Domain Wall Fermion Simulations with the Exact One-Flavor Algorithm

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Motivation

- Recent advances in algorithms used by RBC/UKQCD have driven down the cost of simulating degenerate light quark pairs:
  1. Extensive tuning of forces via **Hasenbusch mass splitting** [Phys. Lett. B519 177-182]
  2. Shamir DWF → Möbius DWF → **zMöbius DWF** [Izubuchi et al., Lattice 2015]
  3. **Reduced L_s approximation** during molecular dynamics [proposed by Brower et al., arXiv:1206.5214; implemented by G. McGlynn, Lattice 2015]
  4. **Mixed precision CG**: single precision inner solves, double precision defect correction

- RHMC strange and charm quark determinants are now the most expensive part of our evolution strategy

Gauge	5800 s	11.6%
Light quarks ($L_s = 14$)	**18000 s**	**36.1%**
$L_s = 14/L_s = 32$ correction det.	**1600 s**	**3.3%**
Strange and charm quarks ($L_s = 32$)	**24200 s**	**48.5%**
DED	170 s	0.3%
Total	50000 s	—

Table: Timings for one HMC trajectory of $80^2 \times 96 \times 192$ $N_f = 2 + 1 + 1$ physical mass $a^{-1} \approx 3\,\mathrm{GeV}$ ensemble on a 12,288-node BG/Q partition [G. McGlynn, Ph.D. thesis]

Motivation (cont'd.)

- These techniques are of limited use for RHMC:
  - Unclear how to restart inner single-precision solver in the context of multishift CG
  - Cost of multishift $D^\dagger D$ inversions at light quark masses largely negates potential gain from Hasenbusch splitting
- For $I = 0$ $K \to \pi\pi$ calculations with G-parity boundary conditions $D^\dagger D$ describes 4 flavors, and RHMC is needed for light quarks as well [C. Kelly, Thur. @ 15:50]
- **Goal:** Explore the exact one-flavor algorithm as an alternative to RHMC for simulating single quark flavors or degenerate G-parity quark pairs

The Exact One-Flavor Algorithm

- Introduced by TWQCD for efficient one-flavor simulations on GPU clusters
- History:
  - 2009: Introduction [TWQCD, arXiv:0911.5532]
  - 2014: Detailed derivation [Chen and Chiu, Phys. Lett. B738 55-60]
  - 2014: Demonstration of $\sim 20\%$ overall speed-up in $16^3 \times 32 \times 16$ $N_f = 2+1$ simulation with EOFA vs. RHMC for heavy quark [Chen and Chiu, arXiv:1412.0819]
- **Main idea:** Use block manipulations in spin space to write

$$\det\left[\frac{D(m_1)}{D(m_2)}\right] = \frac{1}{\det\left(\mathcal{M}_L\right)} \cdot \frac{1}{\det\left(\mathcal{M}_R\right)}$$

  with $\mathcal{M}_L$ and $\mathcal{M}_R$ Hermitian and positive-definite
- Contrast with RHMC, where we instead compute

$$\det\left[\frac{D(m_1)}{D(m_2)}\right] = \left\{\det\left[\frac{D^\dagger D(m_1)}{D^\dagger D(m_2)}\right]\right\}^{1/2}$$

  using a rational approximation to the square root
- Exact in the sense that one does not need to take a fractional power of the fermion determinant to remove unwanted flavors

Derivation Sketch I [Chen and Chiu, Phys. Lett. B738 55-60]

- We begin by factoring the DWF Dirac operator:
  - D_w: Wilson Dirac operator
  - c,d: Möbius parameters
  - $L_{ss'}$: 5D hopping term

$$(D_{\rm DWF})_{xx',ss'} = \Big((c+d)\, D_w + \mathbb{1} \Big)_{xx'} \delta_{ss'} + \Big((c-d)\, D_w - \mathbb{1} \Big)_{xx'} L_{ss'}$$

$$= \underbrace{\left\{ (D_w)_{xx'}\, \delta_{ss'} + \delta_{xx'} \left(d + c\,(1+L)\,(1-L)^{-1} \right)^{-1}_{ss'} \right\}} \times \left\{ d\,(1-L) + c\,(1+L) \right\}$$

$$\boxed{D_{\rm EOFA} \equiv (D_w)_{xx'}\, \delta_{ss'} + \delta_{xx'} \left(P_+ M_+ + P_- M_- \right)_{ss'}}$$

