Full QCD simulations with milder topological freezing via Parallel Tempering on Boundary Conditions

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Lattice QCD at the large scale on exascale computing facilities

Based on:
"*Full QCD with milder topological freezing*"
CB, G. Clemente, M. D'Elia, L. Maio, L. Parente
JHEP **08** (2024) 236 [2404.14151]

Markov Chan Monte Carlo and Critical Slowing Down

Markov Chain Monte Carlo simulations experience
Critical Slowing Down approaching the continuum limit $a \to 0$

$$\tau(\mathcal{O}) \sim \xi_{\rm L}^z \underset{a\to 0}{\to} \infty \qquad\qquad \xi_{\rm L} = \xi/a$$

$\tau(\mathcal{O}) \to$ updating steps to generate two decorrelated "measures" of $\mathcal{O}$

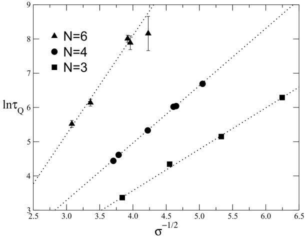
Typically $z \sim 2$ (e.g., Wilson loop)

Not for **Topological Charge** Q:
divergence much more severe

Alles et al. PLB 389 (1996) 107 [hep-lat/9607049]

Del Debbio et al. PLB 594 (2004) 315 [hep-lat/0403001]

ALPHA collab. NPB 845 (2011) 93 [1009.5228]



PLB 594 (2004) 315 [hep-lat/0403001]

Topological Freezing: Markov Chain remains trapped in a fixed topological sector for a long Monte Carlo time.
Standard algorithms (heat-bath, HMC) lose ergodicity as $a \to 0$

Impact of Topological Freezing

Topological freezing prevents proper sampling of $\mathcal{P}(Q)$,

biasing topological quantities, e.g., topological susceptibility $\chi = \frac{\langle Q^2 \rangle}{V}$

Freezing impacts non-topological quantities too, e.g., hadron masses (same considerations apply to n-point correlation functions):

$$\frac{M_Q - M}{M} = \frac{m_2}{\chi}\frac{1}{V}\left[1 + \mathcal{O}\left(\frac{1}{V}\right)\right] \qquad M(\theta) = M\left[1 + m_2\theta^2 + \mathcal{O}(\theta^4)\right]$$

Masses at fixed topology M_Q are biased wrt actual M by $\mathcal{O}\left(\frac{1}{V}\right)$ correction

Brower et al. PLB 560 (2003) 64–74 [hep-lat/0302005] Aoki et al. PRD 76 (2007) 054508 [0707.0396]

After the flow, the energy density $E(t_{\text{flow}})$ becomes highly correlated with the topological background of gauge fields:

- Impact on scale setting (t_0, w_0, …) Bergner et al. EPJP 130 (2015) 11 229 [1411.6995]
- Impact on renormalized coupling Fritzsch et al. PoS Lattice2013 (2014) 461 [1311.7304]

QCD topological susceptibility as a function of the temperature: important for theoretical and phenomenological reasons.

- Dilute Instanton Gas Approximation: $\chi(T) \underset{T\to\infty}{\sim} T^{-8}\ (N_{\rm f}=3)$

What is the size of non-perturbative corrections to DIGA in the high-temperature phase of QCD?

- Axion solution to the strong-CP problem:

$$f_a\, m_a^{(\rm eff)}(T) = \sqrt{\chi(T)}$$

Peccei–Quinn PRL 38 (1977) 1440   Wilczek PRL 40 (1978) 279   Weinberg PRL 40 (1978) 223

Axion Dark Matter: $m_a^{(\rm eff)}(T)$ determines axion cosmological evolution. Necessary input to put a **theoretical** upper bound on f_a.

Preskill et al. PLB 120 (1983) 127   Abbott–Sikivie PLB 120 (1983) 133   Dine-Fischler PLB 120 (1983) 137

In turn, bounding f_a constrains the cold ($T=0$) axion mass: important input for axion detection experiments.

