PACS-CS Project
and
HPCI Strategic Field Program

CCS at U. Tsukuba / RIKEN AICS

Yoshinobu Kuramashi

Plan of talk

§1. PACS-CS Project
§2. Construction of Nuclei
§3. Algorithmic Improvements
§4. HPCI Strategic Field Program
§5. Summary

§1. PACS-CS Project

Machine	2008	2009	2010	2011	2012	2013	2014
PACS-CS (PC-cluster, 14TF) 	Jul. 2006～						
T2K-Tsukuba (PC-cluster, 95TF) 					～Feb. 2014		
HA-PACS (GPU-cluster, 0.8PF) 						+364TF/TCA from fall of 2013	
COMA (MIC-cluster, 1PF) Photo is not yet available							Apr. 2014～

Collaboration members

Physicists:

S.Aoki, N.Ishizuka, D.Kadoh(→KEK), K.Kanaya, Y.Kuramashi, Y.Nakamura(→AICS), Y.Namekawa, Y.Taniguchi, N.Ukita, A.Ukawa, T.Yamazaki(→Nagoya), T.Yoshie	Tsukuba
K.-I. Ishikawa, M.Okawa	Hiroshima
T.Izubuchi	BNL

Computer scientists:

T.Boku, M.Sato, D.Takahashi, Otatebe T.Sakurai, H.Tadano	Tsukuba

Science Target

2+1 flavor QCD simulation at the physical point

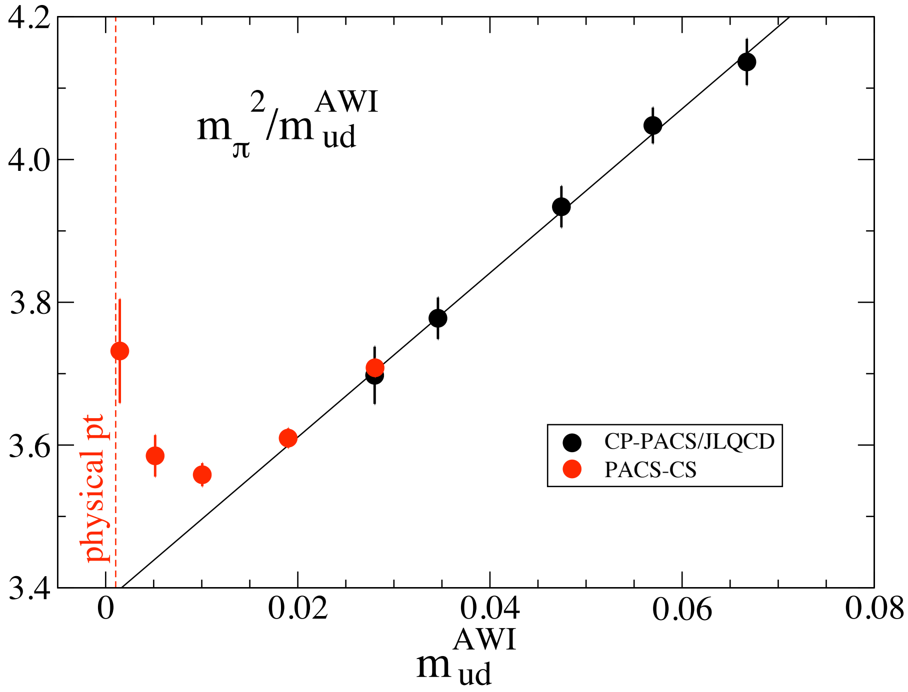
	PACS-CS	CP-PACS/JLQCD
Gauge action	Iwasaki	Iwasaki
Quark action	clover with NP c_{SW}	clover with NP c_{SW}
Lattice spacing a[fm]	$\lesssim$0.1	0.07, 0.1, 0.122
Physical volume	$\gtrsim$(3 fm)3	~(2 fm)3
m_{ud}	physical point	64 MeV ($m_\pi \approx$700 MeV)
Algorithm for ud	DDHMC with some improvements	HMC
Algorithm for s	UV-filtered exact PHMC	exact PHMC

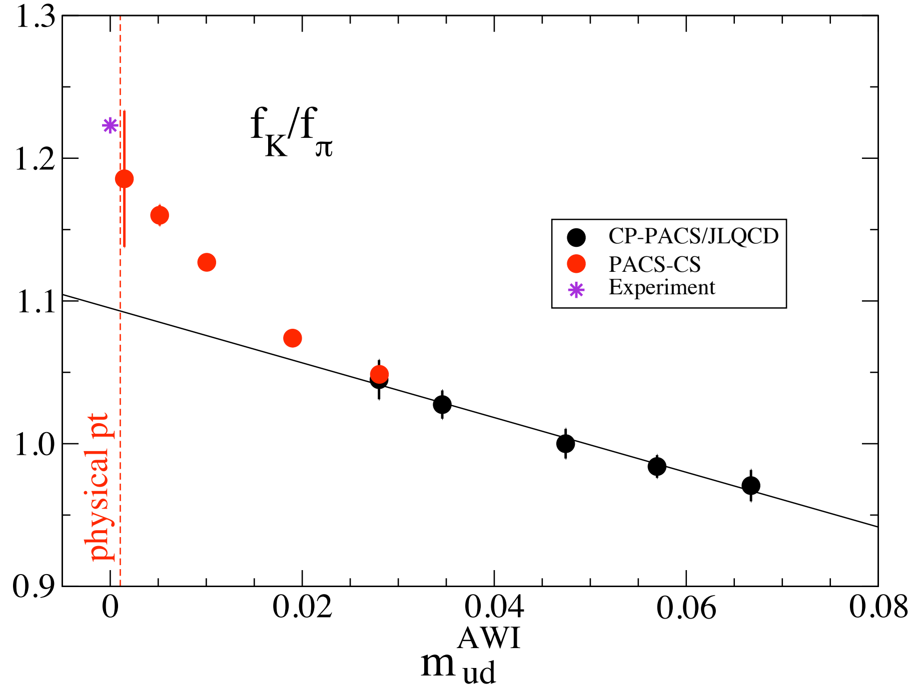
Why physical point simulation?

In my slide @ CERN TH Institute 2010

- Difficult to trace chiral logs for chiral extrapolation
- ChPT is not always a good guiding principle
- Direct treatment of resonances based on phase shift
- Simulations with different up and down quark masses

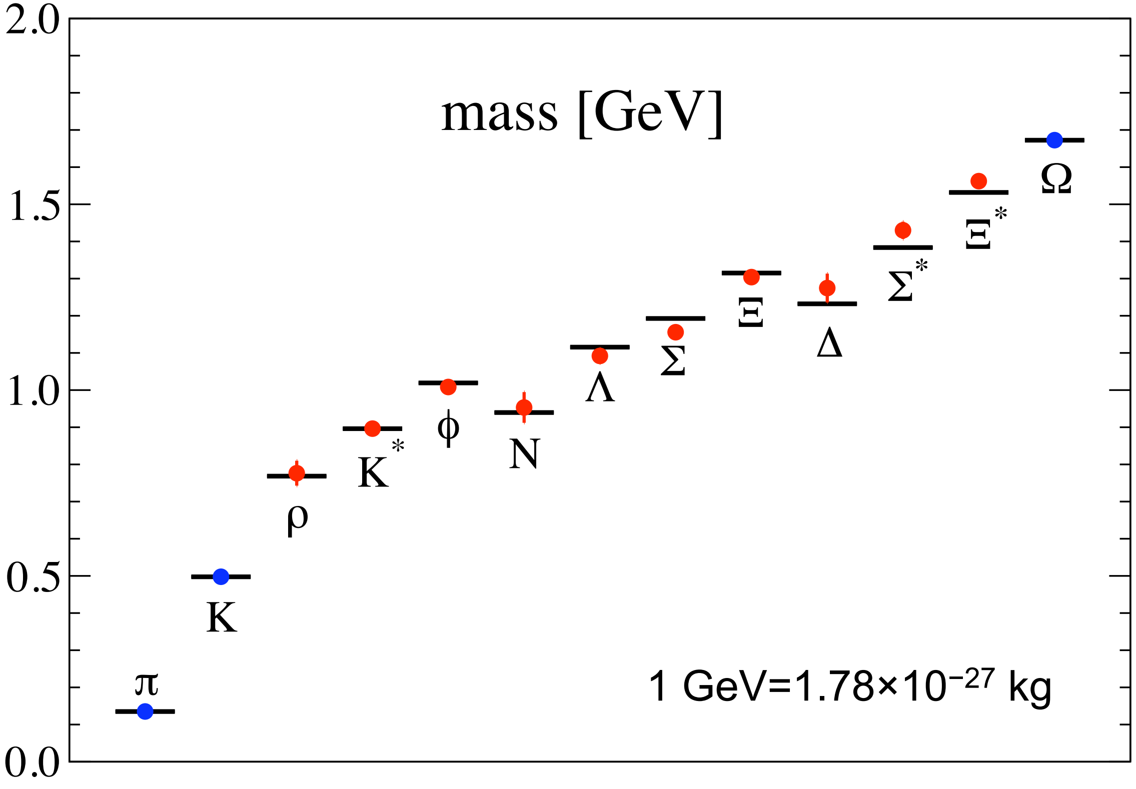
Chiral Behavior





Expected curvature from ChPT ⇒ Determination of LECs of SU(2) ChPT

Hadron masses in 2+1 Flavor QCD



PACS-CS 09

physical input

m_π, m_K, m_Ω

⇩

$m_u=m_d$, m_s, a

consistent within 2～3% error bars

What's Next?

