Sampling $\mathrm{SU}(3)$ pure gauge theory with Stochastic Normalizing Flows

Alessandro Nada

Università degli Studi di Torino

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in collaboration with

Andrea Bulgarelli and Elia Cellini

Critical slowing down in lattice gauge theory

Long autocorrelation times characterize several observables when $a \to 0$

Typical example are **topological observables**: for $a \to 0$ sectors characterized by different values of the topological charge Q emerge

Using standard MCMC algorithms the transition between these sectors is strongly suppressed

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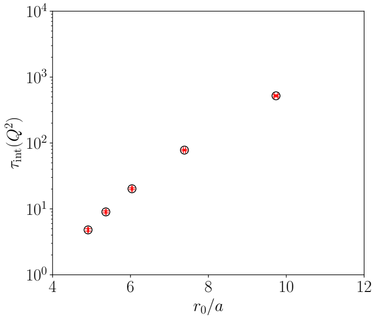
This talk: focus on $\mathrm{SU}(3)$ in 4 dimensions

Update algorithm of choice: 1 heat-bath step + 4 over-relaxation steps

Objective: mitigate freezing at $\beta = 6.5$ ($r_0/a \sim 11$)

$$\tau_{\mathrm{int}}(Q^2) \sim 10^3$$



[Plot courtesy of C. Bonanno]

Re-framing critical slowing down: flowing from one distribution to the other

Flow-based approach

mapping between the target $p(\phi)$ and some tractable distribution $q_0(z)$

$\rightarrow$ novel approach to fight critical slowing down

Lots of progress in Normalizing Flows in the last 5 years!

$\rightarrow$ see **R. Abbott**'s and **K. Javad**'s talks in this session
$+$ **Tej's plenary from Lattice23**

However: NFs do not appear to scale well with the volume (i.e. with the degrees of freedom)

But: same approach is possible stochastically! $\rightarrow$ better scaling?

Out-of-equilibrium Monte Carlo evolutions

Out-of-equilibrium evolutions

sampling each consecutive step from a sequence of distributions

$$q_0 \simeq e^{-S_{c(0)}} \to e^{-S_{c(1)}} \to \cdots \to p \simeq e^{-S_{c(n_{\mathrm{step}})}}$$

Out-of-equilibrium evolutions

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$$q_0 \simeq e^{-S_{c(0)}} \to e^{-S_{c(1)}} \to \cdots \to p \simeq e^{-S_{c(n_{\mathrm{step}})}}$$

- $c(n)$ is a parameter of the action $S_{c(n)}$ of the model
- start **at equilibrium** from a distribution $q_0 = e^{-S_{c(0)}}/Z_0$, the **prior**
- n_{step} intermediate steps
- at each step: MC update with transition probability $P_{c(n)}(U_n \to U_{n+1})$
- $P_{c(n)}$ changes along the evolution according to the **protocol** $c(n)$
- end at the **target** probability distribution $p = e^{-S_{c(n_{\mathrm{step}})}}/Z_{n_{\mathrm{step}}} \equiv e^{-S}/Z$

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"forward" transition probability

$$\mathcal{P}_{\mathrm{f}}[U_0, \ldots, U] = \prod_{n=1}^{n_{\mathrm{step}}} P_{c(n)}(U_{n-1} \to U_n)$$

Crooks' theorem

Crooks' theorem for MCMC **[Crooks; 1999]**: if the update algorithm satisfies detailed balance

$$\frac{q_0(U_0)\mathcal{P}_\mathrm{f}[U_0,\dots,U_{n_\mathrm{step}}]}{p(U)\mathcal{P}_\mathrm{r}[U_{n_\mathrm{step}},\dots,U_0]} = \frac{q_0(U_0)\prod_{n=1}^{n_\mathrm{step}} P_{c(n)}(U_{n-1}\to U_n)}{p(U_{n_\mathrm{step}})\prod_{n=1}^{n_\mathrm{step}} P_{c(n)}(U_n\to U_{n-1})} = \exp(W-\Delta F)$$

