Toward $N_f = 2 + 1$ Lattice QCD Simulation at the Physical Point on PACS-CS

Y. Kuramashi/A. Ukawa (U. Tsukuba) for the PACS-CS collaboration

Oct. 31, 2006
Plan of talk

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§2. Review of previous CP-PACS/JLQCD results

§3. PACS-CS specifications

§4. Preparatory study for production run

§5. Parameter choice and physics plan on PACS-CS

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§1. Introduction

PACS-CS
(Parallel Array Computer System for Computational Sciences)
2560 nodes, 14.3 Tflops peak, 5.12TB memory
installed at U.Tsukuba on 1 July 2006
specifications will be explained later
collaboration members

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N. Ukita, T. Yoshié Tokyo
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T. Izubuchi, M. Tsutsui, KEK
T. Ishikawa, BNL

computer scientists:
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§2. Review of previous CP-PACS/JLQCD results

simulation details
– RG improved gauge + clover quarks with $c_{SW}^{NP}$
– three lattice spacings and continuum extrapolation in $a^2$
  \[ \beta = 1.83(0.12\text{fm}), 1.90(0.10\text{fm}), 2.05(0.07\text{fm}) \]
– fixed physical volume $\sim (2\text{fm})^3$

– conventional HMC for up-down quarks
– exact polynomial HMC for strange quark

encouraging results on meson spectrum and light quark masses
meson spectrum

\[ K\text{-input}(m_\pi, m_\rho, m_K) \rightarrow m_{K^*}, m_\phi \]
\[ \phi\text{-input}(m_\pi, m_\rho, m_\phi) \rightarrow m_{K^*}, m_K \]

clear deviation from quenched results
consistent with experimental values in the continuum
$m_q^{\text{AWI}}$ with perturbative $Z$

smaller than quenced results
$m_s(\phi\text{-input})$ and $m_s(K\text{-input})$ are consistent in the continuum limit
however, light quark masses only down to
\[ \frac{m_{PS}}{m_V} \sim 0.6 \ (m_{ud}^{AWI} \approx 64\text{MeV}) \]
→ long chiral extrapolation to the physical point

wish to go down to lighter quark masses, e.g.
\[ \frac{m_{PS}}{m_V} \sim 0.2 - 0.3 \text{ or less} \ (m_{ud}^{AWI} < 10\text{MeV}) \]
§3. PACS-CS specifications
<table>
<thead>
<tr>
<th><strong>#nodes</strong></th>
<th>2560 (16 × 16 × 10)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>peak speed</strong></td>
<td>14.3 Tflops</td>
</tr>
<tr>
<td><strong>node</strong></td>
<td>single CPU + memory + HDD + 8GB Ethernet ports</td>
</tr>
<tr>
<td><strong>CPU</strong></td>
<td>Intel LV Xeon EM64T, 2.8GHz, 1MB L2 cache</td>
</tr>
<tr>
<td><strong>memory</strong></td>
<td>2GB/node (5.12TB/system)</td>
</tr>
<tr>
<td><strong>network</strong></td>
<td>3 dimensional hyper-crossbar uses dual GBEthernet/link</td>
</tr>
<tr>
<td><strong>network performance</strong></td>
<td>250MB/s/direction 750MB/s/node (3 dim. simultaneous send/receive)</td>
</tr>
<tr>
<td><strong>local HDD</strong></td>
<td>160GB×2 (RAID-1) (410TB×2/system)</td>
</tr>
<tr>
<td><strong>#racks</strong></td>
<td>59 racks</td>
</tr>
<tr>
<td><strong>footprint</strong></td>
<td>100m²</td>
</tr>
<tr>
<td><strong>power</strong></td>
<td>545kW</td>
</tr>
<tr>
<td><strong>OS</strong></td>
<td>Linux, Score</td>
</tr>
<tr>
<td><strong>programming</strong></td>
<td>Fortran, C, C++, MPI for communication</td>
</tr>
</tbody>
</table>
§4. Preparatory study for production run

basic strategy
– Lüscher’s domain-decomposed HMC (LDDHMC) for up-down quarks
– exact polynomial HMC for strange quark

preparatory study at $\beta = 1.9$ on $16^3 \times 32$
1. how light quark masses we can reach with LDDHMC
2. stability study using eigenvalues of the Dirac operator