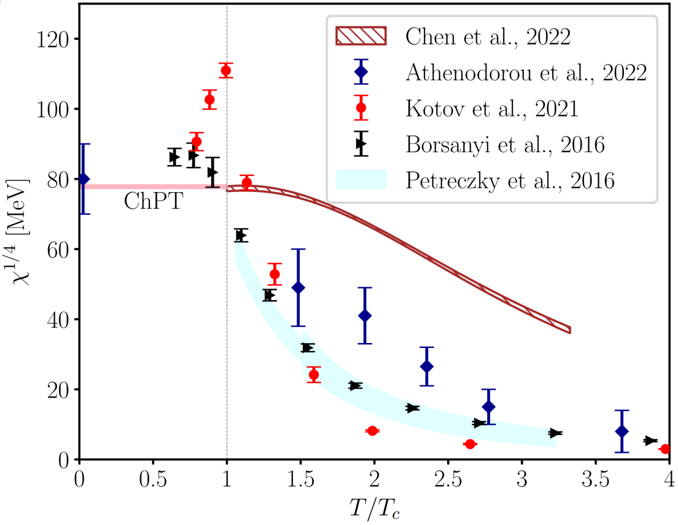


Figure from Aarts et al. PPNP 133 (2023) 104070 [2301.04382] – Sec. 6 (Editor: CB)

No clear consensus yet. Only established fact: $\chi \sim (T/T_c)^{-8}$ (DIGA prediction) describes $\chi(T)$ for $T \gtrsim 300$ MeV $\simeq 2\,T_c$ (but larger prefactor)

Main issue: determining $\chi(T)$ in full QCD at finite temperature is **hard**.

- Most calculations use non-chiral fermions $\Longrightarrow$ large lattice artifacts (several orders of magnitude) Bonati et al. JHEP 03 (2016) 155 [1512.06746]

Systematics on continuum limit under control only with **sufficiently fine lattice spacings** $\Longrightarrow$ Topological Freezing

- At finite T, lattice artifacts controlled by $aT = 1/N_t$.

Simulating very **high temperature with reasonable cut-off effects** require **very fine lattice spacings**.

For example: $N_t = 16$, $T = 1$ GeV $\Longrightarrow$ $a \sim 0.012$ fm
$\Longrightarrow$ Topological Freezing (all direct studies limited to $T < 600$ MeV)

- $\chi \sim (T/T_c)^{-8} \Longrightarrow \langle Q^2 \rangle = \chi V \ll 1$ soon after the chiral crossover.

For example: $T = 570$ MeV, $L_s = 1.5$ fm, $64^3 \times 16$
$\chi^{1/4} \sim 14$ MeV $\Longrightarrow \langle Q^2 \rangle \sim 6 \times 10^{-4}$ CB et al. JHEP 08 (2024) 236 [2404.14151]

Due to the suppression of χ, topological fluctuations are **rare events**
High T $\Longrightarrow$ $\mathcal{P}(Q)$ narrow distribution centered around zero
Issue unrelated to topological freezing! Physical origin, not algorithmic

Parallel Tempering on Boundary Conditions

Several proposals put forward to tackle topological freezing
(not an exhaustive list)

Lüscher & Schaefer CPC 184 (2013) 519 [1206.2809] Laio et al. JHEP 07 (2016) 089 [1508.07270]

Lüscher EPJWC 175 (2018) 01002 [1707.09758] Cossu et al. EPJC 81 (2021) 4, 375

Abbott et al. (2023) [2305.02402] Eichhorn et al. PRD 109 (2024) 114504 [2307.04742]

REVIEWS: Boyle PoS LATTICE2023 (2024) 122 [2401.16620] Finkenrath PoS EuroPLEx2023 (2024) 009

This talk:

Parallel Tempering on Boundary Conditions

This proposal has proved to be very effective in mitigating topological freezing, both in $2d$ models and in $4d$ pure-gauge theories, both at zero and finite temperature.

