Effect of FTHMC with 2+1 Domain Wall Fermions on Autocorrelation Times via Master-Field Technique II

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Review: HMC

Target Distribution

- $Z = \int \mathcal{D}U \, e^{-S(U)} \propto \int \mathcal{D}U\mathcal{D}P \, e^{-P^2/2} e^{-S(U)} = \int \mathcal{D}U\mathcal{D}P \, e^{-H}$
- $H = P^2/2 + S(U)$

HMC

- Momentum Refreshment: A momentum field P is generated randomly with probability density proportional to $e^{-P^2/2}$
- MD: The Hamilton equations are integrated from time $t = 0$ to some later time τ with the initial fields of P and U to obtain a new field U'

$$\dot{U} = PU$$
$$\dot{P} = -\frac{\partial H}{\partial U} = -\frac{\partial S}{\partial U}$$

- Apply the Acceptance-Reject step to decide whether to update U to U_τ or keep U, i.e., $U' = U_\tau$

Field-Transformation HMC

With $U = \mathcal{F}_t(V)$,

$$Z = \int \mathcal{D}U e^{-S(U)} = \int \mathcal{D}V \mathrm{Det}[\mathcal{F}_*(V)]\, e^{-S(\mathcal{F}(V))} = \int \mathcal{D}V\, e^{-S_{FT}(V)}$$

$$S_{FT} = S(\mathcal{F}_t(V)) - \ln \mathrm{Det}\mathcal{F}_*(V).$$

- originally proposed by Luscher for continuous flow [Luscher, 2010]
- perfect trivialization: $S_{FT} = 0$
- Ansatz:

$$\dot{U}_t = Z_t[U_t]U_t$$

- $Z_t(x, \mu) \in \mathfrak{su}(3)$

Field-Transformation HMC

- Luscher: approximate the trivializing map by the Wilson flow

$$Z_t[U]^a(x,\mu) = \partial^a_{x,\mu} P_{\mu\nu}(x,\mu)$$
$$= \frac{P_{\mu\nu}(x,\mu) - P_{\mu\nu}(x,\mu)^\dagger}{2} - \frac{1}{6}\mathrm{tr}\left[P_{\mu\nu}(x,\mu) - P_{\mu\nu}(x,\mu)^\dagger\right]$$

where $P_{\mu\nu}(x,\mu)$ is a sum of plaquettes

$$P_{\mu\nu}(x,\mu) = \sum_{\nu\neq\pm\mu} \rho_{\mu,\nu} U(x,\nu)U(x+\hat{\nu},\mu)U(x+\hat{\mu},\nu)^\dagger U(x,\mu)^\dagger$$

- In our work: discretize the transformation with finite step size $\rho \equiv \rho_{\mu\nu}$

$$U(x,\mu) \to \mathcal{E}_{x,\mu}(y,\nu) = \begin{cases} e^{Z_t(U)(x,\mu)} U(x,\mu) & \text{if } (y,\nu) = (x,\mu) \\ U(y,\nu) & \text{otherwise.} \end{cases}$$

- The number of integration steps for the discretized trivializing map is set to 1

Numerical Integration

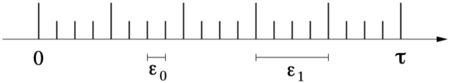
- Elementary updates for P and U

$$I_P(\varepsilon):(P,U) \to (P - \varepsilon F, U)$$
$$I_U(\varepsilon):(P,U) \to (P, e^{\varepsilon P} U)$$

- Leap-frog integrator:

$$\mathcal{J}(\varepsilon, N) = \{I_P(\varepsilon/2) I_U(\varepsilon) I_P(\varepsilon/2)\}^N$$

- Multiple Time-Step Integration:
  - In many cases, $F_0 \gg F_1$
  - We use different integration step sizes for different forces



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Run Parameters

Lattice Parameters:

- on a lattice of size 32^4
- $\beta = 2.37$
- with $2 + 1$ Domain-Wall fermions of mass $m_l = 0.0047, m_s = 0.0186$

HMC Parameters:

