Algorithmic improvements for weak coupling simulations of domain wall fermions

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Motivation: the cost of domain wall fermions

- Domain-wall fermions: good chiral symmetry, but more expensive Dirac operator.
- Cost proportional to L_s, size of fifth dimension.
- Larger L_s gives smaller chiral symmetry breaking but costlier simulations.

Goal: Simulate at large L_s without paying the full cost.

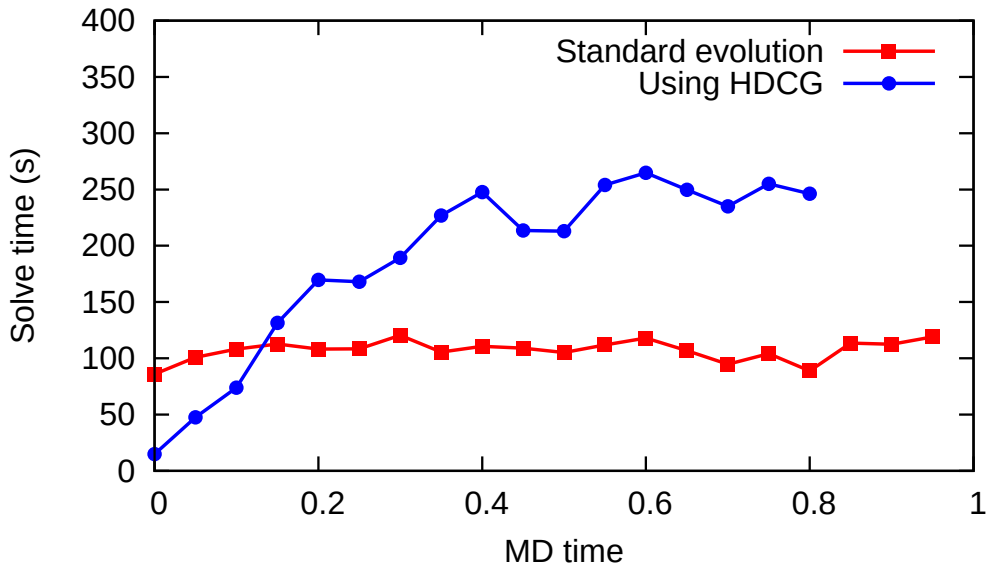
Technique #1: HDCG for deflation in evolution.

Technique #2: We implement an idea suggested by Brower, Neff, and Orginos in arXiv:1206.5214.

HDCG for deflation in evolution

HDCG ("hierarchically deflated conjugate gradient") is a multigrid-like deflation technique for domain-wall fermions. (Boyle, arXiv:1402.2585)

Idea: Calculate a deflation subspace at the beginning of an HMC trajectory and use it to deflate all solves during the trajectory.



Result: No speedup because

- Quality of deflation subspace deteriorates too rapidly as gauge field evolves.
- Matrix elements of the low modes must be reevaluated before each solve.

Future work may overcome these difficulties.

Review of domain wall–overlap correspondence

(see e.g. Brower et al.)

- $D_{\mathrm{DW}}(m, L_s)$ – domain wall Dirac operator with input mass m, acts on 5D vectors.
- Möbius generalization adds more parameters beyond m and L_s.
- For each $D_{\mathrm{DW}}(m, L_s)$ there is a 4D "**effective overlap operator**" $D_{\mathrm{ov}}(m, L_s)$ such that

$$\det\left[\frac{D_{\mathrm{DW}}(m, L_s)}{D_{\mathrm{DW}}(1, L_s)}\right]_{5\mathrm{D}} = \det[D_{\mathrm{ov}}(m, L_s)]_{4\mathrm{D}} \tag{1}$$

- The explicit form of D_{ov} is:

$$D_{\mathrm{ov}}(m, L_s) = [P^{-1} D_{\mathrm{DW}}(1, L_s)^{-1} D_{\mathrm{DW}}(m, L_s) P]_{s=0, s'=0} \tag{2}$$

(P is a simple operator that shifts the chiralities onto the right domain walls).

