Aqtivate Workshop 2024

Generative Machine Learning Methods for the Simulation of 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 QCD

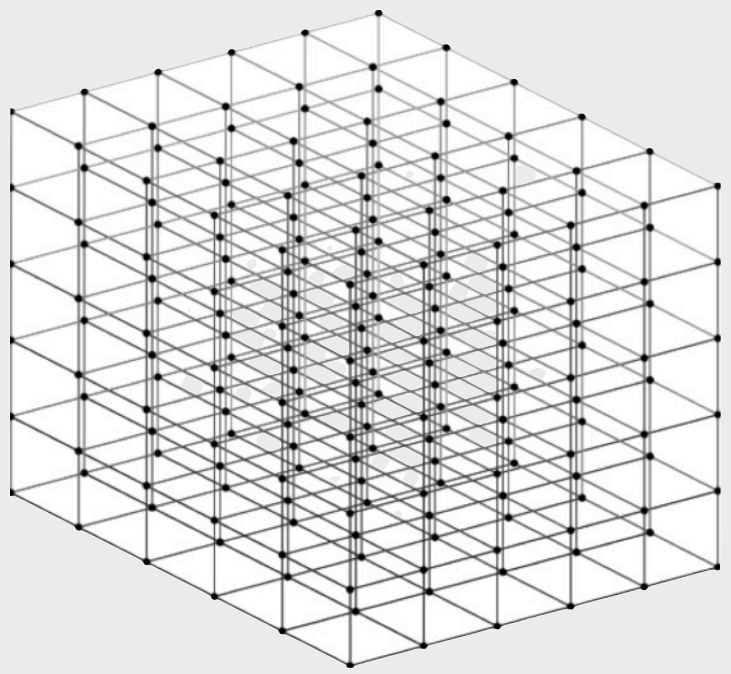
Weak Coupling

Non-Perturbative Methods

Perturbative Methods

Lattice Field Theory

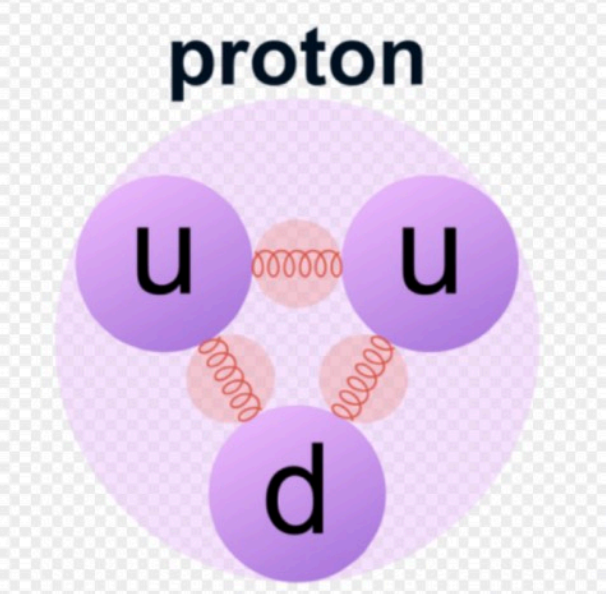
Discrete space time



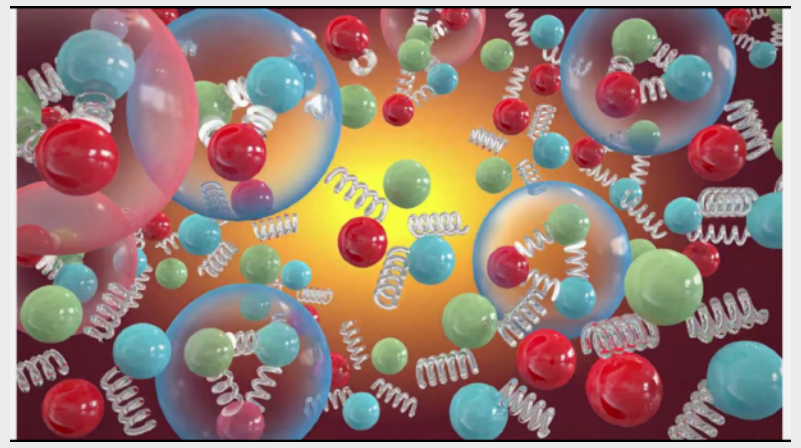
Interested region

Statistical methods of simulation

Prediction: various observables



quark-gluon plasma



Lattice QCD explains

Lattice Field Theory: Sampling task (Phi4 theory)

Continuum QFT action

$$S(\phi) = \int dx^2 \left\{ \frac{1}{2}(\partial_\mu \phi)^2 + \frac{m^2}{2}\phi^2(x) + \frac{\lambda^4}{4!}\phi^4(x) \right\}$$

Feynman path integral

$$\langle \hat{O}_2(\phi(x))\hat{O}_1(\phi(y))\rangle = \frac{\int D\phi e^{-S_E(\phi)} O_2(\phi(x))O_1(\phi(y))}{\int D\phi e^{-S_E(\phi)}}$$

