2+1 flavor lattice QCD simulation with $O(\alpha)$-improved Wilson quarks

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PACS-CS Project:

\( N_f = 2 + 1 \) Simulations at the Physical Point on large enough lattices

(\( \rightarrow \) plenary talk by Kuramashi)

- u-d quarks: Domain-Decomposed HMC (DDHMC) algorithm (Lüscher, 2003)
  + Hasenbusch trick (Hasenbusch, 2001; Hasenbusch, Jansen, 2003) + \cdots

- s quark: UV-filtered Polynomial HMC (UVPHMC) algorithm
  (JLQCD Collaborations, 2002)

• \( O(a) \) improved Wilson quark action with nonperturbative \( c_{SW} \)
  (CP-PACS and JLQCD Collaborations, 2006)

• Iwasaki gauge action (Iwasaki, 1983)

• \( \beta = 1.90 \) (\( a = 0.0907(13) \) fm)

• \( 32^3 \times 64 \) lattice

• \( m_{ud} = 3.5 \sim 67 \) MeV

on the PACS-CS computer (2560 nodes, 14.3 TFLOPS) at University of Tsukuba.
Plan to this talk:

- Introduction

- Algorithm for $N_f = 2$ part: DDHMC, Hasenbusch trick, Solver
  ($\rightarrow$ plenary talk by Ishikawa)

- Simulation Parameters and Data Set

- Run Status

- Conclusion
Here we consider preconditioning for $N_f = 2$ O(a)-improved Wilson-Dirac op.

- Jacobi preconditioning: $|\det(1 + T)|^2 |\det D|^2$
  \[ D = 1 + (1 + T)^{-1}M, \quad T : \text{clover term, } M : \text{hopping term} \]

- Domain decomposition splitting lattice sites into even & odd domains

\[
D = \begin{pmatrix}
D_{EE} & D_{EO} \\
D_{OE} & D_{OO}
\end{pmatrix}
= \begin{pmatrix}
D_{EE} & 0 \\
0 & D_{OO}
\end{pmatrix}
\begin{pmatrix}
1 & D_{EE}^{-1}D_{EO} \\
D_{OO}^{-1}D_{OE} & 1
\end{pmatrix}
\]

\[ \Rightarrow |\det(1 + T)|^2 |\det D_{EE}|^2 |\det D_{OO}|^2 |\det(1 - D_{EE}^{-1}D_{EO}D_{OO}^{-1}D_{OE})|^2 \equiv \hat{D}_{IR} : \text{IR part} \]

- Even-Odd site preconditioning for $D_{EE(0O)}$: $|\det D_{EE}|^2 \Rightarrow |\det \bar{D}_{EE}|^2$
• Further preconditioning by spin & hopping structure: $|\det \hat{D}_{IR}|^2 \Rightarrow |\det D_{IR}|^2$

After all these preconditioning, we have partition function,

$$Z = \int DU e^{-SG} \left( |\det(1 + T)|^2 \right)^{\text{Gauge part}} |\det \tilde{D}_{EE}|^2 |\det \tilde{D}_{OO}|^2 |\det D_{IR}|^2. $$

To reduce the HMC simulation cost, Multi time step integrator is employed for Gauge, UV and IR parts. (Sexton and Weingarten, 1992)

In our simulations, the relative magnitudes of force terms, $F_G, F_{IR}, F_{UV}$, are

$$||F_G|| : ||F_{UV}|| : ||F_{IR}|| \approx 16 : 4 : 1.$$  

We choose the associated step sizes, $\delta \tau_G, \delta \tau_{UV}, \delta \tau_{IR}$ such that

$$\delta \tau_G ||F_G|| \approx \delta \tau_{UV} ||F_{UV}|| \approx \delta \tau_{IR} ||F_{IR}||,$$

$$\delta \tau_G = \tau / N_0 N_1 N_2, \quad \delta \tau_{UV} = \tau / N_1 N_2, \quad \delta \tau_{IR} = \tau / N_2, \quad N_0 = N_1 = 4.$$
For strange quark, we employ UVPHMC algorithm (CP-PACS and JLQCD Collaborations, 2006) where the domain decomposition is not used.

\[ \|F_s\| \approx \|F_{IR}\| \Rightarrow \delta \tau_s = \delta \tau_{IR}. \]

For \( m_{ud} \geq 12 \text{MeV} \), this DDHMC + UVPHMC algorithm works stable, while 3.5 MeV run has large fluctuation of \( \|F_{IR}\| \) and is slow to keep simulation stable.

