Exact Pseudofermion Action for Hybrid Monte Carlo Simulation of One-Flavor Domain-Wall Fermion

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Lattice Dirac Operator for Domain-Wall Fermion (DWF)

For a physical observable $\mathcal{O}(U)$

$$\langle\mathcal{O}(U)\rangle = \frac{1}{Z}\int DqD\bar{q}DU\mathcal{O}(U)\exp\left(-\bar{q}D_f(U)q - S_g(U)\right)$$

$$= \frac{1}{Z}\int DU\mathcal{O}(U)\det[D_f(U)]\exp\left(-S_g(U)\right)$$

If $D_f(U) = K * D(U)$, where the matrix K is independent of the gauge field

$$\frac{\int DU\mathcal{O}(U)\det[D_f(U)]\exp\left(-S_g(U)\right)}{\int DU\det[D_f(U)]\exp\left(-S_g(U)\right)} = \frac{\int DU\mathcal{O}(U)\det[D(U)]\exp\left(-S_g(U)\right)}{\int DU\det[D(U)]\exp\left(-S_g(U)\right)}$$

Lattice Dirac Operator for Domain-Wall Fermion (DWF)

Using the redefined operator $D(U)$

$$\langle \mathcal{O}(U) \rangle = \frac{1}{Z} \int DU \mathcal{O}(U) \det[D(U)] \exp\left(-S_g(U)\right)$$

$$= \frac{1}{Z} \int D\phi D\phi^\dagger DU \mathcal{O}(U) \exp\left(-\phi^\dagger H^{-1}(U) \phi - S_g(U)\right)$$

where H satisfies:

1) $\det[H] = \det[D]$
2) *H is Hermitian*
3) *H is positive-definite*

Lattice Dirac Operator for Domain-Wall Fermion (DWF)

For domain-wall fermion, in general, the lattice Dirac operator reads

$$D_{dwf}(m) = \rho_s D_w + I + [\sigma_s D_w - I\,]L(m)$$

$$= D_w\,[c\omega(I+L) + d(I-L)] + (I - L\,)$$

where $\rho_s = c + d\omega_s,\ \sigma_s = c - d\omega_s$ and $\omega = \mathrm{diag}(\omega_1, \omega_2, \cdots, \omega_{N_s})$, and D_w is the standard Wilson-Dirac operator plus a negative parameter $-\,m_0(0 < m_0 < 2)$,

$$L(m) = P_+ L_+(m) + P_- L_-(m)$$

$$L_+(m)_{s,s'} = \begin{cases} \delta_{s',s-1} & ,1 < s \le N_s \\ -m\delta_{s',N_s} & ,s = 1 \end{cases}$$

$$L_-(m) = L_+(m)^T$$

$$m = rm_q\ ,\ r = 1/[2m_0(1 - dm_0)]$$

Lattice Dirac Operator for Domain-Wall Fermion (DWF)

If ω_s are the optimal weights given in Ref. [1], it gives

Optimal Domain-Wall Fermion

If $\omega_s = 1, c = 0.5, d = 0.5$, it gives

Domain-Wall Fermion with Shamir Kernel

If $\omega_s = 1, c = 1.0, d = 0.5$, it gives

Domain-Wall Fermion with Scaled $(\alpha = 2)$ **Shamir Kernel**

[1] *T. W. Chiu, Phys. Rev. Lett. 90, 071601 (2003)*

Lattice Dirac Operator for Domain-Wall Fermion (DWF)

For DWF, since ω and L are independent of the gauge field,

$$D_{dwf} \rightarrow D(m) = D_w + P_+ M_+(m) + P_- M_-(m)$$

$$M_\pm(m) = \omega^{-1/2}[cN_\pm(m) + \omega^{-1} d]^{-1} \omega^{-1/2}$$

$$N_\pm(m) = [1 + L_\pm(m)][1 - L_\pm(m)]^{-1}$$

The fifth dimensional matrices $M_\pm$ can be rewritten as

$$\boldsymbol{M_\pm(m) = \omega^{-1/2} A_\pm{}^{-1} \omega^{-1/2} + \frac{2cm}{1 + m - 2cm\lambda} R_5 \omega^{-1/2} v_\pm v_\pm{}^T \omega^{-1/2}}$$

where λ and $v_\pm$ are the functions of c, d and ω, and we have defined

$$A_\pm = cN_\pm(0) + \omega^{-1} d$$

Two-Flavor Algorithm (TFA) [2]

For the DWF Dirac operator

$$D(m) = D_w + P_+ M_+(m) + P_- M_-(m)$$

we can apply the *Schur decomposition* with the even-odd preconditioning

$$D(m) = \begin{pmatrix} 4 - m_0 + M(m) & D_w^{eo} \\ D_w^{oe} & 4 - m_0 + M(m) \end{pmatrix}$$

$$= \begin{pmatrix} I & 0 \\ D_w^{oe} M_5(m)^{-1} & I \end{pmatrix} \begin{pmatrix} M_5(m) & 0 \\ 0 & C(m)\, M_5(m) \end{pmatrix} \begin{pmatrix} I & M_5(m)^{-1} D_w^{eo} \\ 0 & I \end{pmatrix}$$

where

$$C(m) = \mathrm{I} - M_5(m) D_w^{oe} M_5(m) D_w^{eo}$$

We then have

$$\det[D(m)] = \det[M_5(m)]^2 \times \det[C(m)]$$

[2] T. W. Chiu, et al. [TWQCD Collaboration],PoS LAT 2009, 034 (2009); Phys. Lett. B 717, 420 (2012) .

