THE TWISTED GRADIENT FLOW STRONG COUPLING WITH PARALLEL TEMPERING ON BOUNDARY CONDITIONS

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The Gradient Flow

Renormalization procedure in which the gauge field $A_\mu(x)$ is replaced by a set of smooth, time-dependent flow fields $B_\mu(x)$ driven by the so-called "flow equations" [arXiv:1101.0963]:

$$\partial_t B_\mu(x, t) = D_\nu G_{\nu\mu}(x, t) \quad B_\mu(x, t = 0) = A_\mu(x)$$

Gauge-invariant composite observables are automatically renormalized quantities for $t > 0$

Renormalized couplings can be introduced trivially, e.g. with the energy density:

$$E(t) = \frac{1}{2} Tr \left( G_{\mu\nu}(x, t) G_{\mu\nu}(x, t) \right)$$

$$\lambda(\mu) = \mathcal{N} \left< t^2 E(t) \right> \bigg|_{\sqrt{8t}=\mu^{-1}}$$
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The Twisted Gradient Flow (TGF) scheme is defined by introducing $SU(N)$ YM theories on an asymmetric hyperbox of size $l^2 \times (Nl)^2$. [arXiv:2107.03747]

**SHORT DIRECTIONS: TWISTED BOUNDARY CONDITIONS**

$$A_\mu(x + l\vec{\nu}) = \Gamma_\nu A_\mu(x)\Gamma_\nu^\dagger, \text{ for } \nu = 1, 2$$

$$\Gamma_1 \Gamma_2 = Z_{12} \Gamma_2 \Gamma_1$$

**LONG DIRECTIONS: PERIODIC BOUNDARY CONDITIONS**

$$\tilde{l} \equiv N \times l$$

The (twisted) gradient flow

$$\lambda_{TGF}(\mu) = \frac{128\pi^2 l^2}{3N\mathcal{A}(\sqrt{c}c^2)} < E(t) >$$

Characterising the scheme ($c = 0.3$)
TWISTED GRADIENT FLOW COUPLING

GEOMETRY AND BOUNDARY CONDITIONS

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\[ \lambda_{TGF}(\mu) = \frac{128\pi^2 t^2}{3N\mathcal{A}(\pi c^2)} \frac{\langle E(t) \delta_Q \rangle}{\langle \delta_Q \rangle} \left| \frac{1}{\sqrt{8t=\tilde{c}=\mu^{-1}}} \right| \]

Projection into the zero charge sector

[arXiv:1311.7304, 1905.05147]
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POSSIBLE SOLUTION: PARALLEL TEMPERING ON BOUNDARY CONDITIONS

Proposed for 2d $\mathbb{CP}^{N-1}$ models [arXiv:1706.04443,1911.03384], and recently implemented for 4d SU(N) pure-gauge theories [arXiv:2205.06190], it alienates open and periodic boundary conditions in a parallel tempered manner.

Implementation

• Consider $N_r$ replicas of the target lattice.
• The boundary conditions in each replica change ONLY along a hypercube: THE DEFECT
• Each replica is updated using a standard algorithm (a combination of heatbatch and overrelaxation steps).
• After updates, propose swaps between configurations via Metropolis test, introducing new plausible topology fluctuations.
• After swaps, update more frequently those links close to the defect (Hierarchical Updates) and move the defect randomly to improve performance.
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Possible Solution: Parallel Tempering on Boundary Conditions

The links closing the defect
Pick a factor $\beta \rightarrow \beta c(r)$
Interpolating between

\[ c(0) = 1 \text{ and } c(N_r - 1) = 0 \]
POSSIBLE SOLUTION: PARALLEL TEMPERING ON BOUNDARY CONDITIONS

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The observables are calculated ONLY in the periodic replica.
A FIRST EXPLORATION: FROZEN VS NON-FROZEN

We will test the parallel tempering in our setup by analyzing two cases, one well-sampled in the standard algorithm, and one suffering from topology freezing, corresponding to the same physical volume.