- different ρ values: 0.1, 0.112, 0.124
- different gauge step sizes $\delta\tau_G = 1/48, 1/96$
- different fermion step sizes $\delta\tau_F = 1/24, 1/16, 1/12, 1/8$

In the following, we focus on the runs with different flow parameters and $\delta\tau_G$ but τ_F is fixed to $1/24$

Statistics

ρ	0.0	0.1	0.112	0.124
$\delta\tau_G = 1/48$	233	230	188	230
$\delta\tau_G = 1/96$	401	232	229	229
$\delta\tau_G = 1/144$	-	230	-	-

Table: The number of configurations for each ensemble after thermalization with $\tau_F = 1/24$

Machine

- Simulation is carried out on Frontier and Andes at Oak Ridge National Laboratory

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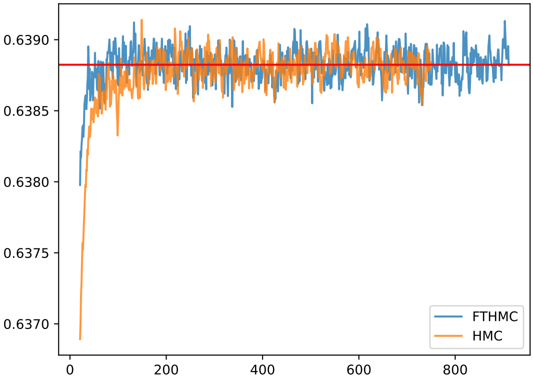
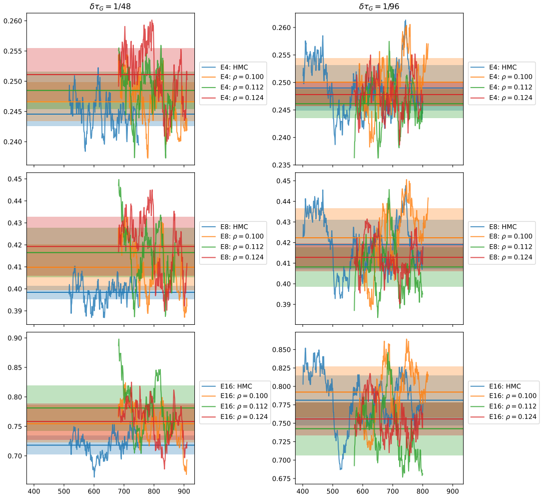
Plaquettes



- The red line is an expected value of plaquette for this lattice from Ref. [Blum et al., 2016]
- Its value is 0.6388238(37).

Wilson flowed energies



- Comparison of Wilson flowed energy with different ρ values for different flow time (raw) and $\delta\tau_G = 1/48, 1/96$ (column)

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Autocorrelation

Notation

- Observable: $A(x)$
- Measurement: $a_i(x)$
- Volume Average: $\langle\!\langle A \rangle\!\rangle = (1/V)\sum_x A(x)$
- Ensemble Average: $a = \langle a_i(x) \rangle = \langle \langle\!\langle A \rangle\!\rangle \rangle$
- Autocovariance: $\Gamma^V(t) = \langle (\langle\!\langle a_i \rangle\!\rangle - a)(\langle\!\langle a_{i+t} \rangle\!\rangle - a) \rangle$
- Autocorrelation Coefficients (ACC): $\rho^V(t) = \Gamma^V(t)/\Gamma^V(0)$

Estimators:

- $\langle a(x) \rangle \to \bar{a}(x) = \frac{1}{T}\sum_{i=1}^{T} a_i(x)$
- $\bar{\Gamma}^V(t) = \frac{1}{T-t}\sum_{i=1}^{T-t}(\langle\!\langle a_i \rangle\!\rangle - \langle\!\langle \bar{a} \rangle\!\rangle)(\langle\!\langle a_{i+t} \rangle\!\rangle - \langle\!\langle \bar{a} \rangle\!\rangle)$
- T: length of Markov chain approximating the ensemble

Volume Autocorrelation

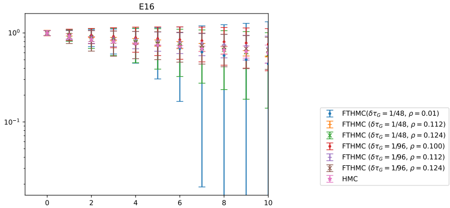

Figure: Autocorrelation coefficient (ACC) as a function of t for Wilson-flowed energy E16.