Science target for post PACS-CS (T2K & K computer)

- 1+1+1($m_u \neq m_d \neq m_s$) flavor QCD+QED simulation
  - EM interactions
  - u-d quark mass defference

Multi-physics toward precision measurement

$K^0(d\bar{s})$ 497.6MeV

1%

$K^+(u\bar{s})$ 493.7MeV

- Hadron-Hadron interactions
  - Resonances（$\rho \rightarrow \pi\pi$ decay etc.）
  - Nuclei based on QCD

Multi-scale physics from quarks to nuclei

1+1+1 flavor QCD+QED

PACS-CS 12

Isospin symmetry breaking

- EM interaction

  $Q_u=+2/3e$, $Q_d=Q_s=-1/3e$, $e=\sqrt{4\pi/137}$

- u-d quark mass difference

  $m_u=m_d\neq m_s$ (2+1フレーバー) $\Rightarrow$ $m_u\neq m_d\neq m_s$ (1+1+1フレーバー)

Physical input:

$m_{\pi+}$(ud), m_{K0}(ds), m_{K+}(us), $m_{\Omega-}$(sss)

Output:

m_u, m_d, m_s, lattice spacing, …

2+1 flavor QCD generation around the physical point → (reweighting method) → 1+1+1flavor QCD+QED on the physical point

K^0-K^+ mass difference

PACS-CS 12

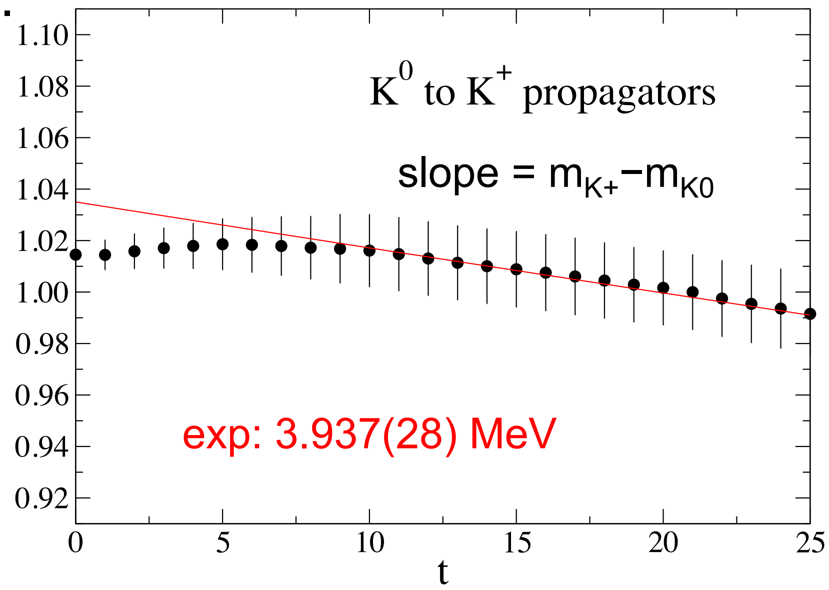
EM interaction + u-d quark mass diff.
⇒ diff. of $m_{K0}(ds)$ and $m_{K+}(us)$

$K^0(d\bar{s})$ 497.6MeV

1%

$K^+(u\bar{s})$ 493.7MeV

lattice size=$32^3 \times 64$, a ~ 0.1 fm



$$\frac{\langle K^0(t)K^0(0)\rangle}{\langle K^+(t)K^+(0)\rangle} \simeq Z\left(1 - \underbrace{(m_{K^0} - m_{K^+})t}_{\text{much smaller than 1}}\right)$$

Slope is consistent with exp. value 3.937(28) MeV within error bars

u, d, s quark masses

PACS-CS 12

Physical input:

$m_{\pi+}$(ud)=139.7(15.5) [MeV] exp: 139.6 [MeV]
m_{K0}(ds)=497.6(8.1) [MeV] exp: 497.6 [MeV]
m_{K+}(us)=492.4(8.1) [MeV] exp: 493.7 [MeV]
m_{Ω}(sss) is fixed at exp. value exp: 1672.5 [MeV]

Quark masses (MSbar scheme at μ=2 GeV):

m_u=2.57(26)(07) [MeV]
m_d=3.68(29)(10) [MeV]
m_s=83.60(58)(2.23) [MeV]

Sizable finite size effects are expected in QCD+QED simulation

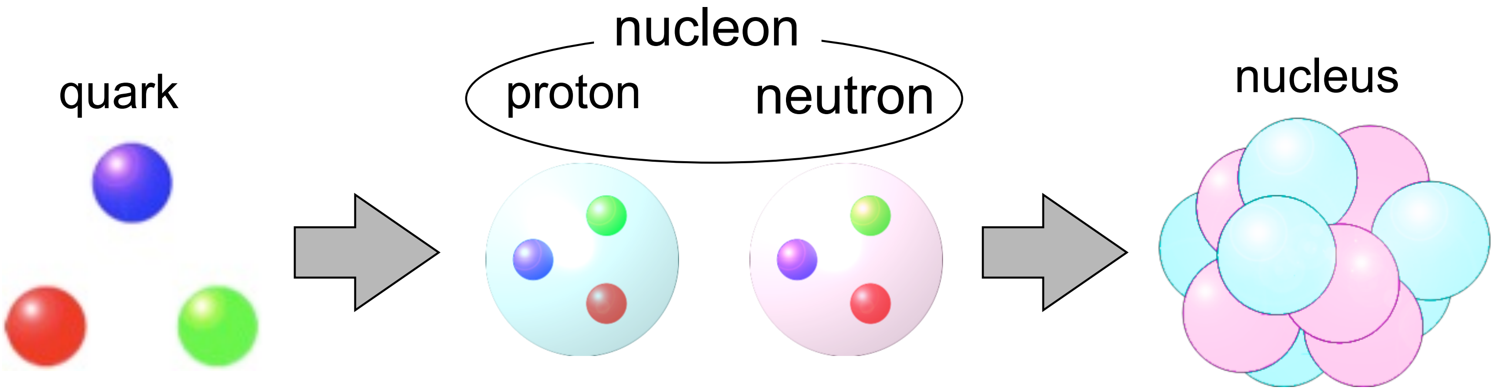
π meson mass(140MeV)@QCD ⇔ photon(massless)@QED

⇒ Simulation with much larger lattice size on K computer
Also useful for calculation of light nuclei and nuclear force

§2. Construction of Nuclei

We are now achieving a precision measurement of hadron masses

Next step is a challenge for multi-scale physics



Exploratory study for ^{4}He and ^{3}He nuclei   Yamazaki-YK-Ukawa 10,12

$$\langle \mathcal{O}_{^4\mathrm{He}}(t)\mathcal{O}^\dagger_{^4\mathrm{He}}(0)\rangle \overset{t\gg 0}{\approx} C\exp\left(-m_{^4\mathrm{He}}t\right)$$

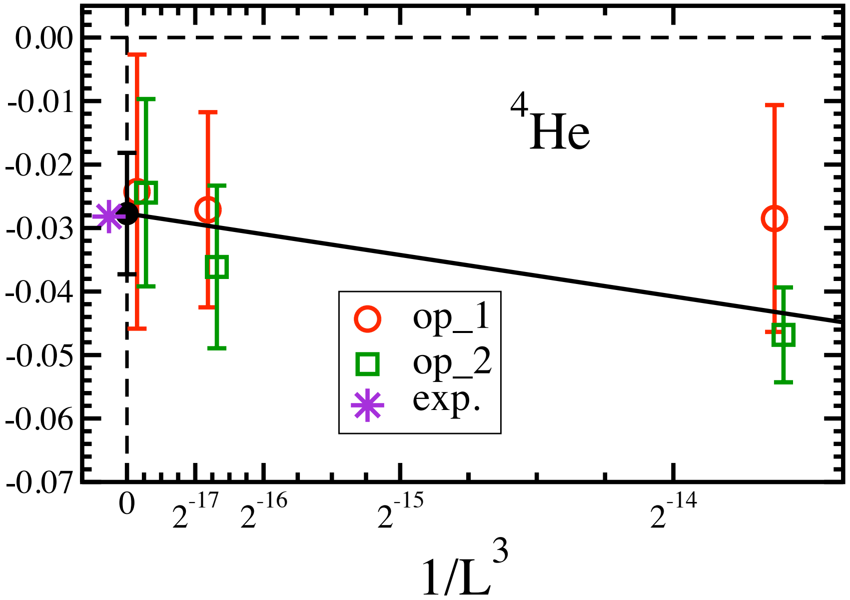
^{4}He: 2 proton+2 neutron ⇒ 12 quark propagators

