Accelerating Metadynamics

...with an eye on full QCD

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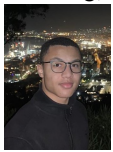
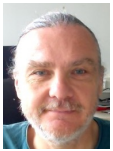
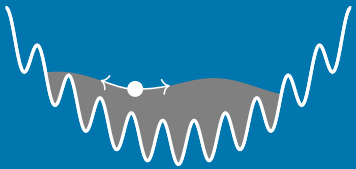




Lattice 2024 01.08.2024



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Extending Metadynamics to QCD

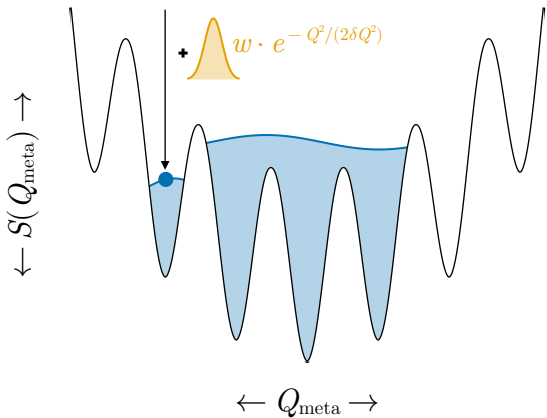
Reminder from previous talk...

- No conceptual difficulties
- HMC already required for dynamical fermions
- Stout smearing often used for fermions
- Compared to fermionic force calculation (especially at physical quark/pion masses), overhead is negligible
- Buildup of potential may take too long
  - $\Rightarrow$ Have to accelerate buildup as much as possible

Building a Metadynamics Bias Potential

Buildup speed determined by three parameters:

- Bin width δQ more or less bounded from above by the standard deviation of the collective variable in unbiased simulations (within a sector)
- Gaussian weight w has to be chosen while weighing speed against smoothness
- CV-space interval $[Q_{\text{min}}, Q_{\text{max}}]$ does not have to be large (*keyword: bias modification*)



Speeding up the Bias Thermalization

1. **Make use of known charge parity symmetry** $Q \leftrightarrow -Q$
   - In practice: Whenever we update the bias potential at some Q_{meta} we also update it at $-Q_{\text{meta}}$
     $\Rightarrow$ approx. 2x speed-up

Speeding up the Bias Thermalization

2. Well-tempered Metadynamics [Barducci' 08]

- Standard Metadynamics

$$V_{t+1}(Q) = V_t(Q) + w \exp\left(-\frac{(Q_t - Q)^2}{2\sigma^2}\right)$$

- Well-tempered Metadynamics

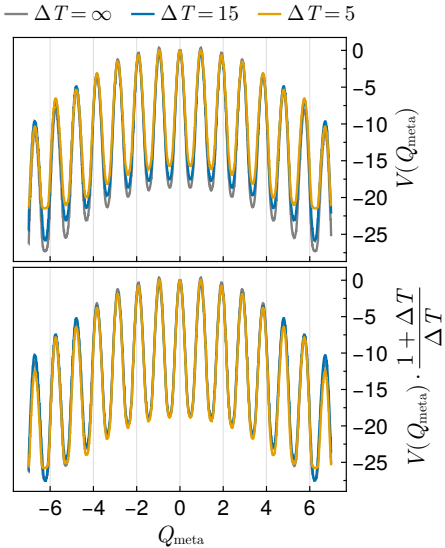
$$V_{t+1}(Q) = V_t(Q) + \exp\left(-\frac{V_t(Q)}{\Delta T}\right) w \exp\left(-\frac{(Q_t - Q)^2}{2\sigma^2}\right)$$

Tunable parameter ΔT:

- $\Delta T \to 0$: No Metadynamics
- $\Delta T \to \infty$: Standard Metadynamics

Speeding up the Bias Thermalization

2. **Well-tempered Metadynamics** [Barducci' 08]
   - Able to choose larger w while maintaining smoothness in the end
   - Quirk: Bias does not converge to $-S(Q)$ but $-\frac{\Delta T}{1+\Delta T}S(Q)$
     $\hookrightarrow$ One has to be careful so as not to decrease the barrier height too much



