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

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Field-Transformed 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 [Luscher, 2010]
- perfect trivialization: $S_{FT} = 0$

In this study,

- approximate the trivializing map by the Wilson flow
- discretize the transformation with step of size ρ
- The number of integration steps for the discretized trivializing map is set to 1

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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 $\delta\tau_G$

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

Machine

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

$\langle dH \rangle$

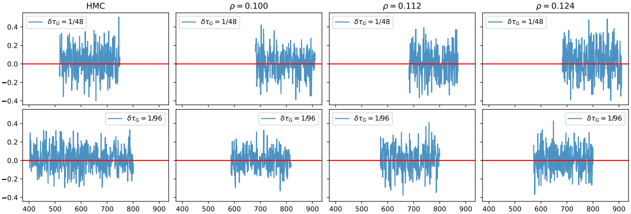

Figure: Histories of dH for different runs

ρ	0.0	0.1	0.112	0.124
$\delta\tau_G = 1/48$	0.026(6)	0.006(6)	0.009(5)	0.03(1)
$\delta\tau_G = 1/96$	0.015(6)	0 ± 0.009	0.009(8)	0.017(7)
$\delta\tau_G = 1/144$	-	0 ± 0.008	-	-

Table: $\langle dH \rangle$ for different runs based on configurations with Metropolis step. $\delta\tau_F$ is fixed to 1/48.

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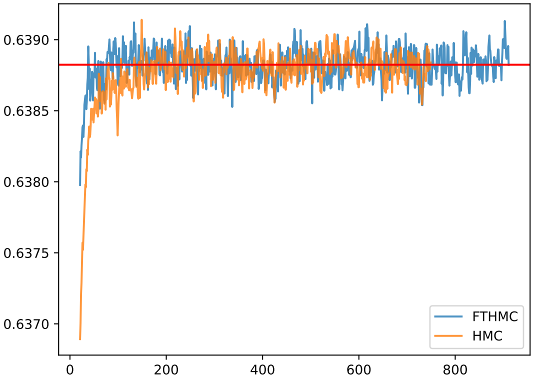
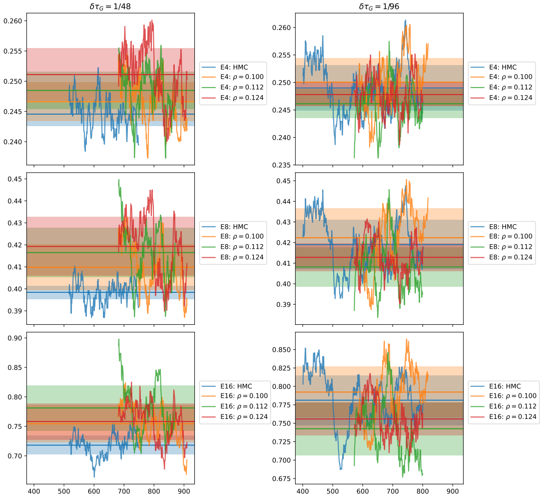
Plaquettes



- 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: $\Gamma^V(t) = \langle \langle\!\langle a_i \rangle\!\rangle \langle\!\langle a_{i+t} \rangle\!\rangle \rangle$
- Autocorrelation Coefficients (ACC): $\rho^V(t) = \Gamma^V(t)/\Gamma^V(0)$

Estimators:

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

Volume Autocorrelation

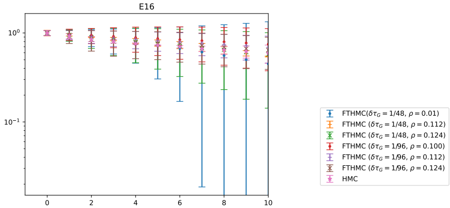


Figure: Autocorrelation coefficient (ACC) as a function of t for Wilson-flowed energy E16.