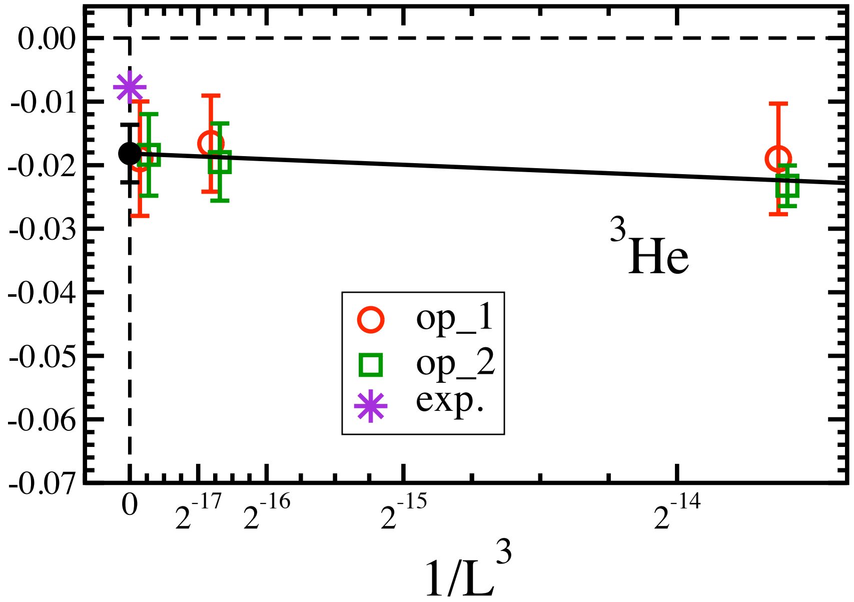
^{3}He: 2 proton+1 neutron ⇒ 9 quark propagators

Exploratory Study in Quenched QCD

Yamazaki-YK-Ukawa 10

m_π=0.8 GeV, m_N=1.6 GeV in quenched QCD
(Real world: m_N=0.94 GeV)





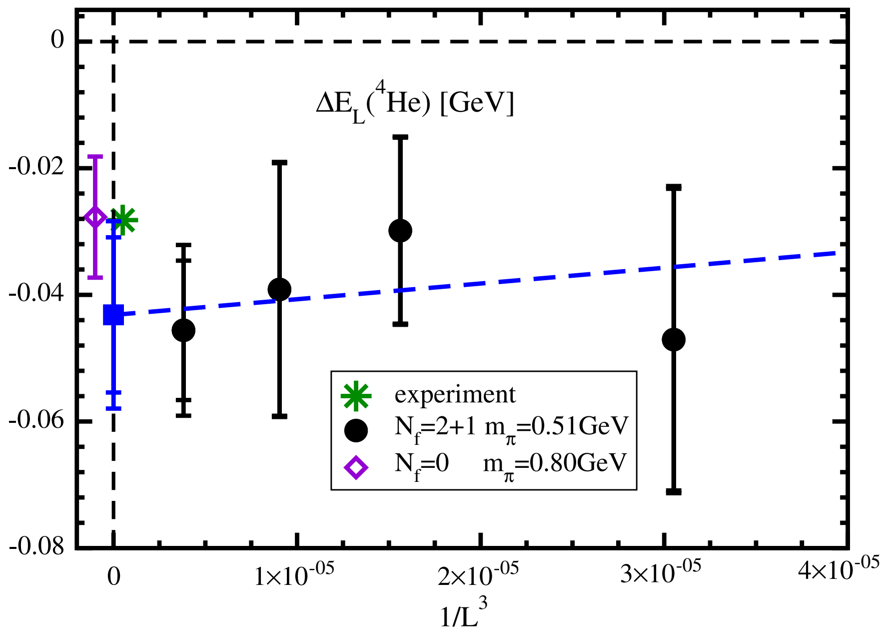
First successful construction of helium nuclei
⇒ 2+1 flavor QCD with lighter quark masses

