Riemannian Manifold Hybrid Monte Carlo in Lattice QCD

Tuan Nguyen
in collaboration with Chulwoo Jung, Yong-Chull Jang, Norman Christ, Peter Boyle, ...

Columbia University

July 2021

This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the US DOE's Office of Science and National Nuclear Security Administration.

Overview

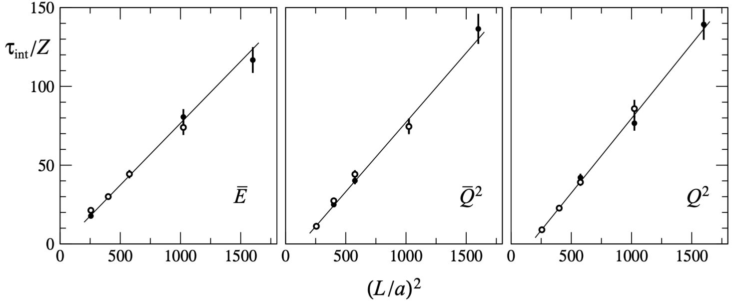
Critical Slowing Down in HMC

Fourier Acceleration

Riemannian Manifold HMC

Next Steps

Autocorrelation Increases as Lattice Spacing Decreases



- Consider fixed physical L with open boundaries in time and $\tau \sim L$
- Lüscher and Schaefer show $\tau_{int} \sim a^{-2}$ for HMC [1]

[1] arXiv: 1105.4749v1 [hep-lat]

Fourier Acceleration: Add Coordinate Dependent Mass Term so All Modes Move at Same Rate

- Free scalar field theory: $H = \frac{1}{2}\pi^2 + \frac{1}{2}\phi\left(m^2 - \nabla^2\right)\phi$
  - $\mathcal{M} = 1$
  - $\ddot{\phi} = -\left(m^2 - \nabla^2\right)\phi$
  - $\omega^2(k) = m^2 + k^2$
- Consider: $H = \frac{1}{2}\pi\left[(1-\kappa) - \kappa\nabla^2\right]^{-1}\pi + \frac{1}{2}\phi\left(m^2 - \nabla^2\right)\phi$
  - $\mathcal{M} = (1-\kappa) - \kappa\nabla^2$
  - $\ddot{\phi} = -\left[(1-\kappa) - \kappa\nabla^2\right]^{-1}\left(m^2 - \nabla^2\right)\phi$
  - $\omega^2(k) = \frac{m^2 + k^2}{(1-\kappa) + \kappa k^2}$
- Adding interactions, we generally want $\mathcal{M}(k) \propto \int \mathrm{d}^4x\, \phi^\dagger \frac{\partial S}{\partial \phi}\bigg|_{\phi = e^{ik\cdot x}}$

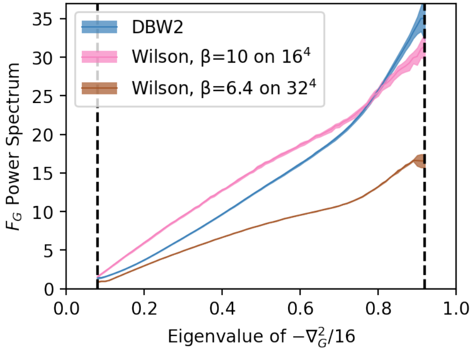
Fourier Acceleration: Add Coordinate Dependent Mass Term so All Modes Move at Same Rate

- Free scalar field theory: $H = \frac{1}{2}\pi^2 + \frac{1}{2}\phi\left(m^2 - \nabla^2\right)\phi$
  - $\mathcal{M} = 1$
  - $\ddot{\phi} = -\left(m^2 - \nabla^2\right)\phi$
  - $\omega^2(k) = m^2 + k^2$
- Consider: $H = \frac{1}{2}\pi\left[(1-\kappa) - \kappa\nabla^2\right]^{-1}\pi + \frac{1}{2}\phi\left(m^2 - \nabla^2\right)\phi$
  - $\mathcal{M} = (1-\kappa) - \kappa\nabla^2$
  - $\ddot{\phi} = -\left[(1-\kappa) - \kappa\nabla^2\right]^{-1}\left(m^2 - \nabla^2\right)\phi$
  - $\omega^2(k) = \frac{m^2 + k^2}{(1-\kappa) + \kappa k^2}$
- Adding interactions, we generally want $\mathcal{M}(k) \propto \int d^4x\, \phi^\dagger \frac{\partial S}{\partial \phi}\Big|_{\phi = e^{ik\cdot x}}$

