Optimization of the Oktay-Kronfeld Action
Conjugate Gradient Inverter

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Motivation

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

\[ |\epsilon_K|^{\text{exp}} = 2.228(11) \times 10^{-3} \quad \text{(PDG)} \]
\[ |\epsilon_K|^{\text{SM}} = 1.6(2) \times 10^{-3} \quad \text{(SWME} \hat{B}_K, \text{FNAL/MILC} V_{cb}) \]

- Error budgets

\[
\frac{\sigma(X)^2}{\sigma(|\epsilon_K^{SM}|)^2} = \left\{ \begin{array}{l} 14\%, \hat{B}_K \\ 51\%, V_{cb} \end{array} \right. 
\]

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

\[ B \rightarrow D^{(*)} l\bar{\nu}_l \]

- 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,  
  - Building blocks
    
    \[B_i, E_i, D_\mu, \psi, \bar{\psi}, \gamma_\mu\]

- full set of \(d = 6\) bilinear 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
  - \(\lambda^3\) of HQET power counting for heavy-light meson
    \[
    \lambda \sim a \Lambda_{QCD} \text{ or } \Lambda_{QCD}/m_Q
    \]
  - \(v^6\) of NRQCD power counting for heavy quarkonium
    \[
    v = p/m_Q
    \]
OK Action
Power Counting

- Number of bilinears

<table>
<thead>
<tr>
<th>$d$</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda^0$</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda^1$</td>
<td>1</td>
<td>3</td>
<td></td>
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</tr>
<tr>
<td>$\lambda^2$</td>
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<td>2(0)</td>
<td></td>
<td></td>
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<tr>
<td>$\lambda^3$</td>
<td></td>
<td>5(4)</td>
<td>12(2)</td>
<td></td>
</tr>
</tbody>
</table>

HQET

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

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


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

[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 \( \gamma \) matrices.
Optimization of the CG Inverter

Strategies

- Combinations of gauge link product (color matrix) in the Dirac operator are precalculated.
- Reflecting the $\gamma$ matrix structure, the Dirac operator is represented by $4 \times 4$ block matrix, the precalculation 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 \textit{backward} direction from the site \(x\), is the \textit{conjugate} of the \textit{forward} precalculation matrix defined on the site \(x - i - j\).
  - Hermitian conjugate in the spin-color space
  - followed by the sign correction
To update the fermion field on the red spot, one needs the fermion fields defined on the yellow sites and the precalculation 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.

Step 1
- Only the nearest neighbor fermion fields are gathered and multiplied to the precalculation matrices. (Step 1)

Step 2
- Then, the multiplication 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
Bi-Stabilized CG solver in the QOPQDP is used.

Mixed precision CG: Single precision iteration followed by a few double precision update

\[\mathcal{D}\text{ function:}
\begin{align*}
\text{matrix multiplication} \\
M_{x,y} \psi_y &= \xi_x \\
\text{precalculation} \\
\text{communication}
\end{align*}

For CPU cluster,

- The \(\mathcal{D}\) function in the QOPQDP is optimized.
- To test the solver, heavy meson correlators are calculated by using the MILC code.
For GPU cluster,

- Only the matrix multiplication module in the optimized QOPQDP 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

<table>
<thead>
<tr>
<th></th>
<th>Naive</th>
<th>Optimized</th>
<th>CUDA</th>
</tr>
</thead>
<tbody>
<tr>
<td>CG total (s)</td>
<td>11814.8</td>
<td>3036.8</td>
<td>891.0</td>
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<tr>
<td>Gain</td>
<td>1</td>
<td>3.9</td>
<td>13.3</td>
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</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Timing (s)</th>
<th>Optimized</th>
<th>CUDA</th>
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<tbody>
<tr>
<td>Matrix Multiplication [SP]</td>
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<td>79.7</td>
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<tr>
<td>Matrix Multiplication [DP]</td>
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<tr>
<td>FLOPS (GF/Nodes)</td>
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<tr>
<td>CUDA Memory Copy, $W$</td>
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<td>CUDA Memory Copy, $\psi$</td>
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<td>FLOPS (GF/Nodes)</td>
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<td>QOPQDP Preparation</td>
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<td>138.9</td>
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<tr>
<td>Precalculation</td>
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<td>67.1</td>
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<tr>
<td>Communication</td>
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<td>7.3</td>
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<td>Gamma Basis Change</td>
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<td>45.2</td>
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<tr>
<td>Spin Decomposition</td>
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<td>62.5</td>
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</table>

- 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.

<table>
<thead>
<tr>
<th>nodes</th>
<th>nx</th>
<th>ny</th>
<th>nz</th>
<th>nt</th>
<th>CPU(GBytes/node)</th>
<th>GPU(GBytes/node)</th>
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<tbody>
<tr>
<td>4</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>64</td>
<td>1.837</td>
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<td>64</td>
<td>64</td>
<td>192</td>
<td>3.762</td>
<td>1.441</td>
</tr>
</tbody>
</table>

- Option: GTX Titan has 6GB global memory.
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!