- Error via Madras-Sokal Approximation [Luscher, 2005]:

$$\langle \delta \bar{\rho}^{(V)}(t)^2 \rangle \simeq \frac{1}{N} \sum_{k=1}^{t+\Lambda} \left[\bar{\rho}^{(V)}(k+t) + \bar{\rho}^{(V)}(k-t) - 2\bar{\rho}^{(V)}(k)\bar{\rho}^{(V)}(t) \right]$$

- $\Lambda \geq 100$ gives a reasonable estimate of the error [Luscher, 2005]

Master-Field Technique

- Instead of ACC of the volume average $\langle\!\langle A \rangle\!\rangle = (1/V)\sum_x A(x)$, consider ACC of local observable $A(x)$
- Subtract the volume average: $A'(x) = A(x) - \langle\!\langle A \rangle\!\rangle$
- Due to translational invariance, $\mu = \langle A'(x) \rangle = a - a = 0$
- Denote autocovariance of $A'(x)$ at x as $\Gamma'_x(t)$
- Then,

$$\begin{aligned}\Gamma'_x(t) &= \langle (a'_i(x) - \mu)(a'_{i+t}(x) - \mu) \rangle \\ &= \langle a'_i(x) a'_{i+t}(x) \rangle \\ &= \langle (a_i(x) - \langle\!\langle a_i \rangle\!\rangle)(a_{i+t}(x) - \langle\!\langle a_{i+t} \rangle\!\rangle) \rangle \equiv \langle \mathcal{O}^i_t(x) \rangle\end{aligned}$$

Master-Field Technique

- Idea: $\langle\langle A(x) \rangle\rangle = \langle A(x) \rangle + \mathcal{O}(V^{-1/2})$
- Approximate $\Gamma'_x(t)$ by $\langle\langle \Gamma'(t) \rangle\rangle$ [Lüscher, 2018]
- Also, $\mathcal{O}^i_t(x) \to \bar{\mathcal{O}}_t(x) \equiv \frac{1}{T-t} \sum_{i=1}^{T-t} \mathcal{O}^i_t(x)$
- Finally, $\rho(t) = \langle\langle \Gamma'(t) \rangle\rangle / \langle\langle \Gamma'(0) \rangle\rangle$

Error via Master-Field Approach

- Need: $\mathrm{Cov}[\langle\!\langle \bar{\mathcal{O}}_s \rangle\!\rangle, \langle\!\langle \bar{\mathcal{O}}_t \rangle\!\rangle] \equiv \langle [\langle\!\langle \bar{\mathcal{O}}_s \rangle\!\rangle - \langle \mathcal{O}_s \rangle][\langle\!\langle \bar{\mathcal{O}}_t \rangle\!\rangle - \langle \mathcal{O}_t \rangle] \rangle =$ $\frac{1}{V}\sum_y \langle [\bar{\mathcal{O}}_s(y) - \langle \mathcal{O}_s \rangle][\bar{\mathcal{O}}_t(0) - \langle \mathcal{O}_t \rangle] \rangle \equiv \frac{1}{V}\sum_y C_{st}(y)$ [Bruno et al., 2023]
- Approximate $C_{st}(y)$ by

$$\langle\!\langle \mathcal{C}_{st}(y) \rangle\!\rangle = \frac{1}{V}\sum_x \delta\bar{\mathcal{O}}_s(x+y)\delta\bar{\mathcal{O}}_t(x),\ \delta\bar{\mathcal{O}}_t(x) \equiv \bar{\mathcal{O}}_t(x) - \langle\!\langle \bar{\mathcal{O}}_t \rangle\!\rangle$$