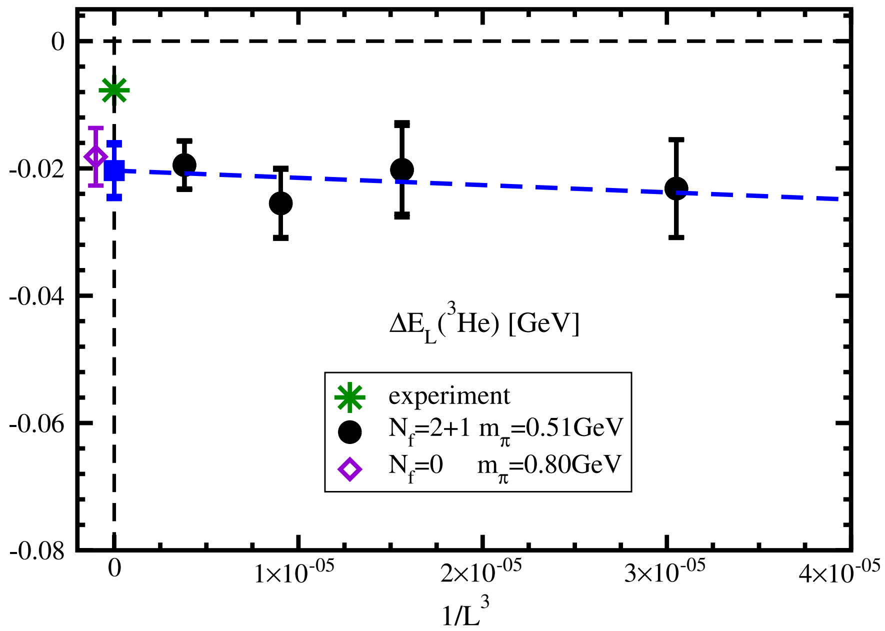
He Nuclei in 2+1 Flavor QCD

Yamazaki-YK-Ukawa 12

2+1 flavor QCD, m_π=0.5 GeV (0.14 GeV in nature), m_N=1.32 GeV

$$\Delta E_{^4\mathrm{He}} = m_{^4\mathrm{He}} - 4m_N$$





ΔE remains finite in the infinite volume limit

Successful construction of helium nuclei in 2+1 flavor QCD

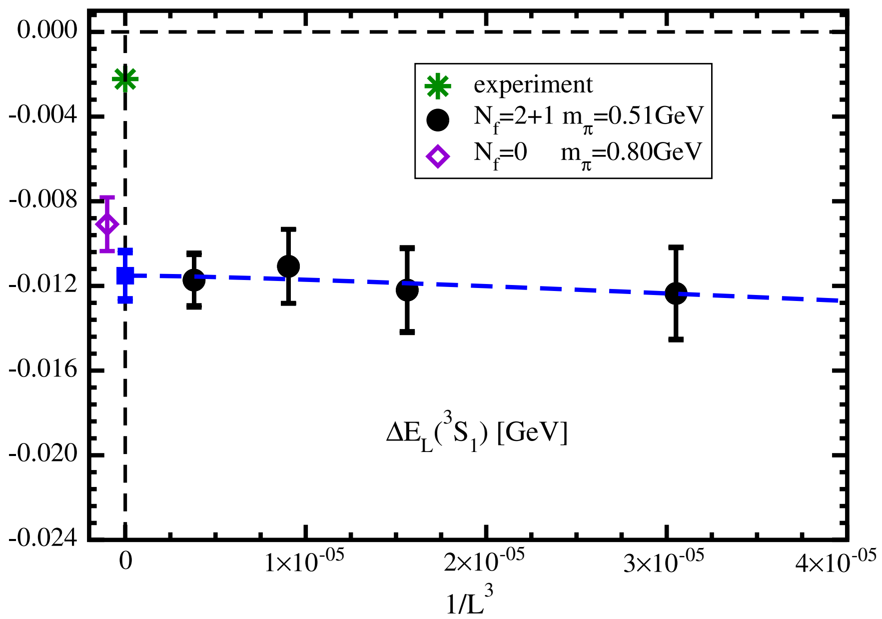
NN Systems in 2+1 Flavor QCD

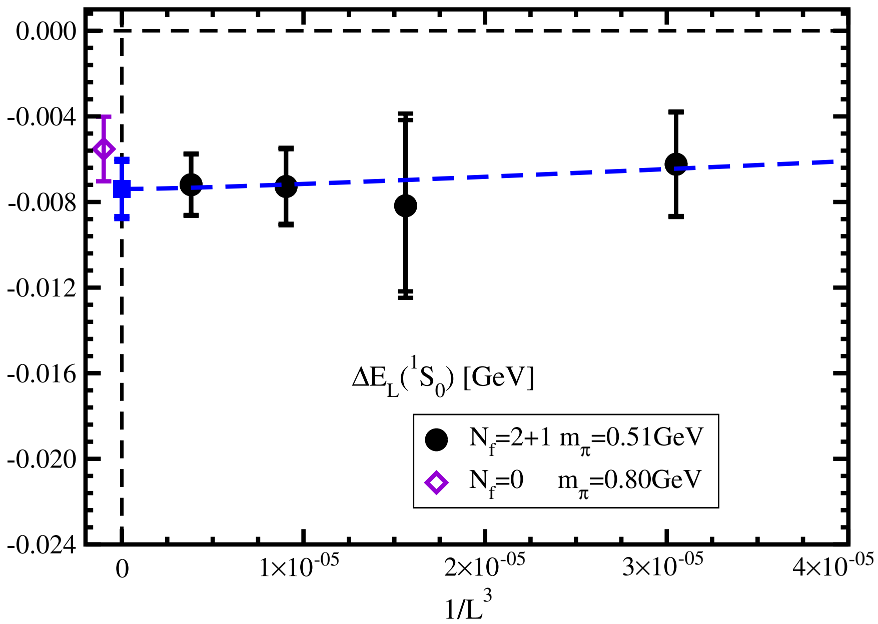
Yamazaki-YK-Ukawa 12

Results obtained in parallel with He calculation
on the same configs

$$NN_{^3S_1}(t) = \frac{1}{\sqrt{2}}[p_+(t)n_+(t) - n_+(t)p_+(t)]$$

$$NN_{^1S_0}(t) = \frac{1}{\sqrt{2}}[p_+(t)p_-(t) - p_-(t)p_+(t)]$$

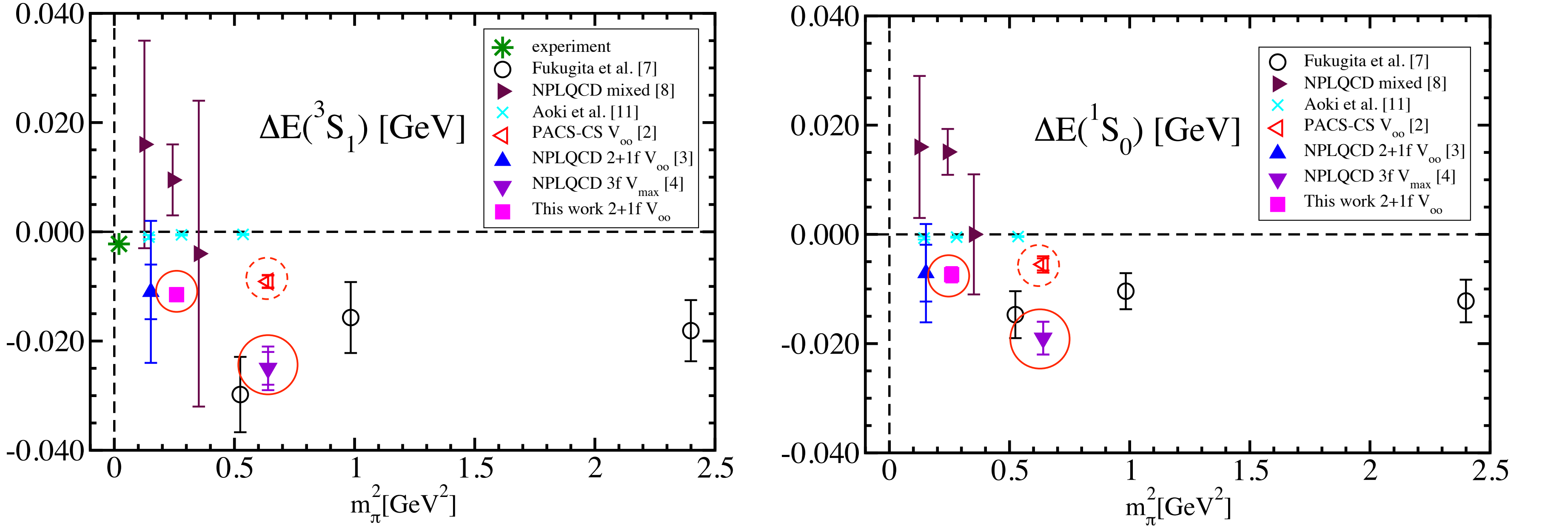




$^1S_0$ channel is also bound ⇔ $^1S_0$ is scattering state in nature

Current Summary for NN Systems

Both $^3S_1$ and $^1S_0$ channels are bound at heavy quark region



$|\Delta E(^3S_1)| > |\Delta E(^1S_0)|$ is suggestive
Important to check quark mass dependence

Target on K computer: construction of nuclei at the physical point

§3. Algorithmic Improvements

Trend of architecture

- PC cluster, multi-core, GPU, …
  - hierarchical parallel structure
  - diminishing B/F

Algorithmic improvements following the architecture trend

- Key points:
  - use of mixed precision
  - reduction of communication

PACS-CS (06～11)

⇒

Mixed precision nested BiCGStab
Modified blocked BiCGStab
Domain-Decomposed HMC(DDHMC)

Developed on PACS-CS and T2K-Tsukuba

T2K-Tsukuba (08～14)

Solver Improvement

Bottle neck for iterative solver of linear eqs.

memory bandwidth

Byte/Flop ≈ 2.1 in MatVec Dx

Advantage in 32bit arithmetic is effective use of

- memory and network bandwidth
- cache size

Maximum use of 32bit arithmetic with the solution kept in 64bit

iterative refinement

1: x:initial guess	(64bit)
2: $r = b - Dx$	(64bit)
3: convert $r_{32} := r$	(64bit $\rightarrow$ 32bit)
4: solve $\delta x_{32} = D^{-1} r_{32}$	(32bit)
5: convert $\delta x := \delta x_{32}$	(32bit $\rightarrow$ 64bit)
6: $r = r - D\delta x$	(64bit)
7: $x = x + \delta x$	(64bit)
8: if $\lvert r \rvert$ is small end else goto 3	

the relation $r = b - Dx$ is kept in 64bit

Mixed Precision Nested BiCGStab

Based on $DMy = b$, $x = My$

x:initial guess, $M \approx D^{-1}$:32bit-preconditioner

$r = b - Dx$, $\tilde{r} = r$, $\rho_0 = |r|^2$, $p = r$

loop

$\nu = Mp$, $q = D\nu$, $\alpha = \rho_0 / \langle \tilde{r} | q \rangle$

$r = r - \alpha q$, $x = x + \alpha \nu$, if $|r|$ is small exit

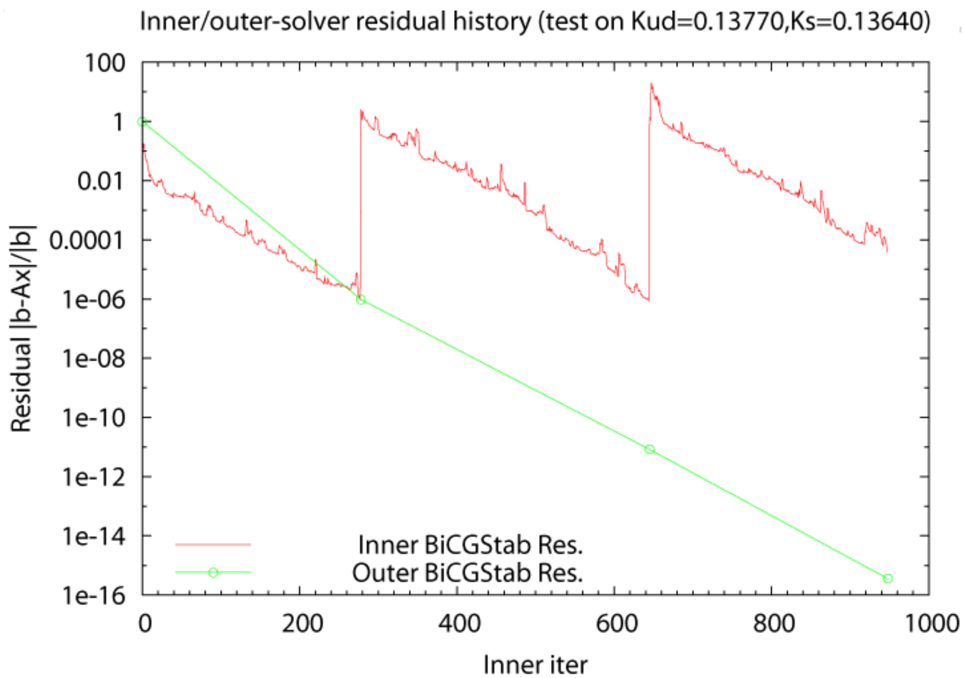
$\nu = Mr$, $t = D\nu$, $\omega = \langle t | r \rangle / \langle t | t \rangle$