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with the generalized **work**

$$W = \sum_{n=0}^{n_\mathrm{step}-1}\left\{S_{c(n+1)}[U_n] - S_{c(n)}[U_n]\right\}$$

and the **free energy** difference

$$\exp(-\Delta F) = \frac{Z_{c(n_\mathrm{step})}}{Z_{c(0)}}$$

Jarzynski's equality for MCMC

Integrating over all paths gives

$$\int [\mathrm{d}U_0 \dots \mathrm{d}U_{n_{\mathrm{step}}}] q_0(U_0) \mathcal{P}_{\mathrm{f}}[U_0, \dots, U_{n_{\mathrm{step}}}] \exp(-(W - \Delta F)) = 1$$

Formal derivation of **Jarzynski's equality [Jarzynski; 1997]** for MCMC

$$\langle \exp(-W) \rangle_{\mathrm{f}} = \exp(-\Delta F) = \frac{Z}{Z_0}$$

Ratio of partition functions computed directly with an average over "forward" non-equilibrium evolutions

→ **see talk by A. Bulgarelli (Tue 14:35)**

Jarzynski's equality for MCMC

Integrating over all paths gives

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$\rightarrow$ **see talk by A. Bulgarelli (Tue 14:35)**

Using Jensen's inequality $\langle \exp x \rangle \geq \exp \langle x \rangle$

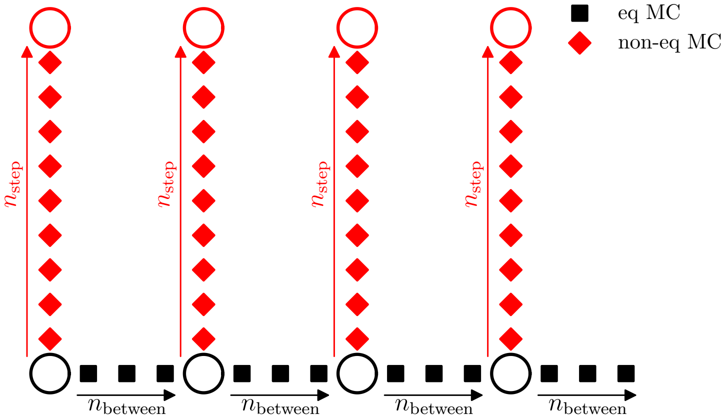
$$\langle W \rangle_{\mathrm{f}} \geq \Delta F$$

$\rightarrow$ **Second Law of Thermodynamics**

The same derivation holds if you want to compute v.e.v. of an observable for the target distribution p

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} \, \exp(-W) \rangle_{\mathrm{f}}}{\langle \exp(-W) \rangle_{\mathrm{f}}} = \langle \mathcal{O} \, \exp(-W_d) \rangle_{\mathrm{f}}$$

A non-equilibrium paradigm to perform MCMC



How far are we from equilibrium?

However we can measure the **similarity of forward and reverse** processes

$$\tilde{D}_{\mathrm{KL}}(q_0\mathcal{P}_{\mathrm{f}}\|p\mathcal{P}_{\mathrm{r}}) = \int [\mathrm{d}U_0 \ldots \mathrm{d}U]\, q_0(U_0)\mathcal{P}_{\mathrm{f}}[U_0, \ldots, U] \log \frac{q_0(U_0)\mathcal{P}_{\mathrm{f}}[U_0, \ldots, U]}{p(U)\mathcal{P}_{\mathrm{r}}[U, U_{n_{\mathrm{step}}-1}, \ldots, U_0]}$$

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Clear "thermodynamic" interpretation

$$\tilde{D}_{\mathrm{KL}}(q_0\mathcal{P}_{\mathrm{f}}\|p\mathcal{P}_{\mathrm{r}}) = \langle W\rangle_{\mathrm{f}} + \log\frac{Z}{Z_0} = \underbrace{\langle W\rangle_{\mathrm{f}} - \Delta F \geq 0}_{\text{Second Law of Thermodynamics!}}$$

$\rightarrow$ measure of how reversible the process is!

