

2+1 flavor Lattice QCD with Lüscher's Domain-Decomposed HMC Algorithm

Y.Kuramashi (U.Tsukuba)
for PACS-CS collaboration

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Plan of talk

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§2. Initial physics plan for PACS-CS

§3. Lüscher's domain-decomposed HMC (LDDHMC) algorithm

§4. 2+1 flavor scaling study with LDDHMC

§5. CPU-time estimate on PACS-CS

§6. Parameter choice for production run on PACS-CS

§7. Summary

§1. Introduction

PACS-CS

(Parallel Array Computer System for Computational Sciences)

2560 nodes, 14.3 Tflops peak, 5.12TB memory

operation started on 1 July 2006

→ Ukawa's talk(Tue)

PACS-CS collaboration

S.Aoki, K-I.Ishikawa, T.Ishikawa, N.Ishizuka, T.Izubuchi, K.Kanaya,
Y.Kuramashi, M.Okawa, K.Sasaki, Y.Taniguchi, N.Tsutsui,
A.Ukawa, T.Yoshié

§2. Initial physics plan for PACS-CS

complete the Wilson-clover $N_f = 2 + 1$ program

CP-PACS and JLQCD joint project

- RG improved gauge + clover quarks with $c_{\text{SW}}^{\text{NP}}$
- three β values: $\beta = 1.83(0.12\text{fm}), 1.90(0.10\text{fm}), 2.05(0.07\text{fm})$
- fixed physical volume $\sim (2\text{fm})^3$
- light quark masses down to $m_{\text{ud}}^{\text{AWI}} \approx 64\text{MeV}$ ($m_{\text{PS}}/m_V \sim 0.6$)

→ wish to go down to lighter quark masses,

e.g. $m_{\text{PS}}/m_V \sim 0.3$ or less

using Lüscher's domain-decomposed HMC (LDDHMC) algorithm

§3. LDDHMC algorithm

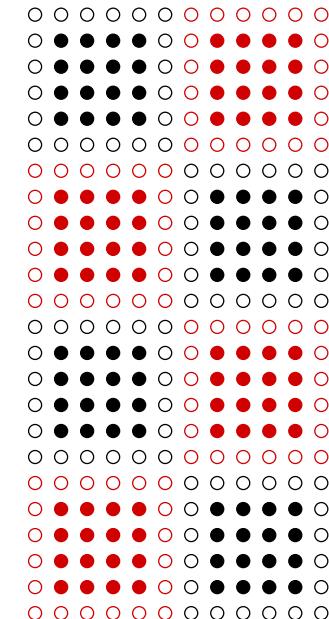
geometric separation of UV and IR modes

$$\begin{aligned} D &= \frac{1}{2} \left\{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - \nabla_\mu^* \nabla_\mu \right\} + m_0 \\ &= D_{\Omega^*} + D_\Omega + D_{\partial\Omega^*} + D_{\partial\Omega} \end{aligned}$$

the quark determinant becomes

$$\det D = \prod_{\text{blocks } \Lambda} \det D_\Lambda \times \det R$$

$$\begin{aligned} R &= 1 - P_{\Omega^*} D_\Omega^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*} \\ R^{-1} &= 1 - P_{\Omega^*} \textcolor{blue}{D^{-1}} D_{\partial\Omega^*} \end{aligned}$$



the pseudo-fermion action

$$S = \sum_{\text{blocks } \Lambda} ||D_\Lambda^{-1} \phi_\Lambda||^2 + ||R^{-1} \phi_R||^2$$

separation of UV and IR modes

molecular dynamics driving force

$$\frac{d}{d\tau} U(x, \mu) = \Pi(x, \mu) U(x, \mu)$$

$$\frac{d}{d\tau} \Pi(x, \mu) = -F_G(x, \mu) - F_\Lambda(x, \mu) - F_R(x, \mu)$$

integration step-sizes

$$\delta\tau_G ||F_G|| \sim \delta\tau_\Lambda ||F_\Lambda|| \sim \delta\tau_R ||F_R||$$

inclusion of strange quark

- **exact PHMC** JLQCD 02
noisy Metropolis test for $\det[D_s P_{N_{\text{poly}}} D_s^{-1}]$ at the end of each traj.
- **UV-filtered PHMC is incorporated in production run**
→ K.Ishikawa's talk for its efficiency(Tue)