$r = r - \omega t$, $x = x + \omega \nu$, if $|r|$ is small exit

$\rho_1 = \langle \tilde{r} | r \rangle$, $\beta = (\alpha/\omega)(\rho_1/\rho_0)$, $\rho_0 = \rho_1$

$p = r + \beta(p - \omega q)$

end loop



- Converged after 1.5 outer iteration
- Almost all the computational cost is spent by 32bit arithmetic
- Time is reduced by a factor 2 on PACS-CS（though, iteration number is slightly increased）

Modified Block BiCGStab (1)

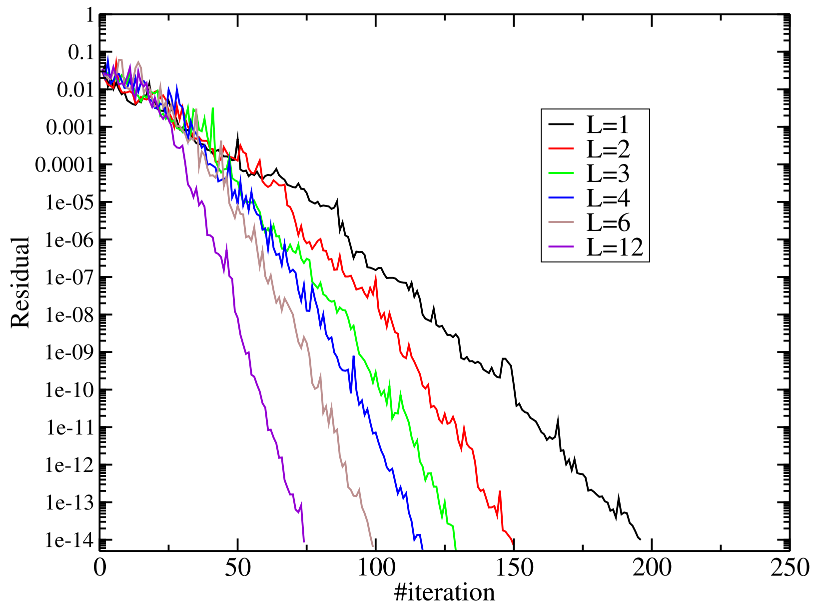
A solver algorithm for linear eqs with multiple right-hand sides

$Dx^{(i)}=b^{(i)}$ (i=1,…,L) ⇒ DX=B

Nakamura et al. 12

1 **initial guess** $X \in \mathbb{C}^{N \times L}$
2 $R = B - AX$
3 $P = R$
4 **choose** $\tilde{R} \in \mathbb{C}^{N \times L}$
while $\max_i(|\boldsymbol{r}^{(i)}|/|\boldsymbol{b}^{(i)}|) \leqslant \epsilon$
do {
4.1 **QR decomposition** $P = Q\gamma, \ P \leftarrow Q$
4.2 $U = MP$
4.3 $V = AU$
4.4 **solve**$(\tilde{R}^H V)\alpha = \tilde{R}^H R$ **for** α
4.5 $T = R - V\alpha$
4.6 $S = MT$
4.7 $Z = AS$
4.8 $\zeta = \mathrm{Tr}(Z_k^H T_k)/\mathrm{Tr}(Z_k^H Z_k)$
4.9 $X \leftarrow X + U\alpha + \zeta S$
4.10 $R = T - \zeta Z$
4.11 **solve**$(\tilde{R}^H V)\beta = -\tilde{R}^H Z$ **for** β
4.12 $P \leftarrow R + (P - \zeta V)\beta$
}
5 **return** (X)

2+1 flavor QCD, $32^3 \times 64$, a∼0.1fm, (κ_{ud},κ_s)=(0.137785,0.13660), point source



Basic idea: blocked version searches the solution vectors with the enlarged Krylov subspace

Modified Block BiCGStab (2)

Performance test on T2K-Tsukuba using 10 configs
$Dx^{(i)}=b^{(i)}$ (i=1,…,12)

$L \times 12/L$	Time [s]	T (gain)	NMVM	NM (gain)
1×12	3827 (755)	1	17 146 (3326)	1
2×6	2066 (224)	1.9	12 942 (1379)	1.3
3×4	1619 (129)	2.4	10652 (832)	1.6
4×3	1145 (99)	3.3	9343 (835)	1.8
6×2	1040 (87)	3.7	7888 (663)	2.2
12×1	705 (70)	5.4	6106 (633)	2.8

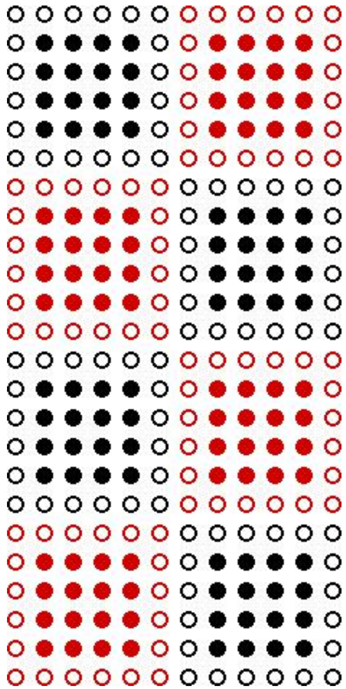
T(gain) > NM(gain) is thanks to effective use of cache

Improvement of Molecular Dynamics

Domain-Decomposed Hybrid Monte Carlo (DDHMC) Lüscher 03

4-dim. lattice is decomposed into small blocks

⇒ introduction of hierarchy



$$\frac{d}{d\tau}P_\mu(n,\tau) = -\frac{\delta\mathcal{H}_{\mathrm{HMC}}}{\delta U_\mu(n,\tau)}$$
$$= F_\mu^{\mathrm{UV}}(n,\tau) + F_\mu^{\mathrm{IR}}(n,\tau) + \cdots$$

domain (single core) — full lattice (many nodes)

F_μ^{UV}: $x = (D_{\mathrm{UV}}[U_\mu])^{-1} b$ within domain

⇒ small condition number w/o communication

F_μ^{IR} : $x = (D_{\mathrm{IR}}[U_\mu])^{-1} b$ on full lattice

⇒ large condition number w/ communication

Multiple Time Step MD Integrator

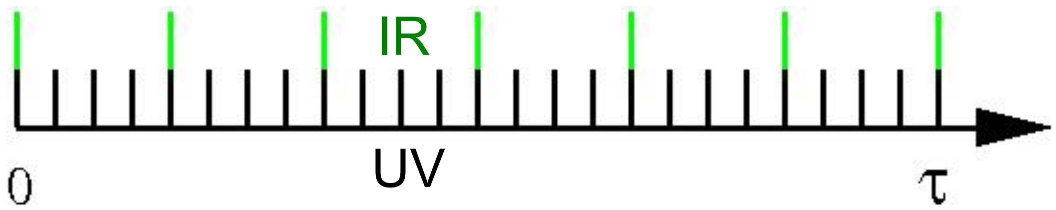
Sexton-Weingarten 92

Adjust step size according to the magnitude of force

$$\delta\tau^{\mathrm{UV}}||F_\mu^{\mathrm{UV}}|| \approx \delta\tau^{\mathrm{IR}}||F_\mu^{\mathrm{IR}}||$$