- 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,

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

- 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

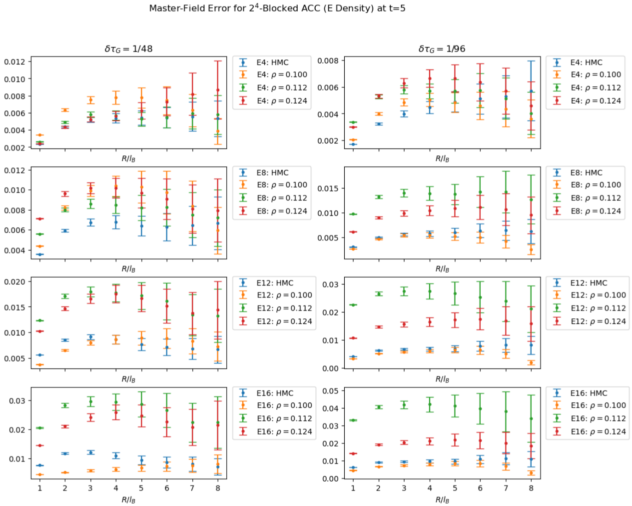
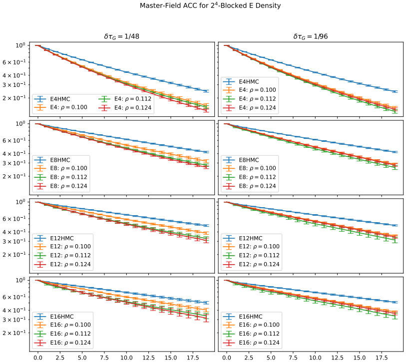


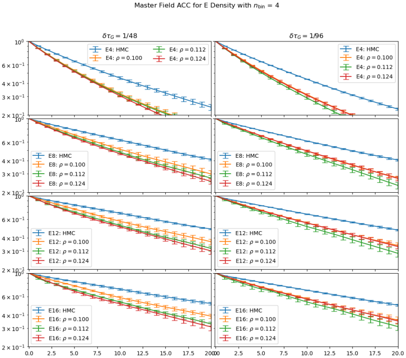
Figure: R: Summation Radius, b: block size

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





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	$\tau_W = 4$	$\tau_W = 8$	$\tau_W = 12$	$\tau_W = 16$
0.0	14.28	22.439	26.6961	27.822
0.100	11.2	17.3	20.628	21.68
0.112	10.87	15.62	17.97	19.2
0.124	10.14	14.8	16.96	17.68

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

ρ	$\tau_W = 4$	$\tau_W = 8$	$\tau_W = 12$	$\tau_W = 16$
0.0	14.0	22.768	27.613	29.6098
0.100	10.53	15.776	19.071	20.683
0.112	10.0	14.862	17.25	18.86
0.124	10.4	15.686	18.884	20.453

Table: Fixed $\delta\tau_G = 1/96$, varied Wilson flow time τ_W

Autocorrelation Times

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

ρ	$\tau_W = 4$	$\tau_W = 8$	$\tau_W = 12$	$\tau_W = 16$
0.100	1.275	1.2967	1.2942	1.2832
0.112	1.313	1.436	1.485	1.4487
0.124	1.408	1.516	1.574	1.5736

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

ρ	$\tau_W = 4$	$\tau_W = 8$	$\tau_W = 12$	$\tau_W = 16$
0.0	1.019	0.9855	0.96681	0.93961
0.100	1.356	1.4224	1.3998	1.3451
0.112	1.428	1.5098	1.5476	1.4754
0.124	1.373	1.4305	1.4137	1.3603

Table: Fixed $\delta\tau_G = 1/96$, varied Wilson flow time τ_W

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Summary and Outlook

- FTHMC is shown to reduce autocorrelation times by a factor of around 1.5 as compared to HMC
- Master-Field technique allows us to measure autocorrelation coefficients based on a small number of configurations
- There is an ongoing effort to reduce the computational overhead from field-transformation part of the algorithm
- Prepare production runs at physical quark masses where fermion force calculation dominates simulation cost
- At physical pion mass, we then expect to see full improvement of HMC simulation by a factor of around 1.5
- Generate ensemble with different parameters (*beta*, the number of trivializing steps, etc...)

Thank you!

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Luscher, M. (2010).
Trivializing maps, the Wilson flow and the HMC algorithm.
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Future Plans

- At the current setup ($m_\pi \approx 400$ MeV), the overhead due to computation of Jacobian force from the trivializing map is comparable to that of fermion force calculation
- We expect: at physical pion mass, fermion force calculation is much more computationally expensive than Jacobian force calculation
- We are optimizing the code so that Jacobian force routine is improved by a factor of 4
- At physical pion mass, we then expect to see full improvement of HMC simulation by a factor of around 1.5

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.