Speeding up the Bias Thermalization

3. **Multiple walkers** [Raiteri' 06]
   - Run N_{walkers} simulation streams in parallel, all working on the same potential
   - Minimal communication between processes required (e.g., a single `MPI.Allgather` call per iteration)
     $\hookrightarrow$ speed-up of factor $\sim N_{\text{walkers}}$
   - **Possible Enhancement**: Start each walker in a different topological sector to eliminate time before falling into unexplored sector

Speeding up the thermalization

Some strategies not mentioned in this talk and/or not explored so far:

- On-the-fly parametric optimization (complicated)
- Alternative biased sampling methods, e.g., OPES [Parrinello' 20] (so far only slightly ahead of MetaD in some cases, but might become very useful)
- Using information from previous simulations on coarser lattices (unexplored)

Question to be Answered

Do these improvements enable us to use PT-MetaD in full QCD?

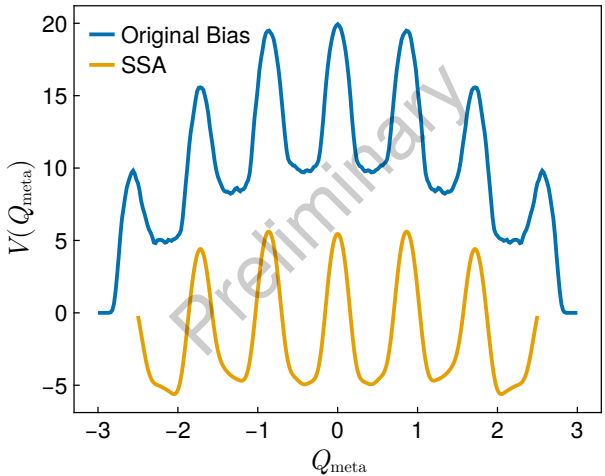
First Unquenched Case Study

- Fermion Action: 4×0.125 Stout-smeared Staggered, $N_f = 2$ @ $am = 0.02$
- Gauge Action: DBW2 @ $\beta = 1.05$
  $\hookrightarrow a^{-1} \approx 3.5\text{-}4$ GeV
- Lattice Volume: $(16a)^4 \approx (0.8\ \text{fm})^4$

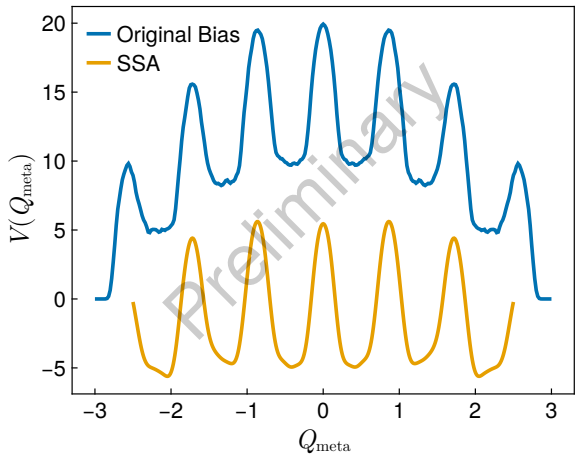
- Collective Variable: Clover-Charge with 6×0.12 Stout smearing
- Bias parameters: $\delta Q = w = 0.02$, $\gamma = \infty$, $[Q_{\text{min}}, Q_{\text{max}}] = [-3, 3]$ and 6 walkers

First Unquenched Case Study — Bias Potential

Bias potential after 5000 HMC trajectories per walker:



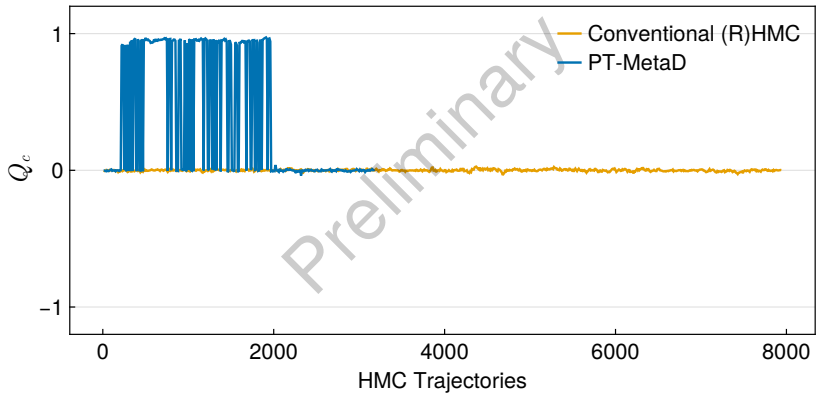
First Unquenched Case Study — Bias Potential



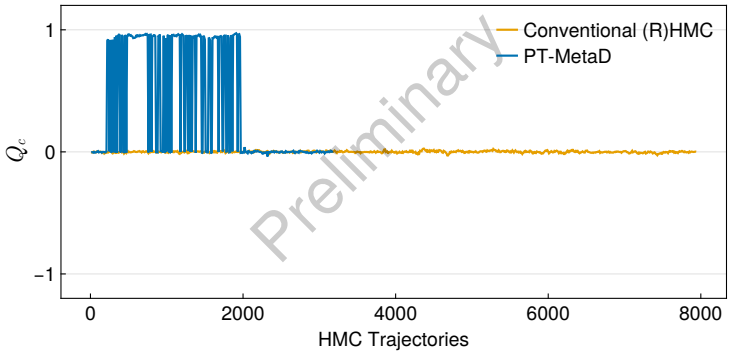
- Very similar shape to pure gauge bias potentials
- Broader valleys most likely caused by longer, possibly excessive, smearing ($4 \times 0.12 \rightarrow 6 \times 0.12$)
- *Maybe possible to guesstimate unquenched potentials from quenched ones?*

First Unquenched Case Study — PT-MetaD

PT-MetaD successfully unfreezes the system:



First Unquenched Case Study — PT-MetaD

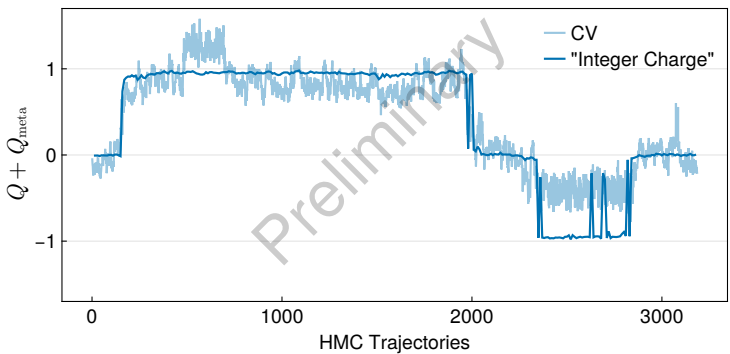


Important to stress:

- All streams use the exact same gauge and fermion actions
  ↪ swap probability only depends on the difference in the bias potential
- Only 2 streams required to facilitate tunneling

First Unquenched Case Study — PT-MetaD

Summed timeseries of measurement stream and biased stream:



- More effective tunneling events than we see in the measurement stream
- Biased stream steps into transition regions, but jumps back instead of tunneling through
  $\Rightarrow$ more tuning of the bias potential required
  (*Better CV and/or higher resolution*)

Summary

- Bias thermalization time can be significantly reduced by combining multiple strategies
- Time scales make it reasonable to use Metadynamics in full QCD (*Further improvements certainly desired and possible*)
- Preliminary case study shows successful unfreezing in full QCD using Staggered Fermions

Outlook

- Scaling of autocorrelation times
- Usage in SU(N) theories and/or with chiral fermions, where topological freezing is even more problematic

Quick Aside...

In case you missed it, check out [part 1 of this talk] by Timo Eichhorn (Thu 9:20)

How was this data generated?

- In-house written Lattice QCD code written in Julia, mainly for prototyping, inspired by [LatticeQCD.jl] by Akio Tomiya et al.:

  [MetaQCD.jl] "*dirac*" branch (still being developed)

Backup