Optimization of the Oktay-Kronfeld Action Conjugate Gradient Inverter

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Heavy Flavor Physics with Lattice QCD

Motivation

- 3σ tension in the neutral Kaon indirect CP violation parameter

$$
\begin{aligned}
|\epsilon_K|^{\text{exp}} &= 2.228(11) \times 10^{-3} && \text{(PDG)} \\
|\epsilon_K|^{\text{SM}} &= 1.6(2) \times 10^{-3} && (\text{SWME } \hat{B}_K, \text{FNAL/MILC } V_{cb})
\end{aligned}
$$

- Error budgets

$$
\sigma(X)^2/\sigma(|\epsilon_K^{SM}|)^2 = \begin{cases} 14\% & , \hat{B}_K \\ 51\% & , V_{cb} \end{cases}
$$

- A way of reducing the V_{cb} error is increasing the precision of lattice form factor calculation.

$$
B \to D^{(*)} l \nu_l
$$

- Heavy quark discretization is a dominant error source.

$$
m_b > a^{-1}, m_c \sim a^{-1}
$$

- Theoretical improvement is needed in contrast to take a brute force approach of reducing a lattice spacing continuously.

OK Action [M. B. Oktay and A. S. Kronfeld, PRD 78, 014504 (2008)]

Construction of LE$\mathcal{L}$

- OK action is the improved Fermilab action,
  [A. El-Khadra, A. S. Kronfeld and P. B. Mackenzie, PRD **55**, 3933 (1997)].
  - Building blocks

$$B_i, E_i, D_\mu, \psi, \bar{\psi}, \gamma_\mu$$

  - full set of $d = 6$ bilnear operators
  - part of $d = 7$ bilinear operators which commensurate to $d = 6$ operators by the power counting
  - No four-fermion operators (tree-level)

- The improvement terms are suppressed by up to
  - λ^3 of HQET power counting for heavy-light meson

$$\lambda \sim a\Lambda_{\mathrm{QCD}} \;\text{ or }\; \Lambda_{\mathrm{QCD}}/m_Q$$

  - v^6 of NRQCD power counting for heavy quarkonium

$$v = p/m_Q$$

OK Action

Power Counting

- Number of bilinears

d	4	5	6	7
λ^0	1			
λ^1	1	3		
λ^2		1	2(0)	
λ^3			5(4)	12(2)

HQET

$\lambda \sim a\Lambda_{QCD}$ or Λ_{QCD}/m_Q

d	4	5	6	7
v^2	2	2		
v^4		2	4(2)	2(1)
v^6			3(2)	8(1)
v^8				2(0)

NRQCD

$v = p/m_Q$

- 4 of 7 dimension 6 operators and

  2 of 12 dimension 7 operators have non-zero coupling after the tree-level matching.

OK Action

Matching: Tree Level

[A. El-Khadra, A. S. Kronfeld and P. B. Mackenzie, PRD **55**, 3933 (1997)]

- On-shell improvement amounts to an expansion in $\mathbf{p}a$
- Each matched coupling has full bare mass dependence, $c_i(m_0 a)$.

[M. B. Oktay and A. S. Kronfeld, PRD **78**, 014504 (2008)]

- Match the on-shell quantities
  - Energy (quark dispersion relation)
  - Current (quark-gluon vertex)
  - Quark-quark scattering
  - Compton scattering

- The tree-level matched action has 12 **operators**.

- **Use this action with the tree-level tadpole improvement.**

Form of the Dirac Operator

$$M_{x,y}\psi_y = \xi_x$$

- In temporal direction, only the *nearest neighbors* are involved.

$$M_{x,x\pm 4} \neq 0$$

- All of the *next-nearest neighbors* in spacial directions participate in. $(i, j = 1, 2, 3)$

$$M_{x,x\pm i},\ M_{x,x\pm i\pm j},\ M_{x,x\pm i\mp j} \neq 0$$

- Dirac operator receives *on-site* contribution from the clover term and the mass term.

$$M_{x,x} \neq 0$$

- Each terms $M_{x,y}$ consist of products of $1 \sim 5$ gauge links and γ matrices.

Optimization of the CG Inverter

Strategies

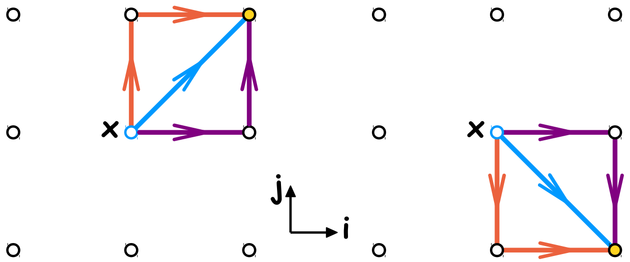
- Combinations of gauge link product(color matrix) in the Dirac operator are precalculated.
- Reflecting the γ matrix structure, the Dirac operator is represented by 4×4 block matrix, the precalcuation matrix.
- Each block is color matrix.

- $M^\dagger M$ preconditioning
- Even-Odd preconditioning
- Spin projection

Precalculation

Reduce the Floating Point Operations

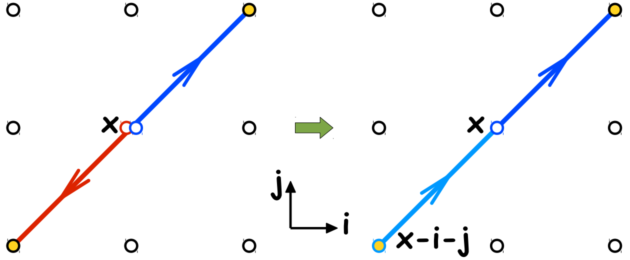
- The precalculation matrices connect the off-diagonal sites are symmetrized.



