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Gauge-Fixed Fourier Acceleration

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Overview

- Background and Motivation
- Preliminary Results with Periodic B.C.
- Current Results with Fixed B.C.

Background and Motivation

Motivation

- In the continuum limit ($a \to 0$), high-energy modes ($\omega \propto \frac{1}{a}$) enter the simulation

- **Problem:** HMC Algorithm needs small step size for high-energy modes, needs many steps for low-energy, physical modes … Critical Slowing Down

- **Upshot:** In the continuum limit, gauge fields enter the action quadratically

$$S_{wilson} = \frac{\beta}{3} \sum_{x,\mu<\nu} Re\, tr[1 - P_{\mu\nu}(x)]$$

$$\to^{U=e^{iA}} (\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial^\mu A^\nu - \partial^\nu A^\mu)$$

⟹ Can apply **Fourier Acceleration** to eliminate Critical Slowing Down

Gauge-Fixing

- Fourier modes are mixed by gauge-symmetry. Need gauge-fixing to identify the modes

- Need Faddeev-Popov term to preserve gauge-invariant observables

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

Gauge-Fixing Action

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

$$S_{GF} = -\beta M^2 \sum_{x,\mu} Re\, tr\big[U_\mu(x)\big]$$ ⟹ softly-fixed Landau gauge [S. Fachin 1993]

$$S_{FP} = \ln \int dg\, e^{-S_{GF1}[U^g]}$$ ⟹ $$\frac{\partial S_{FP}}{\partial U} = \frac{\int dg\, e^{-S_{GF}[U^g]} \frac{\partial S_{GF}[U^g]}{\partial U}}{\int dg\, e^{-S_{GF}[U^g]}} = < \frac{\partial S_{GF}[U^g]}{\partial U} >_g$$

"Inner Monte Carlo": we evaluate $\frac{\partial S_{FP}}{\partial U}$ stochastically using a Heatbath algorithm

$$< \frac{\partial S_{GF}[U^g]}{\partial U} >_g \approx \frac{1}{N} \sum_{i=1}^{N} \frac{\partial S_{GF}[U^{g_i}]}{\partial U}$$

Fourier Acceleration

$$H_p = \sum_k tr[\, P_\mu(-k)\, D^{\mu\nu}\, P_\nu(k)]$$

- To achieve Fourier acceleration, choose the coefficients of the conjugate momenta (the "mass term") as the inverse of coefficients of terms in the action quadratic in gauge-fields

- In the continuum limit, $D_{\mu\nu}$ up to first order is:

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

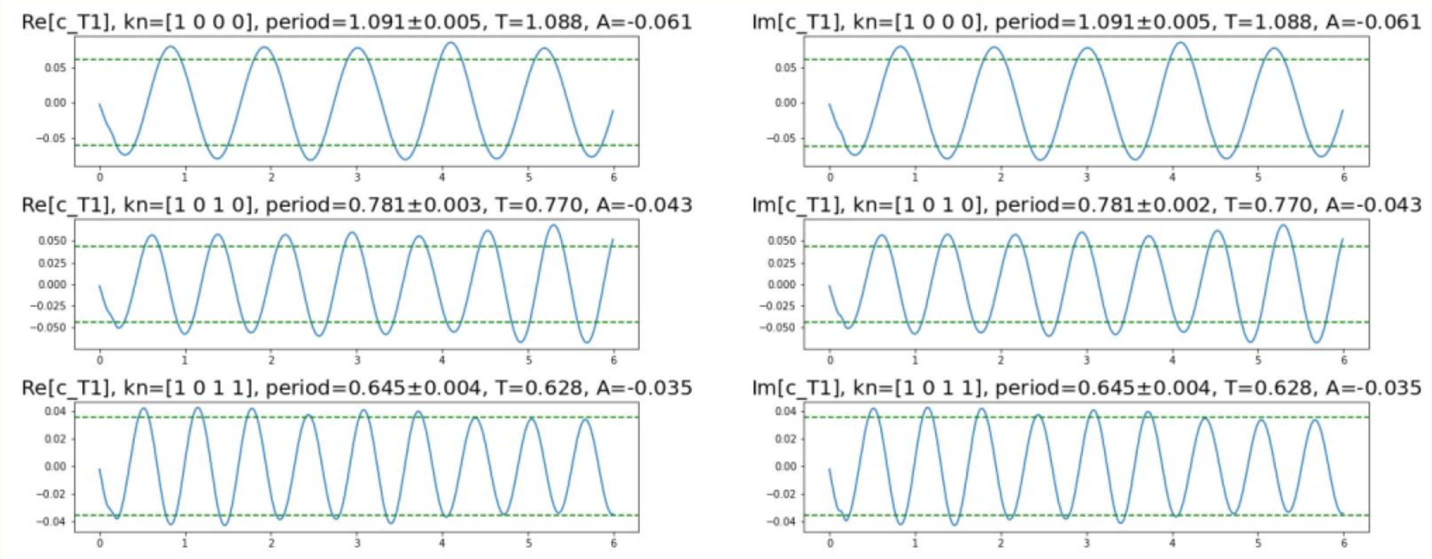
$$P^T_{\mu\nu}(k) = \delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}$$

