New simulation strategies for lattice QCD

Michael G. Endres
(MIT)

Lattice 2016 • Southampton, UK
July 26, 2016
Statistical uncertainties

A reliable determination of statistical uncertainties requires an understanding of correlations in generated configurations

- Arise due to sequential nature of Markov Chain Monte Carlo (MC) algorithms
- Highly dependent on the times scales that govern the Markov process

configuration space
Critical slowing down

*Coarse lattices decorrelate faster than fine lattices*

- Observables are probes for determining decorrelation times
- Autocorrelations are influenced by how well observables couple to slow modes
  - topological charge ($Q$) couples strongly

\[
\tau_{\text{int}}(\mathcal{O}) \sim \left( \frac{1}{a} \right)^{z_{\text{int}}(\mathcal{O})}
\]

\[
cost \sim \left( \frac{1}{a} \right)^{D + \max_{\mathcal{O}} z_{\text{int}}(\mathcal{O})} \sim 9
\]

D=4 with periodic BC; pure gauge theory w/HB

<table>
<thead>
<tr>
<th>Action density ($E(t_0)$)</th>
<th>Topological charge ($Q(t_0)$)</th>
<th>Topological susceptibility ($\chi(t_0)$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z_{\text{int}} \sim 5$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$z_{\text{int}} \sim 2$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Michael G. Endres • MIT • July 26, 2016
Topological charge on a space-time torus

**Continuum:** field space splits into disconnected topological sectors (labeled by quantized $Q$)

**Lattice:** topological sectors are connected, however separated by large action barriers

\[
f(Q) = -\frac{1}{V} \log \langle \delta (Q - Q[U]) \rangle
\]

- Change in topology requires tunneling; probability exponentially suppressed by barrier height
- Barrier height depends on the discretization of the action
Topological freezing

At very fine lattice spacing, the timescale for topology change can exceed the total time of the simulation

• Problem for HB and HMC
• Fixed topology $\rightarrow 1/V$ corrections to observables
• Particularly severe for $a \approx 0.05$ fm


$m_\pi \sim 360 - 480$ MeV
Overcoming topological freezing/critical slowing down

(Some) strategies for attacking the problem

- **Infrared** — choice of boundary conditions
  - open boundary conditions
  - non-orientable manifolds

- **Ultraviolet** — exploiting lattice artifacts, ambiguity in the definition of $Q$
  - metadynamics
  - multiscale methods

References:
- M. Lüscher and S. Schaefer, JHEP 07 (2011) 036
Some recent proposals

Lattice QCD on Non-orientable Manifolds
Theoretical Developments

- July 25, 2016 @ 15:15 (Simon Mages)
- July 25, 2016 @ 15:35 (Balint Toth)

- Open boundary conditions
  - connected field space
  - translational symmetry broken; large boundary effects
- Non-orientable manifolds: P-periodic BCs (parity transformation at boundary)
  - topological charge not quantized; improved scaling of $\tau_{int}(Q)$ with $1/a$
  - suppressed translational symmetry breaking effects
  - non-trivial to implement fermions (but possible)
Some recent proposals

Lattice QCD on Non-orientable Manifolds
Theoretical Developments
  — July 25, 2016 @ 15:15 (Simon Mages)
  — July 25, 2016 @ 15:35 (Balint Toth)

Pure gauge theory
(a=0.04 fm)
Some recent proposals

Metadynamics Remedies for Topological Freezing
Algorithms and Machines
— July 26, 2016 @ 18:10 (Francesco Sanfilippo)

\[ f(Q) = -\frac{1}{V} \log \langle \delta (Q - Q[U]) \rangle \approx -v(Q) \]

- Introduces a MC time-dependent potential bias which disfavors revisiting configurations; effectively fills the potential wells with MC time
- Takes advantage of the fact that MC time-averaged potential bias is an estimator for \(-f(Q)\)
- Recover expectation values via reweighting: \[ \langle O \rangle \approx \frac{\sum_i O(U_i) e^{-Vv(Q(U_i))}}{\sum_i e^{-Vv(Q(U_i))}} \]
Some recent proposals

Metadynamics Remedies for Topological Freezing

*Algorithms and Machines*
— July 26, 2016 @ 18:10 (Francesco Sanfilippo)
Some recent proposals

Multiscale Thermalization

based on

M. G. E., R. C. Brower, W. Detmold, K. Orginos and A. V. Pochinksy

Multiscale thermalization

Can an initial distribution of configurations be constructed such that thermalization is governed only by higher modes of evolution? (Yes!)

\[ \mathcal{P}_s = \mathcal{P}(s) + \sum_{n>0} \langle s | \chi_n \rangle \langle \tilde{\chi}_n | \mathcal{P}_0 \rangle e^{-\tau/s\chi_n} \]

Wanted: \( \mathcal{P}_0 \) such that \( \langle \tilde{\chi}_n | \mathcal{P}_0 \rangle = 0 \) for small \( n \)
Lessons from a toy model

1D Ising model

$H^{[0]} = J \sum_i S_{2i} (S_{2i+1} + S_{2i-1})$

$H^{[1]} = R(J) \sum_i S_{2i+1} S_{2i-1}$

$R(J) = \frac{1}{2} \cosh^{-1} (e^{2J})$
Lessons from a toy model

level | 1D ising model

[0]  

“integrate in?”