Two-Flavor Algorithm (TFA)

The pseudofermion action for HMC simulation of 2-flavor QCD with DWF is

$$S_{pf} = \phi^\dagger C^\dagger(1) \frac{1}{C(m)C^\dagger(m)} C(1)\phi$$

The field ϕ can be generated by the Gaussian noise field η

$$\eta = \frac{1}{C(m)} C(1)\phi \quad \Leftrightarrow \quad \phi = \frac{1}{C(1)} C(m)\eta$$

TWQCD's One Flavor Algorithm (TWOFA)

For one-flavor of domain-wall fermion in QCD, we have devised an exact pseudofermion action for the HMC simulation, without taking square root.

$$\frac{\det[D(m)]}{\det[D(1)]} = \frac{\det[D(m)]}{\det[\widehat{D}\,(m,1)]} \times \frac{\det[\widehat{D}\,(m,1)]}{\det[D(1)]}$$

In Dirac space

$$D(m) = \begin{pmatrix} W - m_0 + M_+(m) & \sigma \cdot t \\ -(\sigma \cdot t)^\dagger & W - m_0 + M_+(m) \end{pmatrix}$$

$$\widehat{D}(m,1) = \begin{pmatrix} W - m_0 + M_+(m) & \sigma \cdot t \\ -(\sigma \cdot t)^\dagger & W - m_0 + M_+(1) \end{pmatrix}$$

TWQCD's One Flavor Algorithm (TWOFA)

Use type I *Schur decomposition* to $\widehat{D}\,(m,1)$, and $D(m)$

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & 0 \\ CA^{-1} & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & I \end{pmatrix}$$

we then have

$$\frac{\det\left[\widehat{D}\,(m,1)\right]}{\det[D(m)]} = \frac{\det[\widetilde{H}(m) + \Delta_-(m)]}{\det[\widetilde{H}(m)]} = \det\left[I + \Delta_-(m)\frac{1}{\widetilde{H}(m)}\right]$$

where

$$\widetilde{H}(m) = R_5\left[W - m_0 + M_-(m) + (\sigma \cdot t)^\dagger \frac{1}{W - m_0 + M_+(m)}(\sigma \cdot t)\right]$$

$$\Delta_-(m) = R_5[M_-(1) - M_-(m)]$$

TWQCD's One Flavor Algorithm (TWOFA)

Use type II *Schur decomposition* to $D(1)$, and $\widehat{D}\,(m,1)$

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} I & 0 \\ D^{-1}C & I \end{pmatrix}$$

we then have

$$\frac{\det[D(1)]}{\det\left[\widehat{D}\,(m,1)\right]} = \frac{\det[\overline{H}(1)]}{\det[\overline{H}(1) - \Delta_+(m)]} = det\left[I + \Delta_+(m)\frac{1}{\overline{H}(1) - \Delta_+(m)}\right]$$

where

$$\overline{H}(1) = R_5\left[W - m_0 + M_+(1) + (\sigma \cdot t)\frac{1}{W - m_0 + M_-(1)} + (\sigma \cdot t)^\dagger\right]$$

$$\Delta_+(m) = R_5[M_+(1) - M_+(m)]$$

TWQCD's One Flavor Algorithm(TWOFA)

Use these relations and some algebra, the pseudofermion action of one-flavor domain-wall fermion can be written as

$$S_{pf} = \begin{pmatrix} 0 & \phi_1{}^{\dagger} \end{pmatrix} \left[I - k v_-{}^T \omega^{-1/2} \frac{1}{H(m)} \omega^{-1/2} v_- \right] \phi_1$$

$$+ \begin{pmatrix} 0 & \phi_2{}^{\dagger} \end{pmatrix} \left[I + k v_+{}^T \omega^{-1/2} \frac{1}{H(1) - \Delta_+(m) P_+} \omega^{-1/2} v_+ \right] \phi_2$$

where $H(m) = \gamma_5 R_5 D(m)$

$$\Delta_{\pm}(m) = k \omega^{-1/2} v_{\pm} v_{\pm}{}^T \omega^{-1/2}$$

$$k = \frac{c}{1 - c\lambda} \frac{1 - m}{1 + m(1 - 2c\lambda)}$$

TWQCD's One Flavor Algorithm (TWOFA)

The initial pseudofermion fields of each HMC trajectory are generated by Gaussian noises as follows.

$$\begin{pmatrix} \xi_1 \\ \phi_1 \end{pmatrix} = \sum_{l=1}^{N_p} \left[\frac{b_l}{1+d_l} I + \frac{b_l}{(1+d_l)^2} k v_-{}^T \omega^{-1/2} \frac{1}{H(m) - \frac{1}{1+d_l} \Delta_-(m) P_-} \omega^{-1/2} v_- \right] \begin{pmatrix} 0 \\ \eta_1 \end{pmatrix}$$

$$\begin{pmatrix} \phi_2 \\ \xi_2 \end{pmatrix} = \sum_{l=1}^{N_p} \left[\frac{b_l}{1+d_l} I - \frac{b_l}{(1+d_l)^2} k v_+{}^T \omega^{-1/2} \frac{1}{H(1) - \frac{d_l}{1+d_l} \Delta_+(m) P_+} \omega^{-1/2} v_+ \right] \begin{pmatrix} \eta_2 \\ 0 \end{pmatrix}$$

Rational Hybrid Monte Carlo(RHMC) Algorithm

A widely used algorithm to do the one-flavor HMC simulation is the rational hybrid Monte Carlo (RHMC)[3], which can be used for any lattice fermion.