Fourier Acceleration: Add Coordinate Dependent Mass Term so All Modes Move at Same Rate

- Free scalar field theory: $H = \frac{1}{2}\pi^2 + \frac{1}{2}\phi\left(m^2 - \nabla^2\right)\phi$
  - $\mathcal{M} = 1$
  - $\ddot{\phi} = -\left(m^2 - \nabla^2\right)\phi$
  - $\omega^2(k) = m^2 + k^2$
- Consider: $H = \frac{1}{2}\pi\left[(1-\kappa) - \kappa\nabla^2\right]^{-1}\pi + \frac{1}{2}\phi\left(m^2 - \nabla^2\right)\phi$
  - $\mathcal{M} = (1-\kappa) - \kappa\nabla^2$
  - $\ddot{\phi} = -\left[(1-\kappa) - \kappa\nabla^2\right]^{-1}\left(m^2 - \nabla^2\right)\phi$
  - $\omega^2(k) = \dfrac{m^2 + k^2}{(1-\kappa) + \kappa k^2}$
- Adding interactions, we generally want $\mathcal{M}(k) \propto \int \mathrm{d}^4x\, \phi^\dagger \frac{\partial S}{\partial \phi}\Big|_{\phi = e^{ik\cdot x}}$

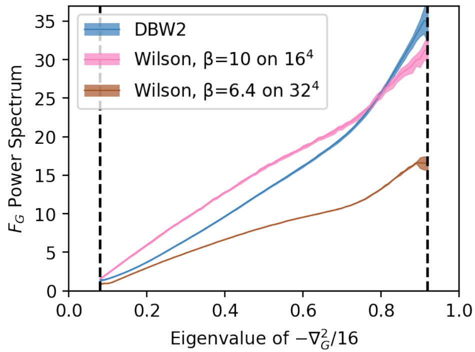
HMC Gauge Force Power Spectrum Is Nearly Linear



- DBW2: $1/a = 2\,\mathrm{GeV}$
- Wilson, $\beta = 10$: $1/a = 270\,\mathrm{GeV}$
- Wilson, $\beta = 6.4$: $1/a = 3.6\,\mathrm{GeV}$

- Define bandpass filter $\mathcal{B}(\lambda) \approx P_{\lambda,\lambda+\Delta\lambda}\left(\nabla_G^2/16\right)$
- Measure $\left\langle F_G^\dagger \middle| \mathcal{B}(\lambda) \middle| F_G \right\rangle / \mathrm{Tr}[\mathcal{B}(\lambda)]$

HMC Gauge Force Power Spectrum Is Nearly Linear



- DBW2: $1/a = 2\,\text{GeV}$
- Wilson, $\beta = 10$: $1/a = 270\,\text{GeV}$
- Wilson, $\beta = 6.4$: $1/a = 3.6\,\text{GeV}$

- Define bandpass filter $\mathcal{B}(\lambda) \approx P_{\lambda,\lambda+\Delta\lambda}\left(\nabla_G^2/16\right)$
- Measure $\left\langle F_G^\dagger \middle| \mathcal{B}(\lambda) \middle| F_G \right\rangle \Big/ \operatorname{Tr}[\mathcal{B}(\lambda)]$

RMHMC: Mass Term Depends Solely on Covariant Laplace Operator

- MD Hamiltonian: [2]

$$H = \frac{1}{2}\,\mathrm{Tr}\left\{P_\mu^\dagger(x)\mathcal{M}^{-1}[U_\mu(x)]P_\mu(x)\right\} + S[U_\mu(x)] + \log|\mathcal{M}| \tag{1}$$

- Duane and Pendleton: [3] $\mathcal{M} = (1-\kappa) - \kappa\frac{\nabla_G^2}{16}$
- Generalize to:

$$\mathcal{M} = \left[c + \sum \frac{a_0 + a_1\left(-\nabla_G^2/16\right)}{b_0 + b_1\left(-\nabla_G^2/16\right) + \left(-\nabla_G^2/16\right)^2}\right]^{-2}$$

[2] https://doi.org/10.1111/j.1467-9868.2010.00765.x
[3] https://doi.org/10.1016/0370-2693(86)90940-8

RMHMC: Mass Term Depends Solely on Covariant Laplace Operator

- MD Hamiltonian: [2]

$$H = \frac{1}{2}\,\mathrm{Tr}\left\{P_\mu^\dagger(x)\mathcal{M}^{-1}[U_\mu(x)]P_\mu(x)\right\} + S[U_\mu(x)] + \log|\mathcal{M}| \tag{1}$$