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

Preliminary Results with Periodic Boundary Conditions

Gauge-Modes ($A = \ln U$)

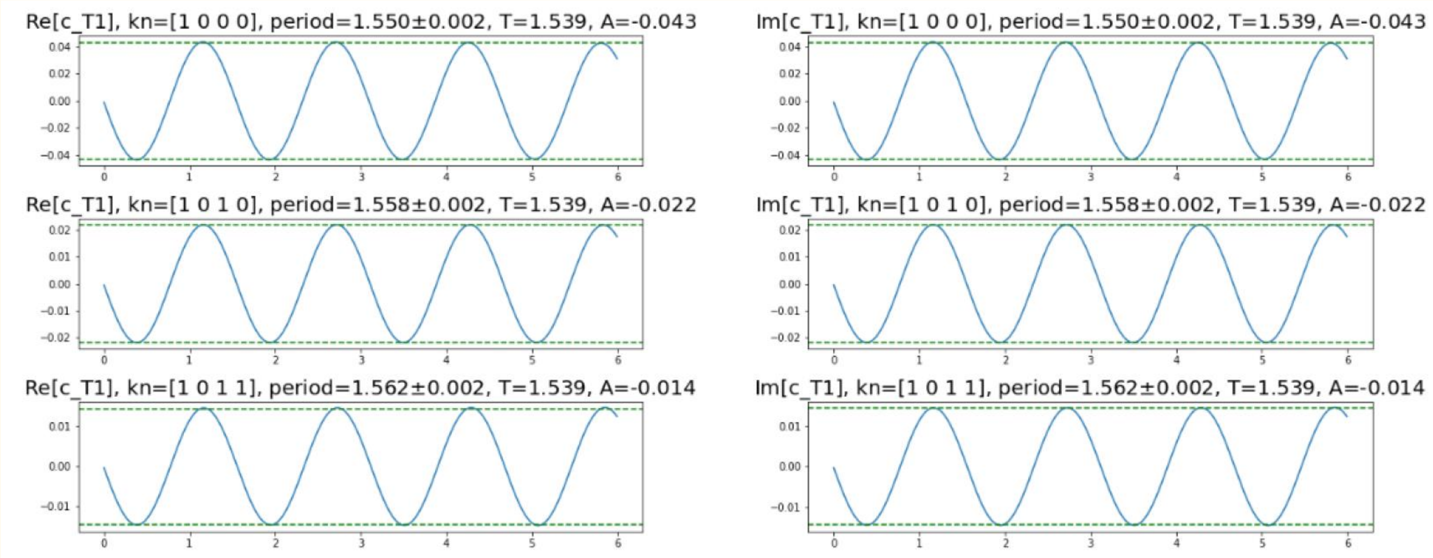
- With gauge-fixing, perturbative gauge modes perform SHO motion with known frequencies
  - With **regular HMC kinetic** term, transverse modes have k-dependent frequencies: $\omega_k = \sqrt{\frac{\beta}{6}}\,\mathrm{k}$