- $M_\pm$ does not involve the gauge field and can be worked out explicitly
- Shamir kernel:
  - $(c,d) = (1/2, 1/2)$
  - $D_{\rm DWF}$ and $D_{\rm EOFA}$ are the same operator
- Möbius kernel:
  - $(c,d) = (\alpha/2, 1/2)$
  - $D^{\perp}_{\rm EOFA}$ is dense but has a somewhat better condition number than $D^{\perp}_{\rm DWF}$
- $H \equiv \gamma_5 R_5 D_{\rm EOFA}$ is Hermitian, but not positive-definite

Derivation Sketch II [Chen and Chiu, Phys. Lett. B738 55-60]

- Consider a slight generalization of $D_{\rm EOFA}$, in the chiral representation of γ^{μ}:

$$\widetilde{D}(m_1, m_2) = \begin{pmatrix} W - M_5 + M_+(m_1) & (\sigma \cdot t) \\ -(\sigma \cdot t)^{\dagger} & W - M_5 + M_-(m_2) \end{pmatrix}$$

- Applying the Schur det. identity to $D_{\rm EOFA}(m) = \widetilde{D}(m, m)$, and taking a ratio:

$$\frac{\det\left(D_{\rm EOFA}(m_1)\right)}{\det\left(D_{\rm EOFA}(m_2)\right)} = \frac{\det\left(W - M_5 + M_+(m_1)\right) \cdot \det\left(H_-(m_1)\right)}{\det\left(W - M_5 + M_-(m_2)\right) \cdot \det\left(H_+(m_2)\right)}$$

Schur complements

- Defining $\Delta_{\pm} \equiv R_5 \left(M_{\pm}(m_2) - M_{\pm}(m_1) \right) = k \Omega_{\pm} \Omega_{\pm}^{\dagger}$ ($\propto m_2 - m_1$), also have:

$$\frac{\det\left(\widetilde{D}(m_1, m_2)\right)}{\det\left(\widetilde{D}(m_1, m_2)\right)} = 1 \quad \Longrightarrow \quad \frac{\det\left(W - M_5 + M_+(m_1)\right)}{\det\left(W - M_5 + M_-(m_2)\right)} = \frac{\det\left(H_+(m_2) - \Delta_+\right)}{\det\left(H_-(m_1) + \Delta_-\right)}$$

- Finally, using Sylvester's determinant identity ($\det(\mathbb{1} + AB) = \det(\mathbb{1} + BA)$):

$$\frac{\det\left(D_{\rm EOFA}(m_1)\right)}{\det\left(D_{\rm EOFA}(m_2)\right)} = \left[\det \underbrace{\left(\mathbb{1} + k \Omega_-^{\dagger} \frac{1}{H_-(m_1)} \Omega_- \right)}_{\equiv \mathcal{M}_L} \right]^{-1} \cdot \left[\det \underbrace{\left(\mathbb{1} + k \Omega_+^{\dagger} \frac{1}{H_+(m_2) - \Delta_+ P_+} \Omega_+ \right)}_{\equiv \mathcal{M}_R} \right]^{-1}$$

Hermitian and pos.-def.!

Derivation Sketch III [Chen and Chiu, Phys. Lett. B738 55-60]

- To simulate, we express the determinant as a path integral:

$$\frac{1}{\det\left(\mathcal{M}_L\right)} \cdot \frac{1}{\det\left(\mathcal{M}_R\right)} = \int \mathcal{D}\phi_L \mathcal{D}\phi_L^\dagger \mathcal{D}\phi_R \mathcal{D}\phi_R^\dagger e^{-\phi_L^\dagger \mathcal{M}_L \phi_L - \phi_R^\dagger \mathcal{M}_R \phi_R}$$