Calculate observables

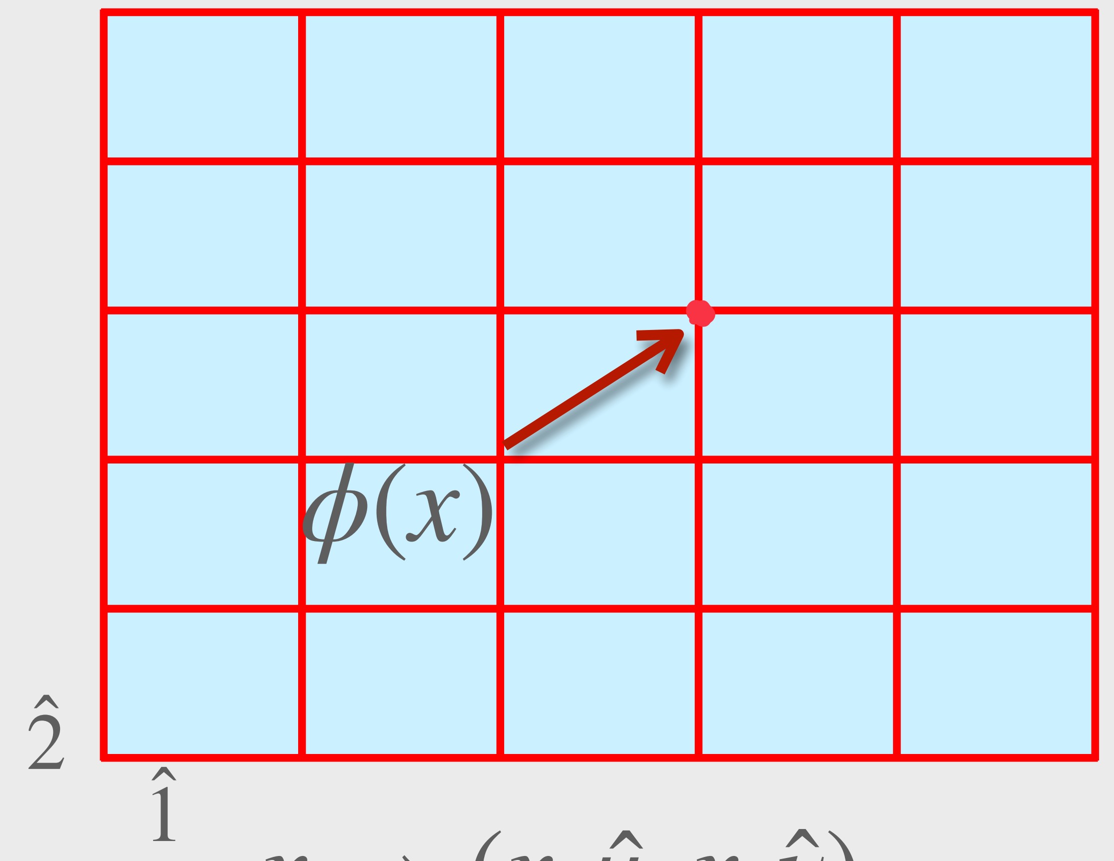
On lattice: After discretising spacetime

Observable :

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

Lattice action :

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

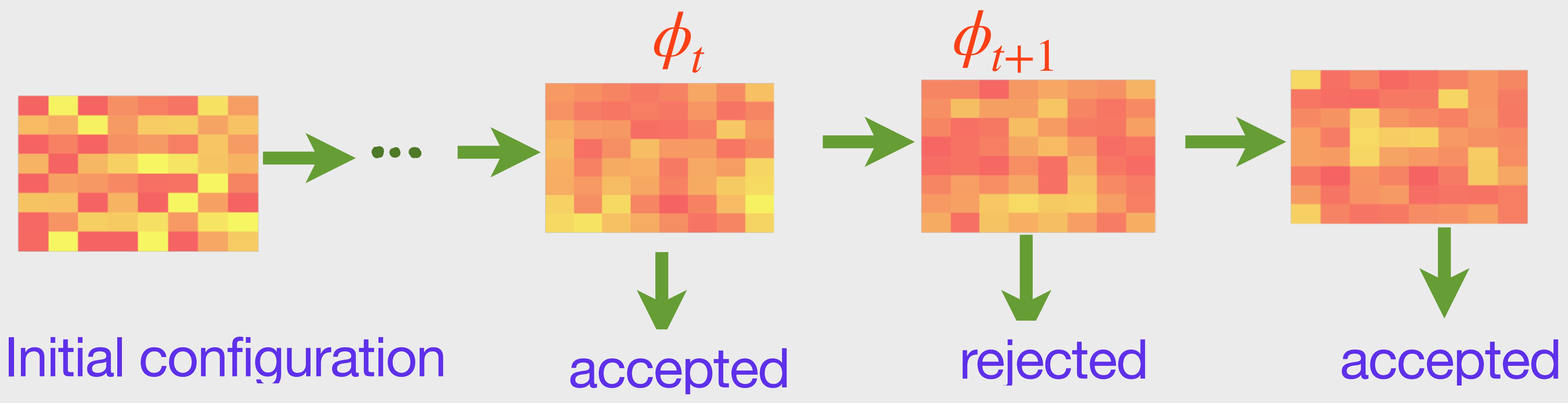


$x \rightarrow (x_1\hat{\mu}, x_2\hat{\nu})$

Lattice Field Theory $\xrightarrow{\text{Sampling task}}$ $P(\phi) = \dfrac{e^{-S(\phi)}}{Z}$

Markov chain Monte Carlo (MCMC) Simulation

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



Markov chain

- ✓ Initialize the lattice
- ✓ Propose a new lattice: $\tilde{\phi} \sim p_{prop}(\phi_{t+1} \,|\, \phi_t)$
- ✓ Accept/reject test. $\phi_{t+1} = \tilde{\phi} \; or \; \phi_t$

1. Ergodicity: must move to any state within finite steps

2. Detailed balance: $\dfrac{P(\phi_i)}{P(\phi_f)} = \dfrac{T(\phi_f \longrightarrow \phi_i)}{T(\phi_i \longrightarrow \phi_f)}$

❖ **Different MCMC algorithm: Metropolis Hasting, Gibbs Sampling, Hybrid Monte Carlo (HMC) etc.**

Hybrid Monte Carlo (HMC)

✓ ***The proposals are constructed by Hamiltonian dynamics using the lattice action.***

