PACS-CS Results for
2+1 Flavor Lattice QCD Simulation
on and off the Physical Point

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(Univ. of Tsukuba)

July 18, 2008
Plan of talk

§1. The PACS-CS project

§2. Simulation details
   – Algorithms ⇒ Ishikawa’s talk (Wed)
   – Simulation parameters

§3. SU(3) and SU(2) ChPT analyses
   – PS sector (Low energy constants, FSE)
   – Baryon

§4. Results of the physical point simulation
   – Comparison with the extrapolated results

§5. Summary
§1. The PACS-CS project
Parallel Array Computer System for Computational Sciences
operation started on 1 July 2006 at CCS in U.Tsukuba
collaboration members

physicists:
S.Aoki, N.Ishii, N.Ishizuka, D.Kadoh, K.Kanaya, Tsukuba
Y.Kuramashi, K.Sasaki, Y.Taniguchi, A.Ukawa,
N.Ukita, T.Yoshié Hiroshima
K-I.Ishikawa, M.Okawa
T.Izubuchi Kanazawa

computer scientists:
T.Boku, M.Sato, D.Takahashi, O.Tatebe Tsukuba
T.Sakurai, H.Tadano
Physics plan

aim: 2+1 flavor QCD simulation at the physical point
strategy: reduce $m_{ud}$ keeping $m_s$ around the physical value
by-product: investigate viability of extrapolation method with ChPT

<table>
<thead>
<tr>
<th>PACS-CS</th>
<th>CP-PACS/JLQCD</th>
</tr>
</thead>
<tbody>
<tr>
<td>gauge action</td>
<td>Iwasaki</td>
</tr>
<tr>
<td>quark action $a$ [fm]</td>
<td>clover with $c_{SW}^{NP}$</td>
</tr>
<tr>
<td>volume</td>
<td>0.07, 0.1, 0.122</td>
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<tr>
<td>$m_{AWI}^{ud}$</td>
<td>$(3\text{fm})^3$</td>
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<tr>
<td>algorithm for ud</td>
<td>physical point</td>
</tr>
<tr>
<td>algorithm for s</td>
<td>DDHMC with improvements</td>
</tr>
<tr>
<td></td>
<td>UV-filtered exact PHMC</td>
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<tr>
<td></td>
<td>Iwasaki</td>
</tr>
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<td></td>
<td>clover with $c_{SW}^{NP}$</td>
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<tr>
<td></td>
<td>0.07, 0.1, 0.122</td>
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<tr>
<td></td>
<td>$(2\text{fm})^3$</td>
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<tr>
<td></td>
<td>$64\text{MeV}$</td>
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<td></td>
<td>HMC</td>
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<td>exact PHMC</td>
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## 2. Simulation details

### parameters

<table>
<thead>
<tr>
<th>$\kappa_{ud}$</th>
<th>$\kappa_S$</th>
<th>ud algorithm</th>
<th>$m_\pi L$</th>
<th>$\tau$</th>
<th>MD time</th>
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<tr>
<td>0.13700</td>
<td>0.13640</td>
<td>DDHMC</td>
<td>10.3</td>
<td>0.5</td>
<td>2500</td>
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<td>0.13727</td>
<td>0.13640</td>
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<td>0.13754</td>
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<td>0.5</td>
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<td>0.13754</td>
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<td>0.13770</td>
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<td>MP2DDHMC</td>
<td>–</td>
<td>0.25</td>
<td>–</td>
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<td>0.13781</td>
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<td>MPDDHMC</td>
<td>2.3</td>
<td>0.25</td>
<td>990</td>
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</tbody>
</table>

$m_{PS} = 156\text{MeV}$ ($m_{ud}^{AWI} = 3\text{MeV}$) is reached

$\kappa_{ud} \geq 0.13754$ for ChPT fits
unitary points with \( m_\pi \lesssim 400 \text{MeV} \)
Further improvements on DDHMC for $m_\pi \lesssim 200\text{MeV}$
⇒ Ishikawa’s talk(Wed)

- Mass-preconditioned DDHMC (MPDDHMC, MP2DDHMC)
  $\kappa_{ud}' = \rho \kappa_{ud}$ for the preconditioner of IR part
  \[
  \det R = \det R' \cdot \det \left( \frac{R}{R'} \right)
  \]
  tame the fluctuation of $||F_{\text{IR}}||$