- ϕ_L and ϕ_R are bosonic pseudofermion fields with two spin components
- $\mathcal{M}_L$ and $\mathcal{M}_R$ contain nested matrix inverses $\rightarrow$ expensive to compute with CG
- Easier to work with block form:

$$\mathcal{M}_{\mathrm{EOFA}} = \mathbb{1} - k P_- \Omega_-^\dagger \frac{1}{H(m_1)} \Omega_- P_- + k P_+ \Omega_+^\dagger \frac{1}{H(m_2) - \Delta_+ P_+} \Omega_+ P_+$$

for which we have, in terms of an ordinary four-component spinor:

$$\frac{\det\left(D_{\mathrm{EOFA}}(m_1)\right)}{\det\left(D_{\mathrm{EOFA}}(m_2)\right)} = \int \mathcal{D}\phi \mathcal{D}\phi^\dagger e^{-\phi^\dagger \mathcal{M}_{\mathrm{EOFA}} \phi}$$

- EOFA evolution requires inversions of the general form $\Big(H(m) + \alpha \Delta_\pm P_\pm\Big)\psi = \phi$

The Hybrid Monte Carlo Algorithm

- We perform dynamical QCD simulations using the HMC algorithm
- **Idea:** Generate a Markov chain of gauge field configurations by evolving a Hamiltonian system in (unphysical) molecular dynamics "time"
  - Generalized coordinate: Gauge field $(U_{x,\mu})$
  - Conjugate momentum: $\pi_{x,\mu} \in \mathfrak{su}(3)$
  - Hamiltonian: $H = \frac{1}{2}\pi^2 + S_g[U] + S_f[U]$
  - Equations of motion:

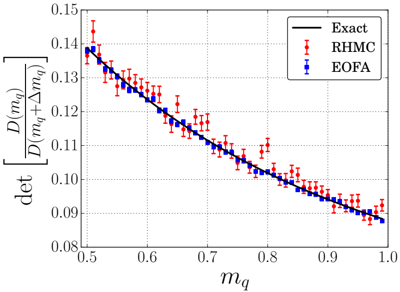
$$\begin{cases} \partial_\tau U_{x,\mu} = \pi_{x,\mu} U_{x,\mu} \\ \partial_\tau \pi_{x,\mu} = -T^a \partial^a_{x,\mu} \left(S_g[U] + S_f[U] \right) \end{cases}$$

- Metropolis accept/reject step corrects for finite precision integration
  - Accept new gauge field $U'_{x,\mu}$ with probability $P_{\text{accept}} = \min\left(1, e^{-\Delta H}\right)$
- Implementing this for EOFA requires:
  1. Action $S_f[U]$
  2. Pseudofermion heatbath
  3. Pseudofermion contribution to momentum update $\pi_{x,\mu} \leftarrow \pi_{x,\mu} - T^a \left(\partial^a_{x,\mu} S_f[U] \right) \Delta\tau$
- Tests performed on two $N_f = 2+1$ Shamir DWF ensembles:
  - 16I: $16^3 \times 32 \times 16$, $\beta = 2.13$, $(am_l, am_h) = (0.01, 0.032)$ [Phys. Rev. D**76**, 014504]
  - 32I: $32^3 \times 64 \times 16$, $\beta = 2.25$, $(am_l, am_h) = (0.004, 0.03)$ [Phys. Rev. D**93**, 054502]

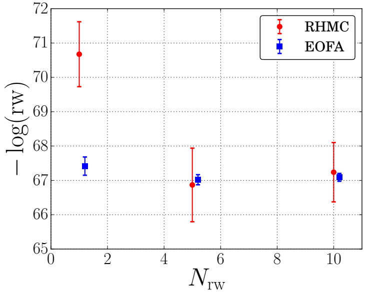
I. Action: Equivalence of EOFA and RHMC for Möbius DWF

- Relation between RHMC determinant ratios and EOFA determinant ratios:

$$\left\{ \det \left[\frac{D^\dagger D_{\rm DWF}(m_1)}{D^\dagger D_{\rm DWF}(m_2)} \right] \right\}^{1/2} = \left(\frac{(c+d)^{L_s} + m_1 (c-d)^{L_s}}{(c+d)^{L_s} + m_2 (c-d)^{L_s}} \right)^{12L^3T} \det \left[\frac{D_{\rm EOFA}(m_1)}{D_{\rm EOFA}(m_2)} \right]$$



(a) Free 4^5 lattice, $\Delta m_q = 0.01$, $\alpha = 4.0$ (Möbius scale), 20 stochastic hits.