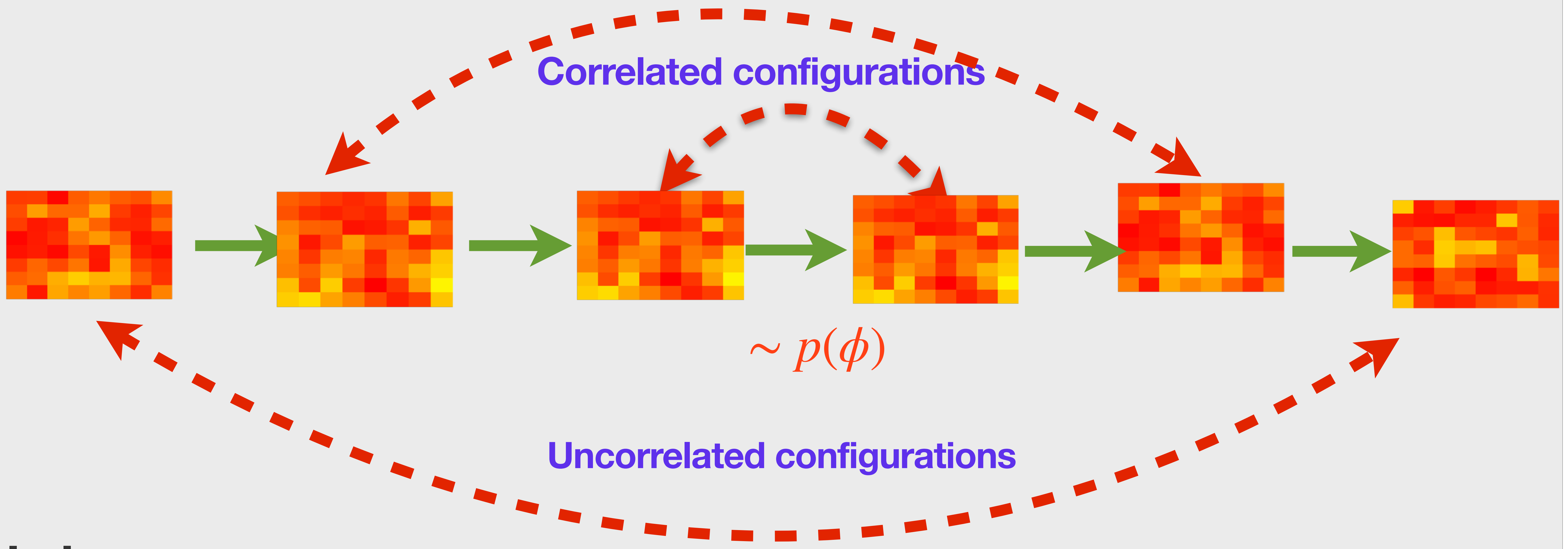
✓ ***Updates are non-local hence explore the parameter space faster, and also provide high acceptance rate.***

Critical Slowing Down (CSD)

$(t+1)^{th}$ proposal depends on previous state $\phi \sim p_{prop}(\phi_{t+1} \mid \phi_t)$

$$[\phi_i,\ \phi_{1+1},\ \phi_{i+2},\ \phi_{i+3}\ \ldots\ \phi_{N-1},\ \phi_N]$$

Markov chain become correlated



Integrated autocorrelation time:

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

$$\rho(t) = \frac{1}{N-t} \sum_{r=1}^{N-t} (O_r - \bar{O})(O_{r+1} - \bar{O})$$

Larger τ_{int} : **Error in estimator: Observable become biased.**

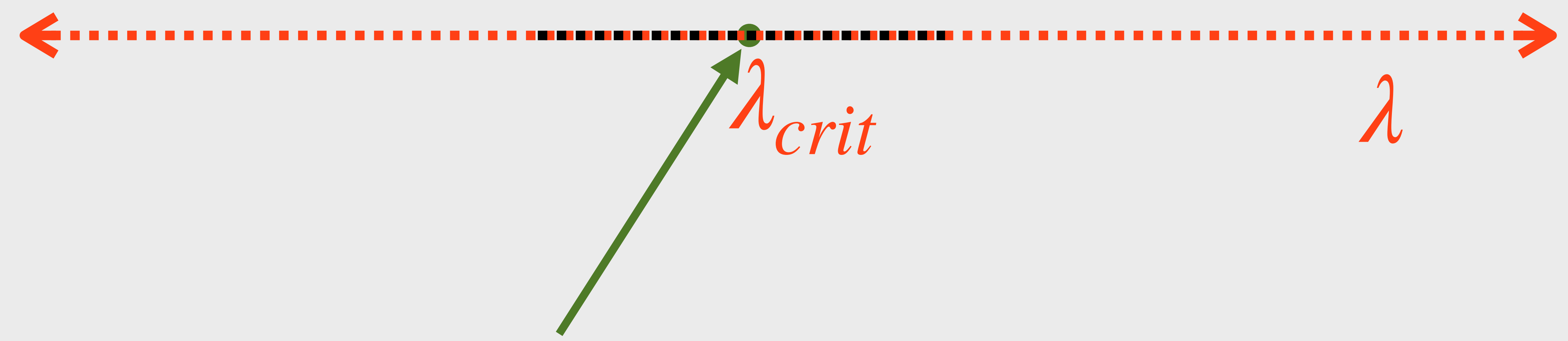
One generate longer Markov chain and use intermediate samples

Requires $2 \times \tau_{int}$ longer simulation run

Action parameter dependence of Critical Slowing Down (CSD)

Phi4 lattice action : $$S[\phi, m, \lambda] = \sum_{x} \sum_{\mu=1,2} [(2+m)\phi^2(x) - \phi(x)\phi(x+a\hat{\mu}) - \phi(x)\phi(x-a\hat{\mu}) + \lambda\phi^4(x)]$$

$S(\phi, m_{fixed}, \lambda);$ **Distribution:** $$P(\phi) = \frac{e^{-S(\phi, m_{fixed}, \lambda)}}{Z}$$



Action parameter

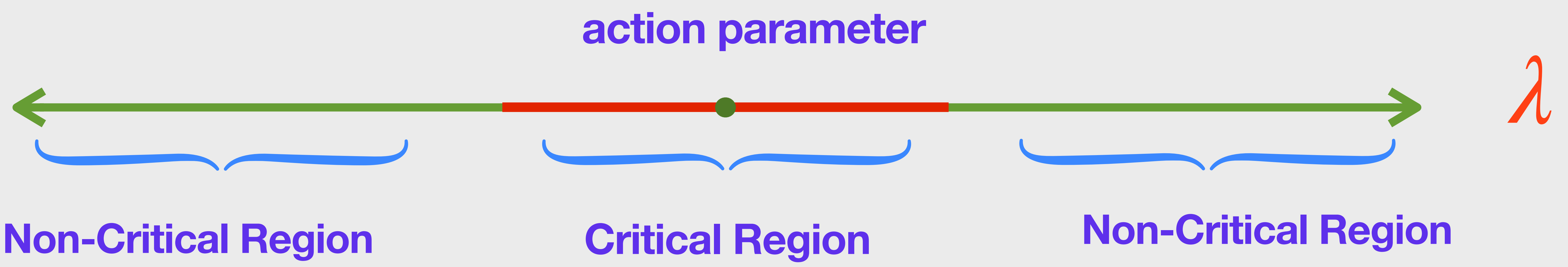
Monte Carlo simulations generate highly correlated lattice samples