- Duane and Pendleton: [3] $\mathcal{M} = (1-\kappa) - \kappa\frac{\nabla_G^2}{16}$
- Generalize to:

$$\mathcal{M} = \left[c + \sum \frac{a_0 + a_1\left(-\nabla_G^2/16\right)}{b_0 + b_1\left(-\nabla_G^2/16\right) + \left(-\nabla_G^2/16\right)^2}\right]^{-2}$$

[2] https://doi.org/10.1111/j.1467-9868.2010.00765.x
[3] https://doi.org/10.1016/0370-2693(86)90940-8

RMHMC: Mass Term Depends Solely on Covariant Laplace Operator

- MD Hamiltonian: [2]

$$H = \frac{1}{2} \mathrm{Tr} \left\{ P^{\dagger}_{\mu}(x) \mathcal{M}^{-1}[U_{\mu}(x)] P_{\mu}(x) \right\} + S[U_{\mu}(x)] + \log |\mathcal{M}| \tag{1}$$

- Duane and Pendleton: [3] $\mathcal{M} = (1-\kappa) - \kappa \frac{\nabla^2_G}{16}$
- Generalize to:
$$\mathcal{M} = \left[c + \sum \frac{a_0 + a_1\left(-\nabla^2_G/16\right)}{b_0 + b_1\left(-\nabla^2_G/16\right) + \left(-\nabla^2_G/16\right)^2} \right]^{-2}$$

[2] https://doi.org/10.1111/j.1467-9868.2010.00765.x
[3] https://doi.org/10.1016/0370-2693(86)90940-8

Instead of Autocorrelation Studies, Investigate Long-Scale Observables

- Full many-trajectory autocorrelation studies take months
- Instead, study movement of long-distance observables
- Wilson flowed observables, such as Wilson flowed energy $E(\tau) = \sum_P \mathrm{Re}\,\mathrm{Tr}[1 - V(\tau)_P]$, probe length scales $\mathcal{O}(\sqrt{\tau})$ [4]

[4] arXiv: 1006.4518

Instead of Autocorrelation Studies, Investigate Long-Scale Observables

- Full many-trajectory autocorrelation studies take months
- Instead, study movement of long-distance observables
- Wilson flowed observables, such as Wilson flowed energy $E(\tau) = \sum_P \mathrm{Re}\,\mathrm{Tr}[1 - V(\tau)_P]$, probe length scales $\mathcal{O}(\sqrt{\tau})$ [4]

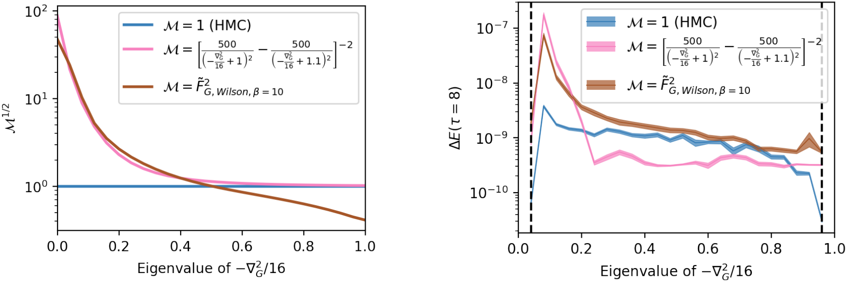
[4] arXiv: 1006.4518

Instead of Autocorrelation Studies, Investigate Long-Scale Observables

- Full many-trajectory autocorrelation studies take months
- Instead, study movement of long-distance observables
- Wilson flowed observables, such as Wilson flowed energy $E(\tau) = \sum_P \mathrm{Re}\,\mathrm{Tr}[1 - V(\tau)_P]$, probe length scales $\mathcal{O}(\sqrt{\tau})$ [4]

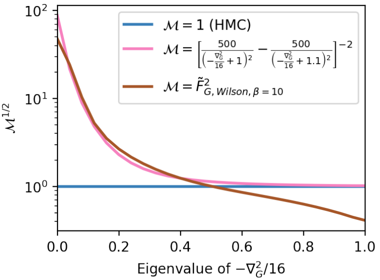
[4] arXiv: 1006.4518

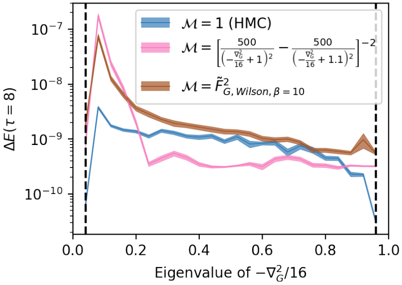
FLOWED WILSON ENERGY PROBES MOVEMENT OF LOW MODES (WILSON $\beta = 10$ ON 16^4 LATTICE)