- Chronological inverter for IR part
  strict tolerance: $|Dx - b|/|b| < 10^{-14}$ both for force and H

- solver improvement
  incorporate deflation technique
3. SU(3) and SU(2) ChPT analyses

NLO SU(3) ChPT formula

\[ m_{\pi}^2 = 2m_{ud}B_0 \left\{ 1 + \mu_\pi - \frac{1}{3} \mu_\eta + 2m_{ud}K_3 + K_4 \right\} \]

\[ m_K^2 = (m_{ud} + m_s)B_0 \left\{ 1 + \frac{2}{3} \mu_\eta + (m_{ud} + m_s)K_3 + K_4 \right\} \]

\[ f_\pi = f_0 \left\{ 1 - 2\mu_\pi - \mu_K + 2m_{ud}K_6 + K_7 \right\} \]

\[ f_K = f_0 \left\{ 1 - \frac{3}{4} \mu_\pi - \frac{3}{2} \mu_K - \frac{3}{4} \mu_\eta + (m_{ud} + m_s)K_6 + K_7 \right\} \]

\[ \mu_P = \frac{1}{16\pi^2} \frac{m_P^2}{f_0^2} \ln \left( \frac{m_P^2}{\mu^2} \right) \]

unknown parameters: \( B_0, f_0, K_{3,4,6,7}, L_{4,5,6,8} \)

should use the formula of WChPT?
NLO WChPT formula in terms of $m^\text{AWI}_q$

Aoki-Bär-Takeda-Ishikawa

\[
m^2_\pi = 2m_{ud} B_0 \left\{ 1 + \mu_\pi - \frac{1}{3} \mu_\eta + 2m_{ud} K_3 + K_4 \frac{2H''}{f_0^2} \right\}
\]

\[
m^2_K = (m_{ud} + m_s) B_0 \left\{ 1 + \frac{2}{3} \mu_\eta + (m_{ud} + m_s) K_3 + K_4 \frac{2H''}{f_0^2} \right\}
\]

\[
f_\pi = f_0 \left\{ 1 - 2\mu_\pi - \mu_K + 2m_{ud} K_6 + K_7 \frac{2H'}{f_0^2} \right\}
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\[
f_K = f_0 \left\{ 1 - \frac{3}{4} \mu_\pi - \frac{3}{2} \mu_K - \frac{3}{4} \mu_\eta + (m_{ud} + m_s) K_6 + K_7 \frac{2H'}{f_0^2} \right\}
\]
NLO WChPT formula in terms of $m_q^{\text{AWI}}$

\[
m_{\pi}^2 = 2m_{ud}B_0 \left\{ 1 + \mu_\pi - \frac{1}{3}\mu_\eta + 2m_{ud}K_3 + K_4\frac{2H''}{f_0^2} \right\}
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m_K^2 = (m_{ud} + m_s)B_0 \left\{ 1 + \frac{2}{3}\mu_\eta + (m_{ud} + m_s)K_3 + K_4\frac{2H''}{f_0^2} \right\}
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f_\pi = f_0 \left\{ 1 - 2\mu_\pi - \mu_K + 2m_{ud}K_6 + K_7\frac{2H'}{f_0^2} \right\}
\]

\[
f_K = f_0 \left\{ 1 - \frac{3}{4}\mu_\pi - \frac{3}{2}\mu_K - \frac{3}{4}\mu_\eta + (m_{ud} + m_s)K_6 + K_7\frac{2H'}{f_0^2} \right\}
\]

redefinition: \(B_0' = B_0 \left\{ 1 - \frac{2H''}{f_0^2} \right\}, \ f_0' = f_0 \left\{ 1 - \frac{2H'}{f_0^2} \right\}\)

\(O(a^2)\) terms can be absorbed in \(B_0'\) and \(f_0'\)
expected chiral behavior parameters are determined by experimental inputs

Amorós-Bijnens-Talavera, 01

curvature due to logarithmic function
⇒ good test ground for light quark mass simulations
chiral behavior

\[ m_{\pi}^2 / m_{ud} \]

\[ f_K / f_\pi \]

Curvature is clearly observed

⇒ try SU(3) ChPT fit
simultaneous fit for $\frac{m_\pi^2}{m_{ud}^{AWI}}, \frac{m_K^2}{(m_{ud}^{AWI} + m_s^{AWI})}, f_\pi, f_K$