✓ τ_{int} **Divergent, CSD dominates**

✓ **Simulation cost is too high**

Our approach: Conditional generative models

Generic lattice action : $S(\phi, \lambda)$



Training in the non-critical region

$\phi_i \sim p(\phi \,|\, \lambda_i)$ **using HMC**

Train Generative models

Sampling in the critical region

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

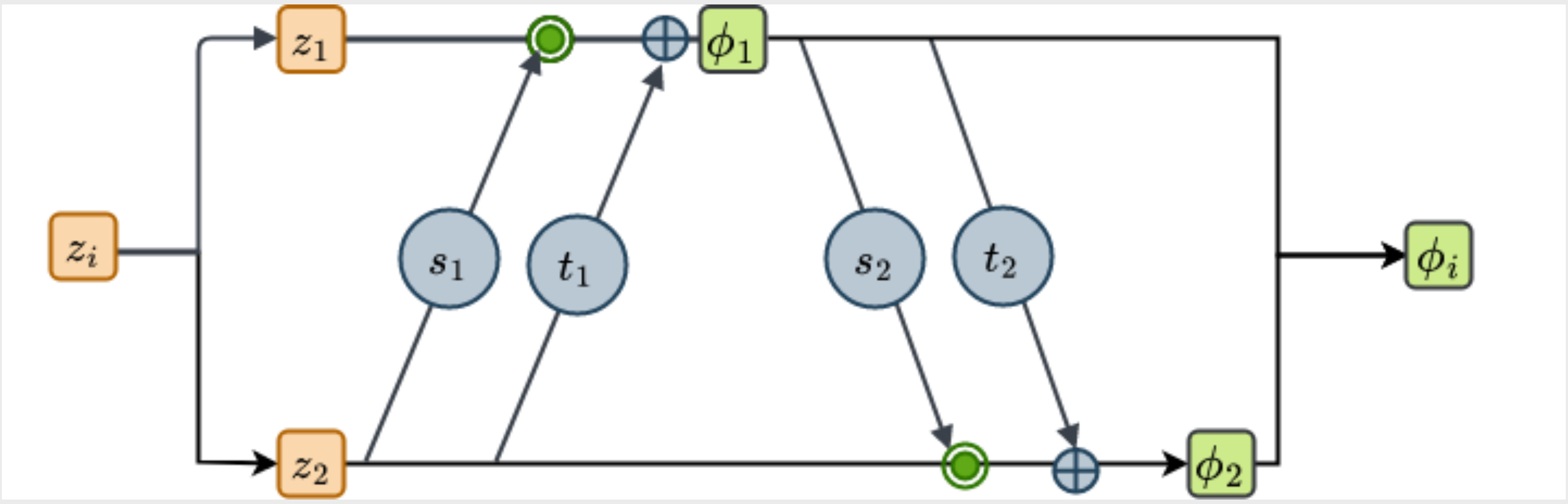
- Uses training samples which are genereted by HMC at low cost
- Model generates samples at multiple parameter values
- Avoids mode collapse problems.

Architecture of NF

Affine coupling layer architecture:

$$\phi_1 = z_1 \odot \exp(s_1(z_2)) + t_1(z_2)$$

$$\phi_2 = z_2 \odot \exp(s_2(\phi_1)) + t_2(\phi_1)$$



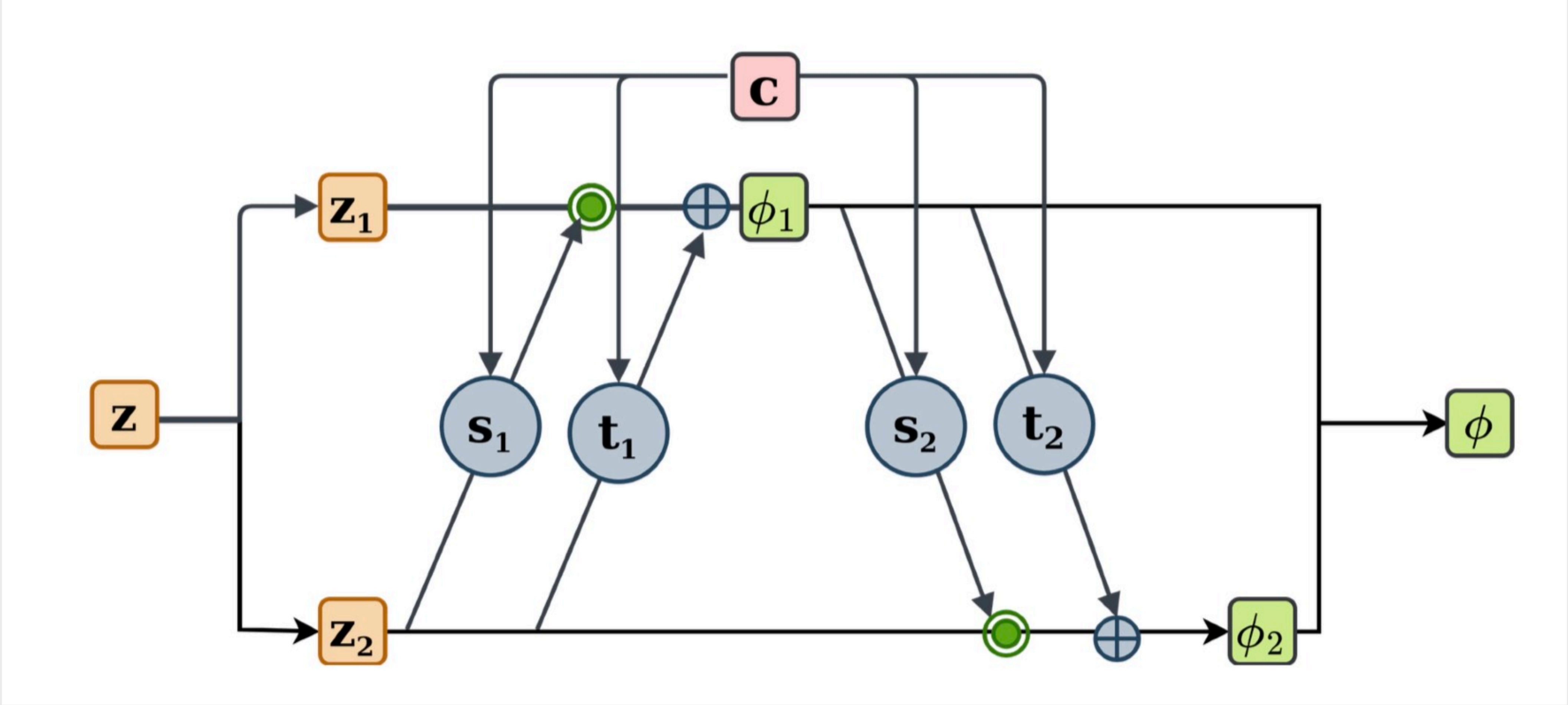
s_i, t_i **are the neural networks**

c is the condition parameter

Condition on Affine coupling layer architecture:

$$\phi_1 = z_1 \odot \exp(s_1(z_2, c)) + t_1(z_2, c)$$

$$\phi_2 = z_2 \odot \exp(s_2(\phi_1, c)) + t_2(\phi_1, c)$$



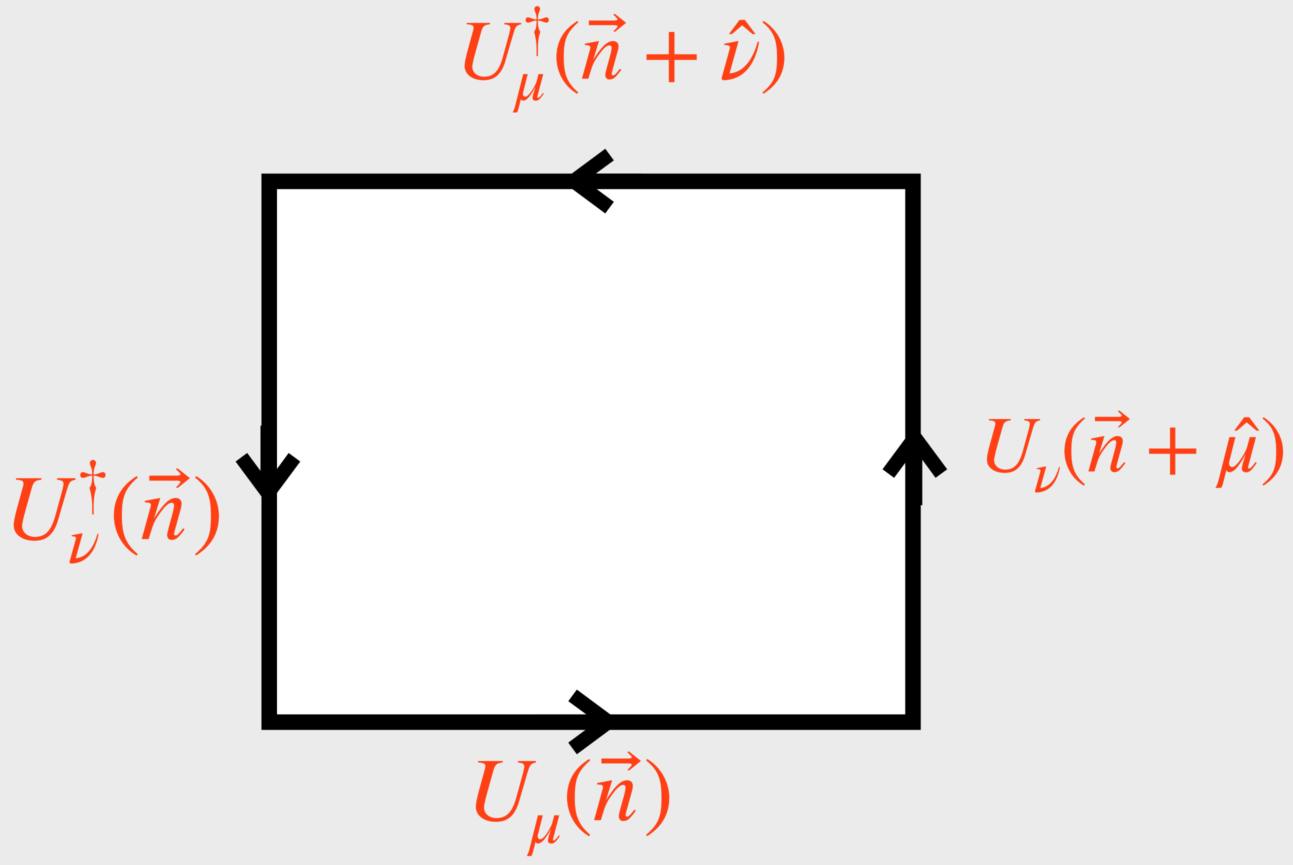
Normalising Flow for U(1) Gauge Theory

The lattice action for U(1) Gauge Theory:

$$S^E_{\mathrm{latt}}[U] = -\beta \sum_{\vec{n}} \left[\sum_{\mu<\nu} \mathrm{Re} P_{\mu\nu}(\vec{n}) \right]$$

where $\quad P_{\mu\nu}(\vec{n}) \equiv U_\mu(\vec{n})\ U_\nu(\vec{n}+\hat{\mu})\ U^\dagger_\mu(\vec{n}+\hat{\nu})\ U^\dagger_\nu(\vec{n})$