§4. 2+1 flavor scaling study with LDDHMC

preliminary study for production run on PACS-CS

1. efficiency of LDDHMC
2. how light quark masses we can go down with LDDHMC
3. CPU-time estimate on PACS-CS

resources

SR11K/J1@CC, Univ. of Tokyo

60.8 Gflops/node peak, 8 nodes shared with other users

parameter choice

RG improved gauge + clover quarks with $c_{\text{SW}}^{\text{NP}}$

lattice spacing $\sim 0.1 \text{ fm}$, lattice size = $16^3 \times 32$

κ is chosen based on the previous CP-PACS/JLQCD results

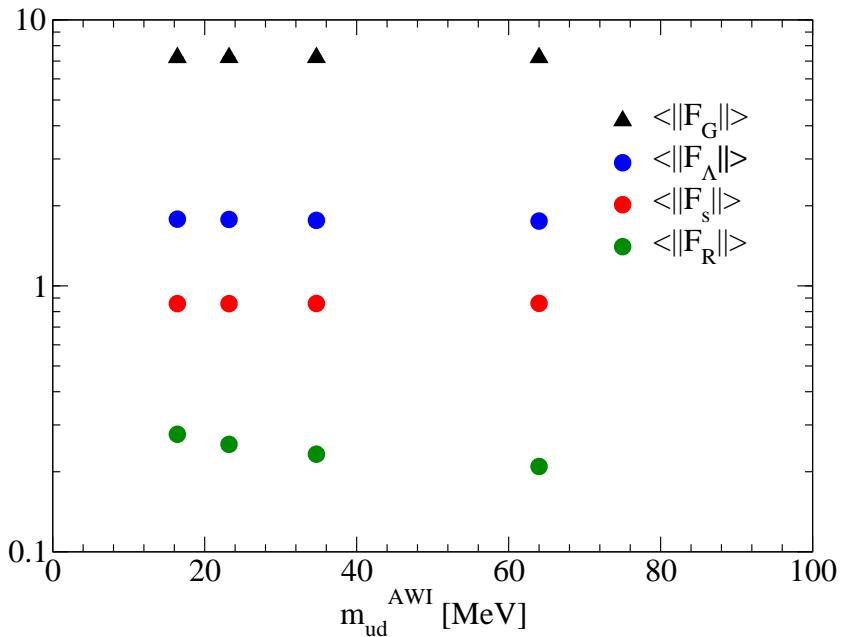
β	κ_s	κ_{ud}	$(m_P/m_V)_{\text{exptd}}$
		0.13700	0.62
1.9	0.1364	0.13741	0.5
	$(\kappa_s^{\text{ph}} = 0.136412(50))$	0.13759	0.4
		0.13770	0.3

simulation details

- $\tau = 0.5/\sqrt{2}$, thermalization=1500-2000 trajs.
- ud quarks: block size= 8^4 , $\delta\tau_\Lambda = \tau/(N_1 N_2)$, $\delta\tau_R = \tau/N_2$
- s quark: polynomial, not domain-decomposed, $\delta\tau_s = \tau/(N_1 N_2)$
- BiCGStab both for force and H
- tolerance: $|\text{residual}|/|\text{source}| \leq \epsilon$, $\epsilon = 10^{-9}(\text{force}), 10^{-14}(H)$