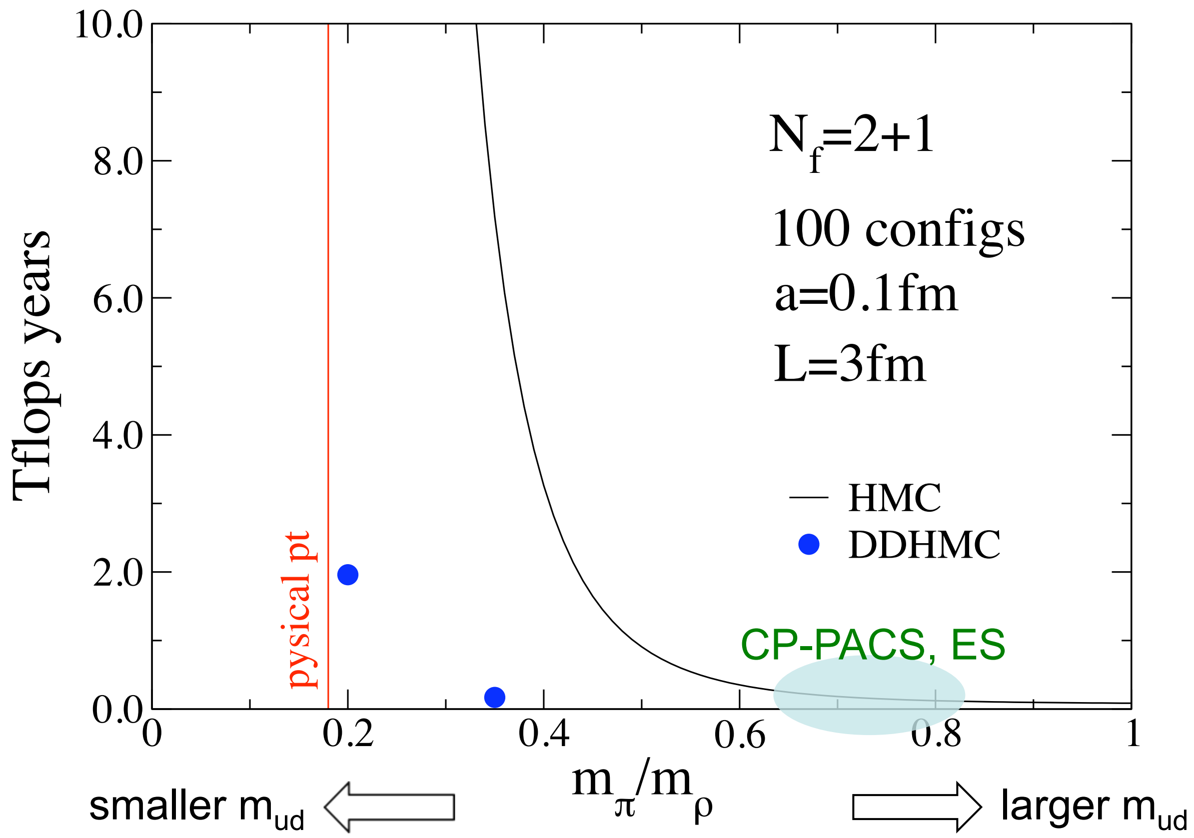
For example

$$||F_\mu^{\mathrm{UV}}|| \ : \ ||F_\mu^{\mathrm{IR}}|| = 4 \ : \ 1 \quad \Rightarrow \quad \delta\tau^{\mathrm{UV}} \ : \ \delta\tau^{\mathrm{IR}} = 1 \ : \ 4$$



Less frequent calculation of F_μ^{IR} ⇒ save computational cost

Cost Reduction due to DDHMC

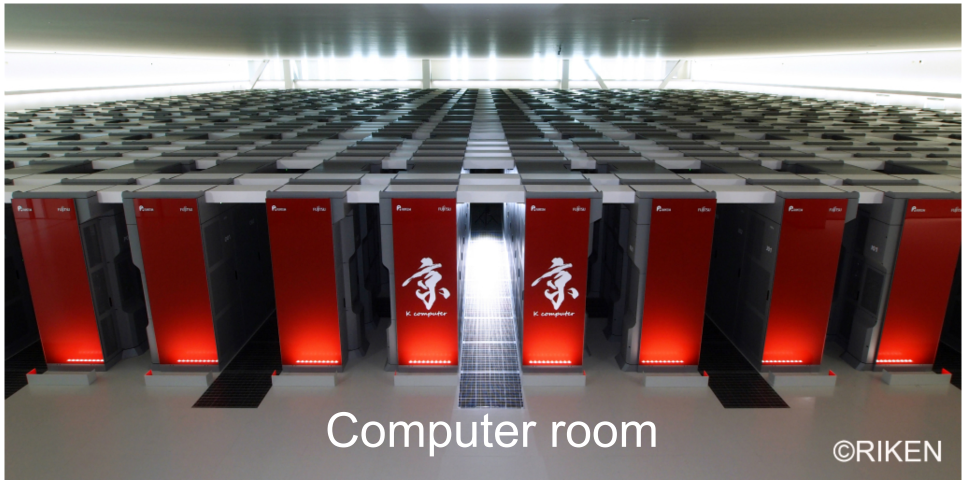


⇒ Physical point simulation is possible on PACS-CS and T2K-Tsukuba

§4. HPCI Strategic Field Program

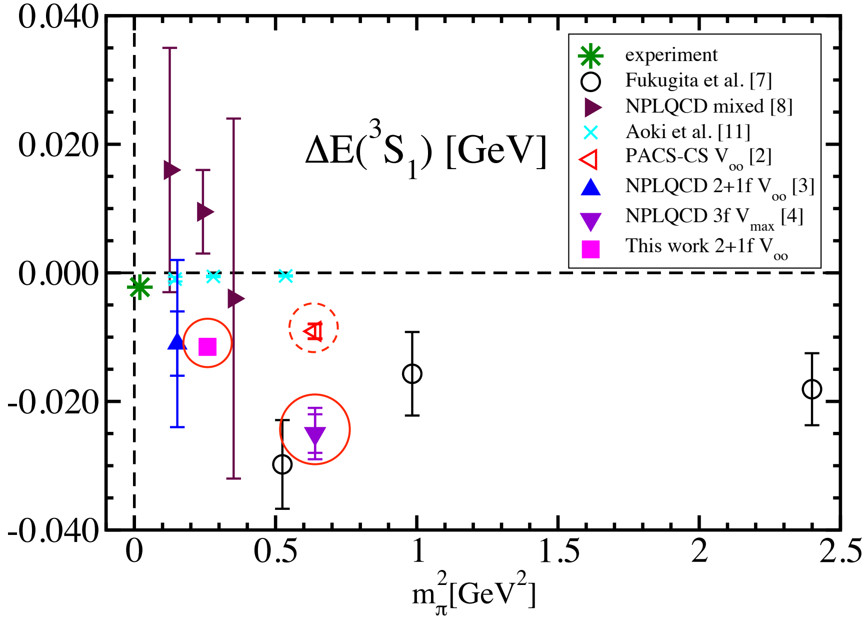
Scientific target

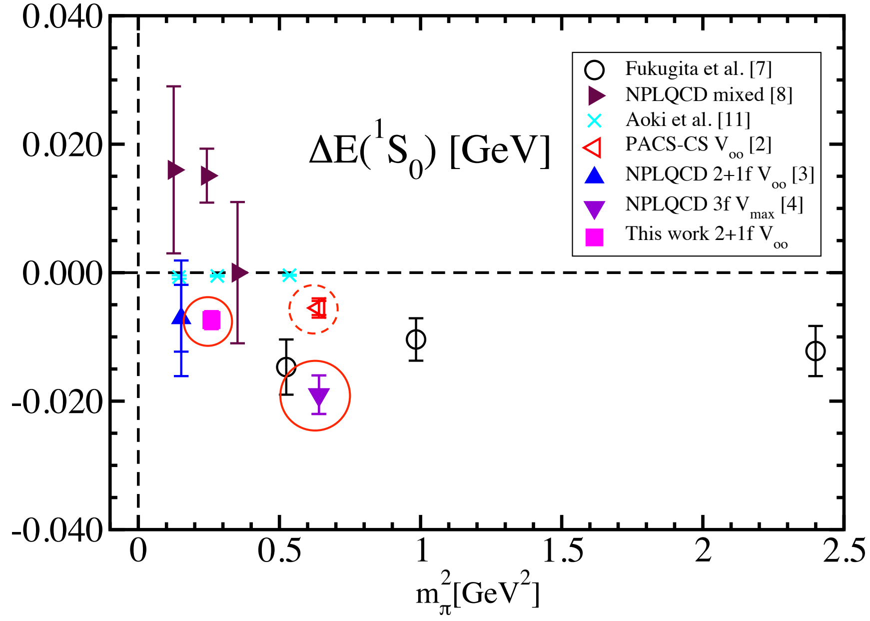
- 2+1 flavor QCD ⇒ 1+1+1 flavor QCD+QED
- Various physical quantities
- Investigation of resonances
- Direct construction of light nuclei
- Determination of baryon-baryon potentials



Current Summary for NN Systems (Reminder)