Upper bound for the divergence used for NFs

$$\tilde{D}_{\mathrm{KL}}(q\|p) \leq \tilde{D}_{\mathrm{KL}}(q_0\mathcal{P}_{\mathrm{f}}\|p\mathcal{P}_{\mathrm{r}})$$

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Another figure of merit is the Effective Sample Size

$$\mathrm{E\hat{S}S} = \frac{\langle \exp(-W)\rangle_{\mathrm{f}}^2}{\langle \exp(-2W)\rangle_{\mathrm{f}}}$$

Out-of-equilibrium evolutions in β for $\mathrm{SU}(3)$ in 4 dimensions

Non-equilibrium evolutions in β

Evolution from thermalized MC at β_0 to a target β

$$q_0 \simeq e^{-S_{\beta(0)}} \to e^{-S_{\beta(1)}} \to \cdots \to p \simeq e^{-S_{\beta(n_{\mathrm{step}})}}$$

Objectives

- Analyze scaling with volume $(L/a)^4$
- Set MCMC standard for flow-based approach
- No topology yet (charge not frozen yet)

Setup

- Increasingly large lattices, from $L/a = 10$ to $L/a = 20$
- "Jump" in β:

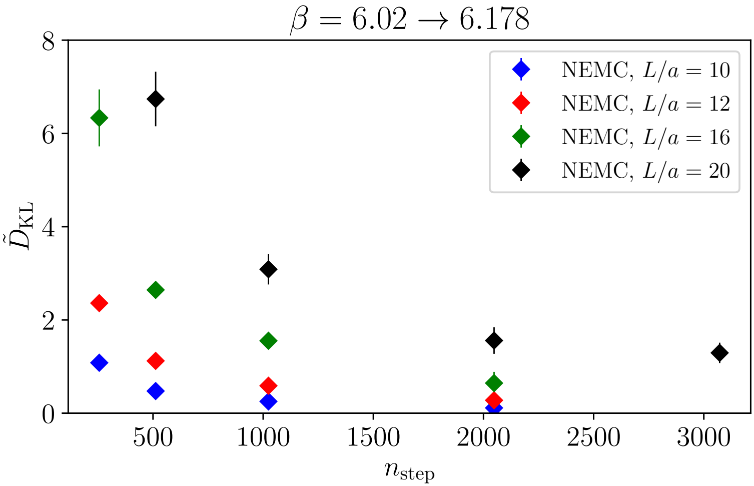
$$6.02 \to 6.178$$

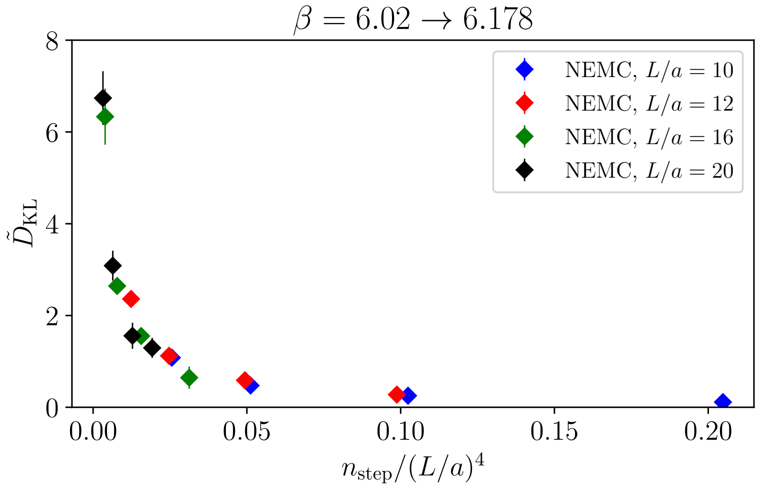
  corresponding to $(1.8\mathrm{fm})^4 \to (1.4\mathrm{fm})^4$ for $L/a = 20$

This work: inverse coupling increased linearly

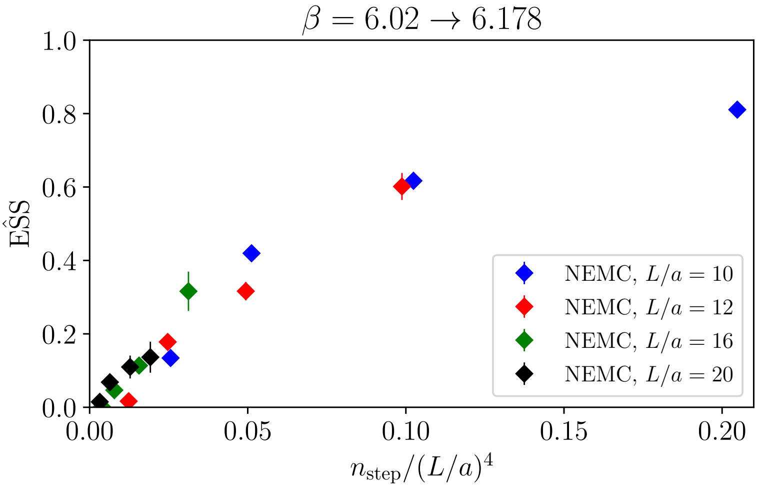
$$\beta(n) = \beta_0 + (\beta - \beta_0)\frac{n}{n_{\mathrm{step}}}$$