I will discuss recent implementation in state-of-the-art QCD simulations

Our Open Source GPU code: `GPU-LQCD/OpenStaPLE`

- Originally proposed by M. Hasenbusch Hasenbusch PRD 96 (2017) 054504 [1706.04443]
I have since then extensively used it in the last few years for several studies

- Topological susceptibility and higher-order moments of the topological charge distribution up to Next-to-Leading Order (NLO) in θ and $1/N$

Berni, CB, D'Elia PRD 100 (2019) 114509 [1911.03384] CB, Bonati, D'Elia JHEP 03 (2021) 111 [2012.14000]

- Impact of topological freezing on glueball mass computations

CB, D'Elia, Lucini, Vadacchino PLB 833 (2022) 137281 [2205.06190]

- Moments of the topological charge correlator up to NLO in p^2 and $1/N$

CB PRD 107 (2023) 1, 014514 [2212.02330]

- Deconfinement temperature up to NLO in θ and $1/N$

CB, D'Elia, Verzichelli JHEP 02 (2024) 156 [2312.12202]

- Lightest glueball mass and string tension up to NLO in θ and $1/N$

CB, Bonati, Papace, Vadacchino JHEP 05 (2024) 163 [2402.03096]

- Impact of topological freezing on the determination of the renormalized strong coupling using gradient flow and step scaling

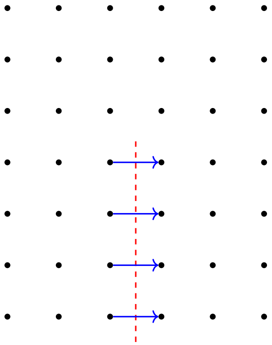
CB, Dasilva Golán, D'Elia, García Pérez, Giorgieri EPJC 84 (2024) 9, 916 [2403.13607]

- **This talk**: first implementation in full QCD with dynamical fermions

CB, Clemente, D'Elia, Maio, Parente JHEP 08 (2024) 236 [2404.14151]

PTBC enjoys improvement of Open Boundaries Lüscher & Schaefer CPC 184 (2013) 519 [1206.2809] while avoiding its main shortcoming (boundary effects)

- consider a collection of N_r lattice replicas
- replicas differ for boundary conditions on **small** sub-region: *the defect*
- each replica is updated with standard methods
- after updates, propose swaps among configurations via Metropolis test
- translation of periodic replica to effectively move around position of defect



Links crossing the defect: $\beta \to \beta \cdot c(r)$

Periodic: $c(0) = 1$ Open: $c(N_r - 1) = 0$
Interpolating replicas: $0 < c(r) < 1$

$c(r)$ tuned to achieve almost uniform swap acceptance
$\to$ configuration does random walk among replicas

Improved decorrelation of Q with open boundaries transferred towards periodic replica

Observables computed on **periodic** replica $\to$ avoids boundary effects

- Fermion determinant does not participate to tempering of boundary conditions.
Our proposal is general and can be applied to any fermion discretization (we chose rooted stout-smeared staggered)

$$K_{\mu}^{(r)}(x) = \begin{cases} c(r), & \mu = 1, \quad x_1 = N_s - 1, \quad 0 \le x_0, x_2, x_3 < L_d, \\ 1, & \text{elsewhere}, \end{cases}$$

$$Z_{\mathrm{LQCD}}^{(r)} = \int [\mathrm{d}U_r] \mathrm{e}^{-S_{\mathrm{YM}}^{(r)}[U_r]} \det\left\{\mathcal{M}_l^{(\mathrm{stag})}[U_r]\right\}^{\frac{1}{2}} \det\left\{\mathcal{M}_s^{(\mathrm{stag})}[U_r]\right\}^{\frac{1}{4}},$$