$$S_{pf} = \sum_n {\phi_n}^\dagger \left(C(1)C^\dagger(1)\right)^{1/4n} \frac{1}{\left(C(m)C^\dagger(m)\right)^{1/2n}} \left(C(1)C^\dagger(1)\right)^{1/4n} \phi_n$$

The fields ϕ_n are generated by the Gaussian noise fields η_n

$$\phi_n = \frac{1}{\left(C(1)C^\dagger(1)\right)^{1/4n}} \left(C(m)C^\dagger(m)\right)^{1/4n} \eta_n$$

[3] M. A. Clark and A. D. Kennedy, Phys. Rev. Lett. 98, 051601 (2007)

TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ Lattice

I. Memory Usage :

We list memory requirement (in unit of bytes) for links, momentum and 5D vectors as follows,

1) $M_S \equiv 8 * {N_x}^3 * N_t$
2) $M_U = 48 * M_S$, link variables
3) $M_P = 32 * M_S$, momentum
4) $M_V = 24 * N_s * M_S$, 5D vector

Then the ratio of the memory usage for RHMC and TWOFA is

$$\frac{M_{RHMC}}{M_{TWOFA}} = \frac{20 + 3(3 + 2N_p)N_s}{32 + 10.5N_s}$$

where N_p is the number of poles for MMCG in RHMC algorithm

TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ Lattice

II. Efficiency:

The lattice setup is

$$\beta = 5.95, \quad m_q = 0.01, \quad L^3 = 8^3, \quad T = 16, \quad N_s = 16,$$

$$N_p = 12 \text{ for RHMC}$$

We compare RHMC and TWOFA for the following cases:

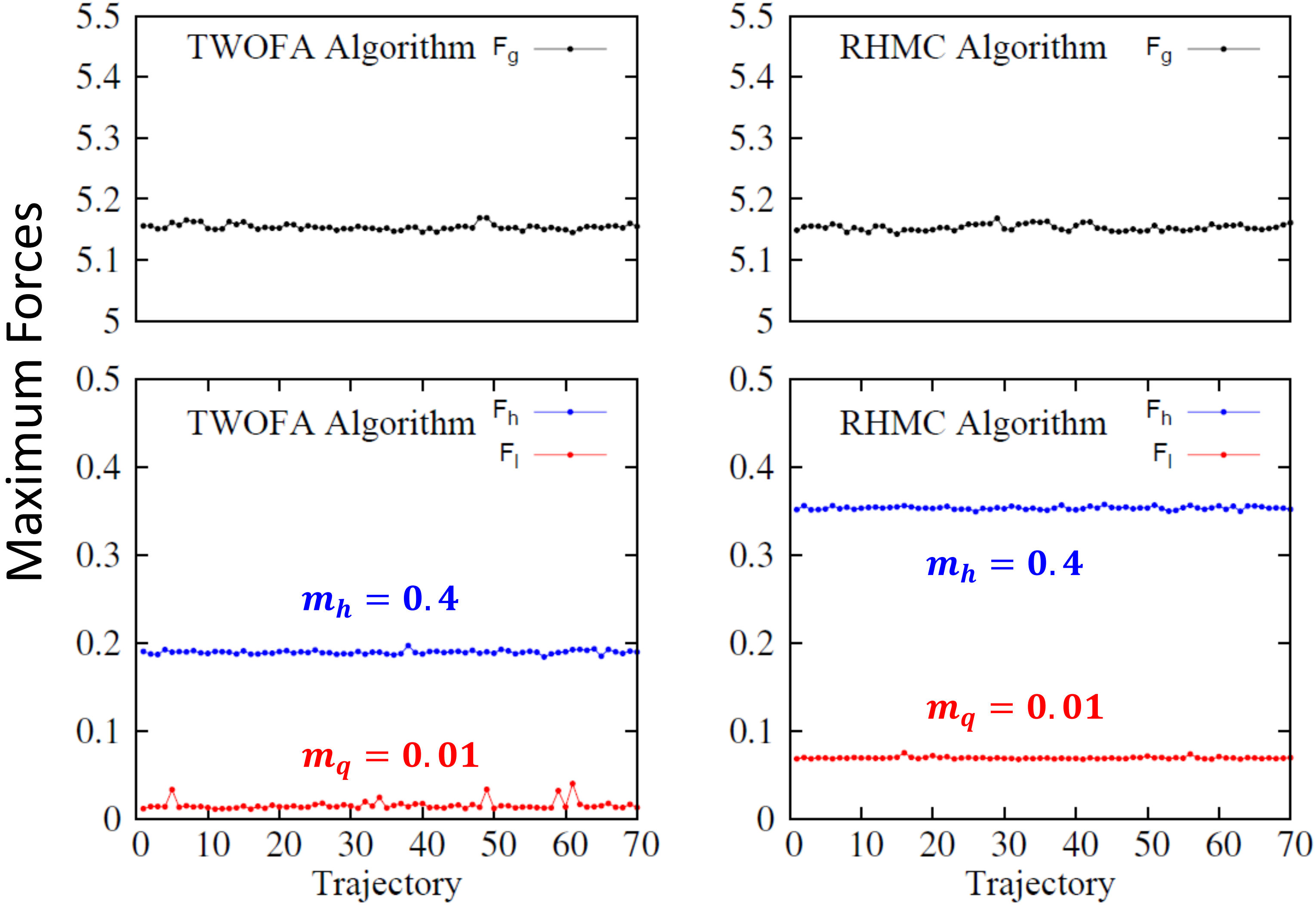
1) DWF *with* $c = 1.0, d = 0.0$ *and* $\lambda_{min}/\lambda_{max} = 0.05/6.2$ *(Optimal DWF)*