Evolutions in β: volume scaling




$\beta = 6.02 \to 6.178$
$\tilde{D}_{\mathrm{KL}}$
$n_{\mathrm{step}}/(L/a)^4$
0
2
4
6
8
0.00
0.05
0.10
0.15
0.20
NEMC, $L/a = 10$
NEMC, $L/a = 12$
NEMC, $L/a = 16$
NEMC, $L/a = 20$

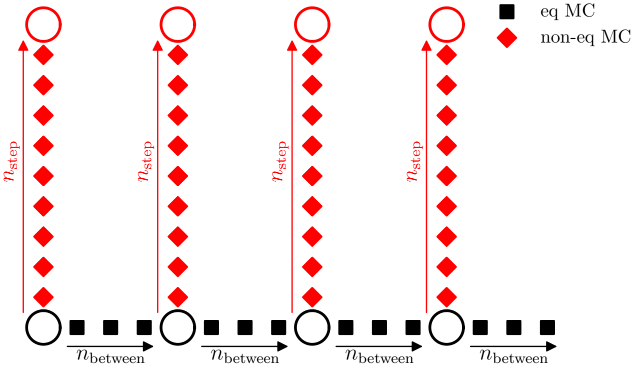
Evolutions in β: volume scaling



Stochastic Normalizing Flows

SNFs as systematic improvement of non-equilibrium evolutions

What if you introduce the same transformations used in NFs **between** the non-equilibrium Monte Carlo updates?



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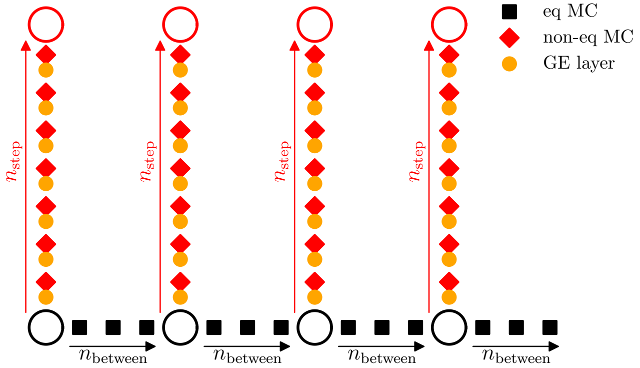
Stochastic Normalizing Flows (introduced in **[Wu et al.; 2020]**)

$$U_0 \xrightarrow{g_1} g_1(U_0) \xrightarrow{P_{c(1)}} U_1 \xrightarrow{g_2} g_2(U_1) \xrightarrow{P_{c(2)}} U_2 \xrightarrow{g_3} \dots \xrightarrow{P_{c(n_{\text{step}})}} U_{n_{\text{step}}}$$



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The (generalized) work now is

$$W = \sum_{n=0}^{n_\mathrm{step}-1} \underbrace{S_{c(n+1)}(g_n(U_n)) - S_{c(n)}(g_n(U_n))}_{\text{stochastic}} - \underbrace{\log|\det J_n(U_n)|}_{\text{deterministic}}$$

- use gauge-equivariant layers to effectively decrease n_step
- how to do training? advantages from the architecture
- same scaling with the volume?

Implementation of the coupling layers introduced in **[Nagai and Tomiya; 2021]** and the link-level flow used in **[Abbott et al.; 2023]**

Essentially a stout-smearing transformation **[Morningstar and Peardon; 2003]** with masks to make it invertible (and compute $\log J$)

$$U'_\mu(x) = g_l(U_\mu(x)) = \exp\left(Q^{(l)}_\mu(x)\right)\, U_\mu(x)$$

with the algebra-valued

$$Q^{(l)}_\mu(x) = 2\left[\Omega^{(l)}_\mu(x)\right]_{\mathrm{TA}}$$

$$\Omega_\mu(x) = \underbrace{C_\mu(x)}_{\text{frozen}}\underbrace{U^\dagger_\mu(x)}_{\text{active}}$$