$$U_r = \text{gauge conf of } r^{\text{th}} \text{ replica}$$

$$S_{\mathrm{YM}}^{(r)}[U_r] = -\frac{\beta}{3} \sum_{x,\mu\neq\nu} \left\{ \frac{5}{6} K_{\mu\nu}^{(1\times1)}(x;r) \mathcal{P}_{\mu\nu}^{(1\times1)}(x;r) - \frac{1}{12} K_{\mu\nu}^{(1\times2)}(x;r) \mathcal{P}_{\mu\nu}^{(1\times2)}(x;r) \right\}$$

$$K_{\mu\nu}^{(n\times m)}(x;r) = \text{product of } K_{\mu}^{(r)}(x) \text{ along } n\times m \text{ closed path}$$
$$\mathcal{P}_{\mu\nu}^{(n\times m)}(x;r) = \text{product of } U_{\mu}^{(r)}(x) \text{ along } n\times m \text{ closed path}$$

- Since observables are computed on the periodic replica, χ measured from $\langle Q^2 \rangle$ (clover discr. after smoothing)

High T: $\langle Q^2 \rangle \ll 1 \to$ topological fluctuations are rare events

At high temperatures this issue is **on top of Topological Freezing**.

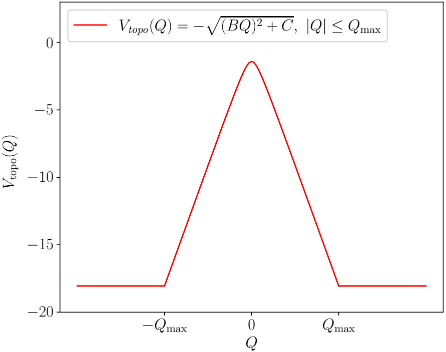
Strategy: **Multicanonic Simulations** (easily combined with PTBC)

$$S_{\mathrm{YM}}[U] \longrightarrow S_{\mathrm{YM}}[U] + V_{\mathrm{topo}}(Q_{\mathrm{mc}}[U])$$

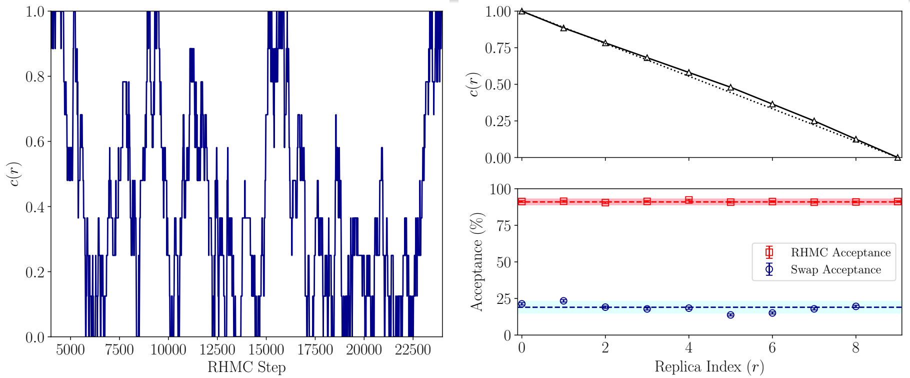
Idea: add bias potential to gauge action to enhance the probability of visiting suppressed topological sectors.

Expectation value wrt original distribution recovered through reweighting

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O}\, \mathrm{e}^{V_{\mathrm{topo}}(Q_{\mathrm{mc}})} \rangle_{\mathrm{mc}}}{\langle \mathrm{e}^{V_{\mathrm{topo}}(Q_{\mathrm{mc}})} \rangle_{\mathrm{mc}}}$$



$T = 570$ MeV $\simeq 3.7\,T_c$ – $a \simeq 0.02145$ fm – $64^3 \times 16$

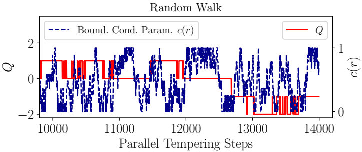


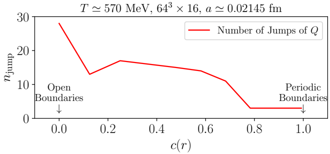
Short test runs are sufficient to tune $c(r)$
to achieve $P_{\mathrm{swap}} \sim 20\%$ almost uniform