(b) 16I. Reweight $am_h = 0.032 \to 0.042$ in N_{rw} steps with 10 hits per step.

- **Observe significantly smaller systematic and statistical errors for EOFA**
  - Cheaper to perform quark mass reweighting with EOFA!

II. Heatbath

- At start of HMC trajectory: draw η with $P(\eta) \propto e^{-\eta^2/2}$, compute $\phi = \mathcal{M}_{\rm EOFA}^{-1/2}\eta$
- Still requires rational approximation $x^{-1/2} \simeq \alpha_0 + \sum_{l=1}^{N_p} \alpha_l/(\beta_l + x)$
- Defining $\gamma_l = (1+\beta_l)^{-1}$, can show

$$\mathcal{M}_{\rm EOFA}^{-1/2} \simeq \alpha_0 \mathbb{1} + \sum_{l=1}^{N_p} \alpha_l \gamma_l \left[\mathbb{1} + k\gamma_l P_- \Omega_-^\dagger \frac{1}{H(m_1) - \gamma_l \Delta_- P_-} \Omega_- P_- - k\gamma_l P_+ \Omega_+^\dagger \frac{1}{H(m_2) - \gamma_l \beta_l \Delta_+ P_+} \Omega_+ P_+ \right]$$

- $\Delta_\pm P_\pm$ has large number of zero modes $\rightarrow$ not invertible! **(no multishift)**

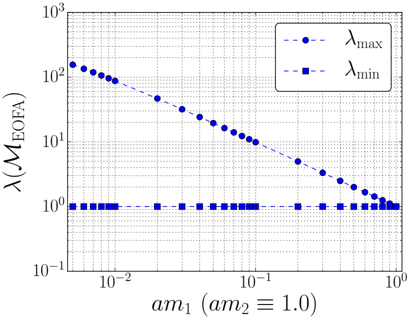


Figure: Spectral range of $\mathcal{M}_{\rm EOFA}$.

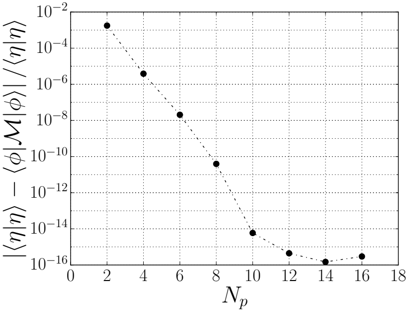


Figure: Heatbath relative error using N_p poles.

III. Momentum Update

- EOFA pseudofermion force is

$$\begin{cases} \partial^a_{x,\mu} S_f[U] = k \chi_L^\dagger \gamma_5 R_5 \left(\partial^a_{x,\mu} D_w \right) \chi_L - k \chi_R^\dagger \gamma_5 R_5 \left(\partial^a_{x,\mu} D_w \right) \chi_R \\ \chi_L = \left[H(m_1) \right]^{-1} \Omega_- P_- \phi, \quad \chi_R = \left[H(m_2) - \Delta_+ P_+ \right]^{-1} \Omega_+ P_+ \phi \end{cases}$$

- Compared to RHMC:
  - Cheaper to evaluate
  - Somewhat smaller total force, with $\langle F \rangle_L \ll \langle F \rangle_R$