<table>
<thead>
<tr>
<th>$\kappa_{ud}$</th>
<th>0.13700</th>
<th>0.13741</th>
<th>0.13759</th>
<th>0.13770</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_0, N_1, N_2$</td>
<td>4,5,6</td>
<td>4,5,8</td>
<td>4,5,12</td>
<td>4,5,14</td>
</tr>
<tr>
<td>$N_{\text{poly}}$</td>
<td>130</td>
<td>140</td>
<td>140</td>
<td>140</td>
</tr>
<tr>
<td>#traj.</td>
<td>2000</td>
<td>2000</td>
<td>2000</td>
<td>900</td>
</tr>
</tbody>
</table>
hadron effective masses

heaviest ud quark mass (left) and lightest (right)

good plateau for $m_{PS}(UD)$

hard to extract $m_V(U)$ in the lightest case
PS meson mass and $m_{ud}^{AWI}$

<table>
<thead>
<tr>
<th>$\kappa_{ud}$</th>
<th>$m_{PS}$ [MeV]</th>
<th>$m_{ud}^{AWI}$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.13700</td>
<td>655(4)</td>
<td>63.7(4)</td>
</tr>
<tr>
<td>0.13741</td>
<td>498(6)</td>
<td>34.8(5)</td>
</tr>
<tr>
<td>0.13759</td>
<td>367(9)</td>
<td>20.7(5)</td>
</tr>
<tr>
<td>0.13770</td>
<td>313(16)</td>
<td>15.4(12)</td>
</tr>
</tbody>
</table>

$m_{ud}^{AWI} \approx 15$MeV ($m_{PS} \approx 300$MeV) is reached
stability study

Wilson fermions break chiral symmetry
→ no protection from small eigenvalues
exceptionally small eigenvalues are source of instabilities

spectral gap distribution
\[ \mu = \min\{ |\lambda| \mid \lambda \text{ is an eigenvalue of } \gamma_5(D_W + m_0) \} \]
investigate probability distribution of \( \mu \)
\[ \mu_{\text{median}}, \mu_{\text{average}}, \text{width } \sigma \]

2 flavor results
\[ \mu_{\text{median}} \propto m_q^{\text{AWI}} \]
\[ \sigma_2 = c_2 a/\sqrt{V}; \quad c_2 \approx 1 \text{ independent of } a, V, m_q^{\text{AWI}} \]

→ how about 2+1 flavor case?
strange quark may change the situation?
roughly symmetric distribution about $\mu_{\text{median}}$

$\mu_{\text{median}}$ and $\mu_{\text{average}}$ are roughly proportional to $m_{\text{ud}}^{\text{AWI}}$
width of the distribution

– smaller width than 2 flavor case: $c_{2+1} < c_2 \approx 1$
– width decreases as $m_q^{AWI}$ becomes smaller

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<th>0.13759</th>
<th>0.13770</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_{ud}^{AWI}$[MeV]</td>
<td>63.7(4)</td>
<td>34.8(5)</td>
<td>20.7(5)</td>
<td>15.4(12)</td>
</tr>
<tr>
<td>$c_{2+1} = \sigma_{2+1} \sqrt{V/a}$</td>
<td>0.755(60)</td>
<td>0.735(53)</td>
<td>0.601(54)</td>
<td>0.501(76)</td>
</tr>
</tbody>
</table>

→ strange quark contributions may stabilize the simulation
§5. Parameter choice for production run on PACS-CS

- Algorithm → K. Ishikawa’s talk
  - LDDHMC with replay trick for ud quarks
    - SAP+GCR solver for IR part
  - UV-filtered PHMC for s quark

- Parameters
  - $\beta = 1.83(0.12\text{fm}), 1.90(0.10\text{fm}), 2.05(0.07\text{fm})$
  - Lattice spatial volume: $(3.0\text{fm})^3$
    - $24^3 \times 48(\beta = 1.83), 32^3 \times 64(\beta = 1.9), 40^3 \times 80(\beta = 2.05)$
  - $m_{ud}^{AWI} = 7, 15, 25, 35, 45\text{MeV or less}$
    - $15\text{MeV on } 16^3 \times 32 \rightarrow 4\text{MeV on } 32^3 \times 64$ from $\sigma \propto a/\sqrt{V}$
  - Two strange quark masses
  - $10^4$ trajs. for 100 indep. cfgs.
physics plan on PACS-CS
- light hadron spectrum including baryon
- heavy quark physics with the relativistic heavy quark action
- $\alpha_s$ and quark masses with nonperturbative renormalization
  Schrödinger functional method (under way)
- physics associated with topology
  $\eta'$ meson mass, NEDM
- hadron matrix elements
- hadron-hadron interactions
  $I = 0, 2$ $\pi$-$\pi$ scattering, $\rho$ resonance
§ 6. Summary

preliminary study with LDDHMC
- \( m_{\text{ud}}^{\text{AWI}} \approx 15 \text{MeV} \) reached
- \( \sigma \sqrt{V/a} \) (2+1 flavor) < \( \sigma \sqrt{V/a} \) (2 flavor)

target of PACS-CS project
- three \( \beta \) values, \((3.0 \text{fm})^3, 10^4\) trajs.
- go down to \( m_{\text{ud}}^{\text{AWI}} = 7 \text{MeV} \) or less
- current status of production runs:
  - \( m_{\text{ud}}^{\text{AWI}} = 7, 15, 25 \text{MeV} \) at \( \beta = 1.9 \) on \( 32^3 \times 64 \)

physical results will be presented in next year