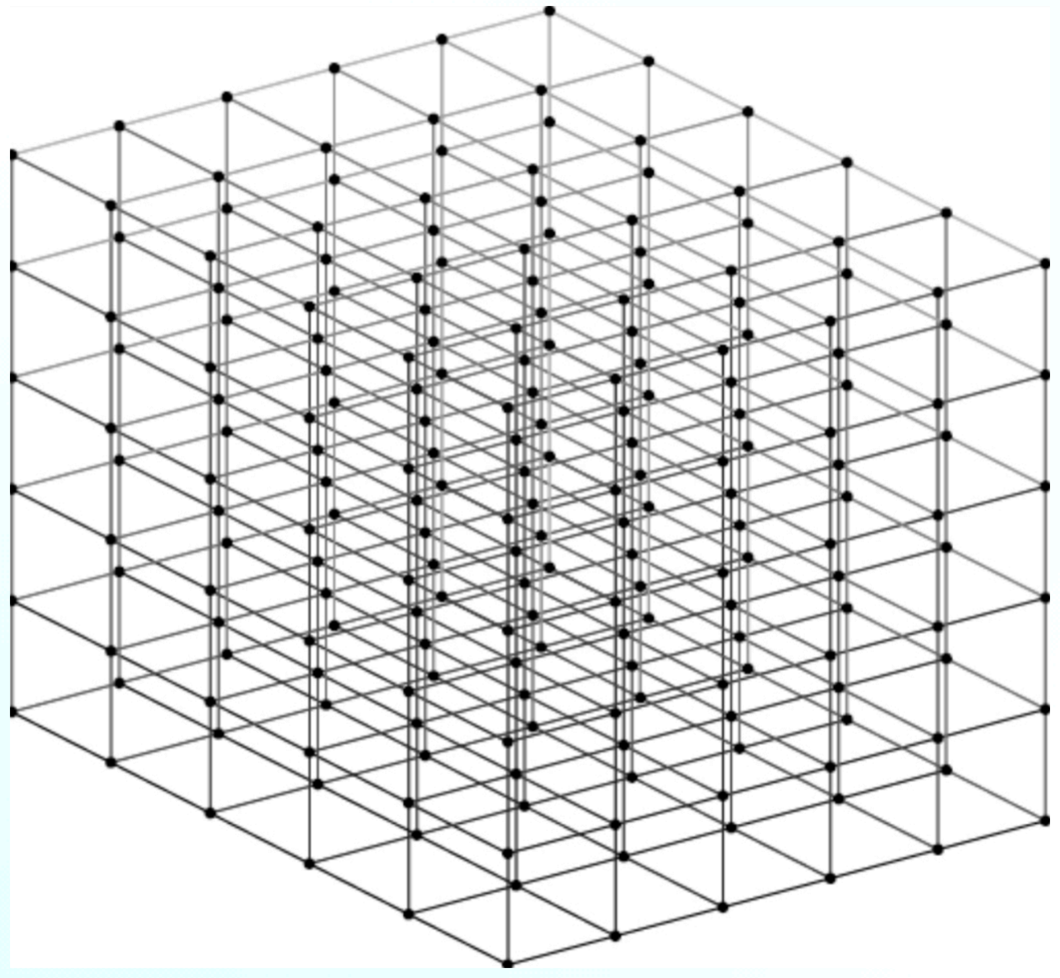
Theory: defined by Action or Lagrangian ;

$$\mathscr{L}(\phi, g_i)$$

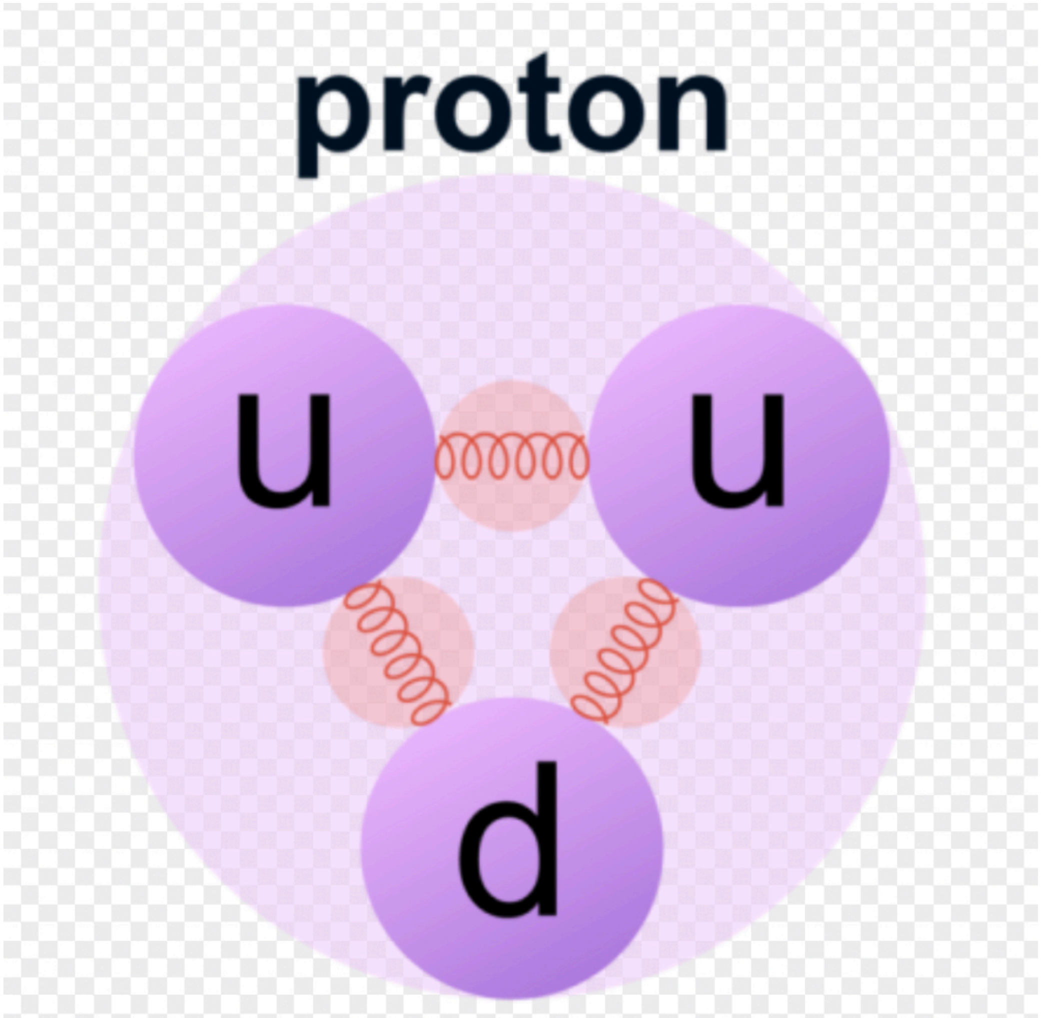
Strong Coupling → **Lattice Field Theory**

Weak Coupling → **Perturbative Methods**

Discrete space time



Computational approach → **QCD: Strong Interaction**



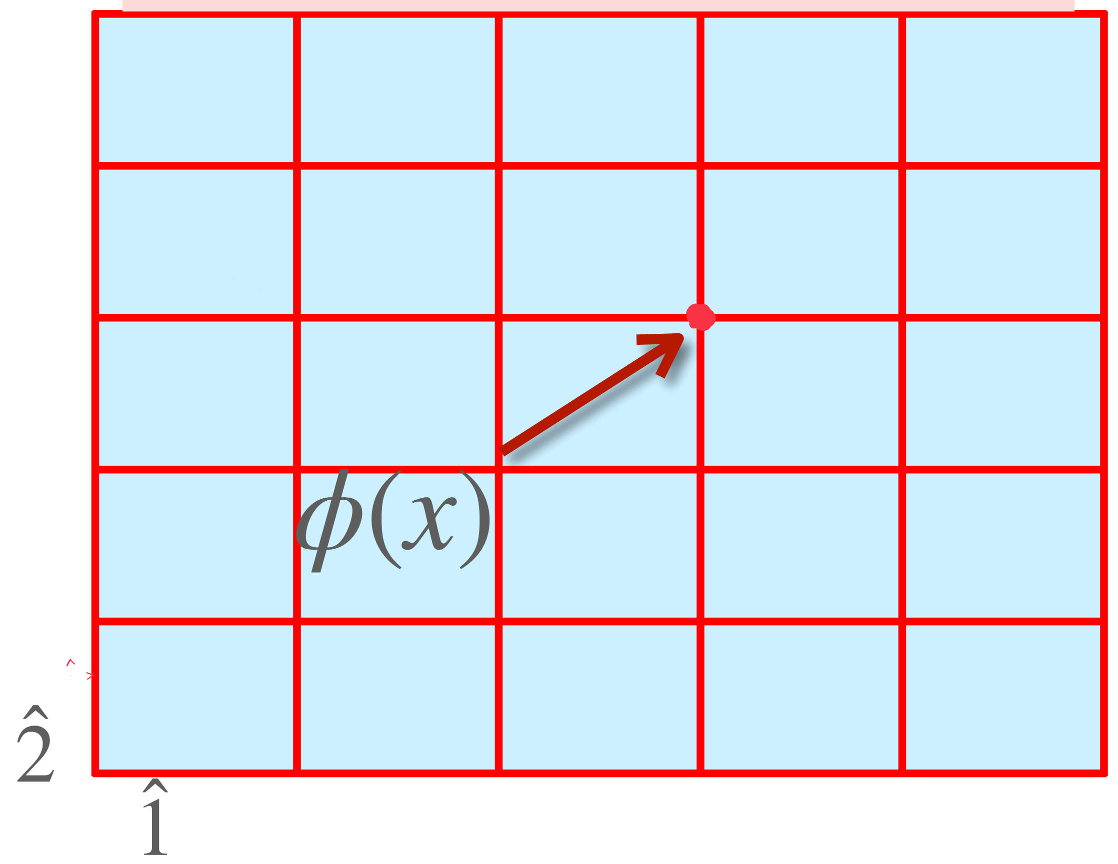
Scalar Lattice Field Theory

Discretized lattice Action:

$$S[\phi, m, \lambda] = \sum_{x} \sum_{\mu=1,2} [(2+m)\phi^2(x) - \phi(x)\phi(x+a\hat{\mu}) - \phi(x)\phi(x-a\hat{\mu}) + \lambda\phi^4(x)]$$

where, m and λ are the parameters of the theory.

2d Lattice



$$x \rightarrow (x_1\hat{\mu}, x_2\hat{\nu})$$

Observable:

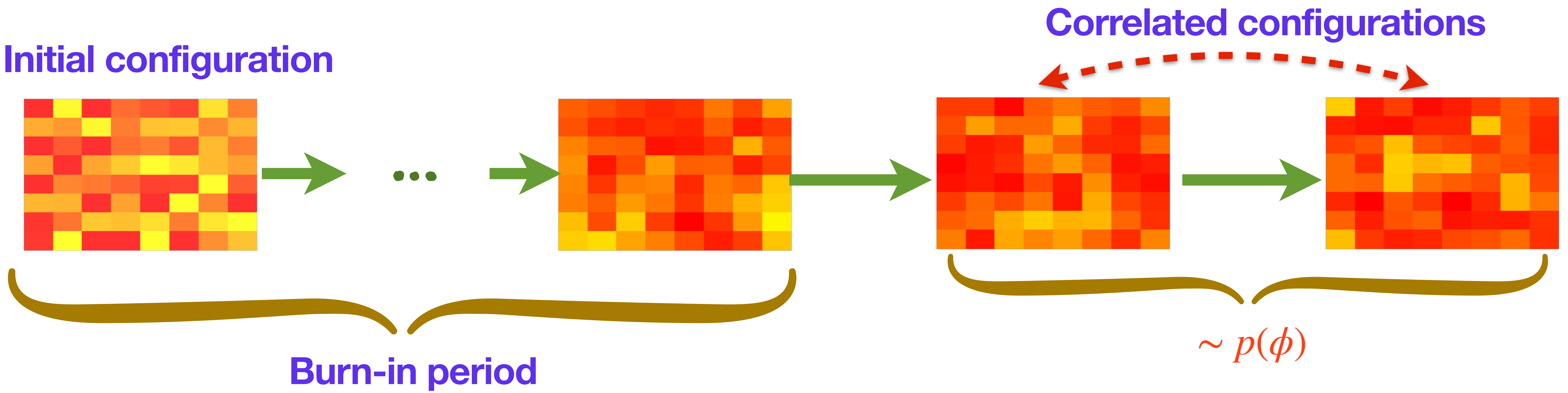
$$\langle O \rangle = \sum_{\phi_i} O(\phi_i) \frac{e^{-S(\phi_i)}}{Z} \rightarrow P(\phi_i)$$

Lattice Field Theory → **Sampling Task**

Distribution

$$P(\phi) = \frac{e^{-S(\phi)}}{Z}$$

MCMC & Critical Slowing Down (CSD)

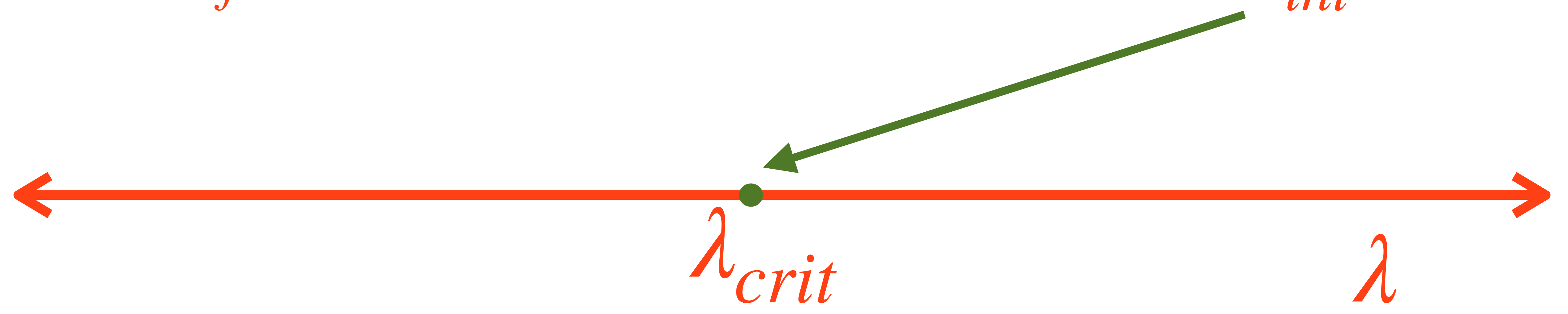


Integrated autocorrelation time:

$$\tau_{int} = \frac{1}{2} + \lim_{\tau \to \infty} \sum_{\tau=1}^{\tau_{max}} \frac{\rho(\tau)}{\rho(0)}$$

For a lattice action : $S(\phi, m_{fixed}, \lambda)$

τ_{int} **Divergent, CSD dominates**



ML based methods for Sampling

- **Generative Adversarial Network (GAN):**
  - Learns a distribution from training samples and generates new unseen data.
  - Can not estimates the density explicitly.

- **Normalizing Flow (NF):**
  - Learns a distribution without any samples as well as with training samples and generates new unseen data.
  - We can estimates the density explicitly.

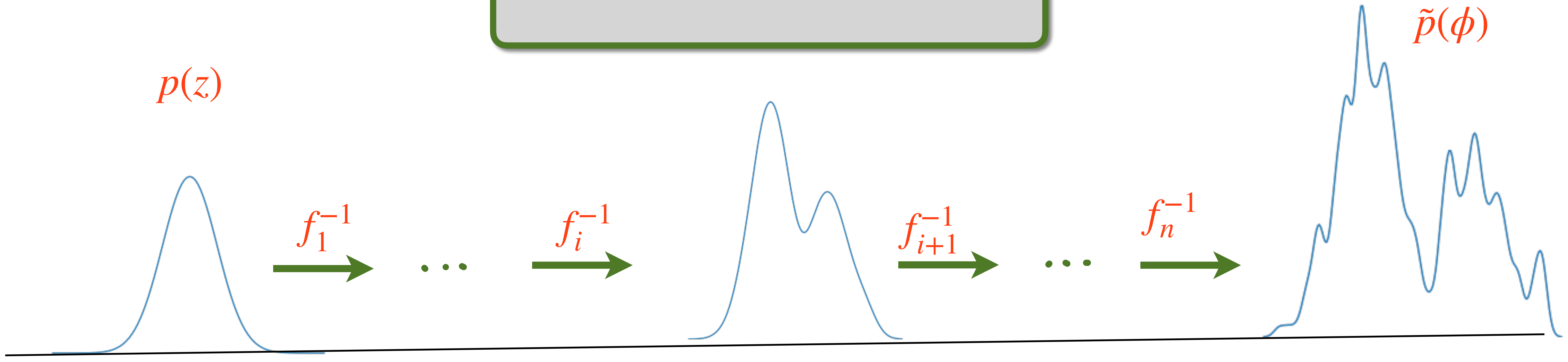
Normalising Flow

$$\phi = f^{-1}(z)$$

Prior distribution: $p(z)$

$$\tilde{p}(\phi) = \left| det \frac{f^{-1}(z)}{\partial z} \right| p(z)$$

Target distribution: $p(\phi)$



$f_i^{-1} \longrightarrow$ **Neural Network**

$\tilde{p}(\phi) \longrightarrow \tilde{p}(\phi;\theta)$

Optimise model so that:
$$\tilde{p}(\phi;\theta) \approx p(\phi)$$

Normalising Flow

Training the NF model can done by minimizing the KL divergence between the $\tilde{p}(\phi;\theta)$ and $p(\phi)$.