We combine DDHMC with Hasenbusch’s mass precondition for IR part (MPDDHMC).

+ Hasenbusch trick (Hasenbusch, 2001; Hasenbusch, Jansen, 2003)

\[ D'_{IR} = D_{IR}(\kappa \to \kappa' = \rho \kappa), \text{ eg. } \rho = 0.9995 \text{ to shift to the heavier mass} \]

\[ |\det D_{IR}|^2 = |\det D'_{IR}| \left| \det \left( \frac{D_{IR}}{D'_{IR}} \right) \right|^2 \]

Step sizes, \( \delta \tau_G, \delta \tau_{UV}, \delta \tau_{IR'}, \delta_{IR/IR'} \), are controlled by \( (N_0, N_1, N_2, N_3) \).

\( N_0 = N_1 = 4, N_2 \text{ and } N_3 \) are chosen to reduce the fluctuation of \( \|F_{IR'}\|, \|F_{IR/IR'}\| \).
For DDHMC algorithm \((12\text{MeV} \leq m_{\text{ud}} \leq 67\text{MeV})\),

- IR solver : SAP(single prec.) preconditioned GCR(double prec.) \((\text{Lüscher, 2004})\)
- UV solver : SSOR(single prec.) preconditioned GCR(double prec.)
- Stopping condition : \(|Dx - b| / |b| \leq 10^{-14}\) for H, \(10^{-9}\) for F

\[ \rightarrow \text{Reversibility : } |\Delta U| \leq 10^{-12}, |\Delta H| \leq 10^{-8} \]
For MPDDHMC algorithm ($m_{ud} = 3.5$ MeV),

★ Chronological guess for IR part (Brower, Ivanenko, Levi, Orginos, 1997)

★ nested BiCGStab solver for IR and UV part:

- Outer solver (double prec.): Solve $Dx = b$ with preconditioner $M \approx D^{-1}$ with strict stopping condition $10^{-14}$ for $F$

- Inner solver (single prec.): Solve $M \approx D^{-1}$ with appropriate preconditioner with automatic tolerance control $tol_{inner} = \min\left(\max\left(\frac{err_{outer}}{tol_{outer}}, 10^{-6}\right), 10^{-3}\right)$

★ Deflation technique (Morgan, Wilcox, 2002; Lüscher, 2007)

- inner BiCGStab stagnant $\rightarrow$ GCRO-DR (Parks et al, 2006)
  (Generalized Conjugate Residual with implicit inner Orthogonalization and Deflated Restarting)
Physical Point simulations require

HMC : $O(100)$ Tflops computer,

MPDDHMC : $O(10)$ Tflops computer.
### Simulation Parameters and Data Set

| Parameter          | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 | Value 7 | Value 8 |
|--------------------|---------|---------|---------|---------|---------|---------|---------|---------|
| $\kappa_{ud}$      | 0.1370  | 0.1372  | 0.1375  | 0.1375  | 0.1377  | 0.1378  | 0.137785|         |
| $\kappa_s$         | 0.1364  | 0.1364  | 0.1364  | 0.1366  | 0.1364  | 0.1366  |         | 0.1366  |
| Algorithm          | DDHMC   | DDHMC   | DDHMC   | DDHMC   | DDHMC   | MPDDHMC | MPDDHMC |         |
| $\tau$             | 0.5     | 0.5     | 0.5     | 0.5     | 0.25    | 0.25    | 0.25    |         |
| $(N_0,N_1,N_2,N_3,N_4)$ | (4,4,10)| (4,4,14)| (4,4,20)| (4,4,28)| (4,4,16)| (4,4,4,6)| (4,4,2,4,4)| (4,4,6,6) |
| $\rho_1$           |         |         |         |         |         |         | 0.9995  | 0.9995  |
| $\rho_2$           |         |         |         |         |         |         |         | 0.9990  |
| $N_{\text{poly}}$  | 180     | 180     | 180     | 220     | 180     | 200     | 220     |         |
| Replay             | on      | on      | on      | on      | on      | off     | off     |         |
| MD time            | 2000    | 2000    | 2250    | 2000    | 2000    | 1400    | 850     |         |
| $m_{ud}[MeV]$      | 67      | 45      | 24      | 21      | 12      | 3.5     | 3.5     |         |
| $m_{\pi}[MeV]$     | 702     | 570     | 411     | 385     | 296     | 156     | 162     |         |
| CPU time [h]/$\tau$ | 0.29    | 0.44    | 1.3     | 1.1     | 2.7     | 7.1     | 6.0     |         |