Sum of frozen staples

$$C_\mu(x) = \sum_{\nu\neq\mu} \rho\, \underbrace{S_{\mu\nu}(x)}_{\text{staple}}$$

Architecture: (1 gauge-equivariant + 1 full MC update) $\times n_{\mathrm{step}}$

Training: minimizing $\tilde{D}_{\mathrm{KL}}(q_0 \mathcal{P}_{\mathrm{f}} \| p \mathcal{P}_{\mathrm{r}}) = \langle W \rangle_{\mathrm{f}} + \mathrm{const}$

Architecture: (1 gauge-equivariant + 1 full MC update) $\times n_{\text{step}}$

Training: minimizing $\tilde{D}_{\text{KL}}(q_0\mathcal{P}_{\text{f}}\|p\mathcal{P}_{\text{r}}) = \langle W\rangle_{\text{f}} + \text{const}$

Short trainings: 200-1000 epochs

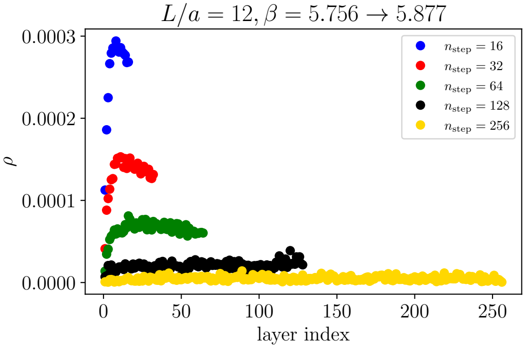
Memory issues for large n_{step} and large volumes

Practical solution: train each layer separately during the non-equilibrium evolution $\rightarrow$ reminiscent of CRAFT **[Matthews at al.; 2022]**

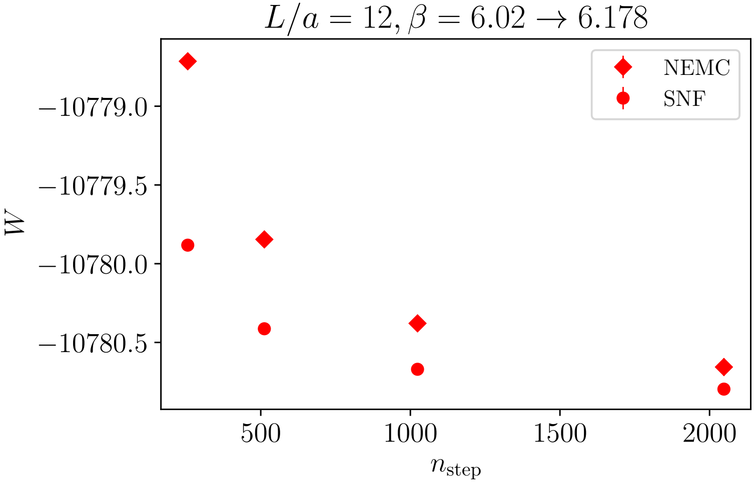
Heavy use of **transfer learning** for each $\beta_0 \rightarrow \beta$ evolution:

- training only at small volumes
- training only with small n_{step}: global interpolation of ρ

No retraining!



Improvements over purely stochastic approach



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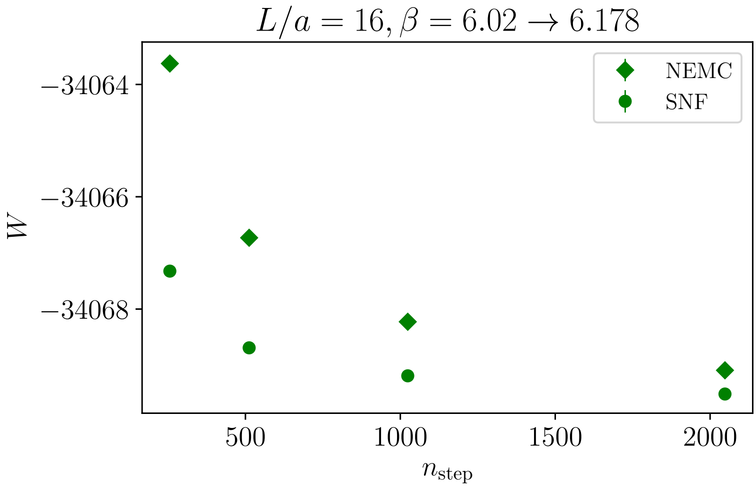