- Define $C_{st}(|y| \le R) \equiv \sum_{|y|\le R} C_{st}(y)$
- Determine the value of R s.t. $C_{st}(|y| \le R)$ saturates
- Truncate the sum in $\mathrm{Cov}[\langle\!\langle \bar{\mathcal{O}}_s \rangle\!\rangle, \langle\!\langle \bar{\mathcal{O}}_t \rangle\!\rangle]$ beyond R_{sat}

$$\mathrm{Var}[\rho(t))] = (\rho(t))^2 \left(\frac{\mathrm{Var}[\langle\!\langle \bar{\Gamma}(t) \rangle\!\rangle]}{\langle\!\langle \bar{\Gamma}(t) \rangle\!\rangle^2} + \frac{\mathrm{Var}[\langle\!\langle \bar{\Gamma}(0) \rangle\!\rangle]}{\langle\!\langle \bar{\Gamma}(0) \rangle\!\rangle^2} - 2\frac{\mathrm{Cov}[\langle\!\langle \bar{\Gamma}(t) \rangle\!\rangle, \langle\!\langle \bar{\Gamma}(0) \rangle\!\rangle]}{\langle\!\langle \bar{\Gamma}(t) \rangle\!\rangle \langle\!\langle \bar{\Gamma}(0) \rangle\!\rangle} \right)$$

Error via Master-Field Approach

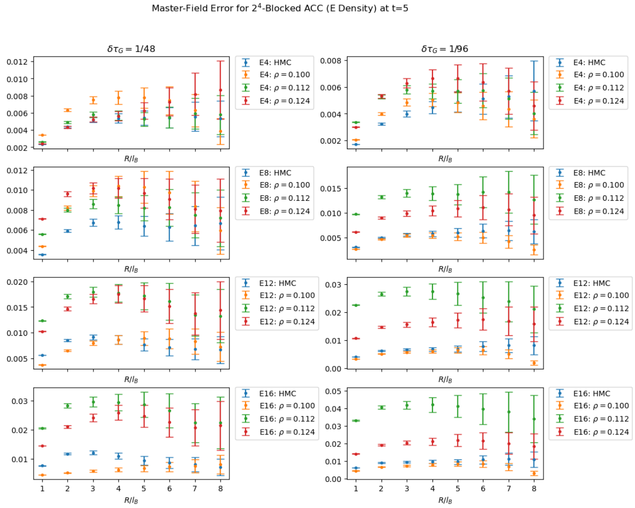

Figure: R: Summation Radius, b: block size

Error via Binning

- Divide the MC into several bins
- Compute $\langle\!\langle \bar{\Gamma}(t) \rangle\!\rangle$ on each bin
- The estimator of the error of $\langle\!\langle \bar{\Gamma}(t) \rangle\!\rangle$ is standard deviation of the mean
- Lattice-correlation is irrelevant