Shifted hopping parameter $\kappa_{ud}' = \rho_1 \kappa_{ud} \sim 0.1377$
\( m_\pi = 570\text{MeV} \)  \( m_\pi = 296\text{MeV} \)  \( m_\pi = 156\text{MeV} \)

\[
\begin{align*}
\text{acc(HMC)} &= 0.87 \\
\text{replay trick} &\sim 0.1\%
\end{align*}
\]

\[
\begin{align*}
\text{acc(HMC)} &= 0.84 \\
\text{replay trick} &\sim 3\%
\end{align*}
\]

\[
\begin{align*}
\text{acc(HMC)} &= 0.88
\end{align*}
\]
\( m_\pi = 570 \text{MeV} \)  \hspace{1cm} \( m_\pi = 296 \text{MeV} \)  \hspace{1cm} \( m_\pi = 156 \text{MeV} \)

\( F_0 : \text{Gauge + clv} \)
\( F_1 : \text{UV} \)
\( F_2 : \text{IR + s} \)
\( F_3 : \text{IR/IR'} \)

\( F_0 : \text{Gauge + clv} \)
\( F_1 : \text{UV} \)
\( F_2 : \text{IR'} + s \)
\( F_3 : \text{IR/IR'} \)
Effective mass : Meson

\[ k_{ud} = 0.13727 \]
\[ m_\pi = 570 \text{MeV} \]

\[ k_{ud} = 0.13770 \]
\[ m_\pi = 296 \text{MeV} \]

\[ k_{ud} = 0.13781 \]
\[ m_\pi = 156 \text{MeV} \]

Fit Range \([t_{\text{min}}, t_{\text{max}}]\) : Pseudoscalar \([13 - 30]\), Vector \([10 - 20]\)
Bin Size Dependence of Jacknife Error for $m_\pi$

plateau: after 100-200τ
same behavior for other masses
jackknife analysis: 250τ (110τ)

$156\text{MeV} \leq m_\pi \leq 411\text{MeV}$
Effective mass : Baryon

\[ k_{ud} = 0.13727 \]
\[ m_\pi = 570\text{MeV} \]

\[ k_{ud} = 0.13770 \]
\[ m_\pi = 296\text{MeV} \]

\[ k_{ud} = 0.13781 \]
\[ m_\pi = 156\text{MeV} \]

Fit Range \([t_{\text{min}}, t_{\text{max}}]\) : Decuplet \([13 - 30]\), Octet \([10 - 20]\)
$\kappa_{ud} = 0.137785, \kappa_{s} = 0.13660$ : Preliminary

$\kappa_{ud} = 0.137785, \kappa_{s} = 0.13660$ is estimated as the physical point from our ChPT analysis. 

(ChPT → talk by Kadoh)

IR part in MPDDHMC : $|\det D_{IR}|^2 = |\det D''_{IR}|^2 \det \left( \frac{D'_{IR}}{D''_{IR}} \right)^2 \det \left( \frac{D'_{IR}}{D''_{IR}} \right)^2$

$F_0 :$ Gauge + clv
$F_1 :$ UV
$F_2 :$ IR'' + s
$F_3 :$ IR'/IR''
$F_4 :$ IR/IR'

acc(HMC) = 0.83, CPU time = 6.0 [h]/$\tau$
Effective mass

\[ m_\pi = 162 \text{MeV} \]
Comparison with Chpt and Experiment

Preliminary
Jackknife analysis = 50τ
at κ_{ud} = 0.137785

|                 | ChPT       | experiment         | κ_{ud} = 0.137785 |
|-----------------|------------|--------------------|--------------------|
| m_{ud}^{MS} [MeV]| 2.53(5)   | –                  | 3.5(3)             |
| m_s^{MS} [MeV]  | 72.7(8)   | –                  | 73.4(2)            |
| f_π [MeV]       | 134.0(4.2)| 130.7 ± 0.1 ± 0.36| 129.0(5.4)         |
| f_K [MeV]       | 159.4(3.1)| 159.8 ± 1.4 ± 0.44| 160.6(1.4)         |
Conclusion

- $N_f = 2 + 1$ full QCD with $O(a)$ improved Wilson quarks on $(2.9\text{fm})^3$
- domain-decomposed HMC + Hasenbusch trick
- $m_{ud} = 3.5 \sim 67[\text{MeV}]$
- $m_\pi = 156 \sim 702[\text{MeV}]$
- $a = 0.0907(13)\text{ fm}$
- Physical Point simulation in progress