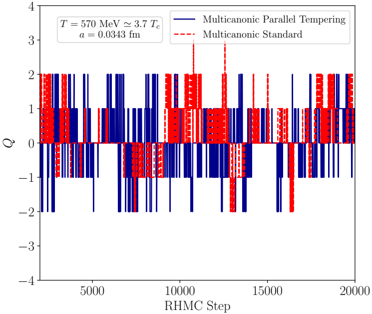
Tuned $c(r)$ appear to deviate from simple linear behavior between
$0.25 < c(r) < 0.6$

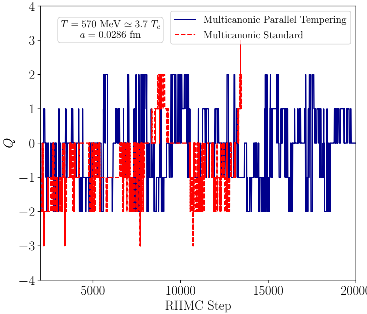
Also HMC acceptance turns out to be constant ($\sim 90\%$) with this choice

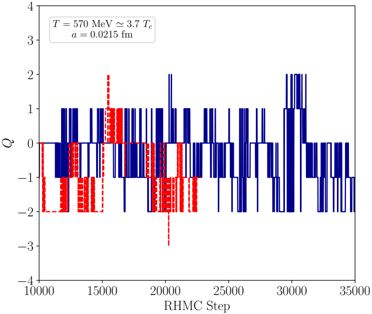
Q-jumps happen when conf explores open boundaries during its random walk.
Non-vanishing correlation between ΔQ and $c(r)$





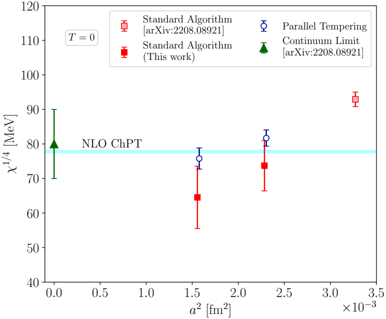


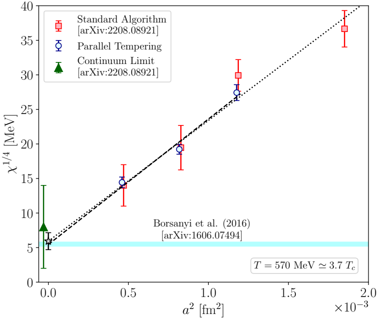




Shown lattices: $40^3 \times 10$ $48^3 \times 12$ $64^3 \times 16$ $\langle Q^2 \rangle \sim 10^{-3}$–$10^{-4}$

a [fm]	L_d	N_r	$\chi^{1/4}$ [MeV] (PTBC)	$\tau_{\rm int}(Q^2)$ (PTBC)	$\chi^{1/4}$ [MeV] (Standard)	$\tau_{\rm int}(Q^2)$ (Standard)
0.0343	1	7	28.2(1.3)	10(3)	29.9(2.3)	30(12)
0.0286	2	10	19.22(71)	27(4)	19.5(3.2)	50(10)
0.0215	2	10	14.44(77)	26(6)	14(3)	$\gtrsim 10^2$





Old continuum results have been obtained with fermionic definition of Q

Athenodorou, CB, Bonati, Clemente, D'Angelo, D'Elia et al. JHEP 10 (2022) 197 [2208.08921]

$T = 0$: $aL_d \sim 0.08$–0.1 fm High temperature: $aL_d \sim 0.03$–0.06 fm

Compatible with expectation from DIGA

$T = 0$: results at 2 finest lattice spacings compatible with NLO χPT

Continuum limit $T = 570$ MeV: $\chi^{1/4} = 6.2(1.2)$ MeV (PTBC) [$\chi^{1/4} = 8(6)$ MeV (old)]

Conclusions and future outlooks

Parallel Tempering on Boundary Conditions (PTBC) has proven to be an effective solution to mitigate topological freezing.
It has allowed substantial progress in the status of several challenging topics.