2) DWF *with* $c = 0.5, d = 0.5$ *and* $\omega_s = 1$ *(Shamir)*

3) DWF *with* $c = 1.0, d = 0.5$ $(\alpha = 2)$ *and* $\omega_s = 1$ *(Scaled Shamir)*

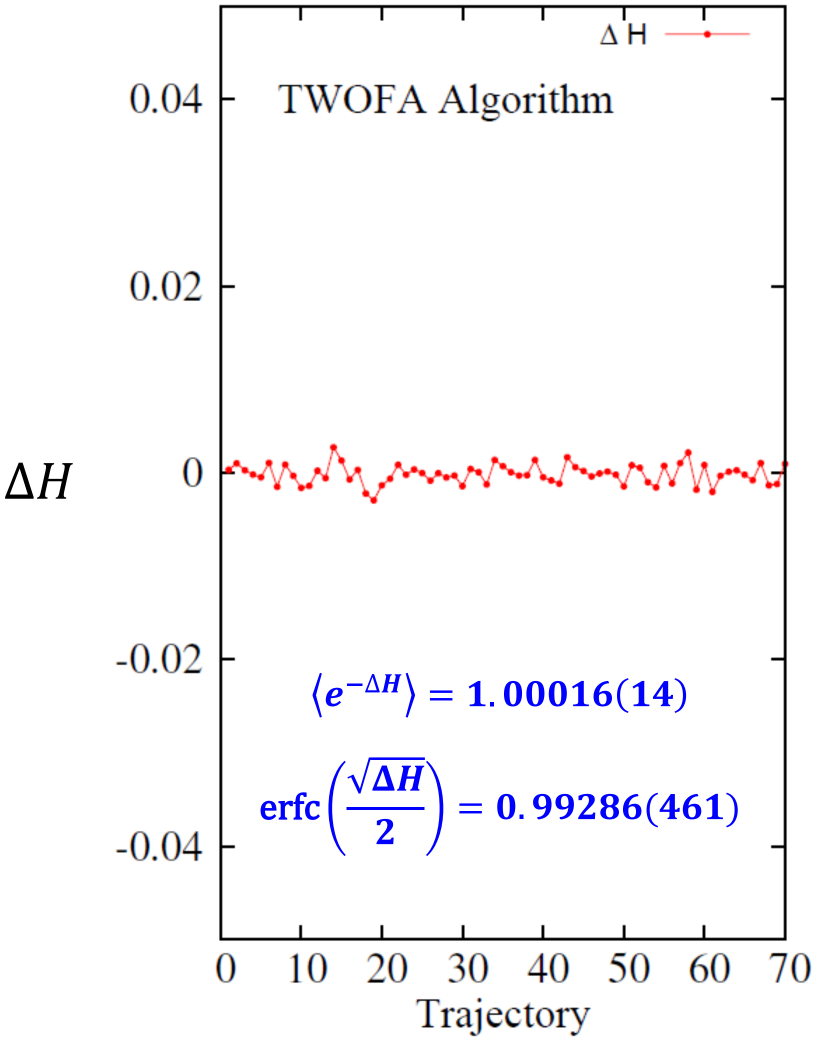
TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ Lattice

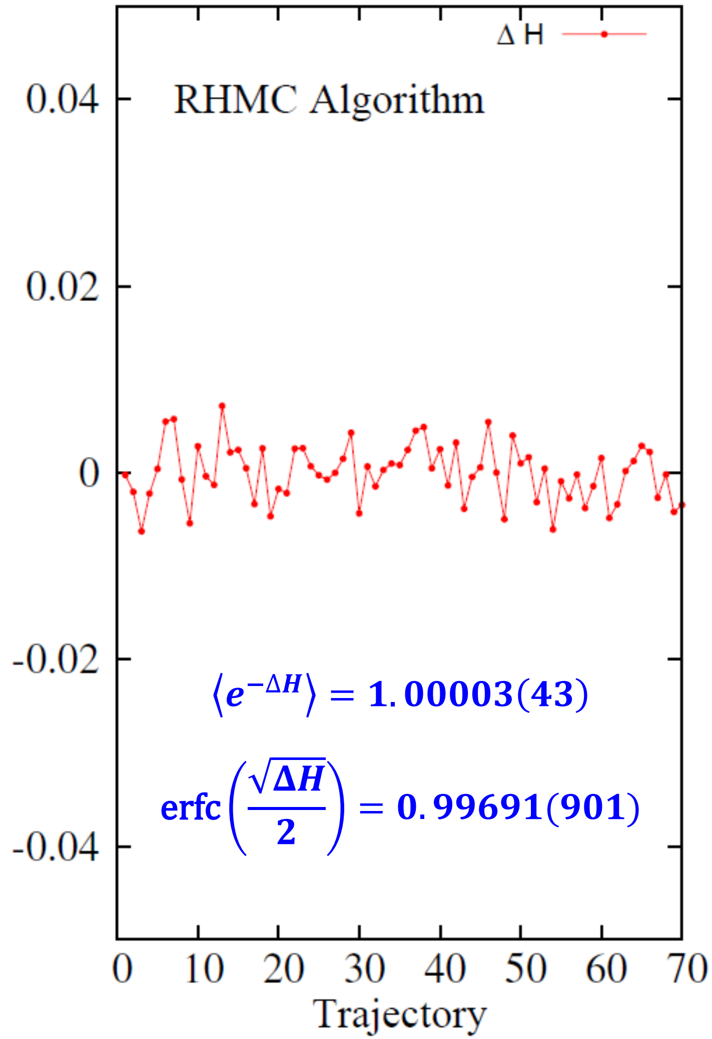
1. Optimal Domain-Wall Fermion : Maximum Forces



TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ Lattice

1. Optimal Domain-Wall Fermion: ΔH





TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ *Lattice*

1. Optimal Domain-Wall Fermion :

$\beta = 5.95, \quad m_0 = 1.3, \quad L = 8, \quad T = 16, \quad N_s = 16,$

$N_p = 12$ for RHMC

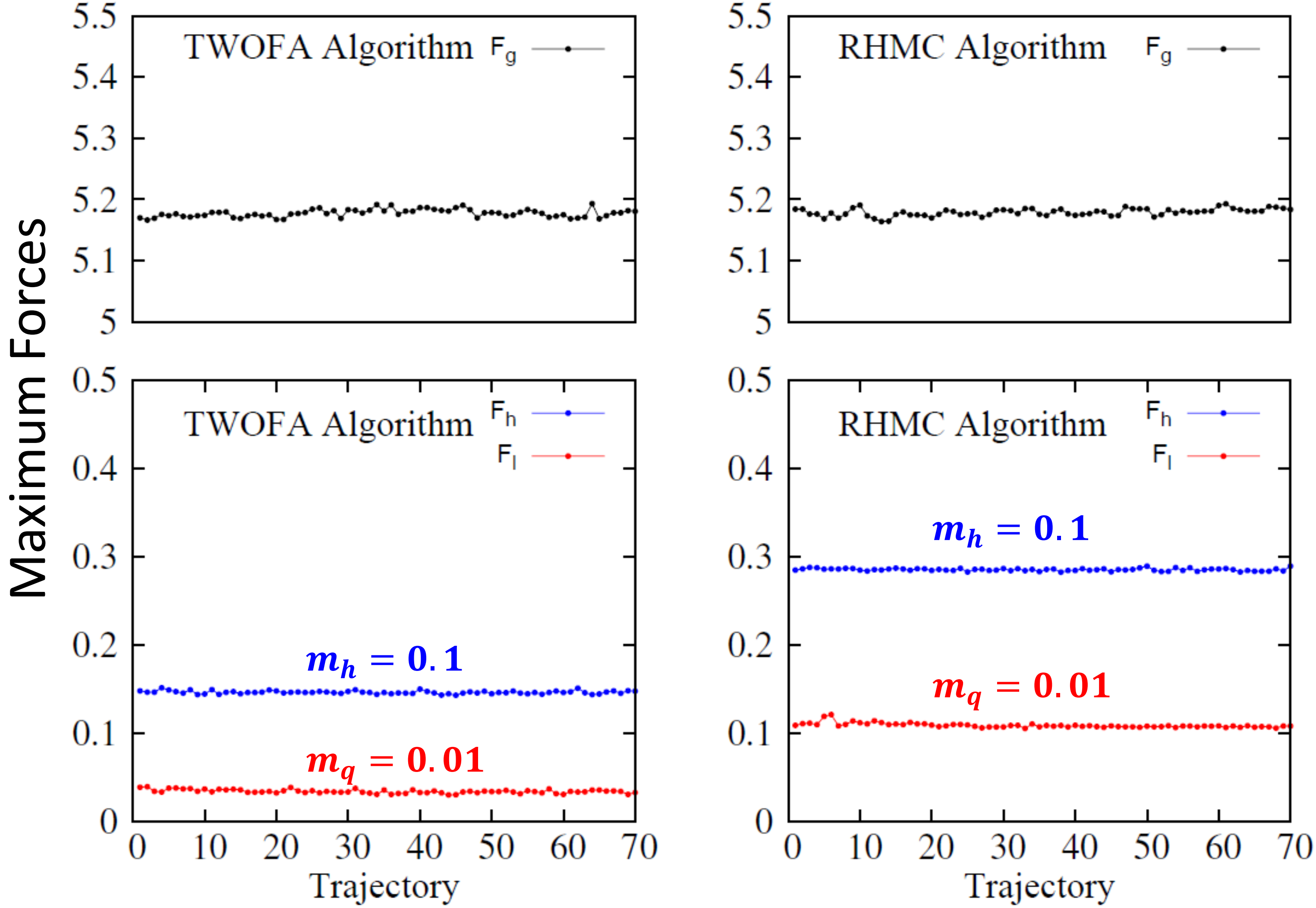
ODWF (kernel H_w) *with* $c = 1.0, d = 0.0$ *and* $\lambda_{min}/\lambda_{max} = 0.05/6.2$

Algorithm	m_q	m_h	Plaquette	Force (Gauge)	Force (heavy)	Force (light)
TWOFA	0.01	0.4	0.57959(23)	5.15418(91)	0.18972(26)	0.01575(63)
RHMC	0.01	0.4	0.58077(25)	5.15343(95)	0.35354(22)	0.06961(17)

Algorithm	Accept	$\mathrm{erfc}(\sqrt{\Delta H}/2)$	$\langle e^{-\Delta H} \rangle$	Memory	$T_{traj.}$	$T_{traj.}$(sec.)
TWOFA	1.0	0.99286(461)	1.00016(14)	**1.0**	**1.0**	**15528(1120)**
RHMC	1.0	0.99691(901)	1.00003(43)	**6.58**	**1.168**	**18137(0776)**