Precalculation

Toward a Memory Budget Solver

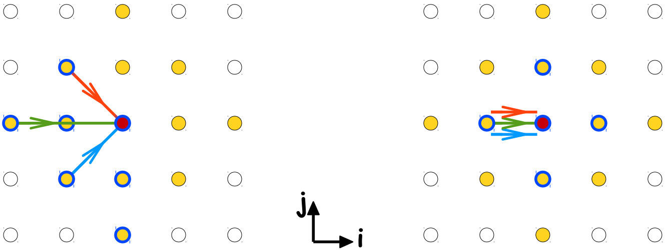
- The precalculation matrix which is pointing to the backward direction from the site x, is the *conjugate* of the forward precalculation matrix defined on the site $x - i - j$.
  - Hermitian conjugate in the spin-color space
  - followed by the sign correction



Precalculation

Simplify the Off-node Communication Pattern

- To update the fermion field on the red spot, one needs
  the fermion fields defined on the yellow sites and
  the precalcuation matrices defined on the blue-circled sites.

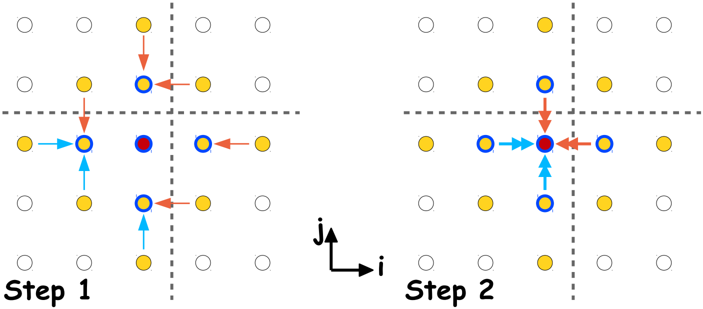


- To simplify this field access pattern, the shifted precalculation matrices are constructed.

Precalculation

Simplify the Off-node Communication Pattern

- Only the nearest neighbor off-node communications are required.
- Matrix multiplications are isolated from the communications.



- Only the nearest neighbor fermion fields are gathered and multiplied to the precalculation matrices.(Step 1)
- Then, the multipication results are gathered from the nearest neighbor sites and added up.(Step 2)

Libraries

Introduction

- **QOPQDP**:

  the implementation of QCD OPerations using QDP
  e.g., fermion inverters

- **QDP**:

  a C implementation of the LQCD suitable Data Parallel interface

- **CUDA**:

  the parallel computing architecture(Compute Unified Device Architecture) and/or programming language implemented by the NVIDIA GPU

- **MILC**:

  a LQCD application package which is hosted by the MILC collaboration

- **QUDA**:

  the QOPQDP analogy which is implemented by using CUDA

Libraries

Development Environments

- Bi-Stabilized CG solver in the QOPQDP is used.
- Mixed precision CG: Single precision iteration followed by a few double precision update

- $\not{D}$ function:
  - matrix multiplication
$$M_{x,y}\psi_y = \xi_x$$
  - precalculation
  - communication

- For CPU cluster,
  - The $\not{D}$ function in the QOPQDP is optimized.
  - To test the solver, heavy meson correlators are calculated by using the MILC code.

Libraries

Development Environments

- For GPU cluster,
  - Only the matrix mutiplication module in the optimized QOPQDP $\not{D}$ function is replaced by CUDA.
  - This matrix multiplication module for GPU is not fully optimized.
  - Precalculation and communication modules belong to the optimized QOPQDP code.

Performance

Time Table

- MILC coarse lattice $20^3 \times 64$ / 4 Nodes

	Naive	Optimized	CUDA
CG total (s)	11814.8	3036.8	891.0
Gain	1	3.9	13.3

- CPU: Intel i7 920@2.67GHz
- GPU: NVIDIA GTX 480
- Network: QLogic InfiniBand, 1 Rail

Timing (s)	Optimized	CUDA
Matrix Multiplication [SP]	2469.3	79.7
Matrix Multiplication [DP]	109.7	10.1
FLOPS (GF/Nodes)	2.1	58.8
CUDA Memory Copy, W		44.1
CUDA Memory Copy, ψ		191.6
FLOPS (GF/Nodes)		18.4
QOPQDP Preparation		138.9
Precalculation	67.1	
Communication	7.3	
Gamma Basis Change	45.2	
Spin Decomposition	62.5	

- Overhead(374.6s) exceeds the floating point calculation(89.8s).

Performance

Memory Requirement

- GTX 480 has 1.5GB global memory.
- Precalculation matrix is quite memory demanding.
- Only the single precision precalculation matrix is saved on the GPU global memory.

nodes	nx	ny	nz	nt	CPU(GBytes/node)	GPU(GBytes/node)
4	20	20	20	64	1.837	0.704
12	28	28	28	96	2.520	0.966
32	40	40	40	96	2.755	1.056
64	48	48	48	144	3.571	1.368
192	64	64	64	192	3.762	1.441

- Option: GTX Titan has 6GB global memory.

Future Work

- Optimize the GPU version of the OK action CG inverter further
- It is expected that the QOPQDP side overhead can be removed by using QUDA.
- The total memory transfer between CPU and GPU should be reduced.
- Use this inverter for the V_{cb} calculation

Thank you for your attention !