Application to full QCD simulations will allow progress in open problems e.g., QCD topological susceptibility and QCD sphaleron rate at finite T

CB et al. PRD 108 (2023) 074515 [2305.17120] PRL 132 (2024) 051903 [2308.01287]

Related ongoing projects:

- Tempering on Boundary Conditions via out-of-equilibrium evolutions (possible application to Stochastic Normalizing Flows)

  CB Nada Vadacchino JHEP 04 (2024) 126 [2402.06561] Bulgarelli Cellini Nada (2024) [2412.00200]

- Topological properties of large-N gauge theories (higher-order moments of topological charge correlator, θ-dependence of the excited spectrum)

  CB JHEP 01 (2024) 116 [2311.06646] CB et al. JHEP 05 (2024) 163 [2402.03096]

- Impact of topological freezing on scale setting, determination of Λ-parameter with gradient flow, step scaling and PTBC in SU(N) gauge theories

  See A. Giorgieri's talk @ Lattice 2024 (Liverpool)

Back-up slides

Practical implementation

Open Source GPU code: `GPU-LQCD/OpenStaPLE`

Cluster: `Leonardo` multi-GPU machine at CINECA (ranked 9^{th} in TOP500 list)

Single replica: lattice partitioned in one space-time direction (the longest) into multiple MPI ranks associated with different GPU devices.

Bonati et al. IJMPC 28 (2017) 1750063 [1701.00426] IJMPC 29 (2018) 1850010 [1801.01473]

Each replica runs same RHMC operations in SIMD fashion.
Only difference: boundary conditions at the defect, depending on replica label.

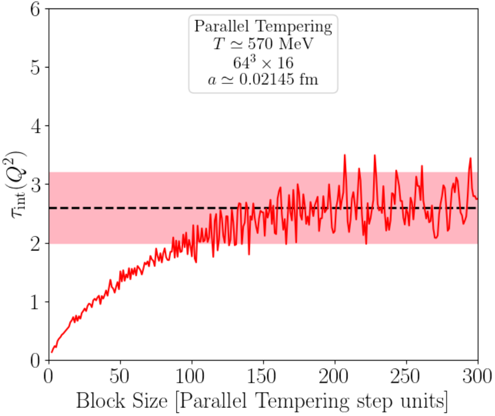
Parallelization: independent MPI communicators for each replica.
Communications only among devices associated with sub-lattices of same replica.

We do not swap configurations, just boundary conditions at the defect.
Labels identifying specific replicas are also swapped among MPI ranks.

Coordination of swaps tests: managed by a single MPI master rank, which gathers action differences from each replica pair and computes acceptances.

τ_{int} from binned analysis Del Debbio Vicari Manca PLB 594 (2004) 315-323 [hep-lat/0403001]

Berg, *Markov Chain Monte Carlo Simulations and their Statistical Analysis* p. 196–235. World Scientific Publishing, Singapore, Oct., 2004



$$\tau_{\text{int}}(Q^2) = \frac{1}{2}\left[\frac{\Delta_{\text{B}}\left(Q^2\right)}{\Delta_1\left(Q^2\right)}\right]^2 - \frac{1}{2}$$

$$\tau_{\text{int}}(Q^2) = 2.6(6) \text{ (PTBC units)}$$

$$N_r = 10$$

$$\Longrightarrow \tau_{\text{int}}(Q^2) = 26(6) \text{ (RHMC units)}$$

No PTBC: $\tau_{\text{int}}(Q^2) \gtrsim 10^2$