- **Forward KL:**

$$\mathscr{L}_R = D_{KL}\big(p(\phi)\,||\,\tilde{p}(\phi;\theta)\big)\,.$$

Require training samples from $p(\phi)$

- **Reverse KL:**

$$\mathscr{L}_F = D_{KL}\big(\tilde{p}(\phi;\theta)\,||\,p(\phi)\big)\,.$$

Require samples from $\tilde{p}(\phi;\theta)$

Application to lattice phi4 theory

Phi4 theory: m **and** λ **fixed** .

$$S[\phi, m, \lambda] = \sum_{x} \sum_{\mu=1,2} [(2+m)\phi^2(x) - \phi(x)\phi(x+a\hat{\mu}) - \phi(x)\phi(x-a\hat{\mu}) + \lambda\phi^4(x)]$$

Generates training data from HMC simulation → **10000 lattice configurations**

✓ **Training the model**

$$z = f(\phi; \theta_{opt})$$

✓ **Generation of lattices**

$$\phi = f^{-1}(z)$$

z **can be easily sampled**

Metropolis-Hastings

Samples from the NF model $\tilde{p}(\phi;\theta)$ cannot be considered for observable calculation.

Cause: → Biases in observable.

We use the samples from NF model as proposal to construct a Markov chain.

Metropolis-Hastings step:

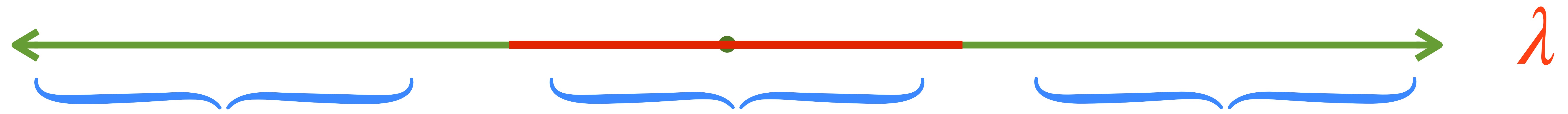
$$A(\phi^{i-1}, \phi') = min\Big(1, \frac{\tilde{p}(\phi^{(i-1)})p(\phi')}{p(\phi^{(i-1)})\tilde{p}(\phi')}\Big)$$

Provides the exactness of the distribution.

Simulation at multiple λ values

For a lattice action : $S(\phi, m_{fixed}, \lambda)$ → $p(\phi\,|\,\lambda_i)$

action parameter



Non-Critical Region

Critical Region

Non-Critical Region

τ_{int} Divergent, simulation cost is high

Utilise information from non-critical regions → Generate lattice configurations in critical regions

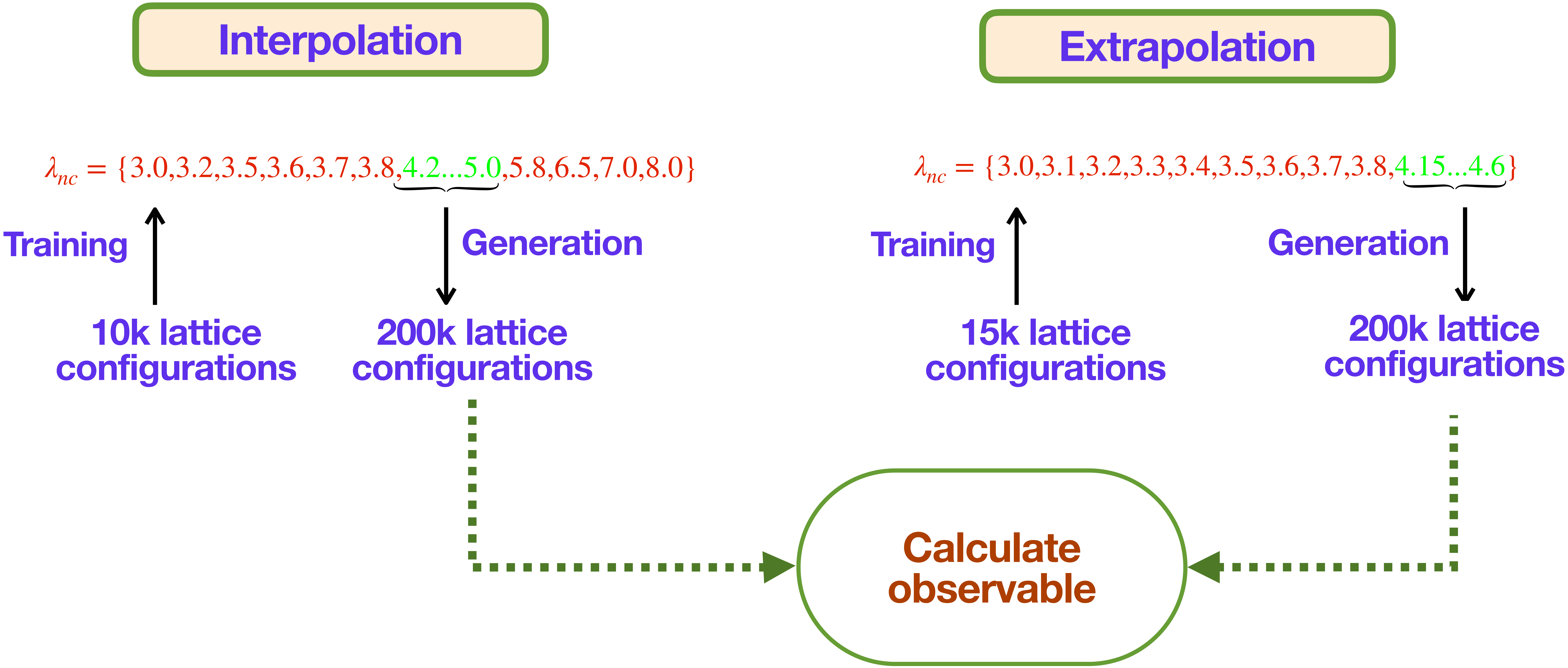
$\phi_{prop} \sim \tilde{p}(\phi; \lambda_c, \theta_{opt})$

Conditional NF

We studied two cases:

- **Interpolation**: generates samples on **both sides** of critical region.
  - Training samples $\phi \sim p(\phi \mid \lambda_{nc})$ where λ_{nc} belong to both non-critical regions.
- **Extrapolation**: generates samples on a **single side** of critical region.
  - Training samples $\phi \sim p(\phi \mid \lambda_{nc})$ where λ_{nc} belong to a single non-critical regions.

C-NF: Training & Generation



Observable

Observable calculated on lattice from HMC and C-NF Model are:

1. $\langle \tilde{\phi}^2 \rangle$: $\tilde{\phi} = \frac{1}{V} \sum_x \phi(x)$
2. Zero momentum Correlation Function:

   $C(t) = \sum_{x_1} G_c(x_1, t)$

   where, $x = (x_1, t)$ and

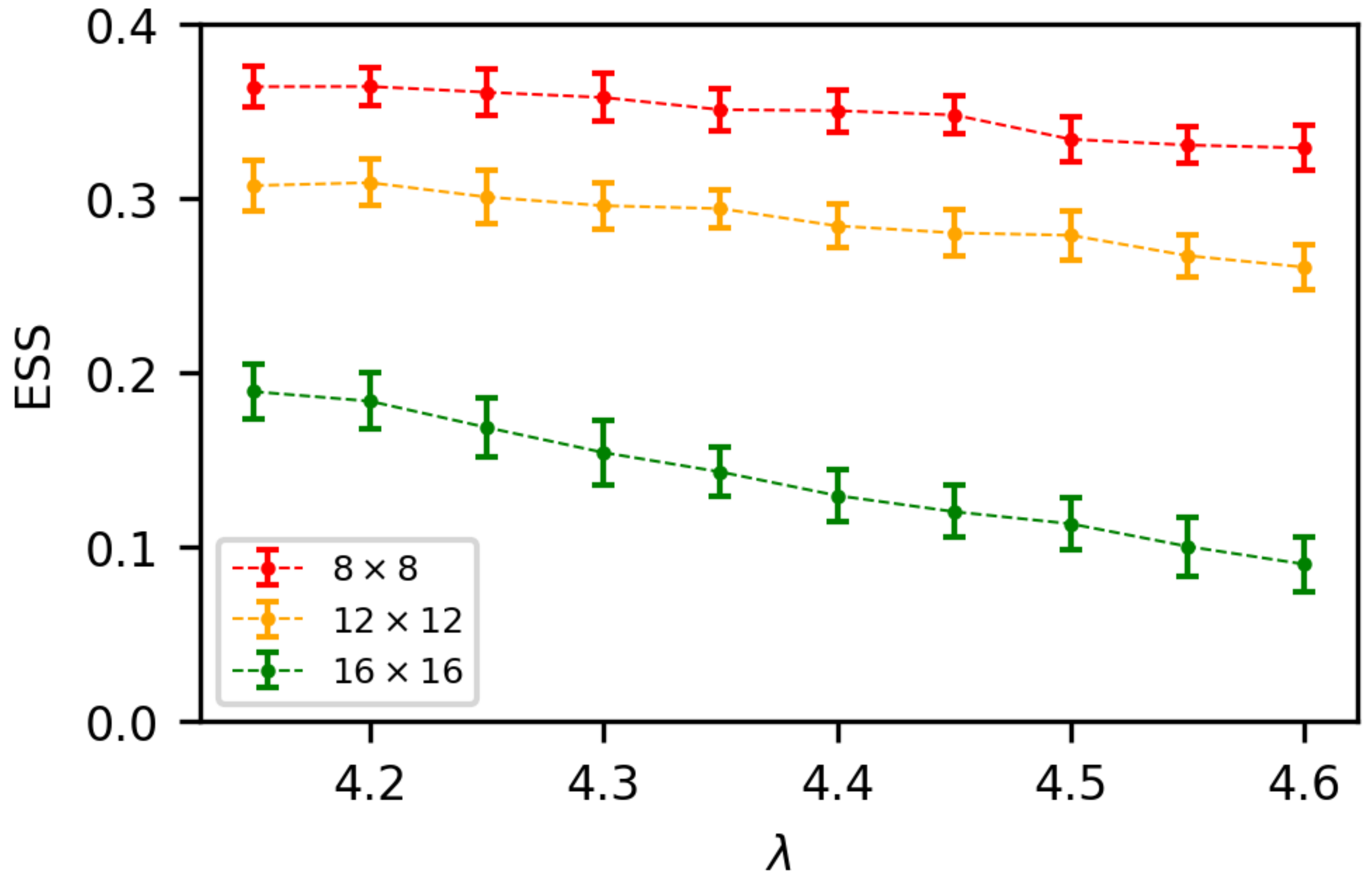
   $G_c(x) = \frac{1}{V} \sum_y [\langle \phi(y)\phi(x+y) \rangle - \langle \phi(y) \rangle \langle \phi(x+y) \rangle]$