$$U_\mu(\vec{n}) = \exp(i\theta_\mu(\vec{n}))$$



$P_{\mu\nu}(\vec{n})$ **is known as Plaquette.**

$U_\mu(\vec{n})$ **is known as Link variable.**

Gauge transformation

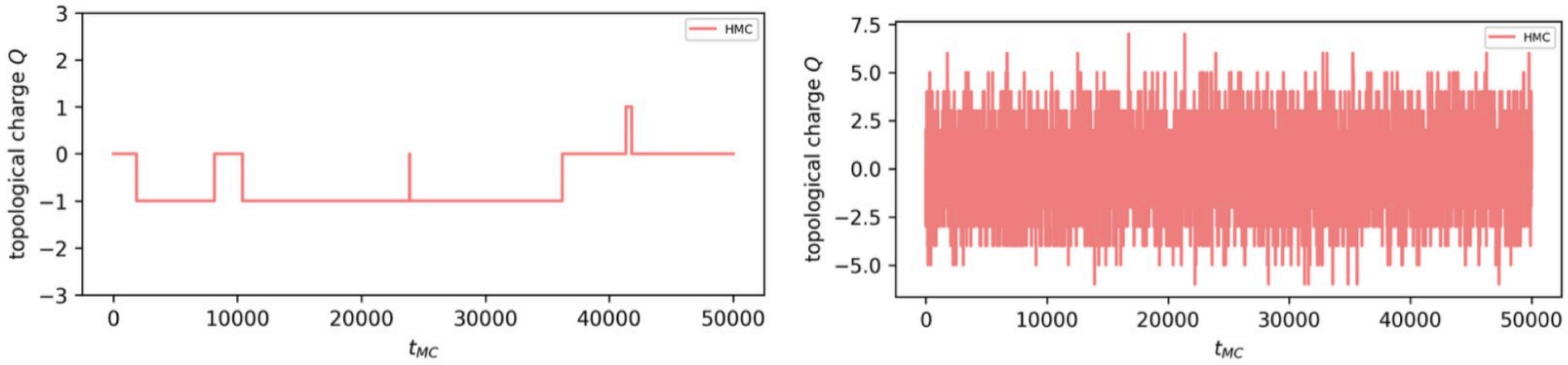
$$\boxed{U_\mu(\vec{n}) \to e^{i\alpha(\vec{n})} U_\mu(\vec{n}) e^{-i\alpha(\vec{n}+\hat{\mu})}}$$

$$P_{\mu\nu}(\vec{n}) = P'_{\mu\nu}(\vec{n})$$

HMC for U(1) Gauge theory

Topological freezing at larger action parameter: Topological Charge

$$Q = \frac{1}{2\pi}\sum_n arg[U_{\mu\nu}(n)],$$
$$\text{where,} \quad arg[(U_{\mu\nu}] \in [-\pi, \pi]).$$



(A) $\beta = 7$ (B) $\beta = 3.5$

Divide the parameter space into two parts

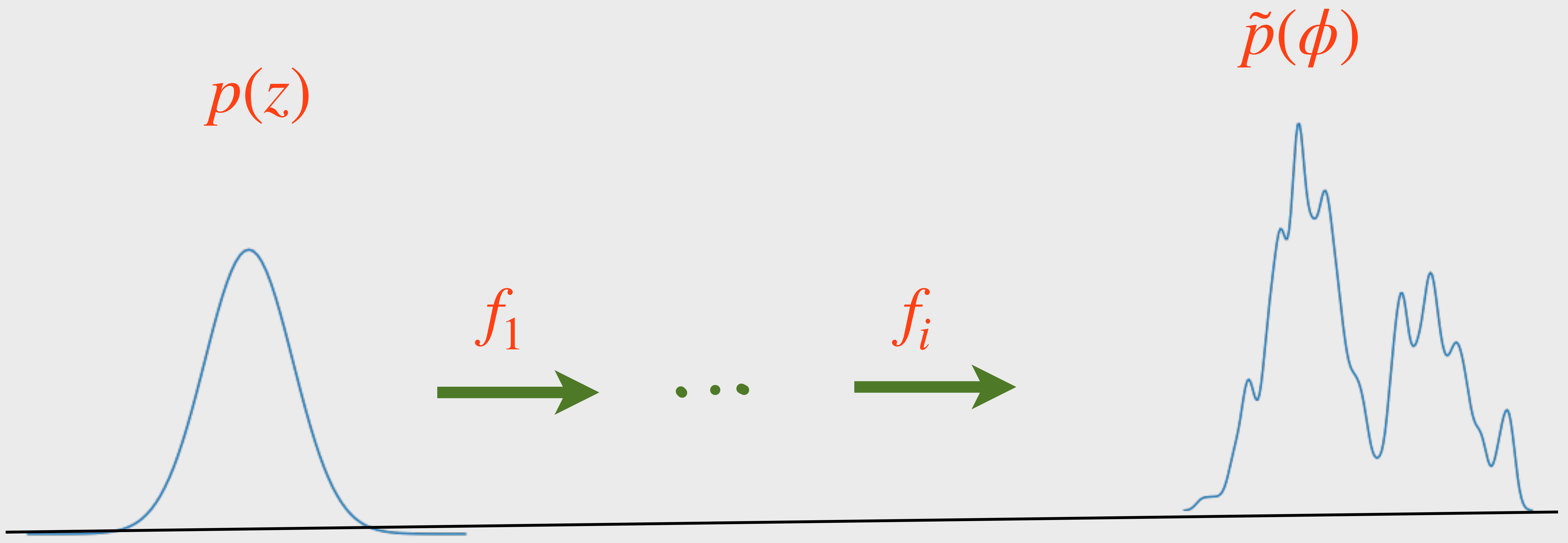
$$\beta_S : \{1.0, 1.5, 1.8, 2, 2.2, 2.5, 2.8, 3, 3.2, 3.5\}$$

$$\beta_L = \{5.5, 6, 6.5, 7, 7.5\}.$$

Implementing gauge symmetries in NF model

This action is invariant under **gauge transformations** G

$$GU_\mu(\vec{n}) \to e^{i\alpha(\vec{n})} U_\mu(\vec{n}) e^{-i\alpha(\vec{n}+\hat{\mu})}$$