$\beta = 100$, 4^4 lattice, regular HMC kinetic energy term

Gauge-Modes ($A = \ln U$)

- With gauge-fixing, perturbative gauge modes perform SHO motion with known frequencies
    - **Fourier Acceleration kinetic term** eliminates k-dependence of transverse mode frequencies: $\omega_k = \sqrt{\frac{\beta}{6}}$



$\beta = 100$, 4^4 lattice, Fourier acceleration kinetic energy term

Periodic Box Results

- $\beta = 10$, 8^4 lattice with periodic boundary conditions. Compare integrated autocorrelation time for the plaquette and Wilson flowed energy, flow time of 4
  - HMC

β	τ_{traj}	steps	trajs	plaq	plaq τ_{int}	E(4) τ_{int}	Accpt
10	0.6	24	10030	0.783295(37)	4.51(82)	20.9(5.4)	75%
10	1.0	50	10030	0.783289(26)	3.41(30)	19.0(4.4)	77.6%
10	4.0	200	8533	0.783363(27)	10.73(61)	13.0(1.4)	78%

  - GFFA

β	τ_{traj}	steps	trajs	plaq	plaq τ_{int}	E(4) τ_{int}	M	MC
10	0.6	24	1911	0.783347(45)	1.26(25)	3.6(1.0)	3.0	200
10	1.0	30	5176	0.783207(16)	0.653(31)	18.6(8.3)	3.0	40
10	0.6	24	3915	0.783404(28)	1.059(81)	5.4(1.3)	5.0	200

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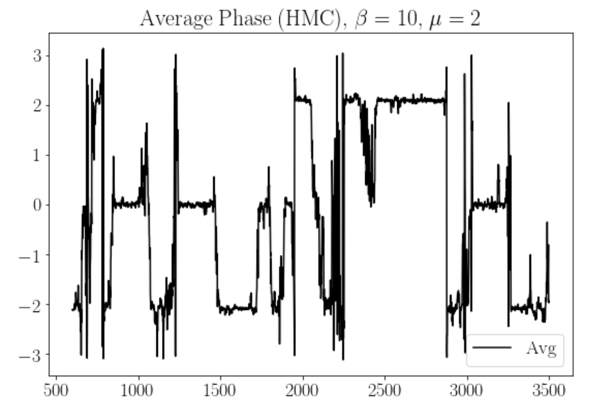
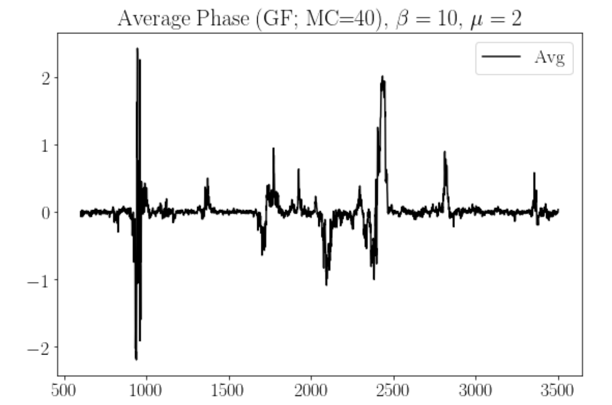
GFFA achieves ≈5x factor acceleration

Polyakov Phases and Z_3 Symmetry

- Recall: $P_\mu \rightarrow e^{2\pi i/3} P_\mu$ is symmetry of action … $\boldsymbol{Z_3}$ **symmetry**

- Evolution (HMC vs GF; **Inner MC sweeps= 40**):