- In the $L_s \to \infty$ limit, D_{ov} becomes the true overlap operator.

L_s-splitting of the determinant

Let's manipulate the fermion determinant for a single domain-wall quark.
Pick a new L_s' smaller than the original L_s.

$$\begin{aligned}
\det\left[\frac{D_{\mathrm{DW}}(m, L_s)}{D_{\mathrm{DW}}(1, L_s)}\right]_{5\mathrm{D}} &= \det[D_{\mathrm{ov}}(m, L_s)]_{4\mathrm{D}} \\
&= \det[D_{\mathrm{ov}}(m, L_s')]_{4\mathrm{D}} \times \det\left[\frac{D_{\mathrm{ov}}(m, L_s)}{D_{\mathrm{ov}}(m, L_s')}\right]_{4\mathrm{D}} \qquad (3) \\
&= \det\left[\frac{D_{\mathrm{DW}}(m, L_s')}{D_{\mathrm{DW}}(1, L_s')}\right]_{5\mathrm{D}} \times \det\left[\frac{D_{\mathrm{ov}}(m, L_s)}{D_{\mathrm{ov}}(m, L_s')}\right]_{4\mathrm{D}}
\end{aligned}$$

First term: the regular 5D DWF determinant at a smaller (cheaper) L_s'.
Second term: a 4D determinant which corrects for $L_s' \neq L_s$.

Correction term is cheap if $D_{\mathrm{ov}}(m, L_s') \approx D_{\mathrm{ov}}(m, L_s)$. Then ratio is ≈ 1 and forces are small, so time step for correction term can be large.

Note that we have NOT changed the overall fermion action, just the strategy for simulating it.

Good reduced-L_s approximations

The speedup relies on finding a $D_{\mathrm{DW}}(m, L_s')$ such that

$$D_{\mathrm{ov}}(m, L_s') \approx D_{\mathrm{ov}}(m, L_s) \tag{4}$$

We have explicitly:

$$D_{\mathrm{ov}}(m) = \frac{1}{2}[1 + m + (1 - m)\gamma_5 \epsilon(H)] \tag{5}$$

$$H = \frac{\gamma_5 D_w(-M_5)}{2 + D_w(-M_5)} \quad \text{(the "Shamir kernel")} \tag{6}$$

For D_{ov} the true overlap operator, $\epsilon(x)$ is the sign function.
For D_{ov} an effective overlap operator, $\epsilon(x)$ is an approximation to the sign function.

$D_{\mathrm{ov}}(m, L_s') \approx D_{\mathrm{ov}}(m, L_s)$ if $\epsilon^{(L_s')}(x) \approx \epsilon^{(L_s)}(x)$.

zMöbius

$$\text{DWF sign function:} \quad \epsilon(x) = \frac{(1+x)^{L_s} - (1-x)^{L_s}}{(1+x)^{L_s} + (1-x)^{L_s}} \tag{7}$$

Möbius fermions generalize DWF to use the sign function approximation

$$\text{Möbius sign function:} \quad \epsilon(x) = \frac{f(x) - f(-x)}{f(x) + f(-x)} \quad ; \quad f(x) = \prod_{i=1}^{L_s} (\omega_i + x) \tag{8}$$