Both $^3S_1$ and $^1S_0$ channels are bound at heavy quark region





$|\Delta E(^3S_1)| > |\Delta E(^1S_0)|$ is suggestive

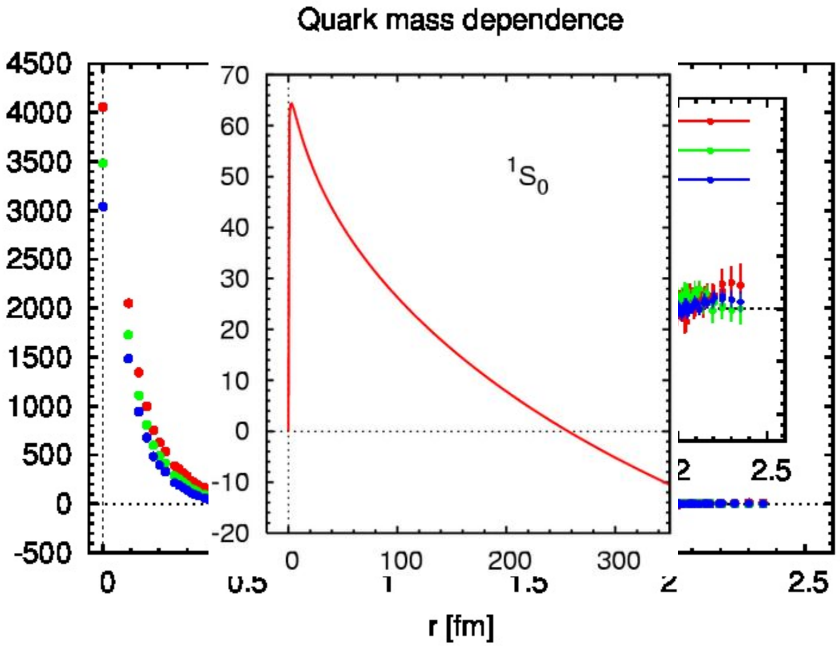
Important to check quark mass dependence

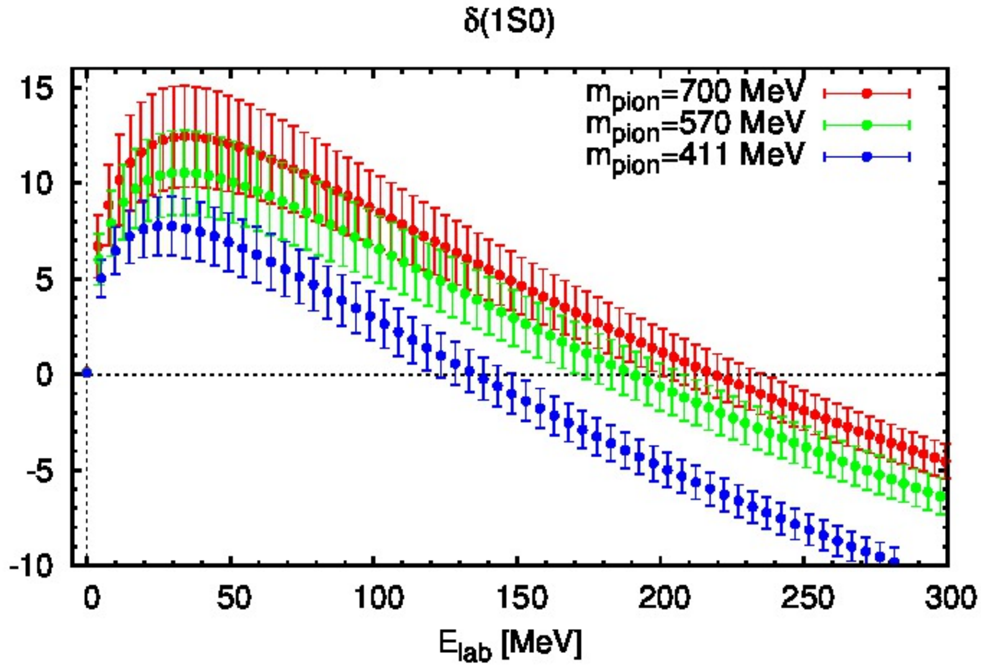
Target on K computer: construction of nuclei at the physical point

Baryon-Baryon Potentials

HAL-QCD @FB12

2+1 flavor QCD, lattice size=$32^3 \times 64$, m_π＝0.70, 0.57, 0.41 GeV





Attractive phase shift, though the magnitude is just 10% of exp. Value

No bound state (He, NN) ⇔ inconsistency against the direct method

Phase shift becomes smaller, as quark mass decreases

⇒ need direct comparison with exp. values at the physical point

Collaboration members

N.Ishii, N.Ishizuka, Y.Kuramashi, Y.Namekawa, H.Nemura, K.Sasaki, Y.Taniguchi, N.Ukita	Tsukuba
T.Hatsuda, T.Doi	RIKEN-Wako
T.Yamazaki	Nagoya
S.Aoki	Kyoto
Y.Nakamura	RIKEN-AICS
K.-I.Ishikawa	Hiroshima

HAL QCD Collab. joins to determine baryon-baryon potential

Simulation Parameters

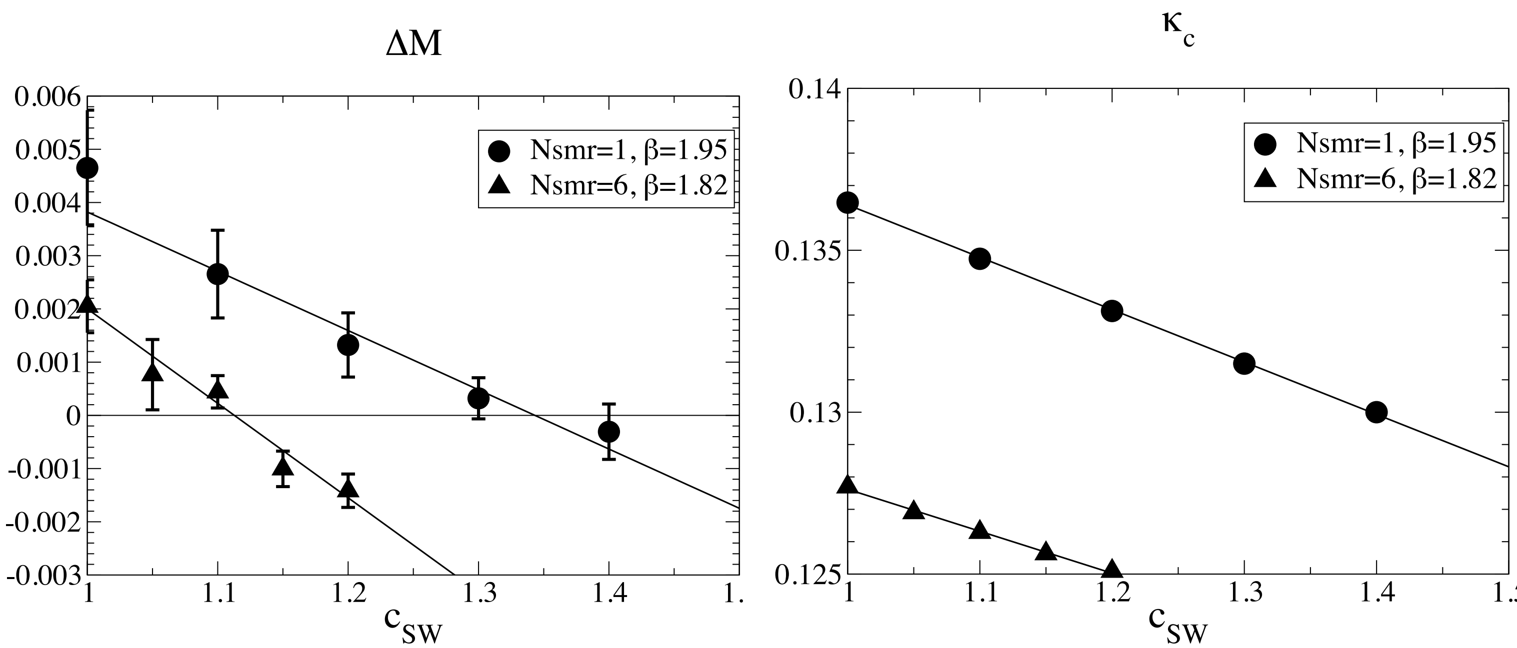
- 2+1 flavor QCD
- Wilson-clover quark action + Iwasaki gauge action
- Stout smearing with α=0.1 and N_{smear}=6
- NP C_{SW}=1.11 determined by SF
- β=1.82 ⇒ a∼0.1 fm
- Lattice size=96^4 ⇒ $(\sim 9\ \mathrm{fm})^4$
- Hopping parameters: (κ_{ud},κ_s)=(0.126117,0.124790)
- Simulation algorithm
  - $(HB)^2$DDHMC w/ active link for ud quarks, UVPHMC for s quark
  - Block size=12^4 ⇒ $(\sim 1\ \mathrm{fm})^4$
  - HB parameters: (ρ_1,ρ_2)=(0.99975,0.9940)
  - Multi-time scale integrator: (N_1,N_2,N_3,N_4,N_5)=(15,2,2,2,8)
  - trajectory length: τ=1
  - N_{poly}=310
  - Chronological inverter guess: N_{chrono}=16
  - Solver: mixed precision nested BiCGStab

Non-Perturbative Determination of C_{SW} (1)