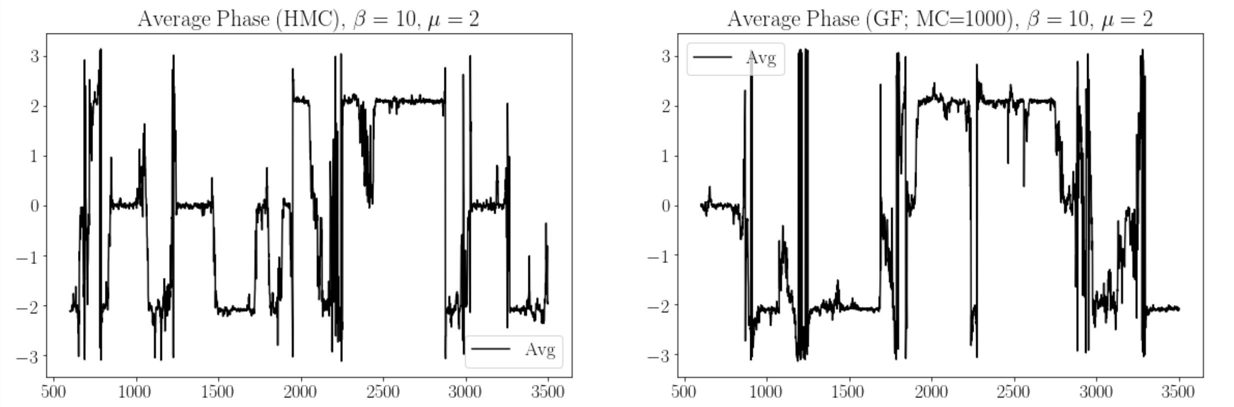


- Gauge-fixed evolution doesn't respect the Z_3 symmetry?

Polyakov Phases and Z_3 Symmetry

- Recall: $P_\mu \rightarrow e^{2\pi i/3} P_\mu$ is symmetry of action … $\boldsymbol{Z_3}$ **symmetry**

- Evolution (HMC vs GF; **Inner MC sweeps= 1000**):



- Gauge-fixed evolution doesn't respect the Z_3 symmetry?
  - Monte Carlo estimate of S_{FP} may fail to adequately compensate lack of Z_3 symmetry in S_{GF}

Change of Setting

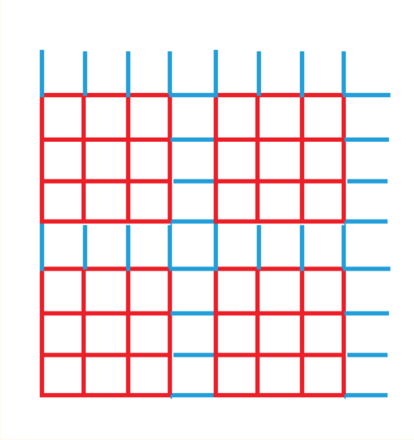
- 1000 Inner MC sweeps are impractical

- Relevance of Polyakov phase?

- Ultimately want to work with fixed boundary conditions
  - Upshot: Eliminate Z_3 symmetry

Fixed Boundaries and Current Results

Looking Forward

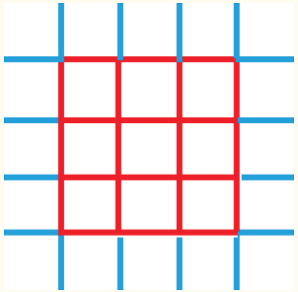


- Ultimate goal: apply Fourier Acceleration to physically relevant, nonperturbatively large volumes

- Fourier acceleration requires:
  - Free modes … Continuum limit ($a \to 0$)
  - Perturbative gauge … Small volume ($L \ll \frac{1}{\Lambda_{QCD}}$)

- Divide large volume into smaller perturbative sub-volumes; and apply Fourier Acceleration independently in each sub-volume

Setup & Evolution Scheme



- Evolve one of the cells
  - Lattice with fixed boundary conditions

- Setup:
  - 1- Entire Lattice equilibriated using Wilson action
  - 2- Sample $g(x)$ according to $\exp\{-S_{GF}[U^g \in B] - S_{FP}[U^g \in B]\}$ and apply it to lattice.