κ_{ud}	0.13700	0.13741	0.13759	0.13770
N_0, N_1, N_2	4,5,6	4,5,8	4,5,12	4,5,14
N_{poly}	130	140	140	140
trajs	2000	2000	2000	900
acc(HMC)	0.88	0.86	0.89	0.86
acc(GMP)	0.94	0.95	0.94	0.93

magnitude of each force term

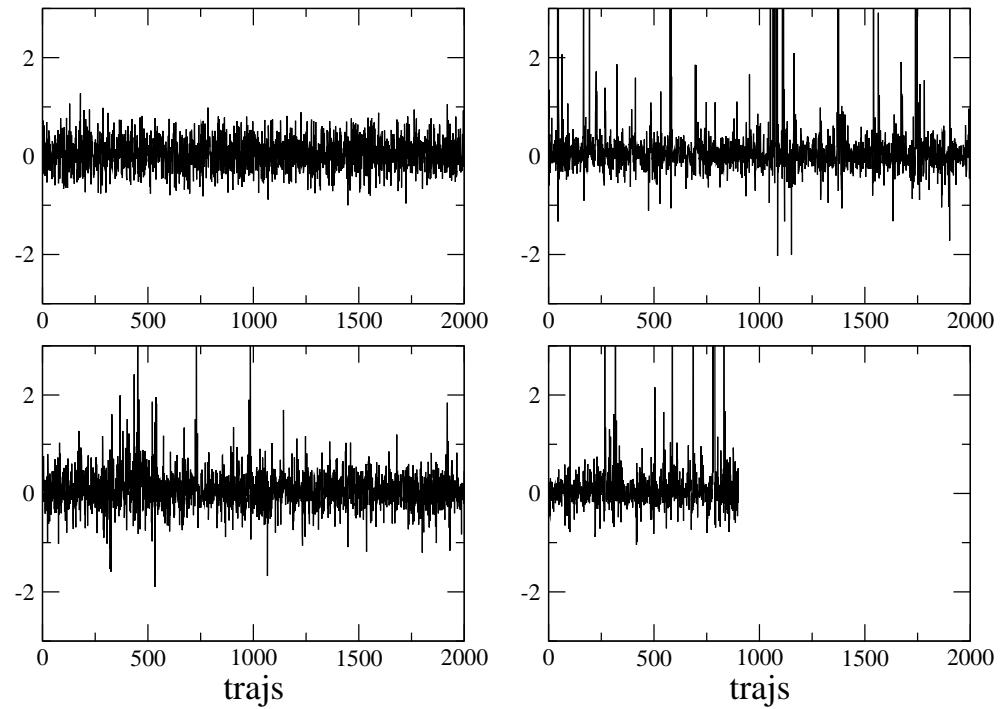


F_G : gauge
 F_Λ : ud quark(UV part)
 F_s : s quark(PHMC)
 F_R : ud quark(IR part)

F_R gradually increases as ud quark mass decreases

$$\|F_G\| : \|F_\Lambda\| : \|F_s\| : \|F_R\| \approx 24 : 6 : 3 : 1 \text{ at } m_{ud}^{AWI} \approx 15 \text{ MeV}$$