3. Two Point Susceptibility: $\chi = \sum_x G(x)$

Results: Effective Sample Size (ESS)

C-NF model quality: ESS

$$ESS = \frac{1}{N}\frac{\left(\sum_{i=1}^{N} p(\phi_i;\lambda)/\tilde{p}(\phi_i;\lambda,\theta)\right)^2}{\sum_{i=1}^{N}\left(p(\phi_i;\lambda)/\tilde{p}(\phi_i;\lambda,\theta)\right)^2}$$

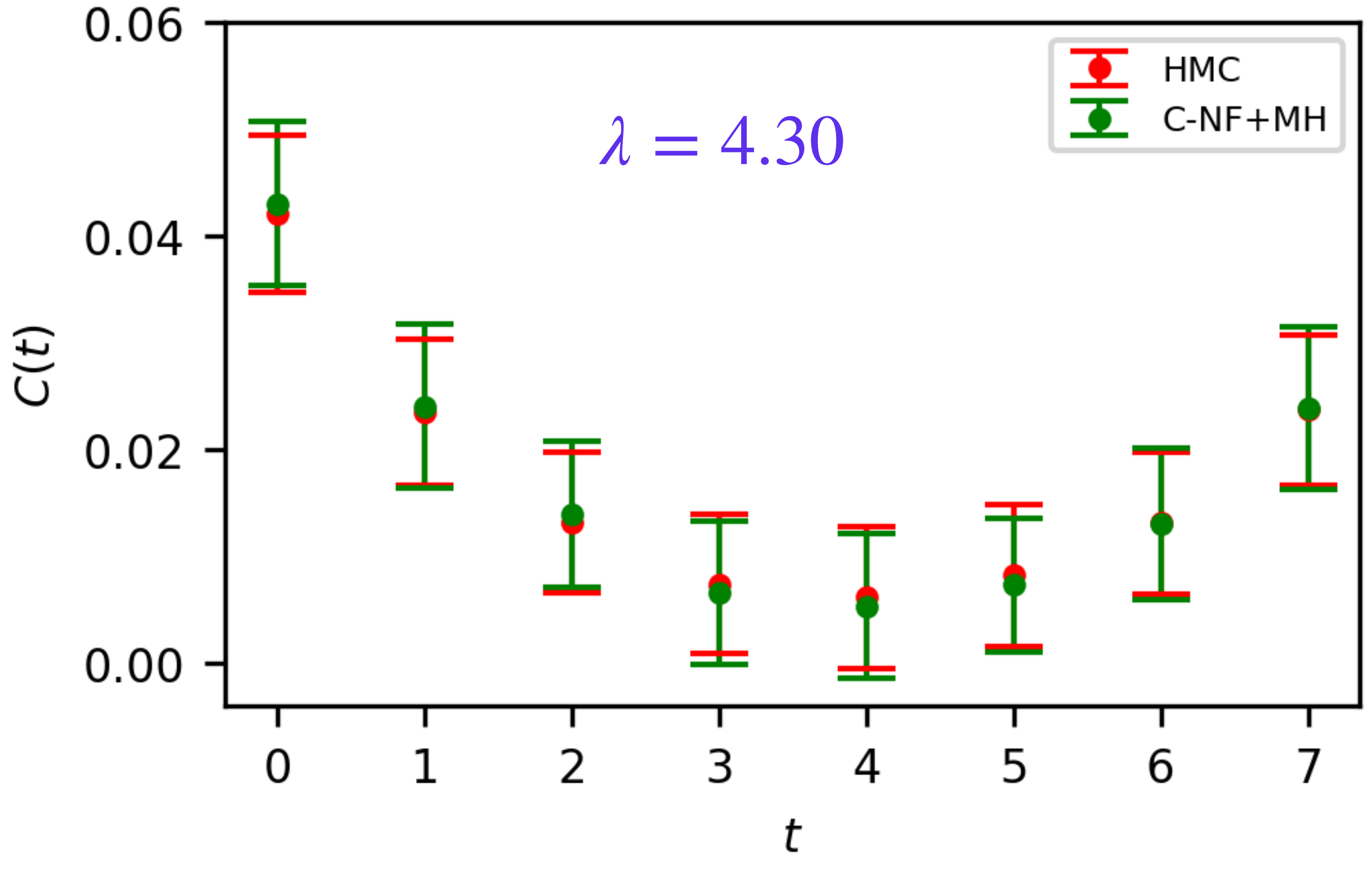


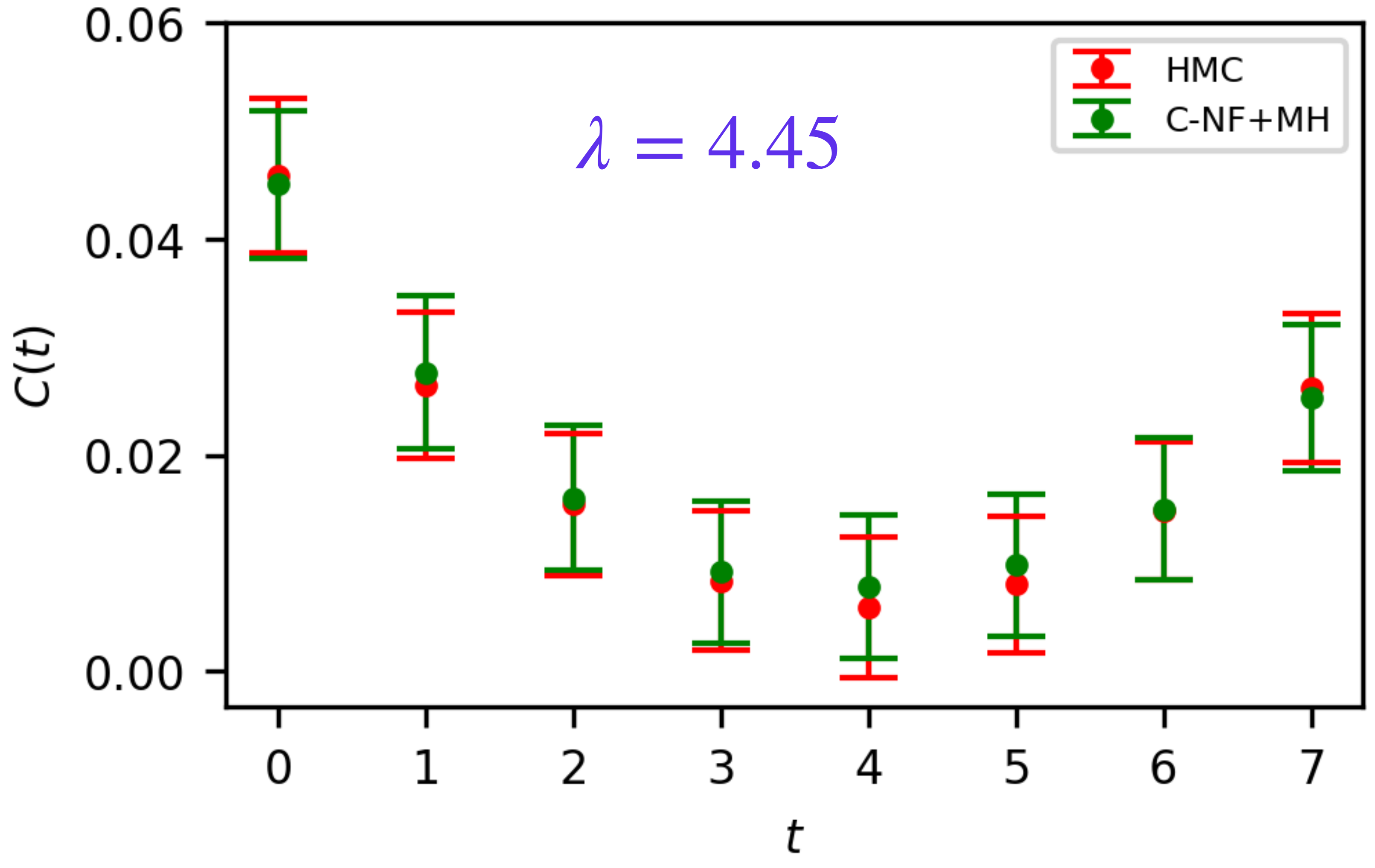
Higher ESS

Better Model → **Higher Acceptance** → **Low Autocorrelation**

Results: Correlation Functions

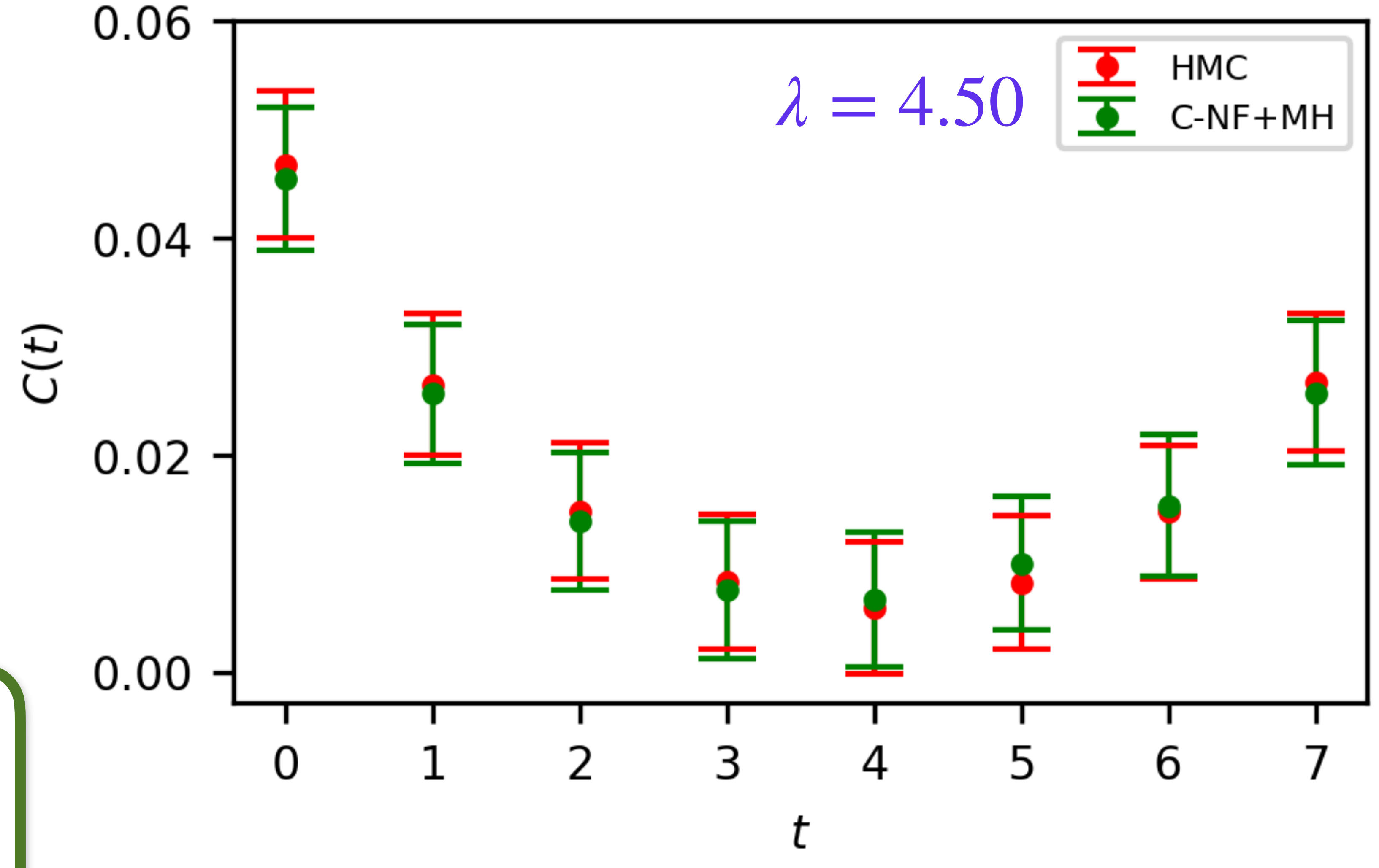
Extrapolation