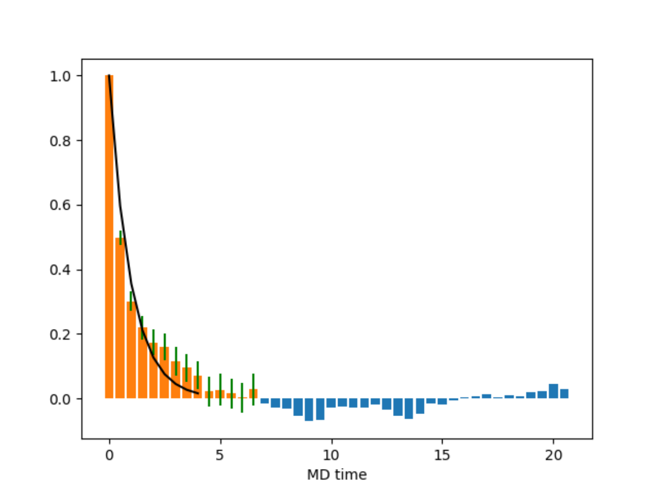
    This fixes Landau gauge in the cell and "squeezes" any nonperturbative effects into the fixed boundary links

- Evolve the cell according to

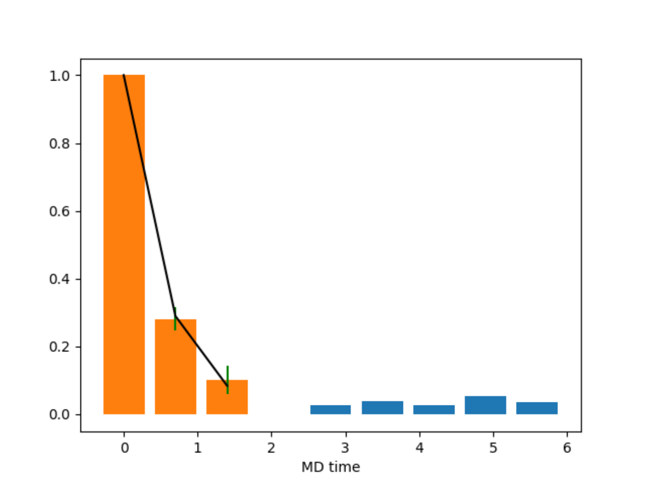
$$H = \sum_k tr[P_\mu(-k)D^{\mu\nu}(k)P_\nu(k)] + S_{wilson}[U] + S_{GF}[U \in B] + S_{FP}[U \in B]$$

Current Results ($\beta = 10$)

- Comparison of plaquette autocorrelation function on the 10^4 cell inside 12^4 lattice



a) HMC, $\tau_{traj} = 0.5$



b) GFFA, $\tau_{traj} = 0.7$

- Observable of interest: autocorrelation time τ_{exp}
- Fit autocorrelation function to exponential $f(t) = e^{-t/\tau_{exp}}$

Current Results ($\beta = 10$)

- 6^4 cell inside 8^4 lattice:
  - HMC

β	τ_{traj}	steps	trajs	plaq	plaq τ_{exp}	Accpt
10	0.5	48	9431	0.783318(56)	0.810(45)	97.2%
10	1.0	96	8481	0.783313(11)	1.540(87)	96.6%

  - GFFA

β	τ_{traj}	steps	trajs	plaq	plaq τ_{exp}	M	MC
10	0.7	48	1518	0.783104(16)	0.579(67)	3.0	200

- 10^4 cell inside 12^4 lattice:
  - HMC

β	τ_{traj}	steps	trajs	plaq	plaq τ_{exp}	Accpt
10	0.5	48	2011	0.783395(13)	0.97(14)	93.3%
10	1.0	96	1807	0.783415(14)	1.97(30)	91.5%

  - GFFA

β	τ_{traj}	steps	trajs	plaq	plaq τ_{exp}	M	MC
10	0.7	60	1009	0.783001(12)	0.565(60)	5.0	200

Conclusion

- 6^4 cell inside 8^4 lattice:
  - HMC

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10	0.7	60	1009	0.783001(12)	0.565(60)	5.0	200

GFFA achieves ≈2x factor acceleration ... expect more on larger volumes

Thank You!