<table>
<thead>
<tr>
<th></th>
<th>PACS-CS</th>
<th>phenom*</th>
<th>RBC/UKQCD08</th>
<th>MILC07</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_0[GeV]$</td>
<td>0.1160(88)</td>
<td>0.115</td>
<td>0.0935(73)</td>
<td></td>
</tr>
<tr>
<td>$f_\pi/f_0$</td>
<td>1.159(57)</td>
<td>1.139</td>
<td>1.33(7)</td>
<td>1.21(5)(+13)</td>
</tr>
<tr>
<td>$L_4$</td>
<td>-0.04(10)</td>
<td>0.00(80)</td>
<td>0.139(80)</td>
<td>0.1(3)(+3)</td>
</tr>
<tr>
<td>$L_5$</td>
<td>1.43(7)</td>
<td>1.46(10)</td>
<td>0.872(99)</td>
<td>1.4(2)(+2)</td>
</tr>
<tr>
<td>$(2L_6 - L_4)$</td>
<td>0.10(2)</td>
<td>0.0(1.0)</td>
<td>-0.001(42)</td>
<td>0.3(1)(+2)</td>
</tr>
<tr>
<td>$(2L_8 - L_5)$</td>
<td>-0.21(3)</td>
<td>0.54(43)</td>
<td>0.243(45)</td>
<td>0.3(1)(1)</td>
</tr>
<tr>
<td>$\chi^2$/dof</td>
<td>4.2(2.7)</td>
<td></td>
<td>0.7</td>
<td></td>
</tr>
</tbody>
</table>

$L_i$ are defined at $\mu = m_\rho$ in units of $10^{-3}$  
* taken from Colangelo-Dürr-Haefeli, hep-lat/0503014

consistent with other groups?
conversion to $\bar{l}_3$ and $\bar{l}_4$ in SU(2) ChPT

\[ m^2_\pi = 2m_{ud}B \left\{ 1 + \frac{2m_{ud}B}{16\pi^2 f^2 \bar{l}_3} \right\} \]

\[ f_\pi = f \left\{ 1 - \frac{2m_{ud}B}{8\pi^2 f^2 \bar{l}_4} \right\} \]

\{ $B_0, f_0, L_4, 5, 6, 8$ \} are converted to \{ $B, f, \bar{l}_{3,4}$ \}

Gasser-Leutwyler, 85
$\bar{l}_3$ and $\bar{l}_4$ in comparison with other groups

MILC result for $\bar{l}_3$ is exceptionally small
what is responsible for $\chi^2/dof=4.2(2.7)$?

$m_{S}^{\text{AWI}}$ dependence is not well reproduced
what about NLO/LO ratio?

NLO/LO ratio is 40∼50%
⇒ NNLO contributions would be considerable
NLO SU(2) ChPT + analytical expansion around the physical $m_s$

\[
m^2_\pi = 2m_{ud}B \left\{ 1 + \frac{2m_{ud}B}{16\pi^2f^2\mu^2} \right\}
\]

\[
f_\pi = f \left\{ 1 - \frac{2m_{ud}B}{8\pi^2f^2\mu^2} \right\}
\]

\[
m^2_K = \alpha + \beta \cdot m_{ud} + \gamma \cdot m_s
\]

\[
f_K = \left( f_s^{(0)} + m_s f_s^{(1)} \right) \left\{ 1 + \beta' \cdot m_{ud} - \frac{3}{4} \left( \frac{2m_{ud}B}{16\pi^2f^2\mu^2} \right) \ln \left( \frac{2m_{ud}B}{\mu^2} \right) \right\}
\]
fit results

simultaneous fit to $m_\pi$, $f_\pi$, $f_K$

3 choices of fit ranges

<table>
<thead>
<tr>
<th></th>
<th>Range I</th>
<th>PACS-CS Range II</th>
<th>Range III</th>
<th>phenom</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f$ [GeV]</td>
<td>0.1248(51)</td>
<td>0.1181(30)</td>
<td>0.1158(28)</td>
<td>0.1219(7)</td>
</tr>
<tr>
<td>$f_\pi/f$</td>
<td>1.063(8)</td>
<td>1.074(5)</td>
<td>1.078(5)</td>
<td>1.072(7)</td>
</tr>
<tr>
<td>$l_3$</td>
<td>3.23(21)</td>
<td>3.32(10)</td>
<td>3.31(10)</td>
<td>2.9(2.4)</td>
</tr>
<tr>
<td>$l_4$</td>
<td>4.10(20)</td>
<td>4.32(9)</td>
<td>4.36(9)</td>
<td>4.4(2)</td>
</tr>
<tr>
<td>$\chi^2$/dof</td>
<td>0.33(68)</td>
<td>2.0(1.0)</td>
<td>2.8(1.8)</td>
<td></td>
</tr>
</tbody>
</table>

results are stable against choice of fit range

$\chi^2$/dof is increased by inclusion of heavier pion
fit ranges

simulation points

CP-PACS/JLQCD
PACS-CS
Physical Point

m_\pi [MeV]

m_K [MeV]