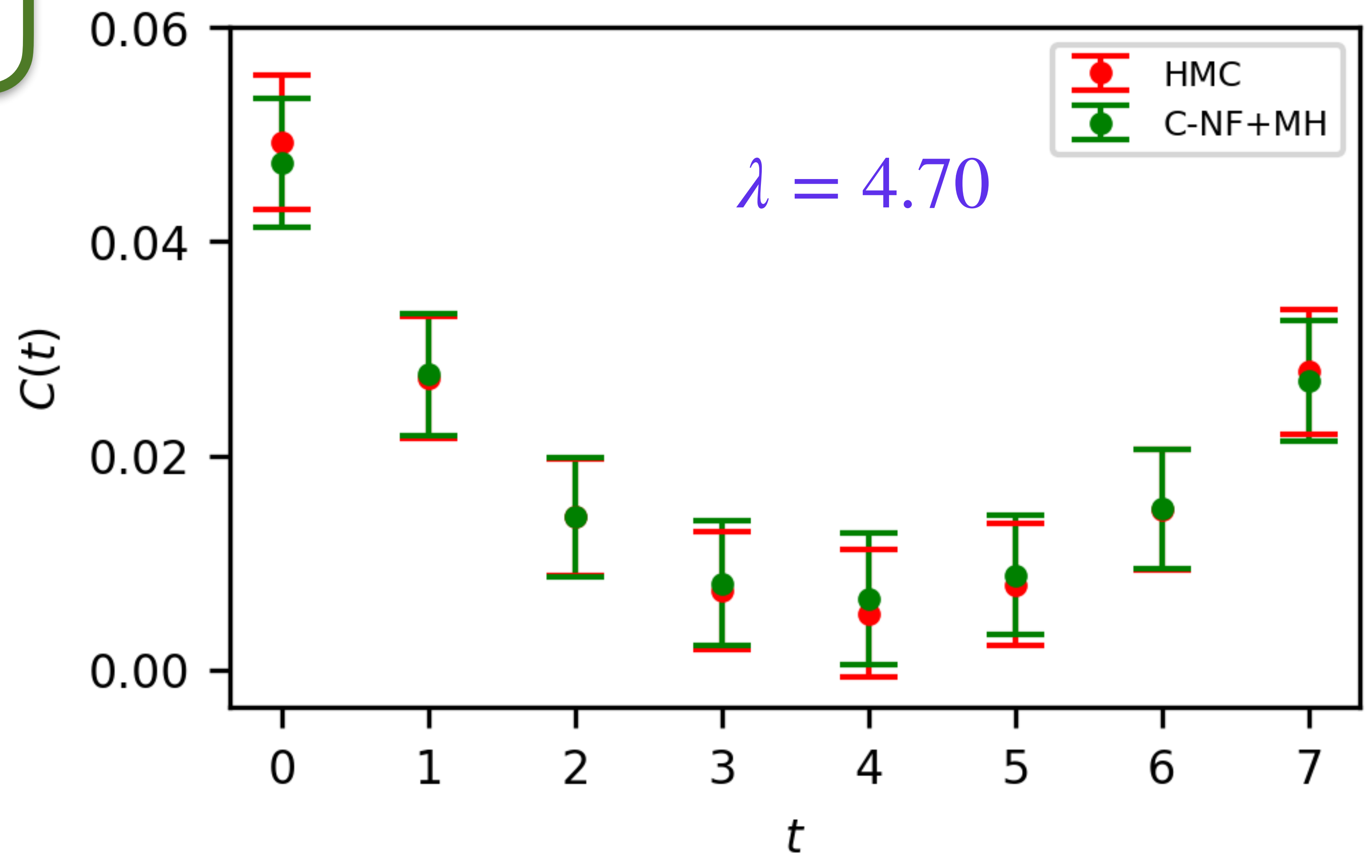




Results only from the critical region

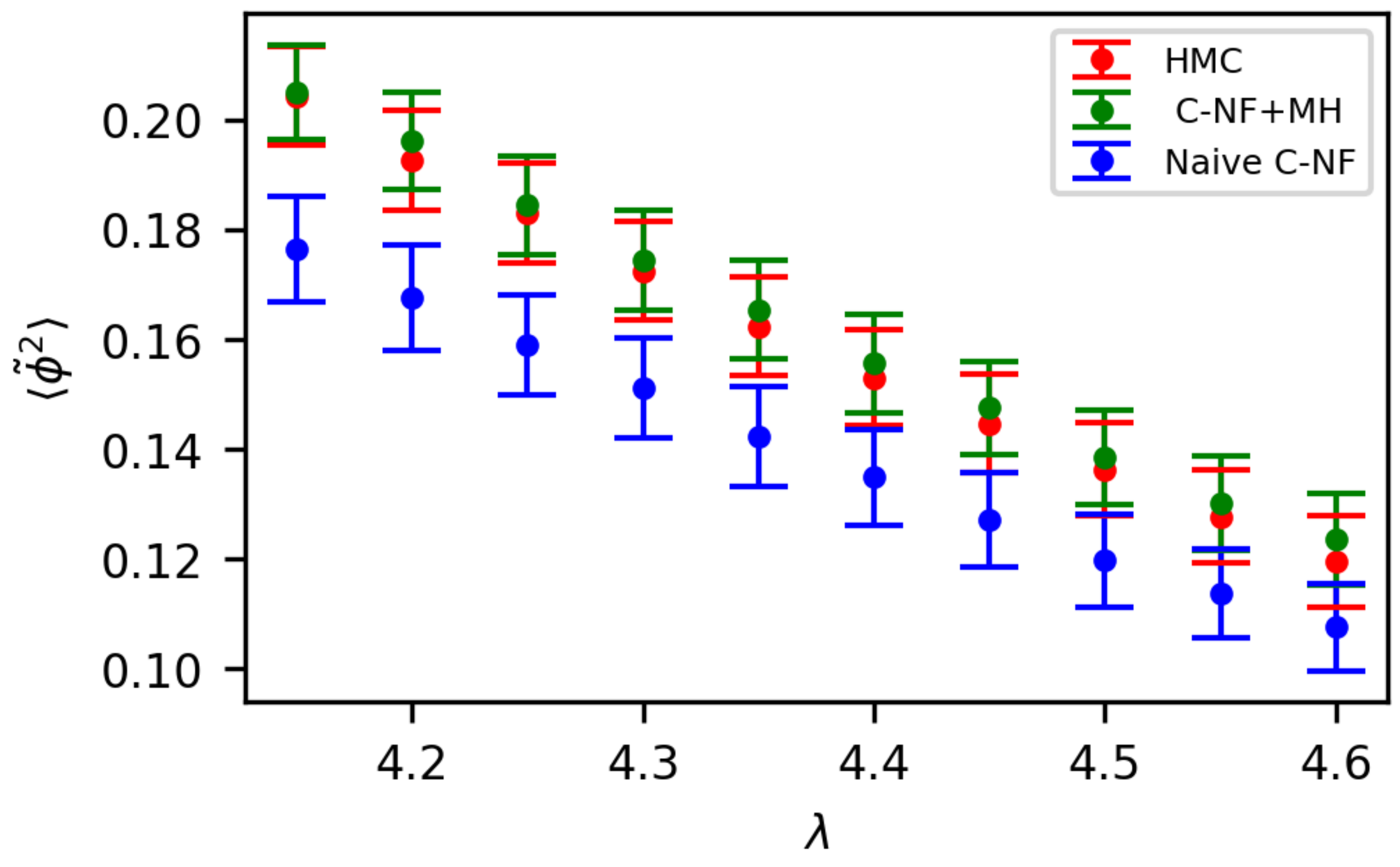
Interpolation

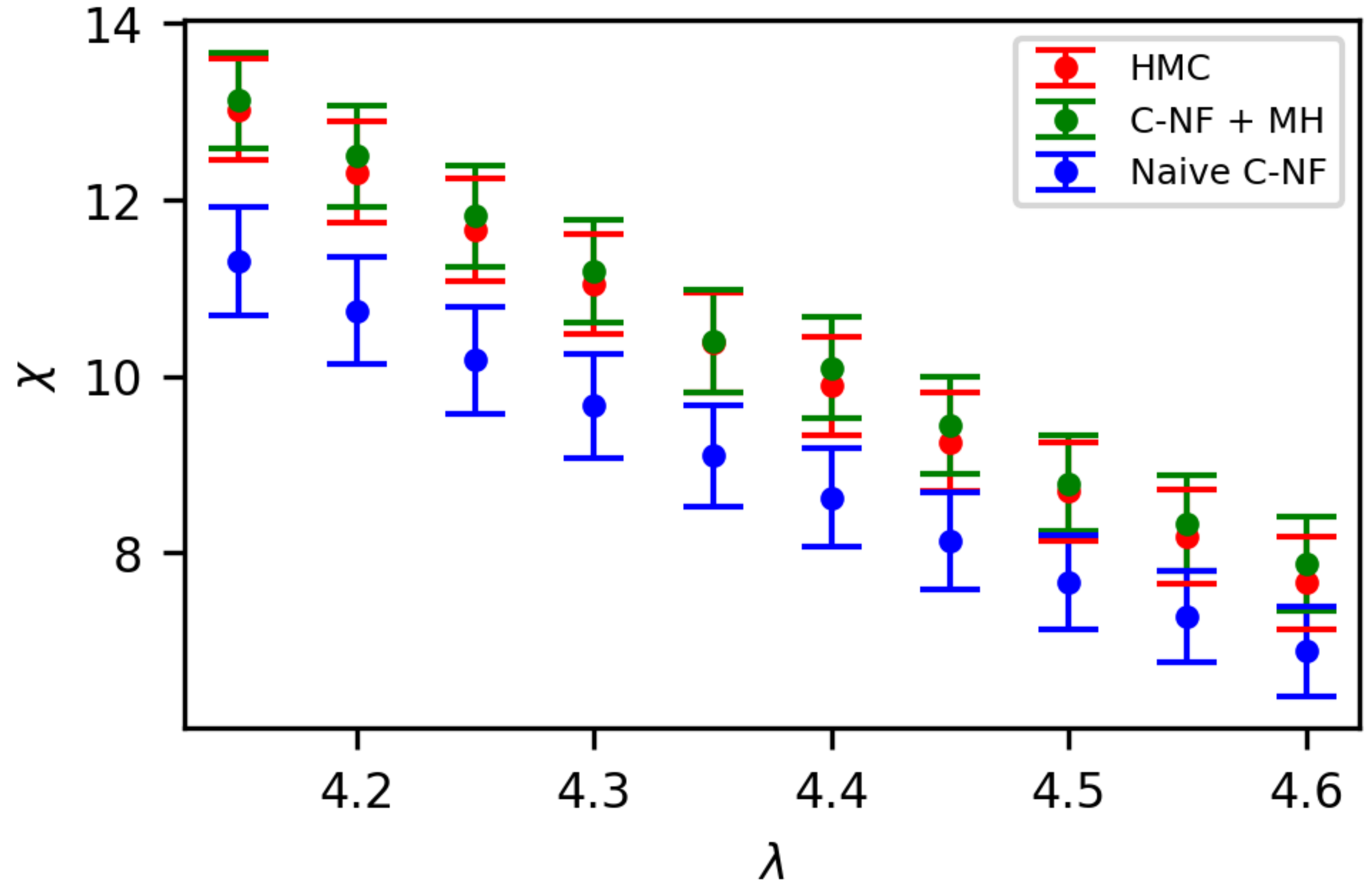




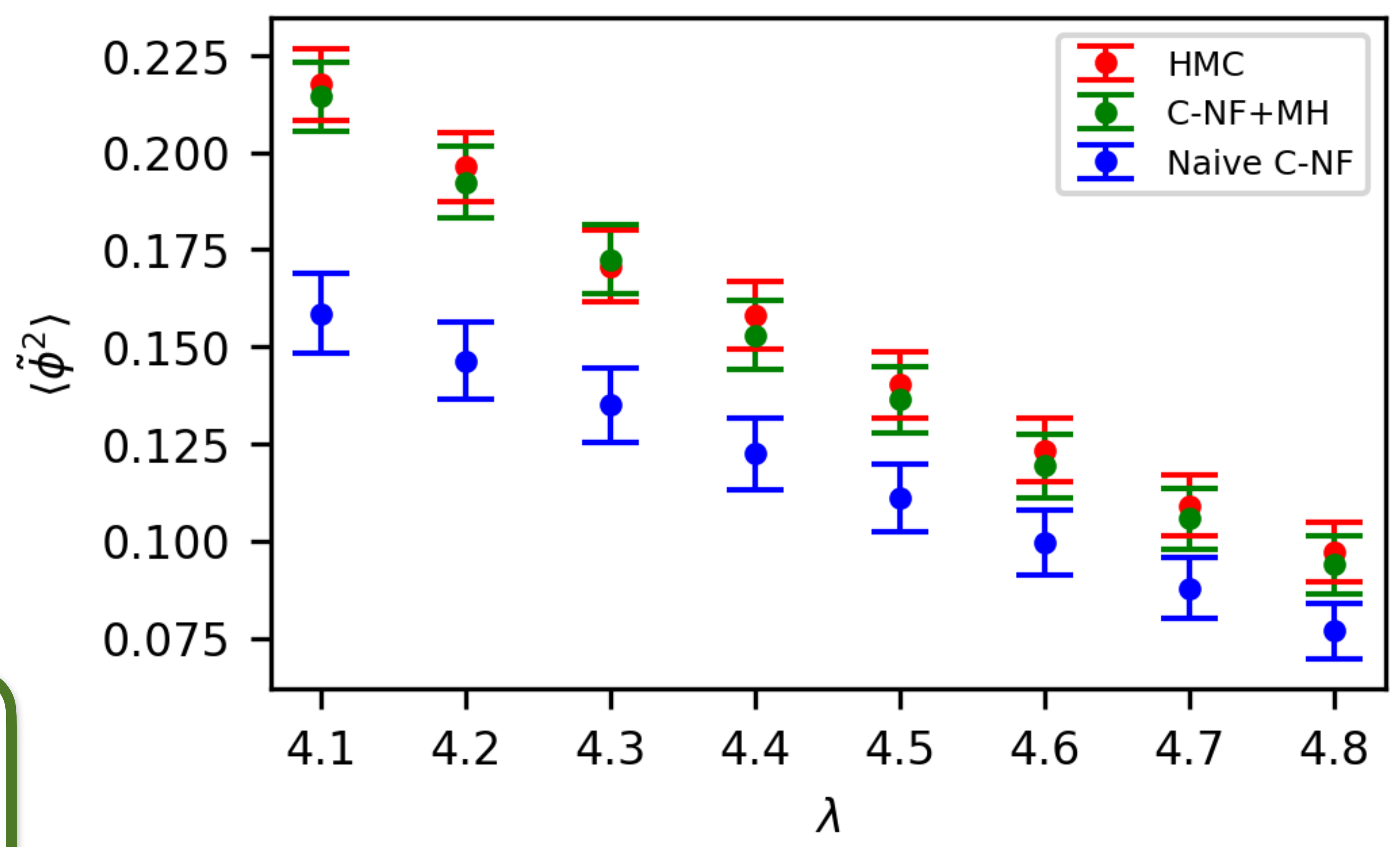
Results : χ *and* $\langle \tilde{\phi}^2 \rangle$

