Metadynamics Remedies for Topological Freezing

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Mainly based on

“Metadynamics Surfing on Topology Barriers: the $CP(N - 1)$ Case“

A.Laio, G.Martinelli, F.S - JHEP 2016(7), 1-21
Summary

The Illness
1. Topological charge
2. Critical Slowing Down

The Treatment
1. Metadynamics
2. A case of investigation: $CP(N - 1)$ model

Side Effects
(and side outcomes!)
1. Measuring the Free Energy
2. Reweighting

Extension and perspectives
1. First checks in $QCD$
2. Extension of the method
Topological charge

**Topological sector:** set of configurations that can be transformed one into the other by means of a continuous deformation

**Winding number**

Topological charge density in QCD

\[ q(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{Tr} [F_{\mu\nu}(x) F_{\rho\sigma}(x)] \]

- Its volume integral define the topological charge

\[ Q = \int d^4x q(x) \]

related to the **winding number** of the field

- Several definitions on the lattice
Topological charge slowing down - two examples

Staggered simulations for Axion Phenomenology (see G. Martinelli talk on Friday@14.20)

- Coarse lattice spacing
- Finer lattice spacing

RBC/UKQCD: Domain Wall simulations for Charm (see T. Tsang talk on Friday@14)

- Coarse lattice spacing
- Finer lattice spacing
Do we have to bother?

Can’t we just ignore the problem?

NO!

[see e.g. M.D'Elia, F.Negro, PRD88 (2013)]

- At finite volume, Observables depends on $Q$
- Bad sampling of $Q$ means to bias observables

Several solutions proposed

- **Lattice QCD without topology barriers**, M.Lüscher, S.Schaefer JHEP 1107 (2011)
- **Simulate at strictly fixed topology**, JLQCD, PRD74 (2006)
- **Encourage tunneling on the point $x^*$ where the $|q(x)|$ is the largest**, P.de Forcrand et al., Nucl.Phys.Proc.Suppl. 63 (1998)
FROZEN

TOPOLOGICAL CHARGE?
Metadynamics
Elixir

“For an immediate relief of your topological paralysis freezing!”

Before

After the treatment
Metadynamics


Similar in spirit to Wang Landau (2001) but applied to Molecular Dynamics
Widely adopted in biochemistry (protein folding, docking, dissociation...)
NEW FRIENDS

CP(N−1)

MODELS
$CP(N - 1)$ models in a nutshell

In the continuum - 2D space

- Commuting complex field $\vec{z} = (z_1...z_N)$ of norm 1
- $U(1)$ gauge symmetry, covariant derivative: $D_\mu = \partial_\mu + iA_\mu$ with $A_\mu \in \mathcal{R}$

\[
S = \beta N \int d^2x \sum_{\mu=1}^{2} |D_\mu \vec{z}(x)|^2, \quad N = 21
\]

Gauge field $A_\mu$ has no kinetic term and could be integrated away, but we’d rather keep it.

On the lattice

\[
S = \beta N \sum_{n \in L^2} \sum_{\mu=1}^{2} |D_\mu \vec{z}_n|^2, \quad D_\mu z_n = \Lambda_{n,\mu} z_{n+\hat{\mu}} - z_n
\]

Like QCD...

- There is a topology $Q$
- There is a mass gap $M \sim 1/\xi$
- The beta-function is negative
- $\beta$ sets the scale: $a \xrightarrow{\beta \to \infty} 0$

But simpler!

- Simulations can be run on a laptop! (actually: Ulisse cluster at Sissa)
- Excellent framework to test new algorithms
MOST IMPORTANT
it suffers from
TOPOLOGICAL FREEZING
Topological charge evolution

$\beta = 0.65, \xi/a \sim 2.7$
Evolution on a finer lattice spacing (same scales)

\[ \beta = 0.70, \quad \xi / a \sim 3.7 \]
Going even finer

\begin{align*}
\beta &= 0.75, \quad \xi/a \sim 5.16
\end{align*}
DOES METADYNAMICS WORK?
And in Metadynamics

\[ \xi \sim 1/a \]

\[ V \sim L/\xi \sim 12 \]

\[ V \sim L/\xi \sim 12 \text{ with metad.} \]
It works at various volumes

\[ \xi \sim \frac{1}{a} \]

\[ 1 \times 10^{-6} \quad 0.0001 \quad 0.01 \]

\[ \frac{L}{\xi} \sim 12 \]

\[ \frac{L}{\xi} \sim 18 \]

\[ \frac{L}{\xi} \sim 25 \]

\[ \frac{L}{\xi} \sim 12 \text{ with metad.} \]

\[ \frac{L}{\xi} \sim 18 \text{ with metad.} \]

\[ \frac{L}{\xi} \sim 25 \text{ with metad.} \]
IT WORKS!!
BUT HOW?
How does it work?

Action dependent on \textbf{simulation time} $S(t) = S(0) + V_{bias}(t)$

**Bias potential**

- $V_{bias}$ built in terms of previous values of a \textbf{collective variable}, here taken to be $Q$
- Example of a possible form of the potential:

$$V_{bias}(t + dt) = V_{bias}(t) + c \cdot \exp \left[ -\frac{1}{2} \left( \frac{Q - Q(t)}{\sigma} \right)^2 \right]$$

To avoid evaluating too many “\text{exp}” we actually use \textbf{triangles on a grid}
How does it work?

Dynamics

- The induced force $F = -\partial_U V_{bias}$ drives the system away from previous values of $Q$
- $V_{bias}$ reduces the probability of occupying previous states
- At large simulation time $V_{bias}$ fills the free energy wells

At convergence (long simulated time)

- $V_{bias}$ provides a negative image of the free energy $F(Q) = -\log Z(Q)$
- The dynamics of the system is completely flat w.r.t $Q$
“What about the sampled distribution of $Q$?”