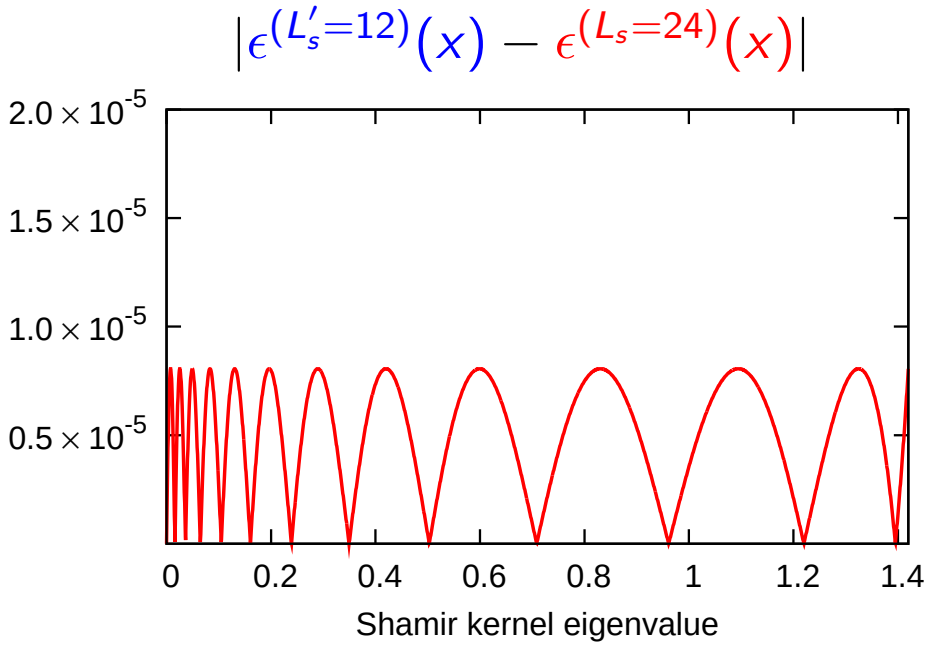
where ω_i are arbitrary complex numbers.

zMöbius: Given original $\epsilon^{(L_s)}(x)$, pick $L_s' < L_s$ and find ω_i to minimize $|\epsilon^{(L_s')}(x) - \epsilon^{(L_s)}(x)|$.

This gives a reduced-L_s approximation $D_{\text{ov}}(m, L_s')$ to the original $D_{\text{ov}}(m, L_s)$.

Approximation shaping

- The Remez algorithm can find good ω_i.
- The accuracy of the approximation can be concentrated in the region of highest eigenvalue density for the kernel operator H.