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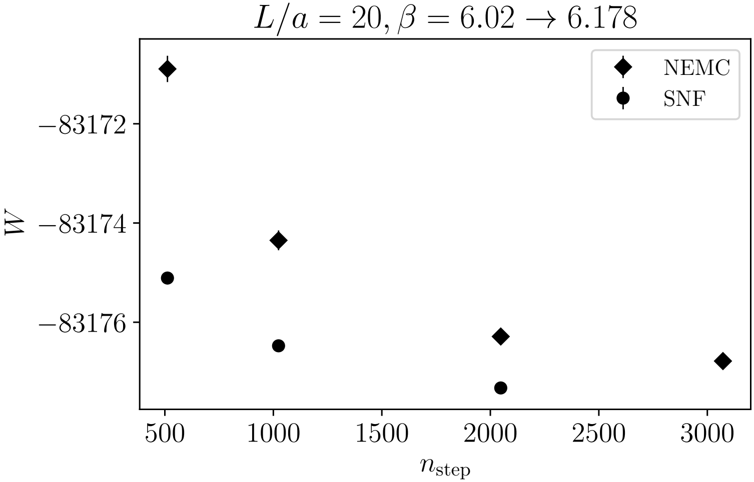
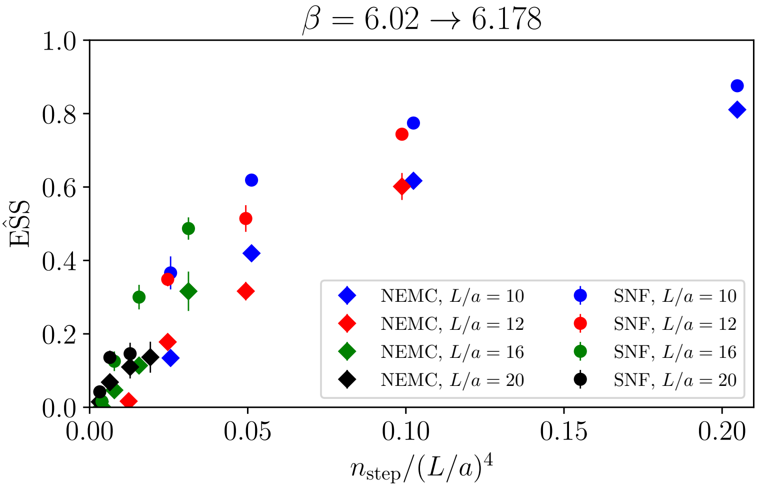


SNF evolutions in β: volume scaling



Conclusions and future prospects

Stochastic approach guarantees a clear scaling with the degrees of freedom

$$n_{\mathrm{step}} \sim \mathrm{d.o.f.} \rightarrow \text{fixed } \tilde{D}_{\mathrm{KL}} \text{ or } \mathrm{ESS}$$

while providing a thermodynamic understanding of the flow

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while providing a thermodynamic understanding of the flow

Overall strategy

systematically improve on stochastic approach by machine-learning deterministic transformations between MC steps

Future improvements

Better protocols (huge literature from non-eq SM): only linear protocols were used in this work!

Better and deeper layers: include larger loops beyond the plaquette + ρ as a neural network **[Abbott et al.; 2023]**

Future implementations

Implement **SNF for evolutions in the BC**

$\to$ **see poster by D. Vadacchino**

Push **SNFs/evolutions in β** at finer lattice spacings

Thank you for your attention!

Applications of Jarzynski's equality in Lattice Field Theory

Several applications in the last 8 years!