0 500 1000

0 500 1000

I

II

III

I

II

III
$\bar{l}_3$ and $\bar{l}_4$ in comparison with other groups

consistent with other groups
how well described by NLO SU(2) ChPT?

$m_{\text{AWI}}$ dependence is well reproduced.
NLO/LO ratio is \( \lesssim 20\% \) in the fit range \( m_{\text{ud}}^{\text{AWI}} \lesssim 0.01 \)

NNLO contributions could be 5\%
FSE based on NLO SU(2) ChPT

\[ R_X = \frac{X(L) - X(\infty)}{X(\infty)} \text{ for } X = \pi^0, f_\pi \]

Colangelo-Dür-Haefeli, 04

\[ R_{\pi^0} = \frac{1}{4} \xi_\pi \tilde{g}_1(m_\pi L), \]
\[ R_{f_\pi} = -\xi_\pi \tilde{g}_1(m_\pi L) \]

\[ \xi_\pi \equiv \frac{m_\pi^2}{(4\pi f_\pi)^2}, \quad \tilde{g}_1(x) = \sum_{n=1}^{\infty} \frac{4m(n)}{\sqrt{n}x} K_1(\sqrt{n}x) \]

valid for \( m_\pi L > 2 \) expected by the authors
$R_{m_{PS}} > 0$ and $R_{f_{PS}} < 0$

at most a few % even at the physical point
ChPT for nucleon

**NNLO SU(2) formula**

\[ m_N = m_0 - 4c_1 m^2_\pi - \frac{3g^2_A}{16\pi f^2} m^3_\pi + \left[ e_1(\mu) - \frac{3}{32\pi^2 f^2} \left( \frac{g^2_A}{m_0} - \frac{c_2}{2} \right) \right. \]
\[ - \frac{3}{16\pi^2 f^2} \left( \frac{g^2_A}{m_0} - 8c_1 + c_2 + 4c_3 \right) \ln \left( \frac{m_\pi}{\mu} \right) \left] m^4_\pi \right. \]
\[ + \frac{3g^2_A}{128\pi f^2 m^5_0} O(m^6_\pi) \]

**fit procedures**

- \( g_A, c_2, c_3 \) given, \( m_0, c_1, e_1(\mu) \) to be determined by fit
- apply to \( \kappa_s = 0.13640 \) series
drastic cancellations between different orders
strange contributions in SU(3) ChPT are significant
Are we satisfied at NLO SU(2) ChPT on the physical $m_s$?
Are we satisfied at NLO SU(2) ChPT on the physical $m_s$?

absolutely NO
Are we satisfied at NLO SU(2) ChPT on the physical $m_s$?

absolutely NO

reasons
– inappropriate for precision measurement
  NNLO contributions could be 5%
– discouraging convergence behaviors for baryons

direct simulation on the physical point is inevitable to control the systematic error
§4. Results of the physical point simulation

practical feasibility

physical point is within our reach
<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>0.137785</td>
<td>0.13660</td>
<td>MP2DDHMC</td>
<td>2.3</td>
<td>0.25</td>
<td>850</td>
</tr>
</tbody>
</table>

slightly off the physical point at the present statistics
interesting to compare the results with the extrapolated values
decay constants

extrapolation ambiguity doesn’t matter at the level of 5% error
vector meson masses

refined with smaller error bars
Ω baryon as physical input

more precise scale determination at the level of < 1%
§4. Summary

what we learn
- large NLO contributions in SU(3) ChPT due to $m_s$
- NLO SU(2) ChPT is not enough for precision measurement
- necessary to simulate the physical point directly

next step
- increasing the statistics on $32^3 \times 64$ at the physical point
- T2K-Tsukuba (95TF peak) started operation in U.Tsukuba on 2 June
- check FSE $\Rightarrow 64^4$ lattice at the physical point
- extension to another lattice spacings