history of dH

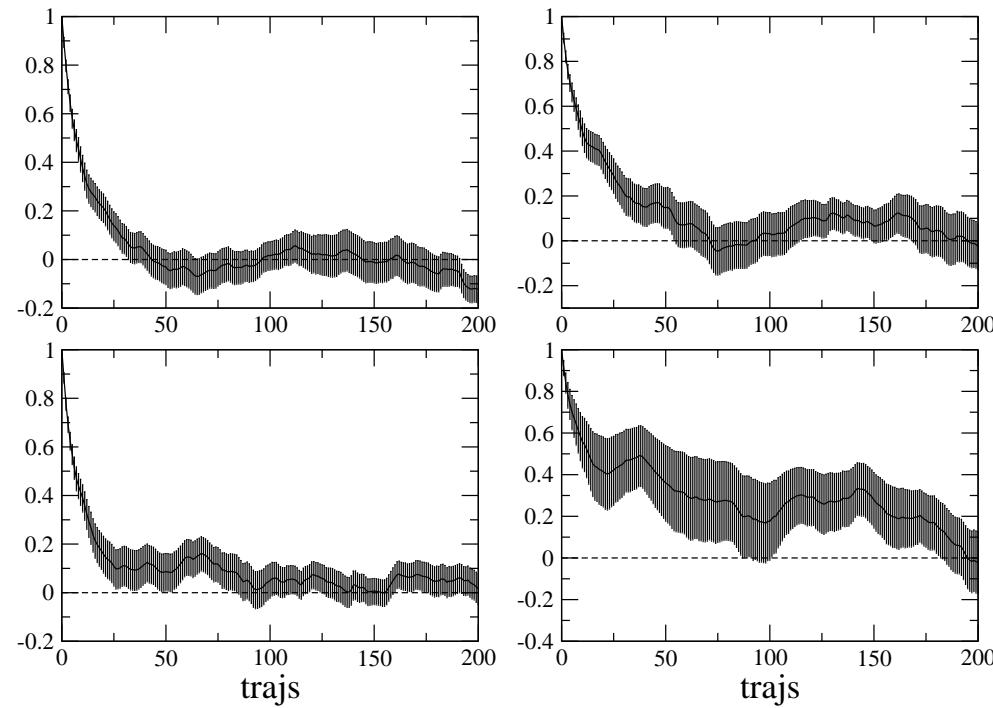


frequency of spike

- less than 2% for $|dH| > 2$
- $\langle e^{-dH} \rangle$ deviates from one by 2σ for $\kappa_{ud} = 0.13759, 0.13770$
- acceptance ratio is sufficiently high
- replay trick is incorporated in production run

κ_{ud}	0.13700	0.13741	0.13759	0.13770
$ dH > 2[\%]$	0	0.2	1.8	1.7
$ dH > 10[\%]$	0	0.05	1.05	0.8
$ dH > 100[\%]$	0	0	0.2	0.3
$\langle e^{-dH} \rangle$	1.003(6)	0.9995(99)	0.9867(92)	0.975(13)
acc(HMC)	0.88	0.86	0.89	0.86

normalized autocorrelation of $\langle P \rangle$



need more statistics for lightest quark mass

comparison of HMC and LDDHMC

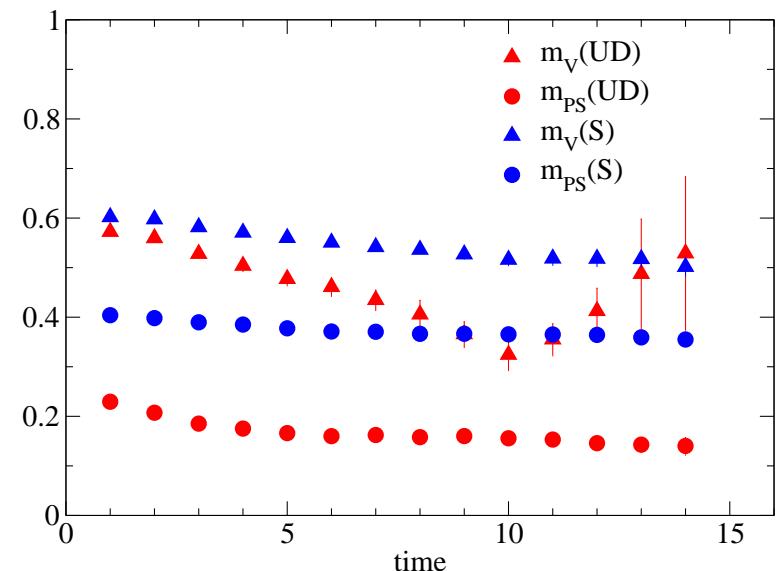
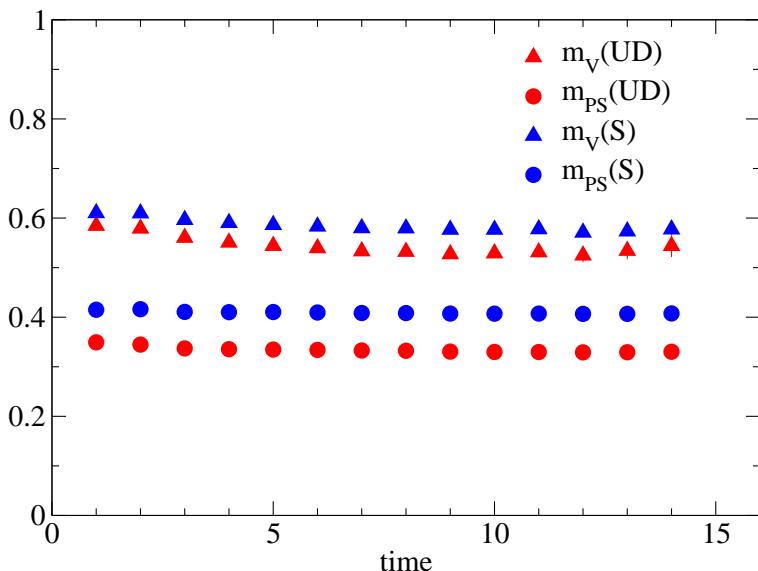
- s quark: exact PHMC
- BiCGStab solver with same tolerances for both algorithms
- $\tau = 1$ for HMC and $\tau = 0.5/\sqrt{2}$ for LDDHMC
measure efficiency by $\tau_{\text{int}}[P] \cdot \#\mathbf{M}_D$