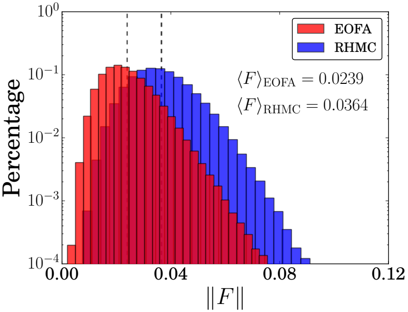


Figure: Lattice-wide distribution of EOFA and RHMC total forces by link

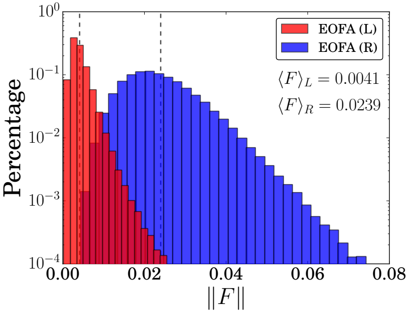
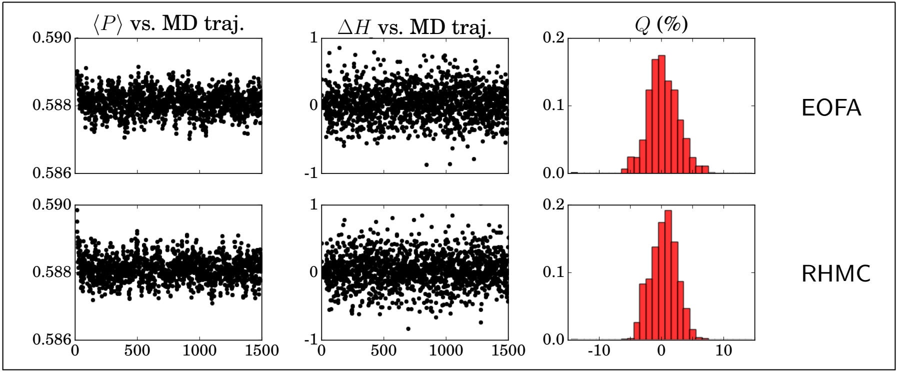


Figure: Lattice-wide distribution of EOFA force contributions from L and R terms by link

- Parallel $N_f = 2 + 1$ evolutions: compare RHMC heavy quark to EOFA heavy quark



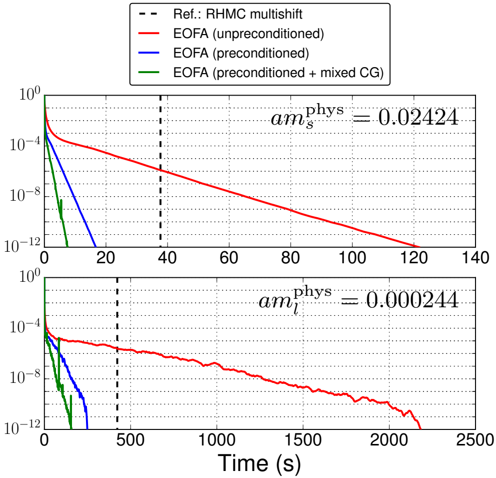
β	2.13
am_l	0.01
am_h	0.032

Table: Parameters

	EOFA	RHMC		EOFA	RHMC
am_π	0.243(2)	0.244(1)	af_π	0.0887(8)	0.0883(6)
am_K	0.326(2)	0.326(1)	af_K	0.0966(6)	0.0963(4)
am_Ω	0.990(9)	0.995(10)	$am'_{\text{res}}(m_l)$	0.00305(4)	0.00306(4)

Table: Spectrum

Optimizations I: Accelerating EOFA Inversions



- EOFA solves accelerated with:
  - Even-odd preconditioning
  - Optimized BG/Q assembly generated by BAGEL [P. Boyle]
  - Mixed-precision CG
- Test on 32I ensemble at physical am_l and am_s determined by chiral fits [Phys. Rev. D**93**, 054502]
- Reference (dashed line): even-odd preconditioned multishift solve of $D^\dagger D$ with same quark mass

	$am_s^{\rm phys}$	$am_l^{\rm phys}$
EOFA	7.6 s	156.5 s
RHMC	37.7 s	422.5 s
Ratio	5.0	2.7

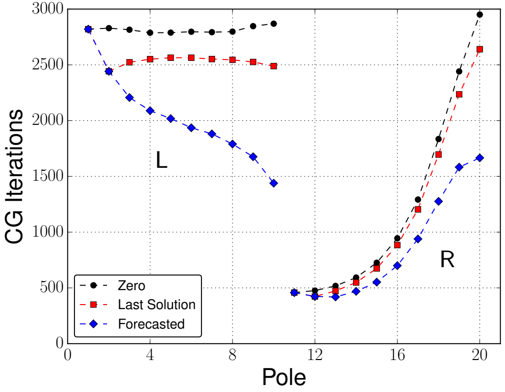
Table: Comparison of total CG inversion time between optimized EOFA and RHMC