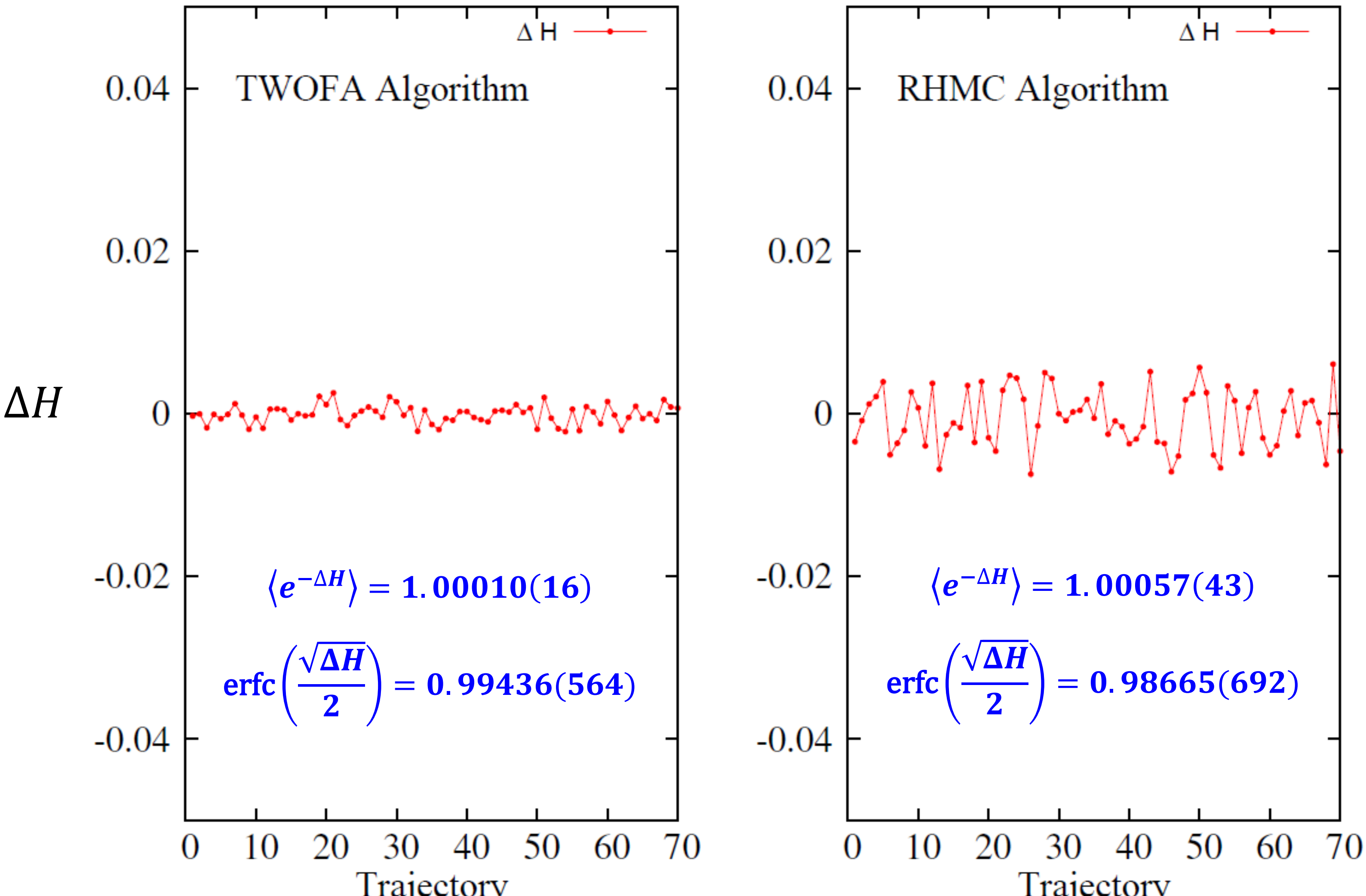
TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ Lattice

