Error reduction with all-mode-averaging in Wilson fermion

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1. Introduction

Lattice QCD is powerful tool to deal with the strong interaction between quark and gluon, however, in order to give a reliable solution, we need to reduce the statistical fluctuation as much as possible. Recently idea of all-mode-averaging (AMA) [1,2] is state-of-the-art algorithm to reduce statistical error of correlation function in Monte-Carlo simulation, and it seems to be broadly applicable. In this poster we present a performance test of AMA using Wilson-Clover fermion.

2. All-mode-averaging (AMA)

The improved estimator is defined as

$$\mathcal{O}^{(\mathrm{imp})} = \mathcal{O}^{(\mathrm{rest})} + \frac{1}{N_G}\sum_{g\in G}\mathcal{O}^{(\mathrm{appx}),g},\ \mathcal{O}^{(\mathrm{rest})} = \mathcal{O} - \mathcal{O}^{(\mathrm{appx})}$$

where $O^{(appx)}$ is approximation whose cost is much smaller than O. *g* denotes the lattice transformation of the symmetry *G*. Here the translational invariance is employed. Using deflation method[2,3], the approximation is defined as the combination of deflation field and truncated solver as

$$\mathcal{O}^{(\mathrm{appx})} = \mathcal{O}^{(\mathrm{AMA})}[S^{(\mathrm{all})}],\ S^{(\mathrm{all})}(x,y) = \sum_{k,l}^{N_\lambda}\Lambda_{kl}\psi_k(x)\psi_l(y) + f_\varepsilon(D(x,y))$$

where two parameters, N_λ and ε, control the quality of approximation and computational cost.

The standard deviation of $O^{(imp)}$ expects to be

$$\frac{\sigma^{\mathrm{imp}}}{\sigma} \simeq \sqrt{\frac{1}{N_G} + 2\Delta r + R^{\mathrm{corr}}},\ R^{\mathrm{corr}} = \frac{1}{N_g^2}\sum_{g\neq g'} r_{gg'},\ \Delta r = 1 - r$$

where with $\Delta O = O - \langle O\rangle$ we have

$$r = \frac{\langle \Delta\mathcal{O}\Delta\mathcal{O}^{(\mathrm{appx})}\rangle}{\sigma\sigma^{(\mathrm{appx})}},\ r_{gg'} = \frac{\langle \Delta\mathcal{O}^{(\mathrm{appx}),g}\Delta\mathcal{O}^{(\mathrm{appx}),g'}\rangle}{\sigma^{(\mathrm{appx}),g}\sigma^{(\mathrm{appx}),g'}},$$

these quantities denote the correlation between O and $O^{(appx)}$,and different g of $O^{(appx)}$. For error reduction, we need to seach the approximation with small Δr and R^{corr}.

3. Approximation with SAP method

Schwartz alternative procedure (SAP) [2] is applied for both generation of deflation field and preconditioning. SAP is approximation to Wilson-Dirac kernel as decomposing lattice into domain Λ and Λ^* in which Dirichlet BC is utilized.

$$D_w \simeq \begin{pmatrix} D_\Lambda & \partial D_\Lambda \\ \partial D_{\Lambda^*} & D_{\Lambda^*}\end{pmatrix} \qquad M_{\mathrm{sap}} = K\sum_{\nu=0}^{n_{\mathrm{cy}}-1}(1-DK)^\nu$$

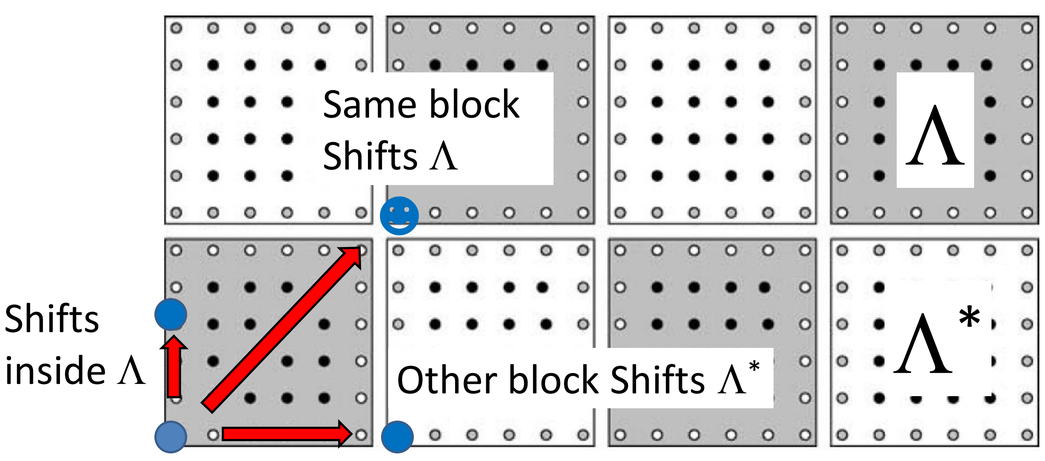
$$K = R_\Lambda^T D_\Lambda^{-1} R_\Lambda + R_{\Lambda^*}^T D_{\Lambda^*}^{-1} R_{\Lambda^*} - R_{\Lambda^*}^T D_{\Lambda^*}^{-1} D_{\partial\Lambda^*} D_\Lambda^{-1} R_\Lambda$$

$$R_\Lambda = \begin{pmatrix} 1 & 0\end{pmatrix},\quad R_{\Lambda^*} = \begin{pmatrix} 0 & 1\end{pmatrix}$$

When we use SAP as an approximation $O^{(appx)}$ in AMA, translational invariance between domains is taken into account:

1. Shift inside domain: NOT translational invariance.
2. Shift other domian: NOT translational invariance.
3. Shift same domain and same local position: **OK.**

It is safe to assure covariance of approximation that source location is set to the next domain Λ and same local position.