Autocorrelation for Local Quantities

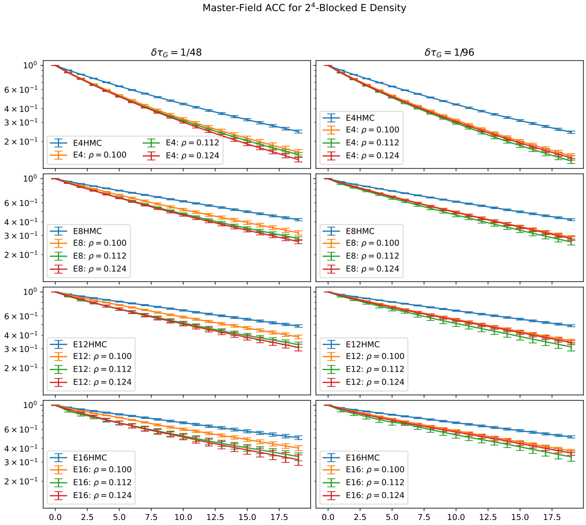

Figure: Autocorrelation based on Master-Field technique

Autocorrelation for Local Quantities

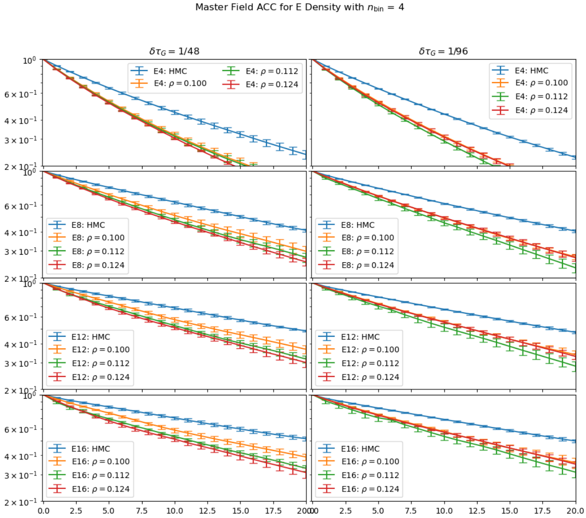

Figure: Autocorrelation based on binning method

Autocorrelation Times

Estimates of exponential autocorrelation times τ_{exp} computed by fitting $e^{-t/\tau_{\text{exp}}}$ to the ACC for different Wilson flow time τ_W, ρ, and $\delta\tau_G$ values:

ρ	$\tau_W = 4$	$\tau_W = 16$
0.0	14.28	27.822
0.100	11.2	21.68
0.112	10.87	19.2
0.124	10.14	17.68

Table: Fixed $\delta\tau_G = 1/48$, varied Wilson flow time τ_W

Autocorrelation Times

The ratios of $\tau_{\mathrm{exp}}(\rho = 0.0, \delta\tau_G = 1/48)$ for HMC to τ_{exp} with other HMC parameters:

ρ	$\tau_W = 4$	$\tau_W = 16$
0.100	1.275	1.2832
0.112	1.313	1.4487
0.124	1.408	1.5736

Table: Fixed $\delta\tau_G = 1/48$, varied Wilson flow time τ_W

- Overhead of field transformation mainly comes from a subroutine `logDetJacobianForceLevel`
- The computer time for this subroutine is reduced by a factor of around 4.

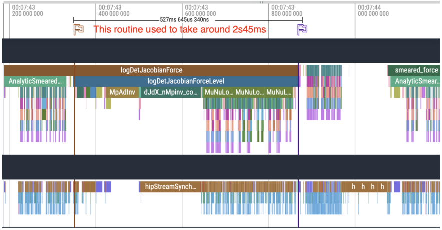

Figure: Snippet of tracing output from `Perfetto` for `logDetJacobianForceLevel` before optimization

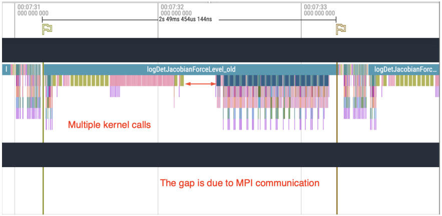

Figure: Snippet of tracing output from `Perfetto` for `logDetJacobianForceLevel` after optimization

Code Optimization

- As a result, the additional cost due to field transformation is reduced by a factor of 4 and now occupies only 2.2% of the total computer time

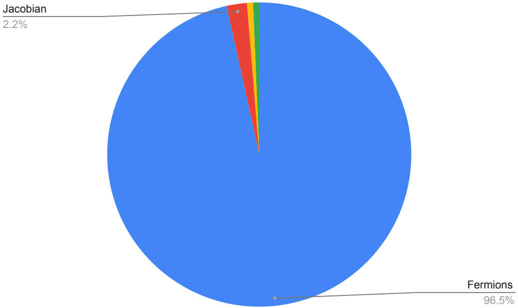

Figure: Breakdown of computer time from various components of FTHMC on a thermalized configuration

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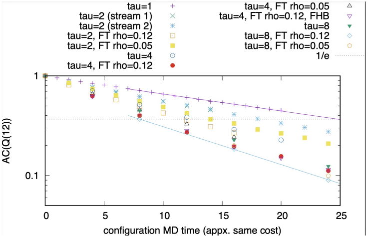
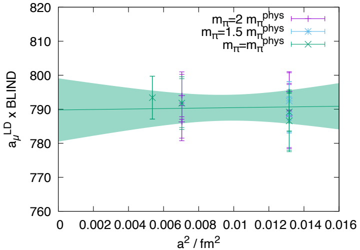
Summary and Outlook