2. Shamir Kernel ($\omega_s = 1$) : Maximum Forces



TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ *Lattice*

2. Shamir Kernel $(\omega_s = 1)$ **:** ΔH



TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ Lattice

2. Shamir Kernel ($\omega_s = 1$) :

$\beta = 5.95$, $m_0 = 1.8$, $L = 8$, $T = 16$, $N_s = 16$,

$N_p = 12$ for RHMC

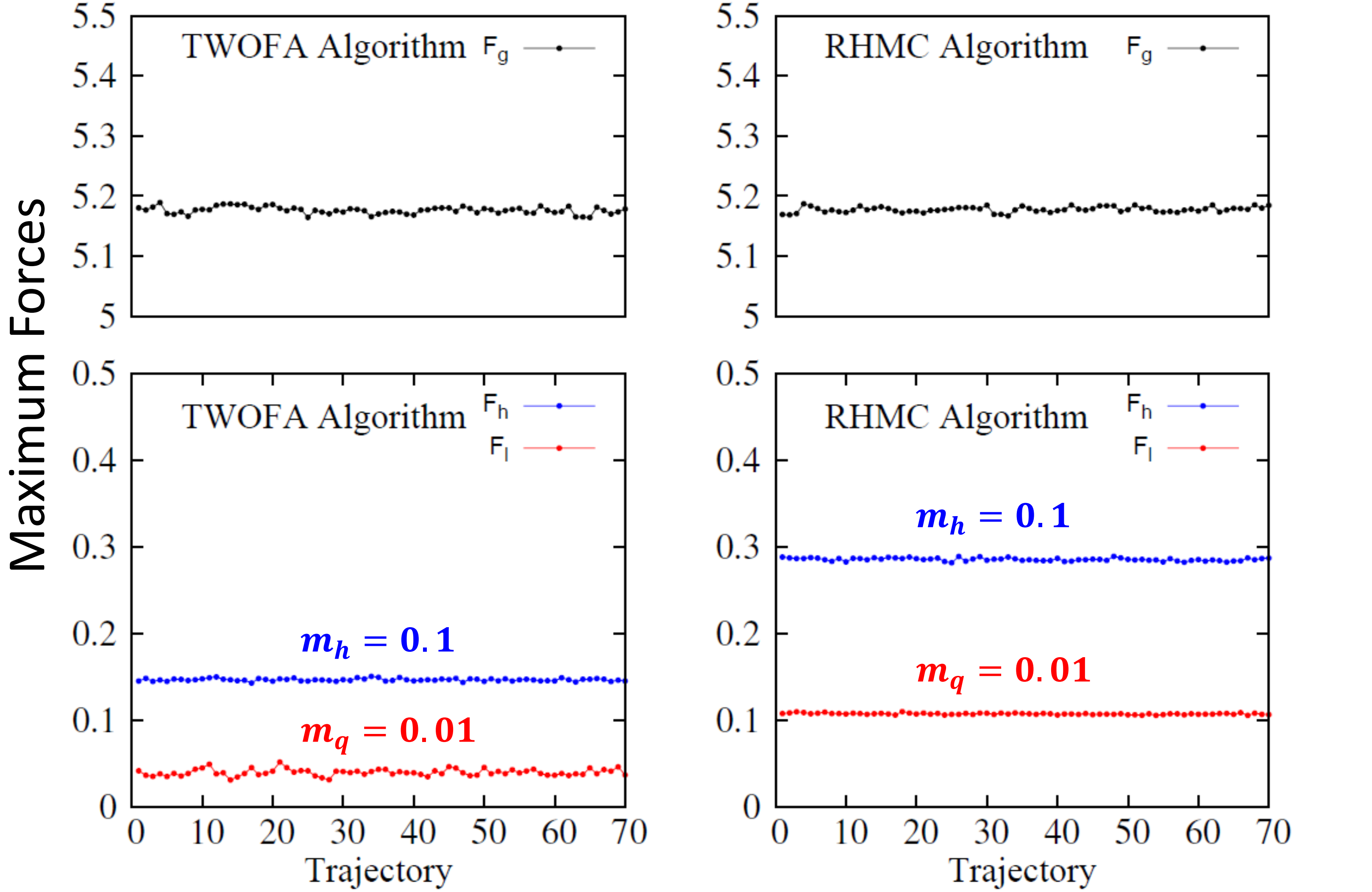
DWF (Shamir kernel) *with* $c = 0.5, d = 0.5$ *and* $\omega_s = 1$

Algorithm	m_q	m_h	Plaquette	Force (Gauge)	Force (heavy)	Force (light)
TWOFA	0.01	0.1	0.59059(35)	5.17758(110)	0.14654(25)	0.03431(39)
RHMC	0.01	0.1	0.59053(20)	5.17917(112)	0.28541(18)	0.10908(53)

Algorithm	Accept	$\mathrm{erfc}(\sqrt{\Delta H}/2)$	$\langle e^{-\Delta H} \rangle$	Memory	$T_{traj.}$	$T_{traj.}$(sec.)
TWOFA	1.0	0.99436(564)	1.00010(16)	1.0	1.0	$10295(088)$
RHMC	1.0	0.98665(692)	1.00060(43)	6.58	1.140	$11732(118)$