- ▶ MD trajectory momenta generated with $p = \mathcal{M}^{1/2}\xi$
- ▶ RMHMC algorithms generate larger momenta corresponding to low Laplace eigvals
- ▶ $E(\tau = 8)$ most sensitive to low Laplace eigval momenta

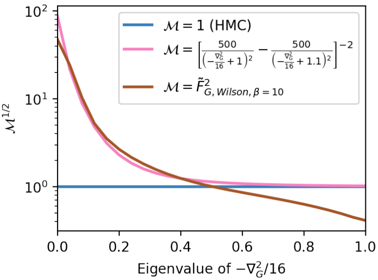
Flowed Wilson Energy Probes Movement of Low Modes (Wilson $\beta = 10$ on 16^4 Lattice)

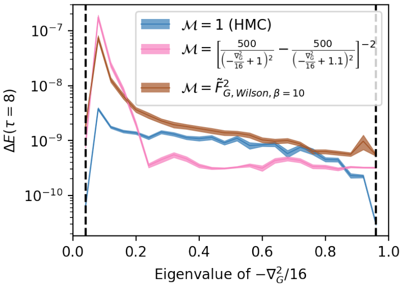




- MD trajectory momenta generated with $p = \mathcal{M}^{1/2}\xi$
- RMHMC algorithms generate larger momenta corresponding to low Laplace eigvals
- $E(\tau = 8)$ most sensitive to low Laplace eigval momenta

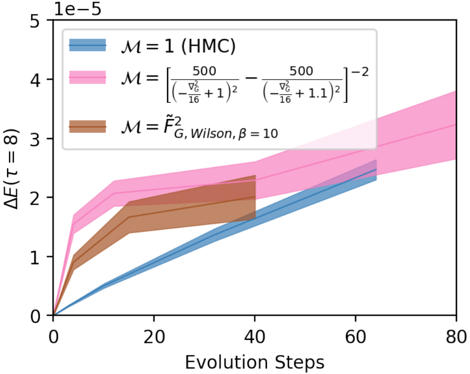
Flowed Wilson Energy Probes Movement of Low Modes (Wilson $\beta = 10$ on 16^4 Lattice)





- MD trajectory momenta generated with $p = \mathcal{M}^{1/2}\xi$
- RMHMC algorithms generate larger momenta corresponding to low Laplace eigvals
- $E(\tau = 8)$ most sensitive to low Laplace eigval momenta

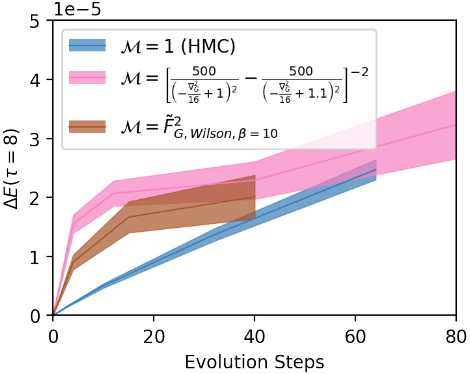
RMHMC Moves Flowed Wilson Energy Faster than HMC (Wilson $\beta = 10$ on 16^4 Lattice)



- HMC: $\Delta\tau = 0.03125$
- RMHMC: $\Delta\tau = 0.025$

- Step sizes tuned to give similar acceptance rates
- Distribution width of $E(8)$ for thermalized configs is $\sim 1 \times 10^{-4}$
- RMHMC moves $E(8)$ same amount as HMC in fewer steps

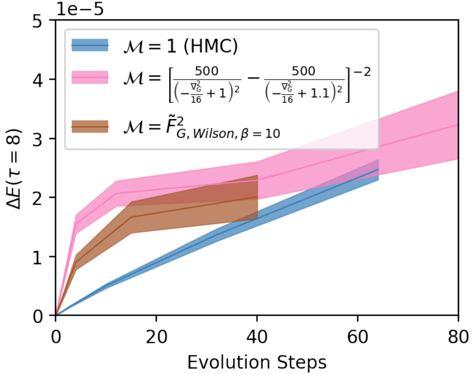
RMHMC Moves Flowed Wilson Energy Faster than HMC (Wilson $\beta = 10$ on 16^4 Lattice)



- HMC: $\Delta\tau = 0.03125$
- RMHMC: $\Delta\tau = 0.025$

- Step sizes tuned to give similar acceptance rates
- Distribution width of $E(8)$ for thermalized configs is $\sim 1 \times 10^{-4}$
- RMHMC moves $E(8)$ same amount as HMC in fewer steps

