Gauge-Fixed Fourier Acceleration to Reduce Critical Slowing Down

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Motive

Consider of a collection of harmonic ocsillators with common mass but varying spring constants. $H = \sum_{i=1}^{N} \frac{p_i^2}{2M} + \frac{1}{2} k_i x_i^2$

- All of the modes evolve with the same time step and the same velocity.
- Modes with small k_i evolve with a smaller time step than needed. Modes with large k_i evolve with more steps than needed.
- Critical slowing down would be removed if different masses $M_j \propto k_j$ are used for each mode.

Motive

- With lattice size $a \to 0$, gauge field enters the action quadratically.

$$S = \frac{\beta}{3} \sum_{n,\mu<\nu} Retr[1 - P_{\mu\nu}] \tag{1}$$

$$\overset{U=e^{iaA}}{\Rightarrow} (\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial^\mu A^\nu - \partial^\nu A^\mu) \tag{2}$$

- Fourier acceleration can be applied.

$$H = \sum_k tr(P_\mu(-k) D^{\mu\nu}(k) P_\nu(k)) + S[U] \tag{3}$$

- Gauge field modes will be mixed by gauge symmetry. To identify different modes, some sort of phsyical gauge fixing is required.

Gauge-Fixing Action

- We introduce a gauge-fixing term into the action.

$$S_{GF1}[U] = -\beta M^2 \sum_{x,\mu} Re\ tr[U_\mu(x)] \tag{4}$$

- Landau gauge is the maximum of $Re\ tr[U_\mu(x)]$. When doing path integral with this new gauge-fixing action, gauge field configurations that obey Landau gauge is favored.
- Gauge-fixing action contains a parameter M. By tuning this parameter, we can control how strongly the gauge fixing condition is imposed.

Gauge-Fixing Action

$$\langle O \rangle = \int dU e^{-S[U]} O[U] \tag{5}$$

$$= \int dU \frac{\int dg' e^{-S_{GF1}[U^{g'}]} e^{-S[U]} O[U]}{\int dg e^{-S_{GF1}[U^g]}} \tag{6}$$

$$= \int dU \frac{\int dg' e^{-S_{GF1}[U^{g'}]} e^{-S[U^{g'}]} O[U^{g'}]}{\int dg e^{-S_{GF1}[U^g]}} \tag{7}$$

$$= \int dU e^{-S[U] \underline{- S_{GF1}[U] - \ln \int dg e^{-S_{GF1}[U^g]}}} O[U] \tag{8}$$

- Using gauge invariance we could add another term into action to compensate gauge-fixing action S_{GF1}, such that the physical observable values are unchanged [C. Parrinello and G. Jona-Lasinio, 1990].

Gauge-Fixing Action

$$H = \sum_k tr(P_\mu(-k)D^{\mu\nu}(k)P_\nu(k)) + S_{wilson}[U] + S_{GF}[U] \qquad (9)$$

$$S_{GF}[U] = S_{GF1}[U] + S_{GF2}[U] \qquad (10)$$

$$S_{GF1}[U] = -\beta M^2 \sum_{x,\mu} Re\ tr[U_\mu(x)] \qquad (11)$$

$$S_{GF2}[U] = \ln \int dg\ e^{-S_{GF1}[U^g]} \qquad (12)$$

- The addition of the logarithm poses computational chanllenges. "Inner Monte Carlo" is needed to calculated both force and difference in Harmiltonian between the beginning and the end of a trajectory.

Gauge-Fixing Action

- Calculate force.

$$\frac{\partial S_{GF2}}{\partial U} = \frac{\int dg\ e^{-S_{GF1}[U^g]} \frac{\partial S_{GF1}[U^g]}{\partial U}}{\int dg\ e^{-S_{GF1}[U^g]}} \approx \frac{1}{N} \sum_{n=1}^{N} \frac{\partial S_{GF1}[U^{g^n}]}{\partial U} \tag{13}$$

- Calculate ΔH. S_{GF2} cannot be calculated directly. But the difference in S_{GF2} is calculable.