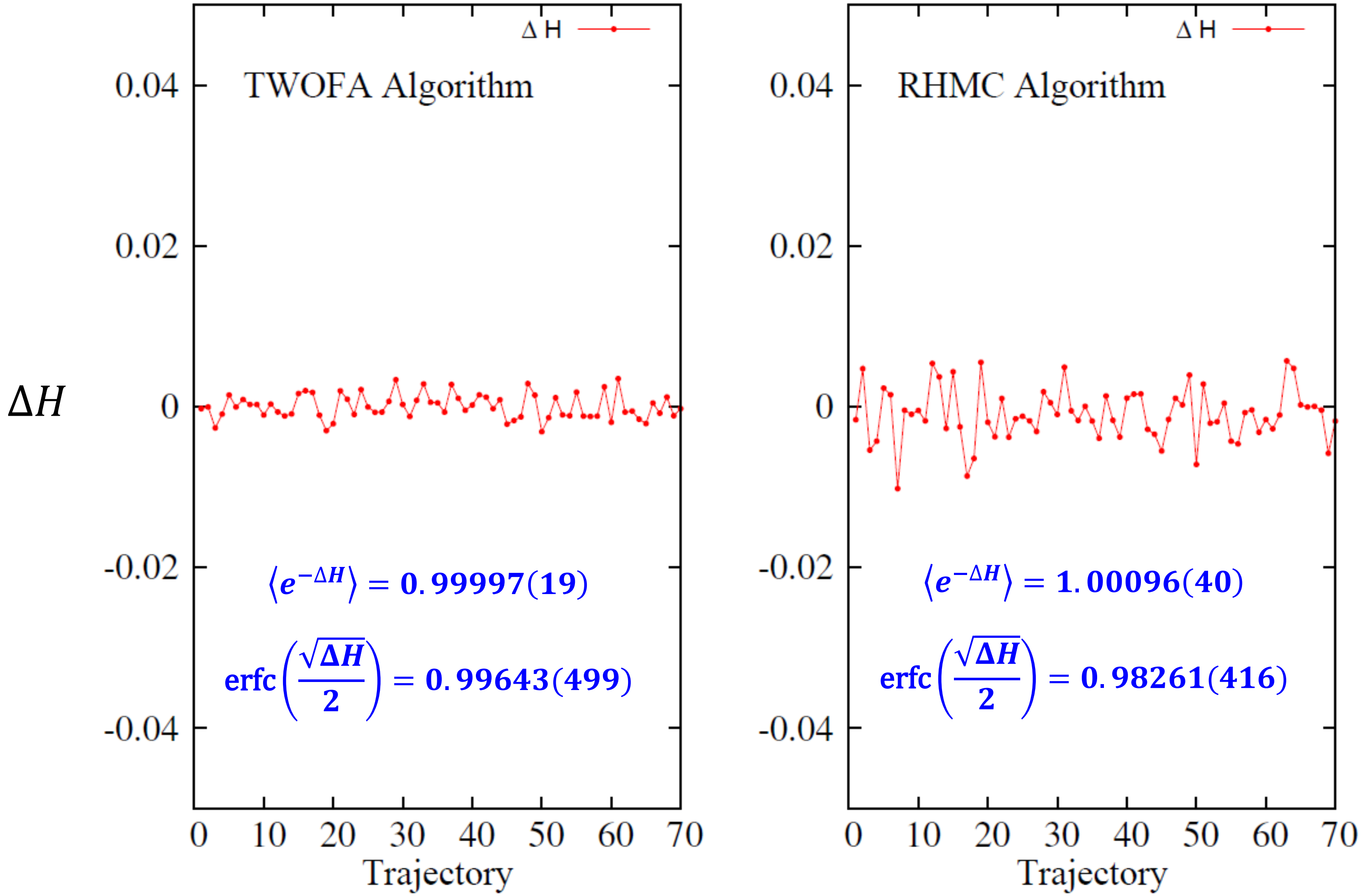
TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ *Lattice*

3. Scaled Shamir Kernel ($\omega_s = 1$ and $\alpha = 2$) : Maximum Forces



TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ Lattice

3. Scaled Shamir Kernel ($\omega_s = 1$ and $\alpha = 2$) : ΔH



TWOFA vs. RHMC with DWF on the $8^3 \times 16 \times 16$ *Lattice*

3. Scaled Shamir Kernel ($\omega_s = 1$ and $\alpha = 2$) :

$\beta = 5.95$, $m_0 = 1.8$, $L = 8$, $T = 16$, $N_s = 16$,

$N_p = 12$ for RHMC

DWF (scaled Shamir kernel) *with* $c = 1.0, d = 0.5$ ($\alpha = 2$) *and* $\omega_s = 1$

Algorithm	m_q	m_h	Plaquette	Force (Gauge)	Force (heavy)	Force (light)
TWOFA	0.01	0.1	0.59044(23)	5.17655(112)	0.14684(20)	0.04003(63)
RHMC	0.01	0.1	0.59054(30)	5.17772(070)	0.28563(30)	0.10758(14)

Algorithm	Accept	$\mathrm{erfc}(\sqrt{\Delta H}/2)$	$\langle e^{-\Delta H} \rangle$	Memory	$T_{traj.}$	$T_{traj.}$(sec.)
TWOFA	1.0	0.99643(499)	0.99997(19)	**1.0**	**1.0**	$\mathbf{10311(199)}$
RHMC	1.0	0.98261(416)	1.00096(40)	**6.58**	**1.168**	$\mathbf{12039(138)}$

Concluding Remarks

1. We have derived a novel pseudofermion action for HMC simulation of one-flavor DWF, which is exact, without taking square root.

2. It can be used for any kinds of DWF with any kernels, and for any approximations (polar or Zolotarev) of the sign function.

3. The memory consumption of TWOFA is much smaller than that of RHMC. This feature is crucial for using GPUs to simulate QCD.

4. The efficiency of TWOFA of is compatible with that of RHMC. For the cases we have studied, TWOFA outperforms RHMC.

5. TWQCD is now using TWOFA to simulate (2+1)-flavors QCD, and (2+1+1)-flavors QCD, on $32^3 \times 64 \times 16,$ and $24^3 \times 48 \times 16$ lattices.

MultiGPUs Simulation of (2+1+1)-Flavors QCD with Domain-Wall Fermion on the $32^3 \times 64 \times 16$ Lattice

- To compute the fermion force (by conjugate gradient) for lattice QCD with DWF on the $32^3 \times 64 \times 16$ lattice, it requires at least 11 GB RAM, exceeding the maximum memory (6 GB) currently available in a single GPU (Nvidia C2070/K20x/GTX-TITAN).

- We use multiGPUs to meet the memory requirement, as well as to speed up the computation.

- TWQCD developed efficient CUDA codes for the computation of entire HMC trajectory with multiGPUs

2*C2070	2*GTX-TITAN	4*GTX-TITAN
340	774	1220

Benchmarks of HMC simulation of (2+1+1) flavors QCD with ODWF on the $32^3 \times 64 \times 16$ lattice. All numbers are in the unit of Gflops/sec.