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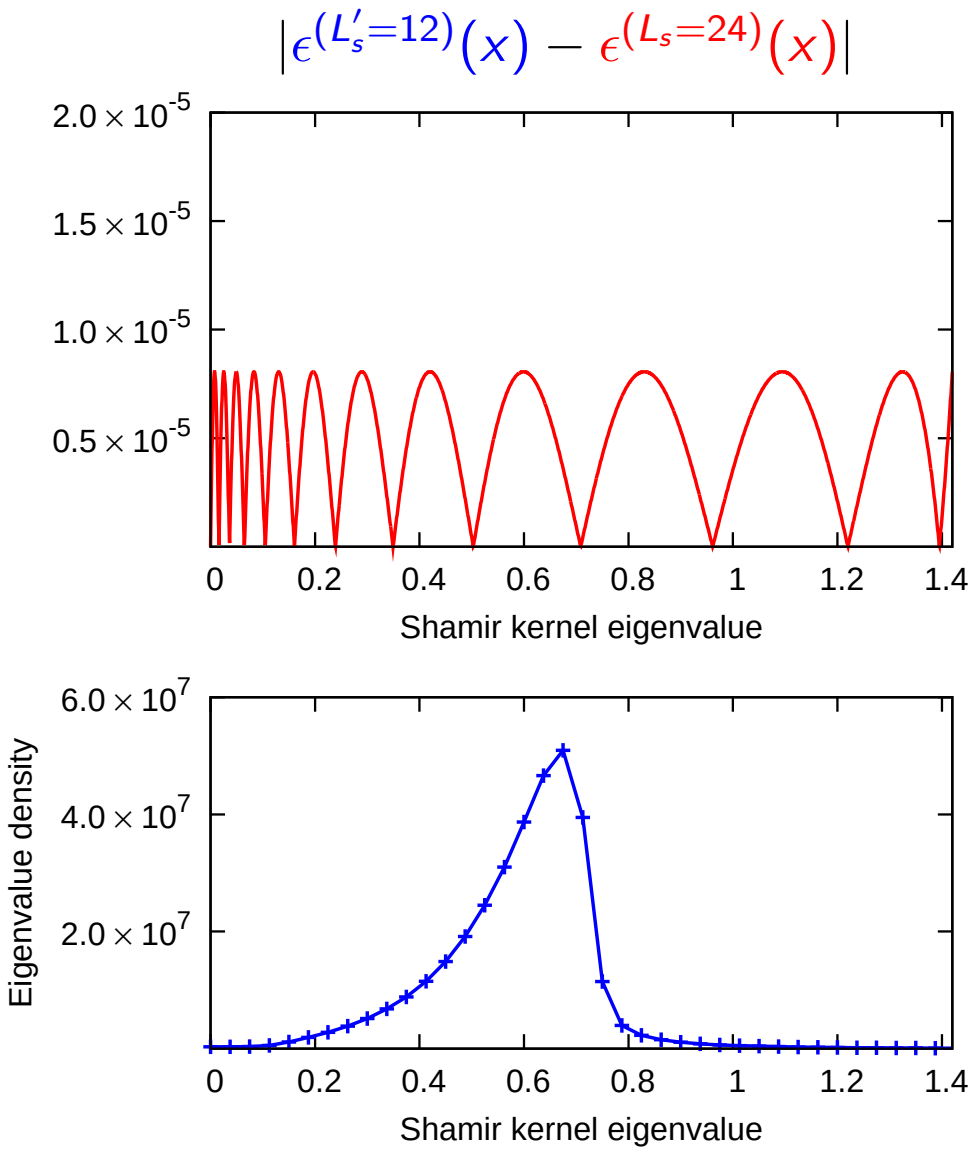

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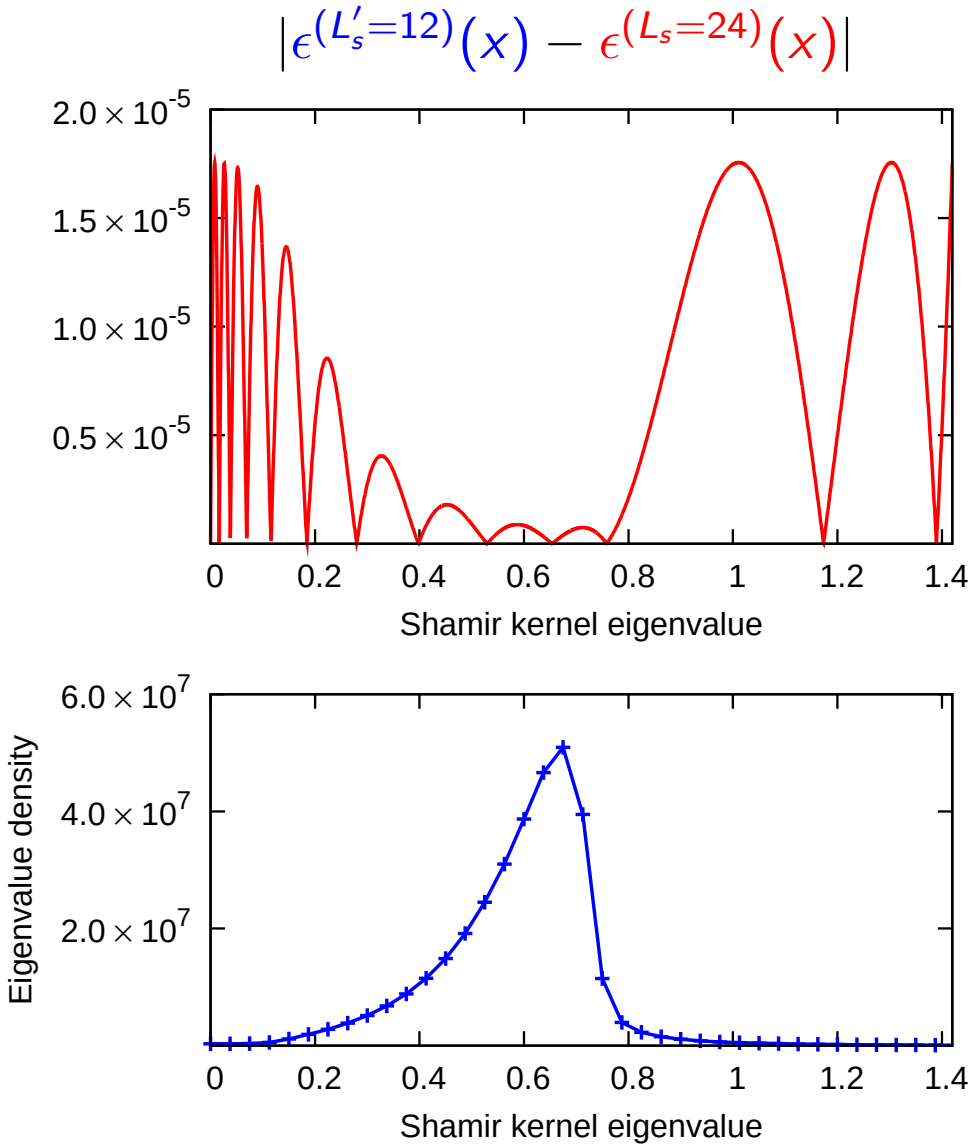