4. Test of covariance in SAP approximation

The covariance is easily checked by consistency test with gauge shift and source shift,

$$O[U](x+\mu, y+\mu) = O[U^g](x,y),\ U^g(x) = U(x-\mu)$$

The precision of discrepancy should be below machine precision (~10^{-16} in double) if the translational symmetry is preserved. We checked same block shift has good consistency.

Table 1: 64×32^3 lattice with 4×4^3 SAP domain in ε~0.01 residue

	Other block shift	(4,0,0,0)	
	Gauge shift	Source shift	diff.
<PsPs>, t=1	2.0810882153191448e-01	2.0814053466832835e-01	1.5e-4
<NN>, t=10	1.9793954905488386e-07	1.9401235321009282e-07	2.0e-2
	Same block shift	(4,4,4,4)	
<PsPs>, t=1	1.9670606430843440e-01	1.9670606430843440e-01	<1e-16
<NN>, t=10	3.5454273713838414e-07	3.5454273713838419e-07	1.4e-16

5. Approximation with SAP+deflation

The left- and right-handed deflation [3] is given as,

$$P_L = 1 - \sum_{k,l}(D\phi_k)\phi_l^\dagger A_{kl}^{-1},\quad P_R = 1 - \sum_{k,l}\phi_k(D\phi_l)^\dagger A_{kl}^{-1},\quad A_{kl} = (\phi_k, D\phi_l),$$

where decomposed matrix A is called as "little Dirac op.". The deflation procedure for solve Dx = b (D is Hermitian) is

1. $P_L D x = P_L b \Rightarrow D P_R x = P_L b,$
2. $P_R x = D^{-1}P_L b = x - \sum_{k,l}\phi_k(D\phi_l, x)A_{kl}^{-1} = x - \sum_{k,l}\phi_k(\phi_l, b)A_{kl}^{-1}$
3. $x = D^{-1}P_L b + \sum_{k,l}\phi_k(\phi_l, b)A_{kl}^{-1}$

The deflation subspace is given from N_s fields generated from smoothing process. Deflation projection with random field in the SAP domain decomposition is given as

$$P = \sum_{\Lambda,\Lambda'}^{N_b}\sum_{kl}^{N_s} R_\Lambda^T\phi_k^\Lambda\phi_l^{\Lambda'\dagger}R_\Lambda(A_{kl}^{\Lambda\Lambda'})^{-1},\quad A_{kl}^{\Lambda\Lambda'} = (\phi_k^\Lambda, R_\Lambda^T D R_{\Lambda'}\phi_l^{\Lambda'})$$

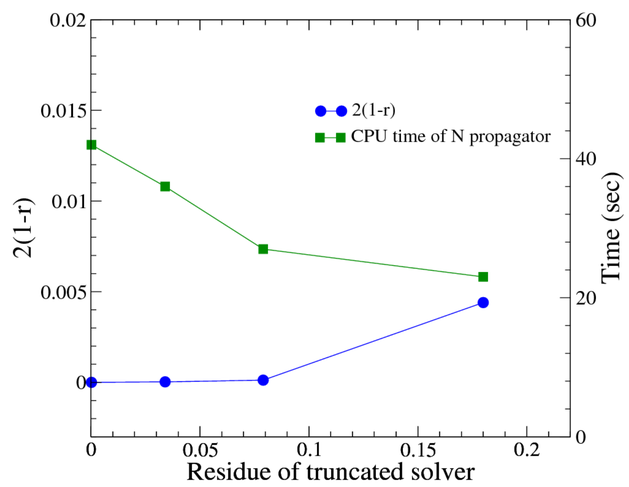
The quality of approximation can be controlled by N_s and SAP domain size in addition to stopping condition ε.

5. Performance test of AMA in SAP+deflation

In this test we use DDHMC library package and GCR algorithm in solver part. Here the mixed precision method is also applied. N_f = 2 Wilson-Clover fermion of CLS is used.

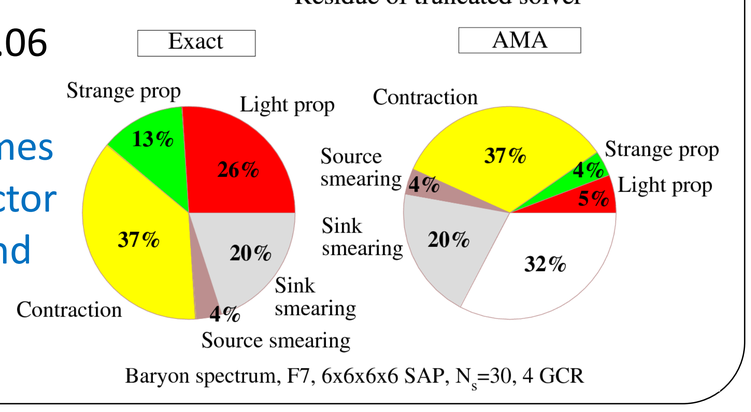
- 64×32^3 lattice at a=0.06 fm in 451 MeV pion.

SAP (TXYZ)	N_s	Fixed GCR	Residue
4x4x4x4	30	5	0.0002
4x4x4x4	10	4	0.18
4x4x8x8	30	3	0.034
8x8x4x4	30	4	0.079



- 96×48^3 lattice at a=0.06 fm at 277 MeV pion.

The solver part becomes sub-dominant after factor 5 reduction in AMA, and total cost is 30% reduction.



References: [1] T. Blum, T. Izubuchi, E. Shintani, PRD88.094503 (2013), 1402.0244 [hep-lat]. [2] M. Luscher, Comp.Phys.Comm.156,209 (2004). [3] M.Luscher, JHEP 07,081(2007).