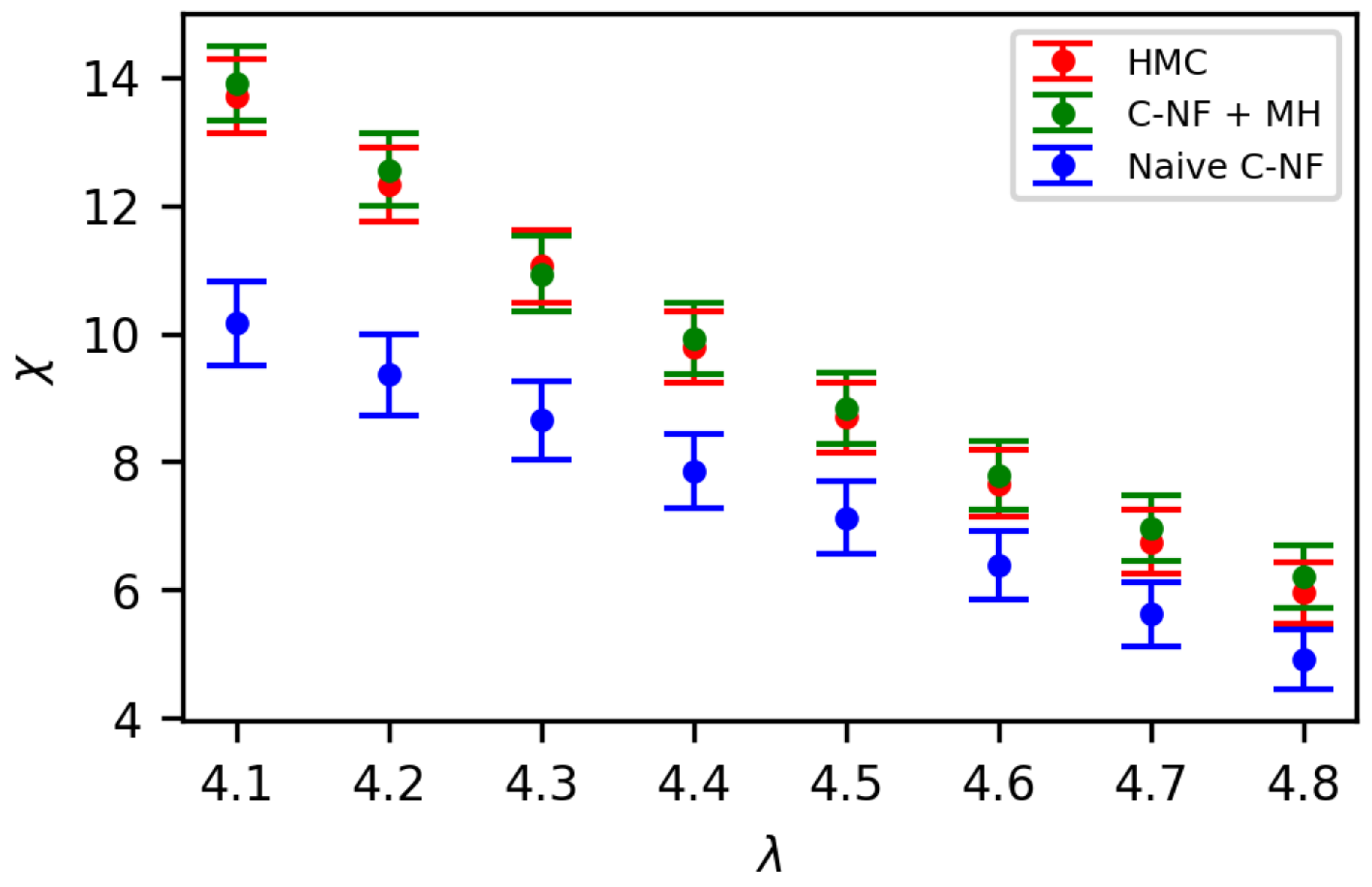
Extrapolation





Interpolation

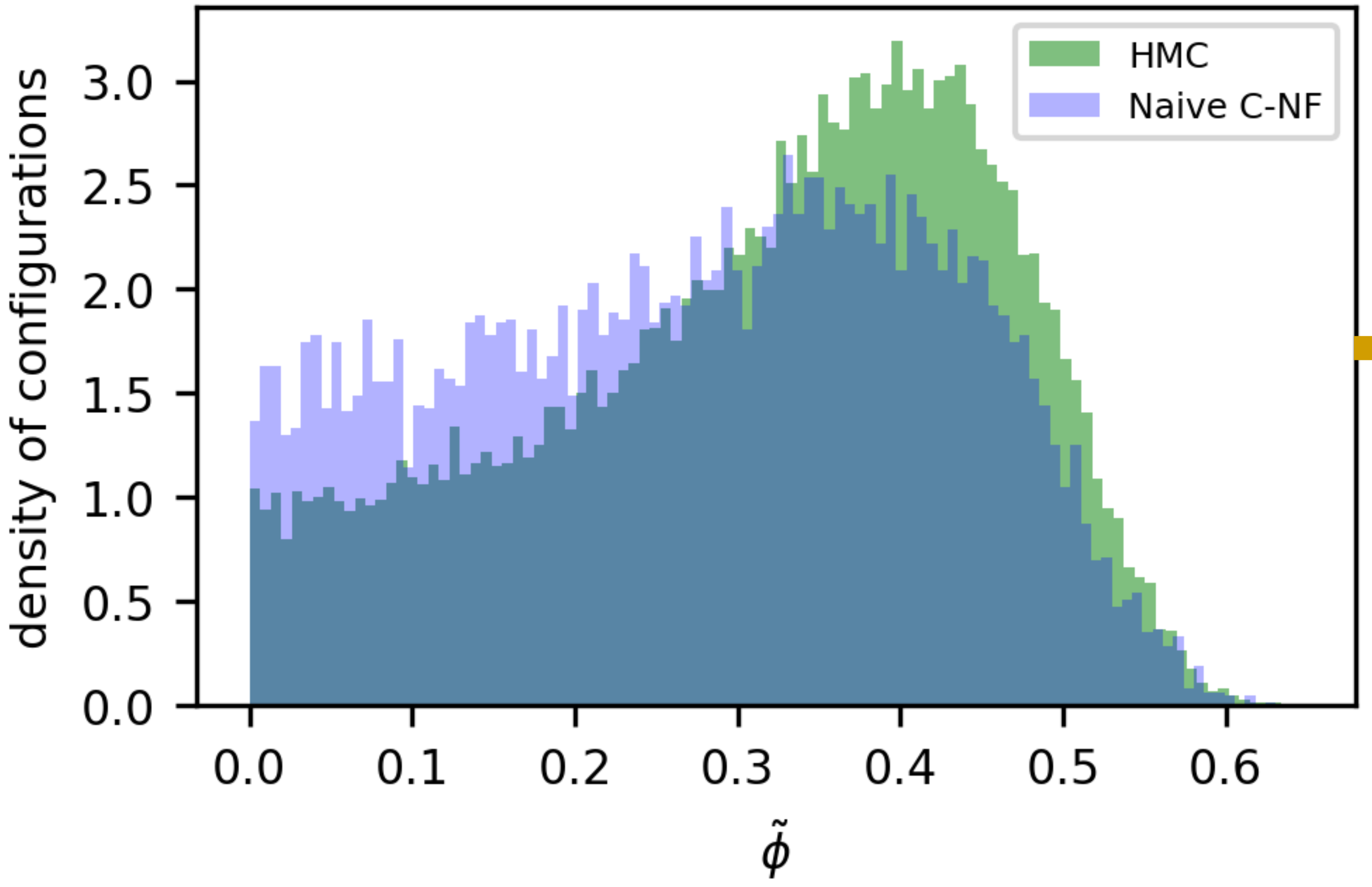




Results matches within statistical uncertainty

Results: artefacts removed by MH

Naive model



MH algorithm

Naive model + MH

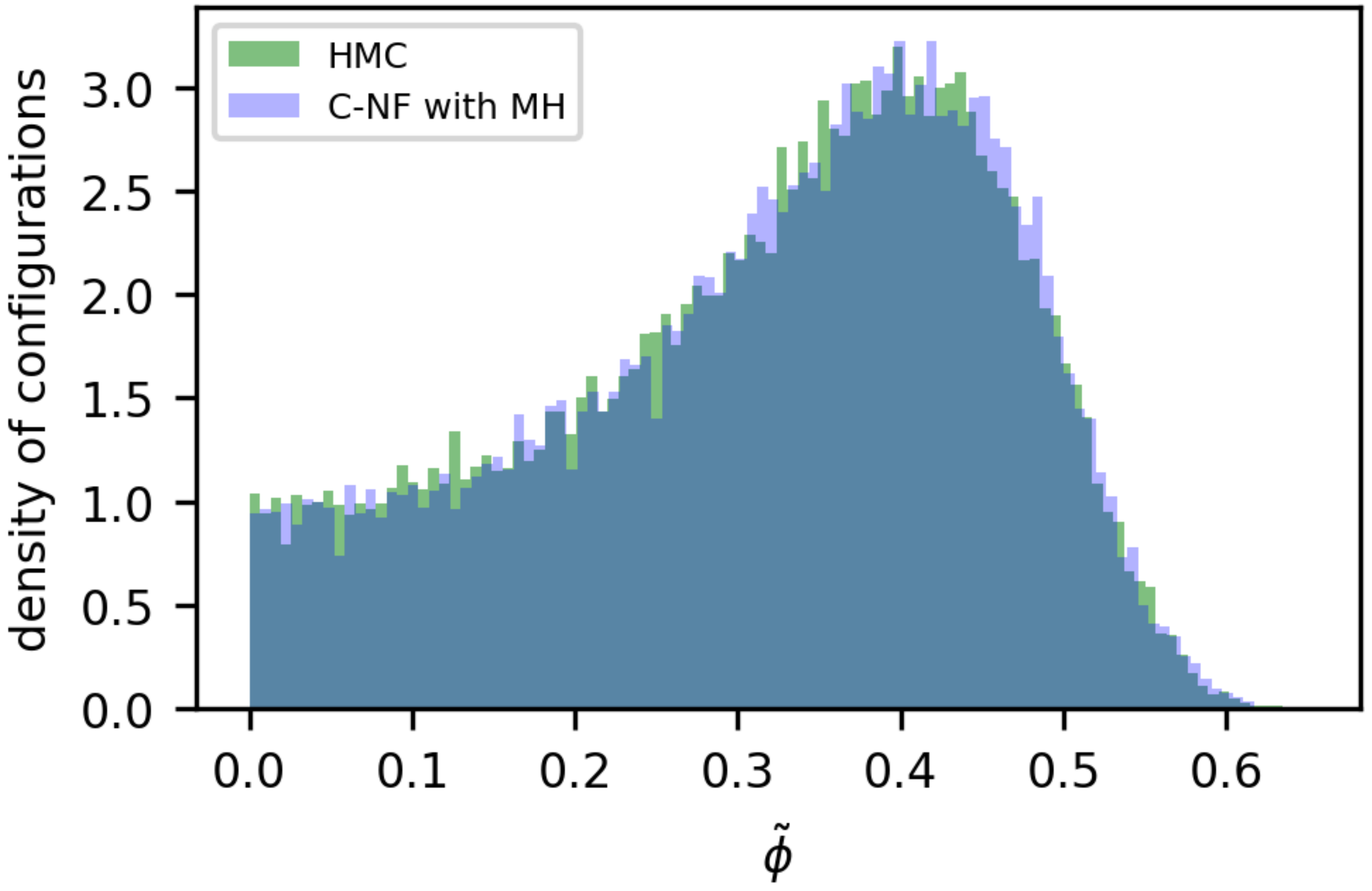


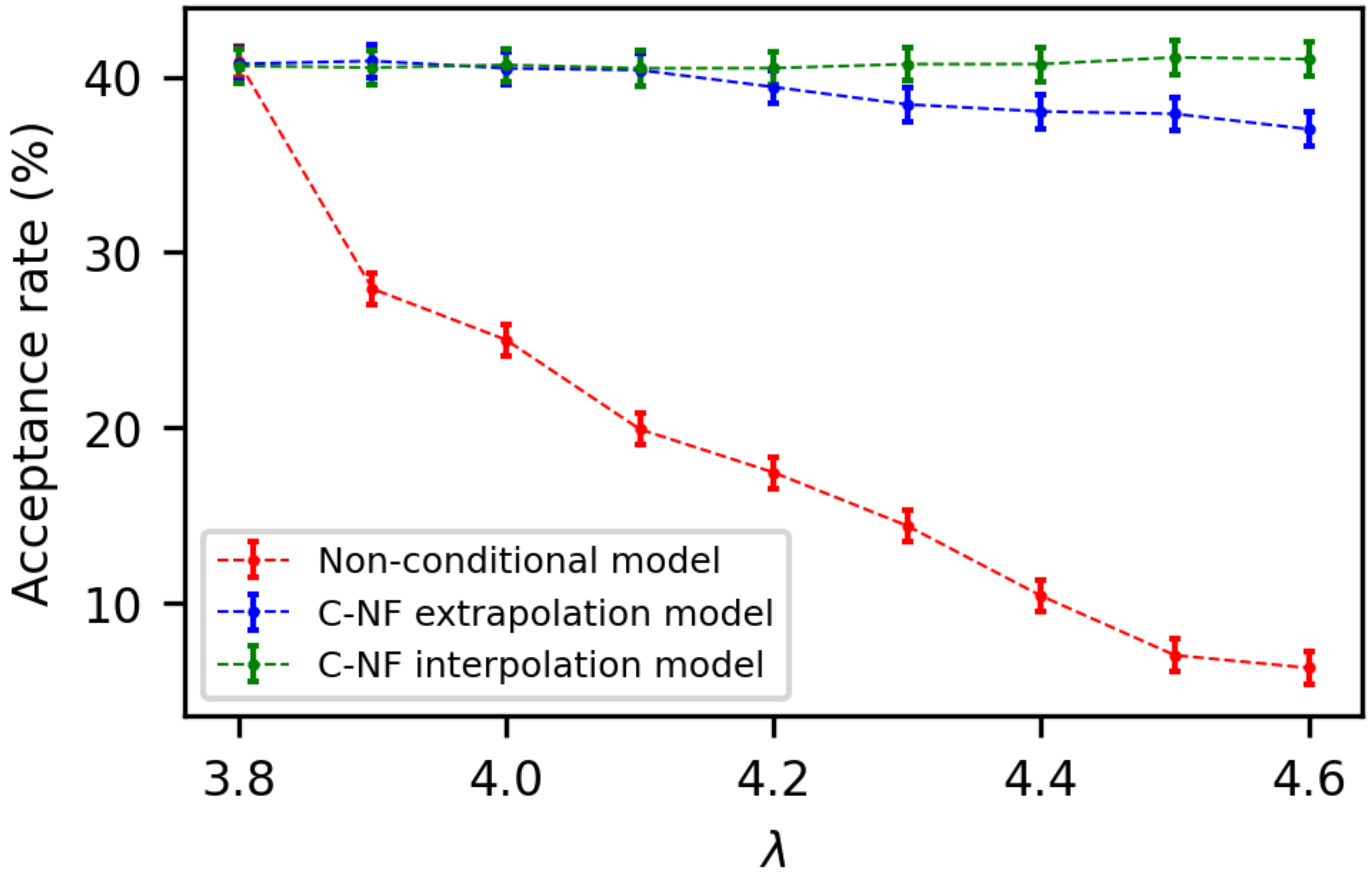
Figure: Histogram of density of lattice configurations for average field value ϕ on a lattice.

Results: compared to a non-conditional model

Acceptance rate in MH: a non-conditional model trained at $\lambda = 3.8$ vs conditional models.

✓ **For interpolation and extrapolation the acceptance rate is almost constant over action parameter.**

✓ **For a non-conditional model the acceptance rate drops faster over the action parameter.**



Summary

Problem: **MCMC simulations are severely affected by CSD.**

Proposed: A conditional NF model.

https://arxiv.org/abs/1904.12072

NF generate proposals for MH

Low Simulation Cost

Utilise samples from non-critical region

Conditional NF generate MH proposals for wide range of action parameter.

THANK YOU !