Gauge invariant distribution

May not be Gauge symmetric

$[f, G] = 0$ $\longrightarrow$ **Equivariant transformation**

Gurtej Kanwar, et al. (2020)

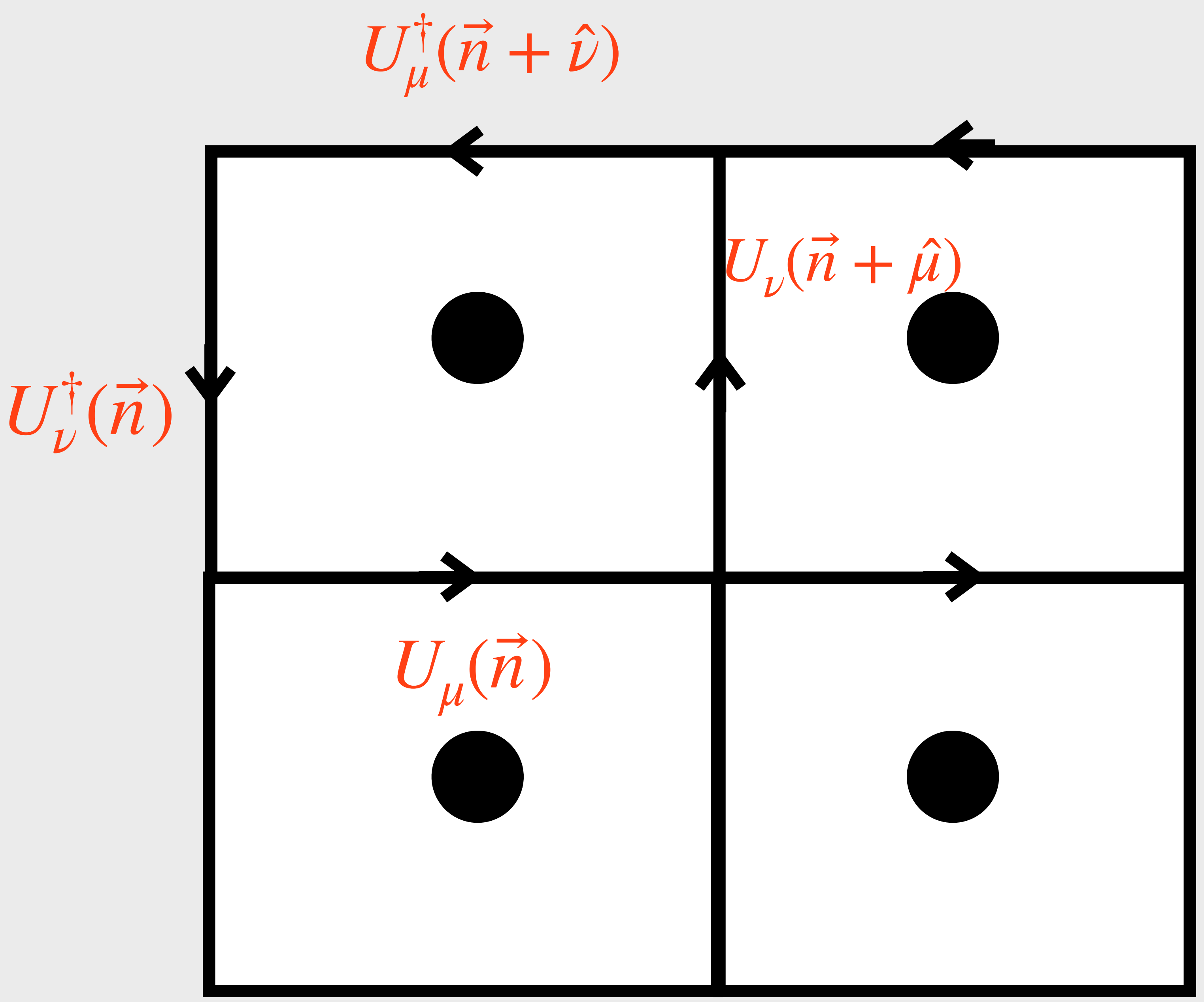
Implementing gauge symmetries in NF model

Flow act on gauge invariant quantity $f : z \longrightarrow \phi$

z gauge invariant quantity

$[f, G] = 0$

Plaqutte in the flow $f : P \longrightarrow P'$



Generate Gauge Field

Translate Plaquette to gauge field:

$$T : P'P^{-1}$$

$$T : U \longrightarrow U'$$

$$P = UV \rightarrow P'P^{-1}UV = P'(V^{-1}U^{-1})UV = P'.$$

Gurtej Kanwar, et al. (2020)