- calculation of the interface free-energy in the Z_2 gauge theory **[Caselle et al.; 2016]**
- $\mathrm{SU}(3)$ pure gauge equation of state in 4d from the pressure **[Caselle et al.; 2018]**
- renormalized coupling for $\mathrm{SU}(N)$ YM theories **[Francesconi et al.; 2020]**
- entanglement entropy **[Bulgarelli and Panero; 2023]**
- connection with Stochastic Normalizing Flows: ϕ^4 scalar field theory **[Caselle et al.; 2022]** and Nambu-Goto effective string model **[Caselle et al.; 2023]**
- Topological unfreezing for $\mathrm{CP}(N-1)$ model **[Bonanno et al.; 2023]**

The effective sample size

Effective Sample Size: defined in general as the ratio between the "theoretical" variance and the actual variance of the NE observable

$$\frac{\mathrm{Var}(\mathcal{O})_{\mathrm{NE}}}{n} = \frac{\mathrm{Var}(\mathcal{O})_p}{n\,\mathrm{ESS}}$$

but difficult to compute

We use the (customary) approximate estimator

$$\mathrm{E\hat{S}S} = \frac{\langle \exp(-W)\rangle_{\mathrm{f}}^2}{\langle \exp(-2W)\rangle_{\mathrm{f}}} = \frac{1}{\langle \exp(-2W_d)\rangle_{\mathrm{f}}}$$

Easy to understand in terms of the variance of $\exp(-W)$:

$$\mathrm{Var}(\exp(-W)) = \left(\frac{1}{\mathrm{E\hat{S}S}} - 1\right)\exp(-2\Delta F) \geq 0$$

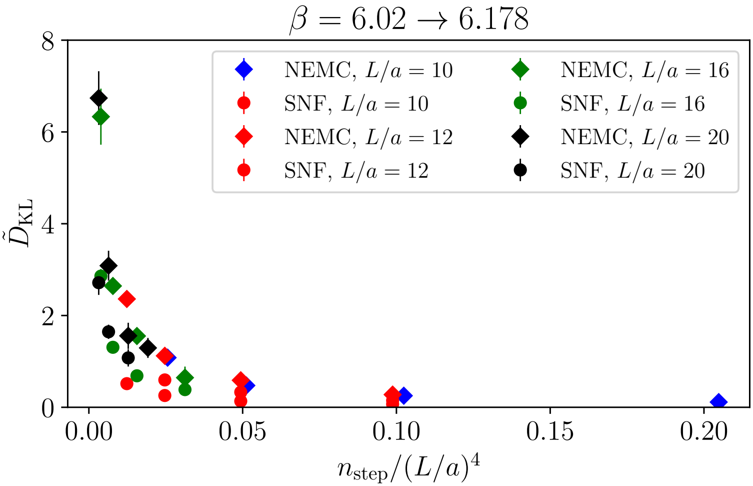
which leads to

$$0 < \mathrm{E\hat{S}S} \leq 1$$

How to sample frozen topological observables at β_{target} on a L^4 lattice?

	Evolution in the boundary conditions	**Evolution in β**
Prior	thermalized Markov Chain at β_{target} with OBC on a L_d^3 defect	thermalized Markov Chain at $\beta_0 < \beta_{\mathrm{target}}$ ($a_0 > a_{\mathrm{target}}$)
Protocol	Gradually switch on PBC	Gradually increase β (compress the volume)
d.o.f.	$\sim (L_d/a)^3$	$\sim (L/a)^4$
Intermediate sampling	—	possible at any intermediate β

SNF evolutions in β: volume scaling



The Second Law of Thermodynamics

Clausius inequality for an (isothermal) transformation from state A to state B

$$\frac{Q}{T} \leq \Delta S$$

If we use

$$\begin{cases} Q = & \Delta E - W \quad \text{(First Law)} \\ F \stackrel{\text{def}}{=} & E - ST \end{cases}$$

the Second Law becomes

$$W \geq \Delta F$$

where the equality holds for reversible processes.

Moving from thermodynamics to statistical mechanics we know that actually

$$\langle W \rangle_f \geq \Delta F = F_B - F_A$$

for a given "forward" process f from A to B

A connection to traditional reweighting

A typical reweighting procedure is meant to sample a distribution p using a (close enough) distribution q_0. It can be written as

$$\langle \mathcal{O} \rangle_{\mathrm{RW}} = \frac{\langle \mathcal{O}(\phi) \exp(-\Delta S) \rangle_{q_0}}{\langle \exp(-\Delta S) \rangle_{q_0}}$$

It is just Jarzynski's equality for $n_{\mathrm{step}} = 1$, see the work

$$W = \sum_{n=0}^{n_{\mathrm{step}}-1} \left\{ S_{c(n+1)}\left[\phi_n\right] - S_{c(n)}\left[\phi_n\right] \right\} = \Delta S(\phi_0)$$

with ϕ_0 sampled from q_0

- It's important to note that there is no issue with the fact that ΔS itself can be large
- The real issue is that the *distribution* of ΔS (and in general of W) can lead to an extremely poor estimate of $\Delta F \rightarrow$ highly inefficient sampling
- The exponential average can be tricky when very far from equilibrium!