Simulation strategy

The only new element of the simulation is the correction determinant, which can be represented by 4D pseudofermions (now we give the 2-flavor version):

$$\begin{aligned} &\det\left[\frac{D_{\text{ov}}(m, L_s)^\dagger D_{\text{ov}}(m, L_s)}{D_{\text{ov}}(m, L_s')^\dagger D_{\text{ov}}(m, L_s')}\right]_{\text{4D}} \\ &\propto \int D\phi^\dagger D\phi \exp\left(-\phi^\dagger \left[\frac{D_{\text{ov}}(m, L_s)^\dagger D_{\text{ov}}(m, L_s)}{D_{\text{ov}}(m, L_s')^\dagger D_{\text{ov}}(m, L_s')}\right]^{-1} \phi\right) \end{aligned} \tag{9}$$

- The zMöbius approximation is extremely accurate for large enough L_s'.
- As a result the correction force is so small that we can completely omit it from the evolution.
- We only include these 4D pseudofermions in the HMC accept/reject step.

Results

Test ensemble: 2+1+1f, $a^{-1} = 3$ GeV, $32^3 \times 64$, $L_s = 24$, $L_s' = 12$, near physical point

- Reduced-L_s simulation strategy gives 30% reduction in cost of light quark determinant.
- Speedup comes from 50% reduction in L_s. Cost reduction is less than 50% because CG iteration count increases somewhat.
- New preconditioning scheme needed to avoid even larger increase in iteration count (see Chulwoo's talk).

Production:
This strategy now in use for $80 \times 80 \times 96 \times 192$, $a^{-1} = 3$ GeV, physical point 2+1+1f simulations by RBC/UKQCD collaboration, using $L_s = 32$, $L_s' = 14$. Here $\Delta H_{\text{correction}} \lesssim 5 \times 10^{-4} \ll 1$.

(L_s is large here because we have included a "dislocation-enhancing determinant" to promote topology change. Dislocations increase the residual chiral symmetry breaking of DWF and we use large L_s to compensate.)

Summary

- We have implemented a version of Brower et al.'s idea for speeding up DWF simulations.
- We achieve a $\sim 30\%$ speedup of the light quark determinant.
- The zMöbius ideas discussed in the next talk are crucial to achieving a speedup.
- We are applying these ideas in a new large-volume physical-point 2+1+1f simulation.

Backup slides