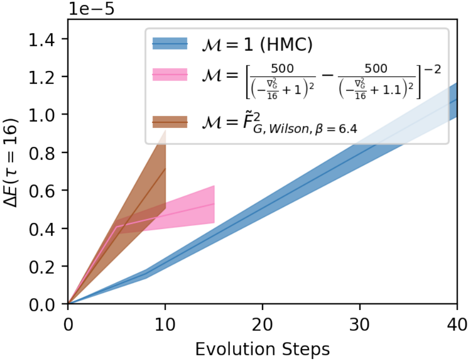
RMHMC Moves Flowed Wilson Energy Faster than HMC (Wilson $\beta = 10$ on 16^4 Lattice)



- HMC:
  $\Delta\tau = 0.03125$
- RMHMC:
  $\Delta\tau = 0.025$

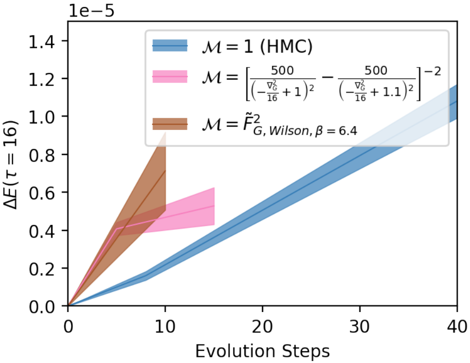
- Step sizes tuned to give similar acceptance rates
- Distribution width of $E(8)$ for thermalized configs is $\sim 1 \times 10^{-4}$
- RMHMC moves $E(8)$ same amount as HMC in fewer steps

Similar Results Seen for Wilson $\beta = 6.4$ on 32^4 Lattice



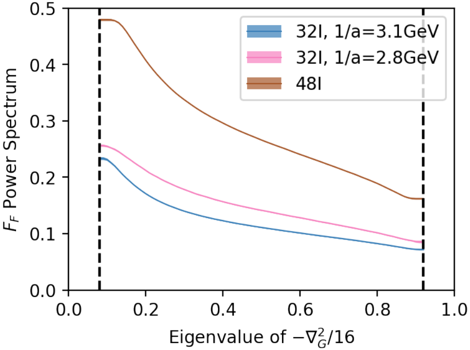
- Step sizes tuned to give similar acceptance rates
- RMHMC moves $E(16)$ faster than HMC

Similar Results Seen for Wilson $\beta = 6.4$ on 32^4 Lattice



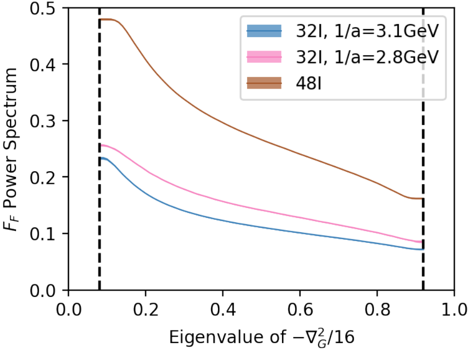
- Step sizes tuned to give similar acceptance rates
- RMHMC moves $E(16)$ faster than HMC

HMC Fermion Force Has a Milder Spectral Dependence



- Fermion force has milder spectral dependence
- In hierarchical scheme, implicit integration only needed in lower (gauge only) levels

HMC Fermion Force Has a Milder Spectral Dependence



- Fermion force has milder spectral dependence
- In hierarchical scheme, implicit integration only needed in lower (gauge only) levels

Next Steps

- Demonstrate reduction in autocorrelation from long evolution time
- Tune and run RMHMC with fermions. Investigate spectral dependence of forces from Hasenbusch ratios.

Bibliography

Martin Lüscher and Stefan Schaefer.
Lattice qcd without topology barriers.
Journal of High Energy Physics, 2011(7), Jul 2011.

Mark Girolami and Ben Calderhead.
Riemann manifold langevin and hamiltonian monte carlo methods.
Journal of the Royal Statistical Society: Series B (Statistical Methodology), 73(2):123–214, 2011.

Simon Duane, Richard Kenway, Brian J. Pendleton, and Duncan Roweth.
Acceleration of gauge field dynamics.
Physics Letters B, 176(1):143–148, 1986.

Martin Lüscher.
Properties and uses of the wilson flow in lattice qcd.
Journal of High Energy Physics, 2010(8):71, Aug 2010.

Thank You!
Questions?