A common framework: Stochastic Normalizing Flows

Jarzynski's equality is the same formula used to extract Z in NFs

$$\frac{Z}{Z_0} = \langle \tilde{w}(\phi) \rangle_{\phi \sim q_N} = \langle \exp(-W) \rangle_{\mathrm{f}}$$

The exponent of the weight is always of the form (note that for NFs $\langle \dots \rangle_{\phi \sim q_N} = \langle \dots \rangle_{\mathrm{f}}$)

$$W(\phi_0, \dots, \phi_N) = S(\phi_N) - S_0(\phi_0) - Q(\phi_1, \dots, \phi_N)$$

Normalizing Flows

$$\phi_0 \to \phi_1 = g_1(\phi_0) \to \cdots \to \phi_N$$

$$\text{"} Q \text{"} = \log J = \sum_{n=0}^{N-1} \log |\det J_n(\phi_n)|$$

stochastic non-equilibrium evolutions

$$\phi_0 \overset{P_{c(1)}}{\to} \phi_1 \overset{P_{c(2)}}{\to} \dots \overset{P_{c(N)}}{\to} \phi_N$$

$$Q = \sum_{n=0}^{N-1} S_{c(n+1)}(\phi_{n+1}) - S_{c(n+1)}(\phi_n)$$

Stochastic Normalizing Flows (introduced in **[Wu et al.; 2020]**)

$$\phi_0 \to g_1(\phi_0) \overset{P_{c(1)}}{\to} \phi_1 \to g_2(\phi_1) \overset{P_{c(2)}}{\to} \dots \overset{P_{c(N)}}{\to} \phi_N$$

$$Q = \sum_{n=0}^{N-1} S_{c(n+1)}(\phi_{n+1}) - S_{c(n+1)}(g_n(\phi_n)) + \log |\det J_n(\phi_n)|$$

Taking cues from the $\mathrm{SU}(3)$ e.o.s.

Large-scale application: computation of the $\mathrm{SU}(3)$ equation of state **[Caselle et al.; 2018]**

Goal: extract the pressure with Jarzynski's equality

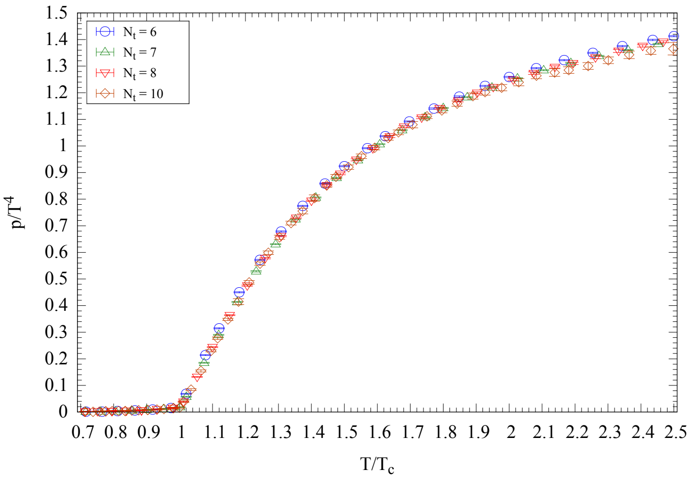
$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \left(\frac{N_t}{N_s}\right)^3 \log\langle e^{-W_{\mathrm{SU}(N_c)}}\rangle_{\mathrm{f}}$$

evolution in β_g (inverse coupling) $\rightarrow$ changes lattice spacing a $\rightarrow$ changes temperature $T = 1/(aN_t)$

Prior: thermalized Markov chain at a certain $\beta_g^{(0)}$

For systems with many d.o.f. (i.e. large volumes), JE works when N is large, i.e. evolution is slow (and expensive)

SU(3) e.o.s. with Jarzynski's equality



Large volumes (up to $160^3 \times 10$) and very fine lattice spacings $\beta \simeq 7$