Our simulations

- $N_r = 18$ replicas.
- Defect of size $d = 4$ in lattice units.
- Acceptance probability for the Metropolis swapping steps of 20 %. [arXiv:2012.14000]

\[ \tilde{L} = 24 \text{ and } \beta = 6.4881 \]

- $N_r = 32$ replicas.
- Defect of size $d = 6$ in lattice units.
- Acceptance probability for the Metropolis swapping steps of 20 %.

\[ \tilde{L} = 36 \text{ and } \beta = 6.7790 \]
FIRST EXPLORATION: FROZEN VS NON-FROZEN

\[ L = 24 \text{ and } \beta = 6.4881 \]

\[ L = 36 \text{ and } \beta = 6.7790 \]
FIRST EXPLORATION: DO WE GAIN SOMETHING USING PT?
Although PT improves the topology fluctuations, $Q = 0$ configurations remain dominant, which has nothing to do with topology freezing, but with a dynamic reduction related to the small volume.
There are two problems of different nature

- **Small Value of $\langle Q^2 \rangle$**
  - Can be mitigated, for instance, with multi canonical approaches

- **Topology Freezing**
  - Can be mitigated with parallel tempering on boundary conditions

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**HISTOGRAMS EXHIBIT SMALL VALUE OF $\langle Q^2 \rangle$**
A FIRST EXPLORATION: FROZEN VS NON-FROZEN

Let us compare the coupling, computed in different projected sectors, and the $< Q^2 >$ value.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>$\lambda_{TGF}(\text{All } Q)$</th>
<th>$\tau_\lambda(\text{All } Q)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tilde{L} = 24$</td>
<td></td>
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<tr>
<td>PT</td>
<td>34.09(32)</td>
<td>37.4(79)</td>
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<tr>
<td>nPT</td>
<td>34.97(20)</td>
<td>43.5(43)</td>
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<tr>
<td>$\tilde{L} = 36$</td>
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<tr>
<td>PT</td>
<td>35.47(26)</td>
<td>149(31)</td>
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<tr>
<td>nPT</td>
<td>35.65(77)</td>
<td>550(274)</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>$\lambda_{TGF}(Q = 0)$</th>
<th>$\tau_\lambda(\text{All } Q)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tilde{L} = 24$</td>
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</tr>
<tr>
<td>PT</td>
<td>31.87(30)</td>
<td>39.1(50)</td>
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<tr>
<td>nPT</td>
<td>32.17(11)</td>
<td>40.1(43)</td>
</tr>
<tr>
<td>$\tilde{L} = 36$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PT</td>
<td>33.37(22)</td>
<td>100(19)</td>
</tr>
<tr>
<td>nPT</td>
<td>33.23(22)</td>
<td>88.7(84)</td>
</tr>
</tbody>
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A FIRST EXPLORATION: FROZEN VS NON-FROZEN

\[ \tilde{L} = 36 \]
\[ \tilde{L} = 24 \]

\[ \langle Q^2 \rangle \]

\[ \tau_{Q^2} \]
A FIRST EXPLORATION: FROZEN VS NON-FROZEN

\[ Q = -1 \]
\[ Q = 1 \]
\[ Q = 0 \]
\[ \text{All } Q \]

\[ \lambda_{TGF} \]

\[ 32.5 \quad 35.0 \quad 37.5 \quad 40.0 \quad 42.5 \quad 45.0 \]

\[ \tau_\lambda \]

\[ 0 \quad 200 \quad 400 \quad 600 \quad 800 \]
A FIRST EXPLORATION: FROZEN VS NON-FROZEN

PT IMPROVES $\lambda$ (All $Q$)
Conclusions

- Parallel Tempering improves the autocorrelation time of the topological charge of our previous TGF calculations.
- At this stage, it appears that topological fluctuations are well sampled once the calculation of the coupling is projected into a specific charge sector.
- Although PT efficiently mitigates topology freezing, \( Q = 0 \) configurations remain dominant because the mean \( < Q^2 > \) is small. This can be solved with other types of algorithms.

Further studies are needed to reproduce the running of the coupling and to extract the pure \( SU(3) \Lambda \) parameter.

Thank you for your attention.
A FIRST EXPLORATION: TOPOLOGICAL SUSCEPTIBILITY

\[ 10^4 t_0^2 \chi \]

\[ \bar{l}/\sqrt{8t_0} \]

\[ a=0.094 \text{ fm} \]
\[ a=0.069 \text{ fm} \]
\[ a=0.059 \text{ fm} \]
\[ a=0.052 \text{ fm} \]
\[ 0.030 \text{ fm} < a < 0.050 \text{ fm} \]