Even site probability measure:  
\[ \mathcal{P}(S_{2i}) = \frac{e^{-JS_{2i}(S_{2i+1}+S_{2i-1})}}{\cosh(J(S_{2i+1} + S_{2i-1}))} \]

“Integrating in” remaining fine degrees of freedom requires only a single update per site
Generalization to more complicated systems

- Higher dimensions/complicated actions:
  - coarse graining induces increasingly complicated interactions
- Gauge theories with fermions:
  - nonlocal actions due to fermion determinants

\[ \text{RG induced interactions} \]
Generalization to more complicated systems

- Generalization is achieved with approximations:
  - truncated coarse action; implies inexact RG matching
  - inexact (one-to-one) refinement prescription
- *Rethermalize* using conventional algorithms to correct errors induced by approximations

\[\text{RG induced interactions}\]
A new proposal for ensemble generation

- Generate *decorrelated* coarse ensemble using an RG matched coarse action

\[\begin{array}{c}
\text{coarse} \quad \rightarrow \\
\text{unthermalized} \quad \rightarrow \\
\text{thermalized} \quad \rightarrow \\
\end{array}\]
A new proposal for ensemble generation

- Generate *decorrelated* coarse ensemble using an RG matched coarse action
- Map coarse ensemble onto a fine lattice, *while preserving long distance properties*

![Diagram showing ensemble generation process](image)
A new proposal for ensemble generation

- Generate *decorrelated* coarse ensemble using an RG matched coarse action
- Map coarse ensemble onto a fine lattice, *while preserving long distance properties*
- Rethermalize and evolve multiple refined streams using fine action
A new proposal for ensemble generation

\[ \tau_{\text{decorr}} \sim \tau_1 \]

**VS.**

\[ \tau_{\text{retherm}} \sim \tau_k \]

want \( k > 1! \)

- unthermalized
- thermalized
- ensemble
Refinement via interpolation of gauge fields (à la ’t Hooft)

\[ U_\mu(x) = e^{iaA_\mu(x)} \]

[1] Coarse lattice variables are transferred to the fine lattice

--- set to unity by a gauge choice

---------- undefined bond variables (set to unity)
Refinement via interpolation of gauge fields (à la ’t Hooft)

[2] Interior links obtained by maximizing boundary plaquette action

--- set to unity by a gauge choice

---------- undefined bond variables (set to unity)
Refinement via interpolation of gauge fields (à la 't Hooft)

[3] Process sequentially repeated for interior cells
Properties of the interpolation

- Implementation is **simple, local and efficient**; preserves hypercubic **symmetries**
- Preserves long distance properties of coarse configurations
  - subset of even-shaped Wilson loops on even sites
  - topological charge/density at sufficiently fine lattice spacing
- Breaks discrete translational symmetry
  - rapidly restored upon rethermalization
Interpolation — topological charge density

(coarse-grain) -> (refine)

(single time slice)
At sufficiently fine lattice spacing, refinement preserves topological charge on a per configuration basis.
Demonstration of the approach — pure SU(3) YM

- Refined ensemble obtained from decorrelated RG matched (using $r_0$) ensemble
- Long distance observables rethermalize on time scales shorter than:
  - thermalization time for hot/cold starts (standard approach)
  - decorrelation time for fine evolution: $\tau_{\text{decorr}} \approx 2 \tau_{\text{int}}(Q)$

\begin{itemize}
  \item $a \sim 0.07 \text{ fm}$
  \item $\tau_{\text{decorr}} \geq 2600$
  \item heat bath (also works for HMC!)
\end{itemize}
Inclusion of fermions — QCD with $N_f=2c=2$

- Coarse/fine actions matched using $t_0$ and $m_\pi$
  - $m_\pi/m_p \sim 0.85$ (isospin limit)
  - differences in Dirac spectrum presumably due to lattice artifacts
- Refinement of coarse action applies **only** to gauge fields...
- what does Dirac spectrum of refined ensemble look like?
Inclusion of fermions — QCD with $N_f=N_c=2$

- Refinement via interpolation: $C \rightarrow R^{(0)}$
  - spurious zero modes; large initial fermion forces in HMC rethermalization

- Short *quenched* evolution of interpolated fields: $R^{(0)} \rightarrow R^{(1)} \rightarrow R^{(2)} \rightarrow \ldots$
  - produce a gap in the Dirac spectrum, eliminate large initial forces
  - only impacts short distance properties of ensemble (if evolution is short)
Demonstration of the approach — QCD with $N_f = N_c = 2$
Conclusion & Outlook

- Several recent promising simulation strategies for addressing critical slowing down and topological freezing:
  - non-orientable manifolds
  - metadynamics
  - multiscale thermalization
- Many remaining open issues for multiscale thermalization:
  - coarse/fine action matching
  - metrics for thermalization
  - removal of inherited lattice artifacts in fine topological charge distribution
  - better understanding of spurious zero-modes of refined Dirac operator and their removal