Taniguchi @Lattice2012

Schördinger functional method

- $L^3 \times T = 8^3 \times 16$ ($L^3 \times T = 12^3 \times 24$ for volume dependence check)
- Choose β such that the lattice spacing becomes around 0.1 fm



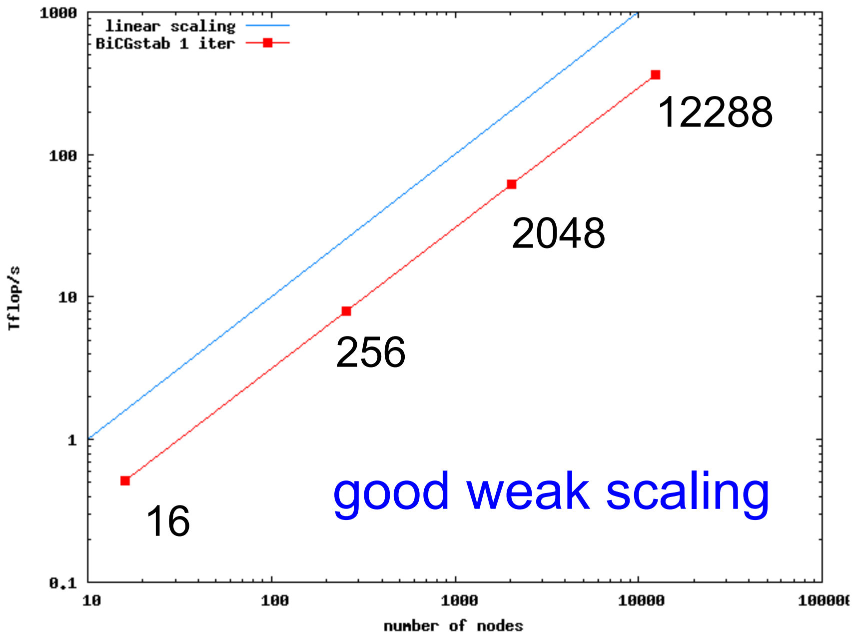
C_{SW}=1.11 at β=1.82 ⇒ 1/a∼2.1 GeV

κ_C is close to 0.125 at β=1.82

Performance on K computer

- Kernel (MatVec) performance: >50%
- Solver performance: ∼26% (mixed precision nested BiCGStab)
- Weak scaling test
  - $6^3 \times 12$/node fixed
  - 16 nodes ($V=12^3 \times 24$) ⇒ 12288 nodes ($V=48 \times 72 \times 96^2$)

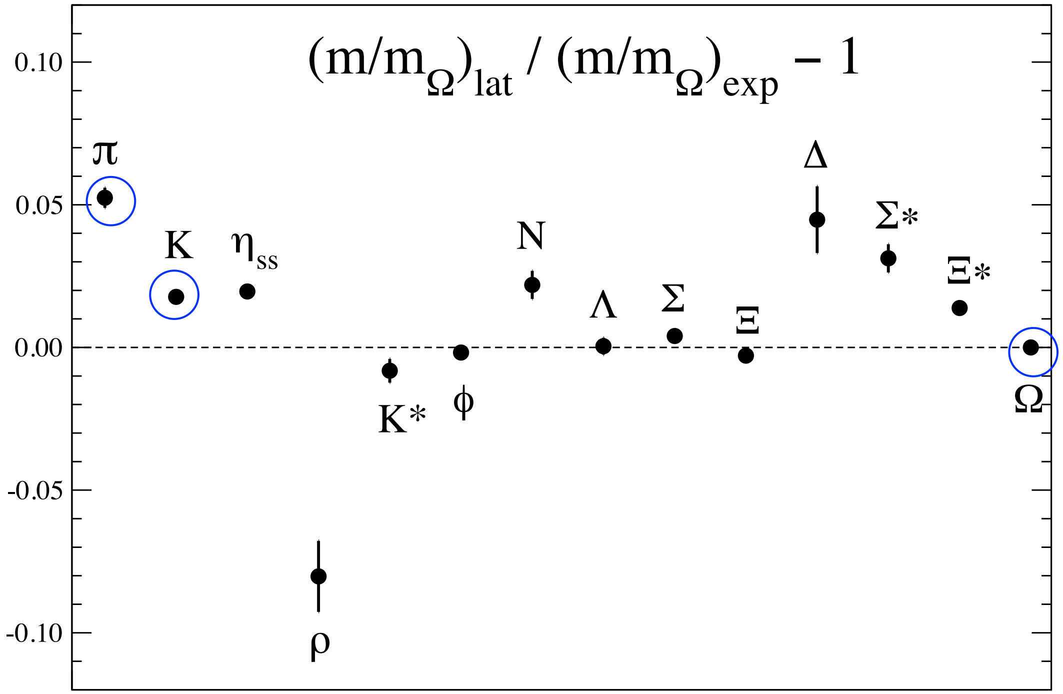
B/F=0.5 on K computer



#node	scalability
16 ⇒ 256	98%
256 ⇒ 2048	98%
2048 ⇒ 12288	96%

Current Status (As of Lattice 2013)

Hadron spectrum in comparison with experiment (normalized by m_Ω)



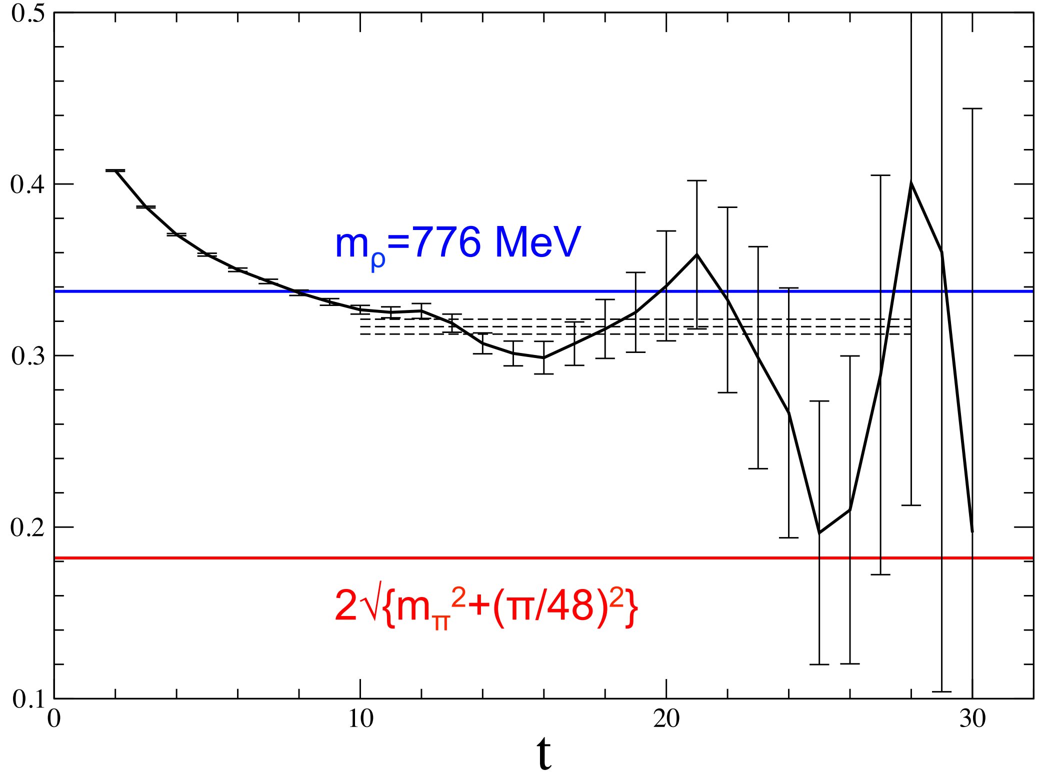
Preliminary

Further tuning to the physical point is planned with reweighting method

Clear deviation is already observed for unstable particles (ρ,K*)

ρ Meson Effective Mass

Decay channel is open: $m_\rho > 2\sqrt{m_\pi^2 + (\pi/48)^2}$



It looks hard to find a reasonable plateau

Analysis of 2×2 correlation matrix (ρ,ππ) is necessary

Summary

Historical role of PACS-CS/T2K-Tsukuba

- Achievement of physical point simulation
- Beginning of precision measurement with EM and u-d quark mass difference
- One-body study of hadron ⇒ Hadron-hadron interaction including Nuclei

Peak	Machine	Scientific Target
<1TF class	CP-PACS	Development of 2+1 flavor QCD simulation
10TFclass	PACS-CS	Physical point simulation
100TFclass	T2K-Tsukuba	Development of 1+1+1flavor QCD+QED simulation Construction of Nuclei with heavy m_{ud}
1PF class 10PF class	HA-PACS K computer	Large scale simulation of 1+1+1 flavor QCD+QED Construction of Nuclei at the physical point