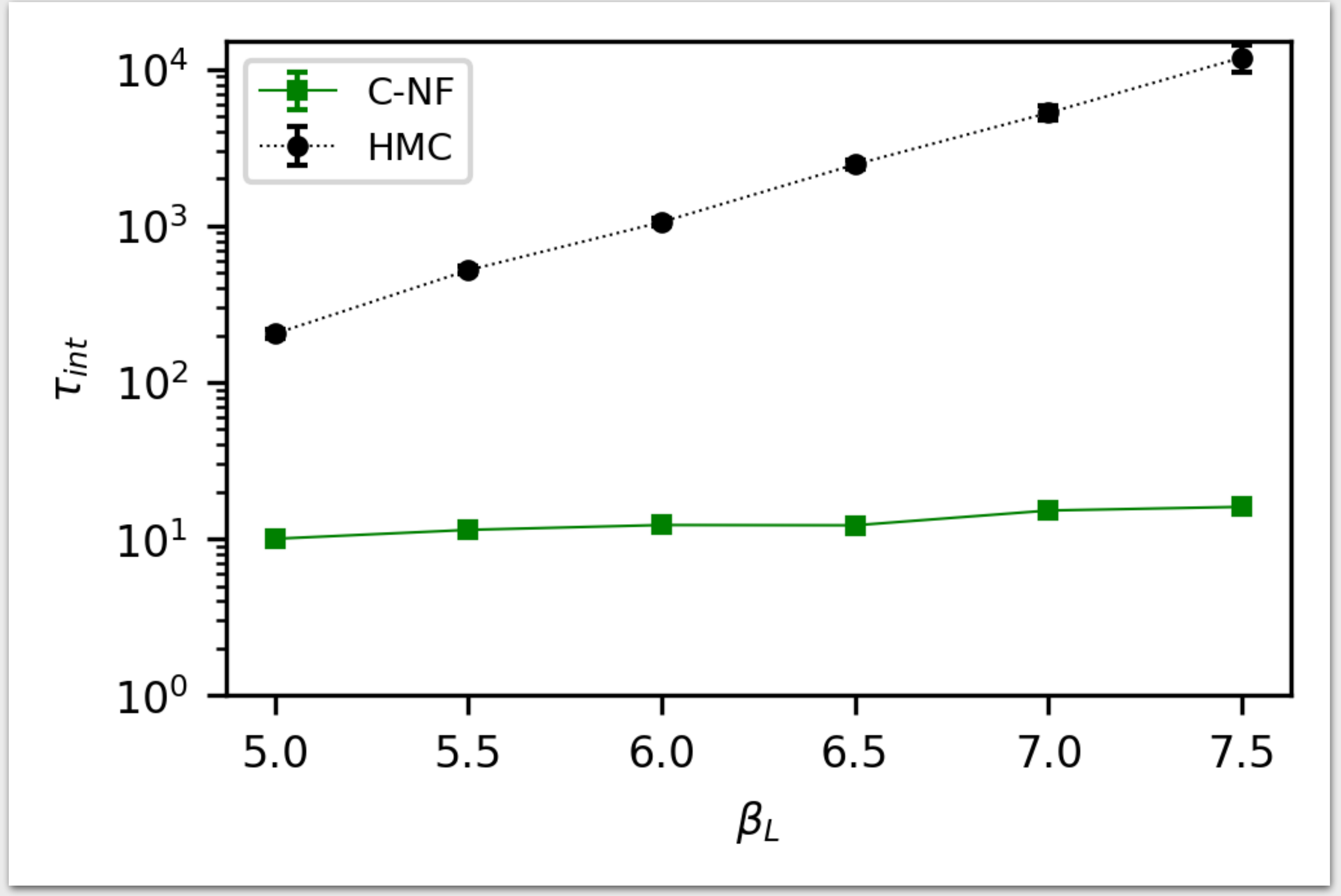
$link\ dimensions\ 2 \times 3 \times 3$

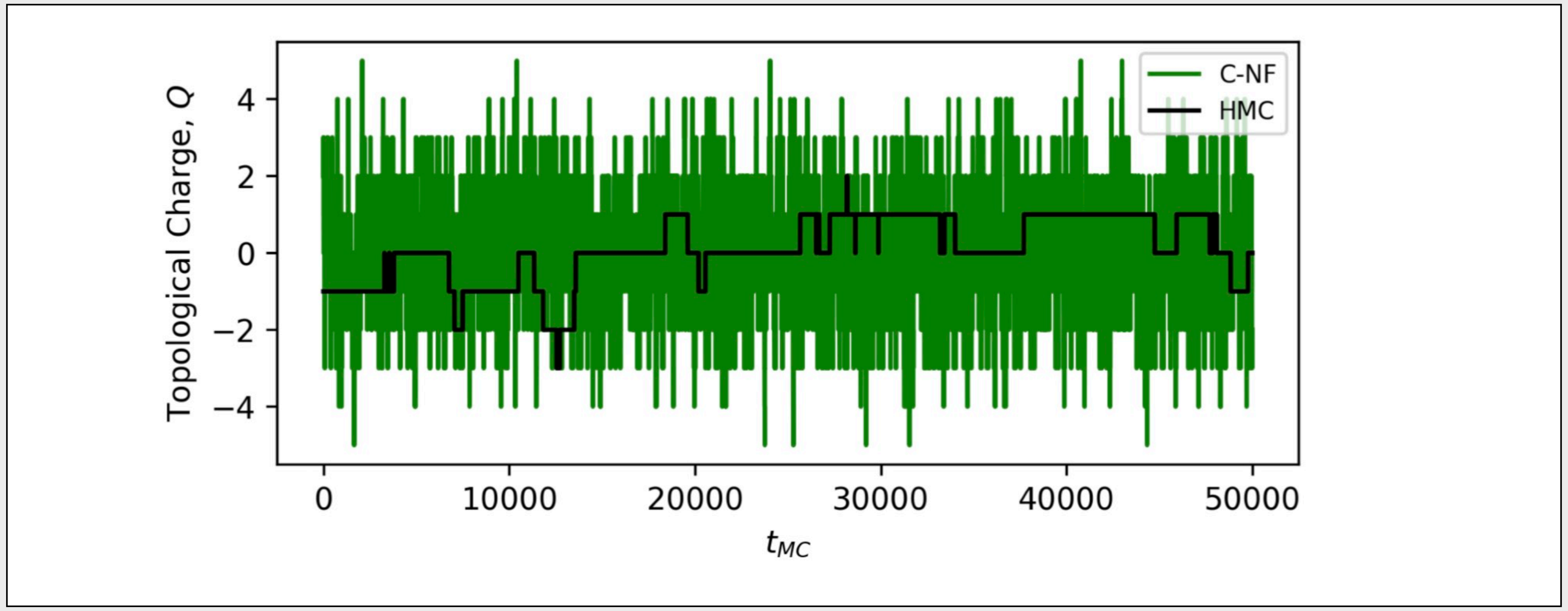
$plaquette\ dimensions\ 3 \times 3$

Actual flow will occur in the plaquette level

We a conditional model on parameters $\beta_S : \{1.0, 1.5, 1.8, 2, 2.2, 2.5, 2.8, 3, 3.2, 3.5\}$

Autocorrelation in topological charge





- A constant autocorrelation over the action parameter, in the C-NF model.
- At much high values HMC completely fails to generate significant ensemble.

Thank you