$$S_{GF2}[U'] - S_{GF2}[U] = \ln \frac{\int dg\ e^{-S_{GF1}[U'^g]}}{\int dg\ e^{-S_{GF1}[U^g]}} \tag{14}$$

$$= \ln \frac{\int dg\ e^{-S_{GF1}[U^g]} e^{S_{GF1}[U^g] - S_{GF1}[U'^g]}}{\int dg\ e^{-S_{GF1}[U^g]}} \tag{15}$$

$$\approx \ln \frac{1}{N} \sum_{n=1}^{N} e^{S_{GF1}[U^{g^n}] - S_{GF1}[U'^{g^n}]} \tag{16}$$

Gauge Fixing action

- Soft guage fixing is achieved by introducing gauge-fixing action S_{GF1} together with compensating term S_{GF2}.
- Soft gauge fixing offers great computational challenges.
  - Inner Monte Carlo makes evolution more computationally demanding.
  - Force and ΔH are calculated statistically, introducing stochastic noise into results.

Fourier Acceleration

- Fourier acceleration can be achieved by choosing the coefficients of conjugate momenta to be the inverse of the coefficients of gauge fields.

$$H_p = \sum_k tr(P_\mu(-k)D^{\mu\nu}(k)P_\nu(k)) \tag{17}$$

- In continuum limit, this inverse is the following propagator up to the first order[S. Fachin, 1993].

$$D^{\mu\nu}(k) = \frac{1}{k^2}P^T_{\mu\nu} + \frac{1}{M^2}P^L_{\mu\nu} \tag{18}$$

$$P^T_{\mu\nu}(k) = \delta_{\mu\nu} - \frac{k^\mu k^\nu}{k^2} \tag{19}$$

$$P^L_{\mu\nu}(k) = \frac{k^\mu k^\nu}{k^2} \tag{20}$$

The Choice of $D^{\mu\nu}$: Lattice version

- How about lattice version?

$\widetilde{A}_\mu(k) = \int \frac{d^4x}{(2\pi)^2} e^{-ikx} A(x)$. For continuum case, $\partial_\mu \to k_\mu$.
For discrete case, forward and backward derivatives:

$$\partial_\mu^+ A_\nu(x) = A_\nu(x+\delta) - A_\nu(x) \quad (21)$$

$$\partial_\mu^- A_\nu(x) = A_\nu(x_1) - A_\nu(x-\delta) \quad (22)$$

So on lattice we have $\partial_\mu^\pm \to 2ie^{\pm i\pi k_\mu/L}\sin(\pi k_\mu/L)$. And projection operator becomes:

$$(P_L)_{\mu\nu} = \frac{\partial_\mu^- \partial_\nu^+}{\sum_\rho \partial_\rho^- \partial_\rho^+} \quad (23)$$

$$\to \frac{e^{-i\pi k_\mu/L}\sin(\pi k_\mu/L) e^{+i\pi k_\nu/L}\sin(\pi k_\nu/L)}{\sum_\rho \sin^2(\pi k_\rho/L)} \quad (24)$$

Fourier Acceleration

- By examining the action carefully, we propose the following kinetic energy term.

$$H_p = \sum_k tr(P_\mu(-k) D^{\mu\nu}(k) P_\nu(k)) \tag{25}$$

$$D_{\mu\nu}(k) = \frac{1}{\sin(\frac{k}{2})^2 + \epsilon^2} P^T_{\mu\nu}(k) + \frac{1}{M^2} P^L_{\mu\nu}(k) \tag{26}$$

$$P^T_{\mu\nu}(k) = \delta_{\mu\nu} - \frac{e^{-i\frac{k_\mu}{2}} \sin(\frac{k_\mu}{2}) e^{i\frac{k_\nu}{2}} \sin(\frac{k_\nu}{2})}{\sin(\frac{k}{2})^2} \tag{27}$$

$$P^L_{\mu\nu}(k) = \frac{e^{-i\frac{k_\mu}{2}} \sin(\frac{k_\mu}{2}) e^{i\frac{k_\nu}{2}} \sin(\frac{k_\nu}{2})}{\sin(\frac{k}{2})^2} \tag{28}$$

Summary

- Fourier acceleration + Soft gauge fixing $\rightarrow$ reduce critical slowing down.
- Gauge fixing action introduces inner Monte Carlo which is computationally expensive. Hopefully it is relatively cheaper compared to dynamical fermions.
- This method affects only the gauge evolution, and thus will work equally well for any fermion formulation.
- Numerical tests are requried to determine appropriate parameters.
- Code has been written and is being tested.