At convergence

By construction $F(Q) = -\log Z(Q)$ which means that

$$P(Q) = \text{const}$$

in the generated sample

“So you are sampling a different distribution!!!”

$F(Q)$ can be used to reweight the distribution:

$$\langle O \rangle = \frac{\sum_i O_i \exp[-F(Q_i)]}{\sum_j \exp[-F(Q_j)]}$$

Reweighting costs

- By reweighting we suppress configurations with non-integer charge
- Nonetheless the configurations generate by metadynamics are uncorrelated
  - We agree with HMC where it works, but we achieve increasingly large speed-up as $a \to 0$
  - We obtain sensible results at reasonable cost, even when the HMC is completely frozen

The associated costs seems to scale well with $a$ and $V$ (see next plots)
$\rho(Q)$, HMC (40M painful trajectories, $\beta = 0.75$, $\xi/a \sim 5.16$, $L/a = 60$)
$\rho(Q)$, metadynamics (700k trajectories)
Reweighting

Without metadynamics
With metadynamics, reweighted

Q
-4  -2   0   2   4

0
0.5
1
1.5
2

Without metadynamics
With metadynamics, reweighted
Topological susceptibility - 3M trajectories $L/\xi_g \sim 12$

Here HMC is completely frozen.
Extension to \( QCD \)

**No conceptual difference**

It amounts to simulate with a time-dependent (imaginary) \( V_{bias} = \theta_{QCD} Q^{stout} \) where

\[
\theta_{QCD}(t) = i F [Q^{stout}(t)]
\]

Tune the \( \sim 5 \) parameters on the basis of the \( CP(N - 1) \) experience

**Ingredients**

- Compute a new force term \( \propto \partial_U Q \)
- Stout smear the configuration (several levels, \( \mathcal{O}(10) \) needed)
- Remap the force iteratively \( F^{non-stout} \rightarrow F^{1-stout} \rightarrow \ldots F^{N-stout} \)

**A first taste - In collaboration also with M.D’Elia, C.Bonati**

Can we unfreeze this?

\[
\begin{align*}
\beta &= 4.36 \\
a &= 0.0397 \text{ fm} \\
M_\pi &\sim 135 \text{ MeV} \\
L/a &= 40 \\
N_f &= 2 + 1 \\
\text{staggered} &\quad \text{small volume} \\
\text{totally frozen}
\end{align*}
\]
It looks promising...
Future improvements

Squeezing the best from the algorithm
- Make use of $Q \rightarrow -Q$ symmetry
- Make use of $Q \rightarrow Q + 2k\pi$ symmetry?
- Precondition the algorithm, feeding-in the information on $F(Q)$
- Improve the convergence starting from a guess of $V_{bias}$
- Include other collective variables

Extending to QCD
- No conceptual problems, just a bit of pain to implement
- Preliminary test shows encouraging results
- Needs more stout: 30-40% overhead (less important towards the continuum limit)

More than topology?
- Can it be used to study Gribov copies problem in Gauge Fixing?
- Can it help computing Spectral Density?
- Can it be used to study Finite Density!
Conclusions

**Topology**
- Different definitions of the Topological charge can be **useful for different reasons**
- Dependency on the topological sector is **non trivial**
- Simulations get frozen close to the continuum limit (**a long history**)

**Metadynamics**

- Coupling **the past** history to reduce the occupancy of already explored states
  - Bias potential inducing a force driving **“away from the past”**
  - Topological charge gets **unfrozen**
  - Distribution of $Q$ at Long Simulation Time is **flat**: $P(Q) = 1$
  - Reweighting restores the proper distribution
  - Several parameters to tune...

**The future**
- Use all the available **symmetries**
- Further test **QCD** simulations
- Apply to **other problems**
...THANKS...

...FOR YOUR ATTENTION!!!
BACKUP
Which definition of $Q$?

Geometrical: sum of the solid angle between $z$ on all triangles

$$Q_g = \frac{1}{2\pi} \sum \nabla, \Delta \arg [(\vec{z}_a, \vec{z}_b) (\vec{z}_b, \vec{z}_c) (\vec{z}_c, \vec{z}_a)]$$

This is matemagically an integer number

✓ perfect to measure the actual topological charge

✗ useless as a collective variable!

In fact $F_z = -\partial_z V_{bias}^g \propto \partial_z Q_g = 0$: the bias would induce no force on the system

Gauge definition: plaquette of $\Lambda$

$$Q = \frac{1}{2\pi} \sum \text{Im} \square = ZQ_g + \eta - \text{Not an integer number}$$

✗ not ideal to measure the actual topological charge

✓ useful as a collective variable: $F_\Lambda = -\partial_\Lambda V_{bias}^Q \propto \partial_\Lambda Q \neq 0$

- Field $\Lambda$ must be smoothed, so that $\sqrt{\langle \eta^2 \rangle} \lesssim 1$ and $Z \sim 1$
- Analytical smoothing easily differentiable: stout smearing

What’s the shape of $F(Q)$?
"You are violating the sacred principles of Monte Carlo methods!"

- In fact the algorithm does not build a Markov Chain of configurations \([z, \Lambda]\) at all!
- You have to think in terms of the enlarged configuration space \([\{z, \Lambda \otimes V_{bias}\}]\)
- Indeed it was rigorously shown that:

The correct sampling of the configuration space is obtained after reweighting

[\textit{Equilibrium Free Energies from Nonequilibrium Metadynamics},
G.Bussi, A.Laio, M.Parrinello, PRL96 (2006)]