algorithm	κ_{ud}	$\tau_{\text{int}}[P]$	$\#\mathbf{M}_D$	$\tau_{\text{int}}[P] \cdot \#\mathbf{M}_D/10^3$
LDDHMC	0.13700	6.6(1.8)	148625(626)	981(268)
	0.13700	10.6(2.7)	20284(61)	215(55)
	0.13741	16.0(6.6)	31776(171)	508(210)
	0.13759	18.0(6.0)	53403(395)	961(320)

→ LDDHMC is 4–5 times more efficient at $m_{PS}/m_V \approx 0.6$

hadron effective masses

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



hard to extract $m_V(UD)$ in the lightest case

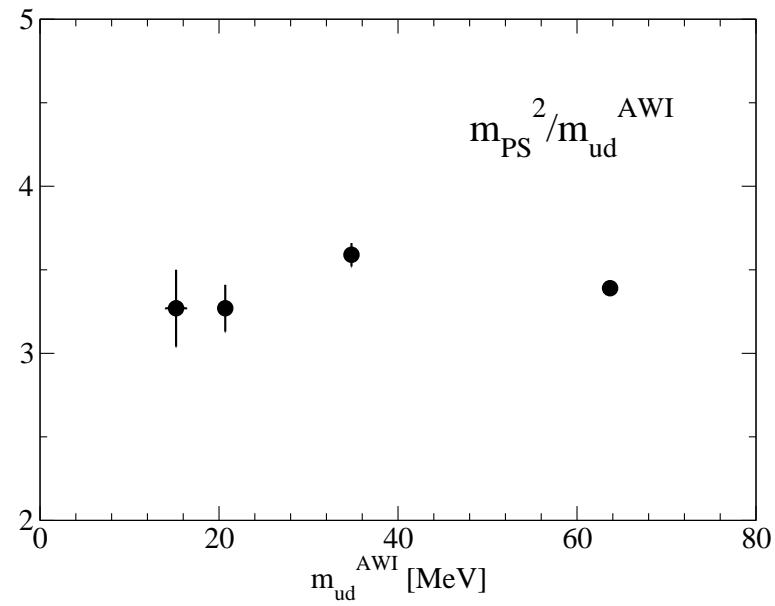
PS meson mass and m_{ud}^{AWI}

κ_{ud}	0.13700	0.13741	0.13759	0.13770
$(m_{PS})_{\text{exptd}}$	0.33	0.23	0.17	0.12
m_{PS}	0.3303(21)	0.2509(29)	0.1851(46)	0.158(8)
$m_{PS} [\text{MeV}]$	655(4)	498(6)	367(9)	313(16)
$m_{ud}^{\text{AWI}} [\text{MeV}]$	63.7(4)	34.8(5)	20.7(5)	15.4(12)