Optimizations II: Accelerating EOFA Heatbath

- Following TWQCD, we use the chronological inversion method introduced by Brower et al. to forecast CG guesses [Nucl. Phys. B**484**, 353-374]
- Forecast solution to $\left(H + \alpha_l \Delta_\pm P_\pm \right) \psi = \phi$ by minimizing

$$\Psi[x] = x^\dagger \left(H + \alpha_l \Delta_\pm P_\pm \right) x - \phi^\dagger x - x^\dagger \phi$$

over the space of accumulated solutions for previous shifts α_l



- Test: 16I, 10 poles in rational approximation
- Find $\sim 30\%$ reduction in total iteration count
- No additional gain from sharing solutions between L and R terms

Conclusions and Next Steps

- We have:
  - Independently implemented TWQCD's EOFA, and performed basic algorithmic tests
  - Reproduced 16I ensemble using EOFA to evolve the heavy flavor
  - Partially implemented and tested a number of optimizations:
    1. Even-odd preconditioning
    2. Optimized BG/Q assembly for sparse matrix applications (BAGEL)
    3. Mixed-precision CG
    4. Forecasted CG guesses for heatbath
    5. Hasenbusch mass splitting
- Next steps:
  - Better ideas to ameliorate the cost of the EOFA heatbath?
  - Tuning Sexton-Weingarten integration and/or Hasenbusch mass splitting?
  - G-parity simulations with EOFA light quarks
  - Port to P. Boyle's Grid library: is a further speed-up possible if we perform deflated sparse matrix inversions with HDCR? [Poster by A. Yamaguchi and P. Boyle]
- We expect a gain over RHMC with a fully optimized and tuned implementation of EOFA, but the exact gain is difficult to predict!

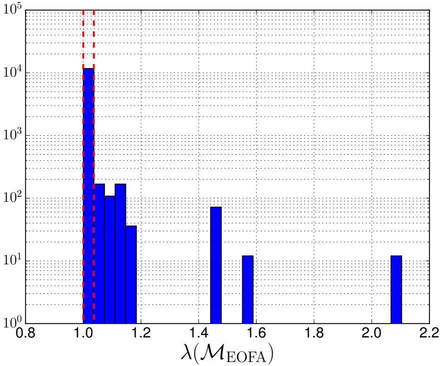
Thank you!

Extra Slides

Spectrum of the EOFA and RHMC actions

- Can think of EOFA as a preconditioning step applied to RHMC action
  - Mapping of eigenvalue spectrum: $(\lambda_{\rm min}, \lambda_{\rm max})_{\rm RHMC} \mapsto (1, \lambda_{\rm max})_{\rm EOFA}$
  - Similar range, but $\mathcal{M}_{\rm EOFA}$ spectrum more densely concentrated near low end
  - Computes same determinant ratio, but easier to stochastically estimate $\mathcal{M}_{\rm EOFA}$!
  - Notation: action is $S = \phi^{\dagger} \mathcal{M} \phi$

$$\mathcal{M}_{\rm EOFA} = \mathbb{1} - k P_{-} \Omega_{-}^{\dagger} \frac{1}{H(m_1)} \Omega_{-} P_{-} + k P_{+} \Omega_{+}^{\dagger} \frac{1}{H(m_2) - \Delta_{+} P_{+}} \Omega_{+} P_{+}$$



$$\mathcal{M}_{\rm RHMC} = \left(D^{\dagger} D(m_2) \right)^{1/4} \left(D^{\dagger} D(m_1) \right)^{-1/2} \left(D^{\dagger} D(m_2) \right)^{1/4}$$

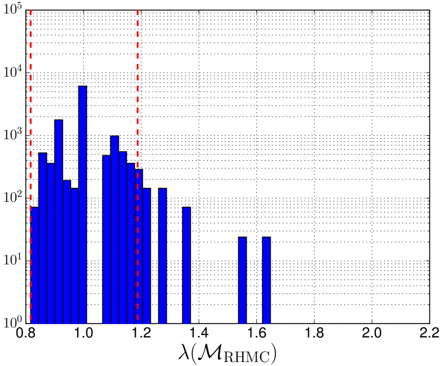


Figure: 4^5 free lattice, $am_1 = 0.1$, $am_2 = 1.0$, $aM_5 = 1.8$. Lines mark 95% of density.