- FTHMC reduces autocorrelation times around 1.5x compared to HMC
- Longer trajectory length + field transformation reduced autocorrelation time around 3.5x
- Enabled simulation at finer lattice spacings, huge volume (3.5 Gev, $128^3 \times 288$ for Iwasaki gauge action and 2+1 DWF)
- $\Rightarrow$ continue with gauge + fermion action: big impact on physics program of RBC-UKQCD
- Basis of INCITE computing proposal for next 3 years





Summary and Outlook

- Master-Field technique allows us to measure autocorrelation coefficients based on a small number of configurations
- Generate ensemble with different parameters (*beta*, the number of trivializing steps, etc...) for tuning
- FTHMC showed potential to reduce autocorelation time for topologial charge
- However, there are a number of parameters for FTHMC to tune for optimal performance
- Better understanding of why and how FTHMC is effective is needed

Thank you!

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Schwarz-preconditioned HMC algorithm for two-flavour lattice QCD.
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Luscher, M. (2010).
Trivializing maps, the Wilson flow and the HMC algorithm.
Commun. Math. Phys., 293:899–919.

Lüscher, M. (2018).

Wilson Flow

- Ansatz:

$$[Z_t(U)]^a(x,\mu) = -\partial^a_{x,\mu}\tilde{S}_t(U)$$

- Insert this to the previous equation:

$$\mathfrak{L}_t\tilde{S}_t = S_G + \dot{C}_t$$
$$\mathfrak{L}_t = \sum_{x,\mu}\{\partial^a_{x,\mu}\partial^a_{x,\mu} + t(\partial^a_{x,\mu}S_G)\partial^a_{x,\mu}\}$$

- Expand: $\tilde{S}_t = \sum_{k=0}^{\infty} t^k \tilde{S}_t^{(k)}$
- Matching t leads to recursive relations

$$\mathfrak{L}_0\tilde{S}^{(0)} = S_G + \dot{C}^{(0)}$$
$$\mathfrak{L}_0\tilde{S}^{(k)} = -\sum_{x,\mu}\partial^a_{x,\mu}S_G\partial^a_{x,\mu}\tilde{S}^{(k-1)} + \dot{C}^{(k)}$$

Wilson Flow

- The solution of the recursion

$$\tilde{S}^{(0)} = \mathfrak{L}_0^{-1} S_G$$
$$\tilde{S}^{(k)} = -\mathfrak{L}_0^{-1} \sum_{x,\mu} \partial^a_{x,\mu} S_G \partial^a_{x,\mu} \tilde{S}^{(k-1)}$$

- Approximation:
  - $\tilde{S} \approx \tilde{S}^{(0)}$
  - $S_G = S_W = -\frac{\beta}{6} \sum_{x,\mu\neq\nu} \mathrm{tr}[P_{\mu\nu}(x)]$
  - Plaquette: $P_{\mu\nu}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x)$

Wilson Flow

- Then,

$$
\begin{aligned}
Z_t(U_t)(x,\mu) = \mathcal{P}(C(x,\mu)) &\equiv \frac{1}{2}(C(x,\mu) - C(x,\mu)^\dagger) \\
&- \frac{1}{6}\mathrm{tr}\,[C(x,\mu) - C(x,\mu)^\dagger] \\
\mathcal{P}(M) &= \frac{1}{2}(M - M^\dagger) - \frac{1}{6}\mathrm{tr}\,(M - M^\dagger) \\
C(x,\mu) &= \sum_{\nu \neq \pm\mu} \rho_{\mu,\nu} U(x,\nu) U(x+\hat{\nu},\mu) U(x+\hat{\mu},\nu)^\dagger U(x,\mu)^\dagger.
\end{aligned}
$$

- Numerical integration
  - discretize the transformation with step of size $\rho \equiv \rho_{\mu\nu}$
  - ρ includes a expansion parameter ε
  - The number of integration steps for the discretized trivializing map is set to 1

Acceptance Rates

	HMC	$\rho = 0.1$	$\rho = 0.112$	$\rho = 0.124$
$\delta\tau_G = 1/48$	0.929(6)	0.944(5)	0.935(6)	0.924(6)
$\delta\tau_G = 1/96$	-	0.956(4)	0.944(5)	0.94(5)

Table: $\langle P_{\mathrm{acc}} \rangle$ for runs with and without FT.