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

m_{PS} at $\kappa_{ud} = 13770$ is much heavier than expected
finite size effect?

check m_{PS}^2/m_{ud}^{AWI}



→ not due to finite size effect, but need more study

§5. CPU-time estimate on PACS-CS

	κ_{ud}	SR11K@CCUT BiCGStab	PACS-CS BiCGStab	SAP+GCR
volume		$16^3 \times 32$		$32^3 \times 64$
sustd. speed		13.8Gflops		4Tflops
days for 10^4 trajs	0.13700	95.8		
	0.13741	146.7		
	0.13759	251.4		
	0.13770	331.7		

– $\beta = 1.9(a \sim 0.1\text{fm})$, $\kappa_s = 0.1364$

§5. CPU-time estimate on PACS-CS

extend the volume to $(3.0\text{fm})^3$ with 10^4 trajs. on PACS-CS

	κ_{ud}	SR11K@CCUT BiCGStab	PACS-CS BiCGStab	SAP+GCR
volume		$16^3 \times 32$		$32^3 \times 64$
sustd. speed		13.8Gflops		4Tflops
days for 10^4 trajs	0.13700	95.8	10.6	
	0.13741	146.7	16.2	
	0.13759	251.4	27.7	
	0.13770	331.7	36.6	

- $\beta = 1.9(a \sim 0.1\text{fm})$, $\kappa_s = 0.1364$
- L^5 dependence assumed

§5. CPU-time estimate on PACS-CS

extend the volume to $(3.0\text{fm})^3$ with 10^4 trajs. on PACS-CS

	κ_{ud}	SR11K@CCUT BiCGStab	PACS-CS BiCGStab	PACS-CS SAP+GCR
volume		$16^3 \times 32$	$32^3 \times 64$	
sustd. speed		13.8Gflops	4Tflops	
days for 10^4 trajs	0.13700	95.8	10.6	8.4
	0.13741	146.7	16.2	11.0
	0.13759	251.4	27.7	18.0
	0.13770	331.7	36.6	19.6

- $\beta = 1.9 (a \sim 0.1\text{fm}), \kappa_s = 0.1364$
- L^5 dependence assumed
- SAP+GCR to BiCGStab acceleration factor is 3 (Lüscher 03)

§6. Parameter choice for production run on PACS-CS

algorithm

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

parameters

- $\beta = 1.83(0.12\text{fm}), 1.90(0.10\text{fm}), 2.05(0.07\text{fm})$
- lattice spatial volume: $(3.0\text{fm})^3$
 $24^3 \times 48(\beta = 1.83), 32^3 \times 64(\beta = 1.9), 40^3 \times 80(\beta = 2.05)$
- $m_{ud}^{\text{AWI}} = 7, 15, 25, 35, 45, 65\text{MeV}$
15MeV is reached in this study
- two strange quark masses
- 10^4 trajs. for 100 indep. cfgs.

physics plan on PACS-CS

– light hadron spectrum including baryon

small chiral extrapolation from 7MeV to m_{ud}^{ph}

→ independent of extrapolation functions(ChPT, poly., etc.)

– heavy quark physics with the relativistic heavy quark action

– quark masses with nonperturbative renormalization

Schrödinger functional method(under way)

– physics associated with topology

η' meson mass, NEDM

– hadron matrix elements

heavy-light, light-light meson weak matrix elements

σ -term, proton decay, g_A

– hadron-hadron interactions

$I = 0$ $\pi\text{-}\pi$ scattering, ρ resonance

§7. Summary

2+1 flavor scaling study with LDDHMC

- factor 4–5 acceleration at $m_{\text{PS}}/m_V \approx 0.6$
- $m_{\text{ud}}^{\text{AWI}} \approx 15\text{MeV}$ reached

target of PACS-CS project

- three β values, $(3.0\text{fm})^3$, 10^4 trajs.
- go down to $m_{\text{ud}}^{\text{AWI}} = 7\text{MeV}$

the production run will start after this conference
details of machine performance and present status
→ Ukawa's talk(Tue)