Recent Results from PACS-CS Collaboration

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Before My Talk

What is Advanced Institute for Computational Science (AICS) ?

- Next-Generation Supercomputer (NGS) Project
- New Institute in Kobe
- Strategic Field Program for NGS

Next-Generation Supercomputer (NGS) Project

Overview of Project

- Development of 10 Pflops-class system in Kobe

  ⇒ named "K computer" by public competition
- Development of grand challenge applications in nano science and life science
- Federation of the 10 Pflops-class and supercomputers installations throughout Japan
- Buildup of a research center in computational science around the 10 Pflops-class system

  ⇒ Advanced Institute for Computational Science (AICS)
- Project period is from Japanese FY 2006 to 2012
- RIKEN is responsible for the computer development

  completely independent from RIKEN-BNL-Colombia Collab.

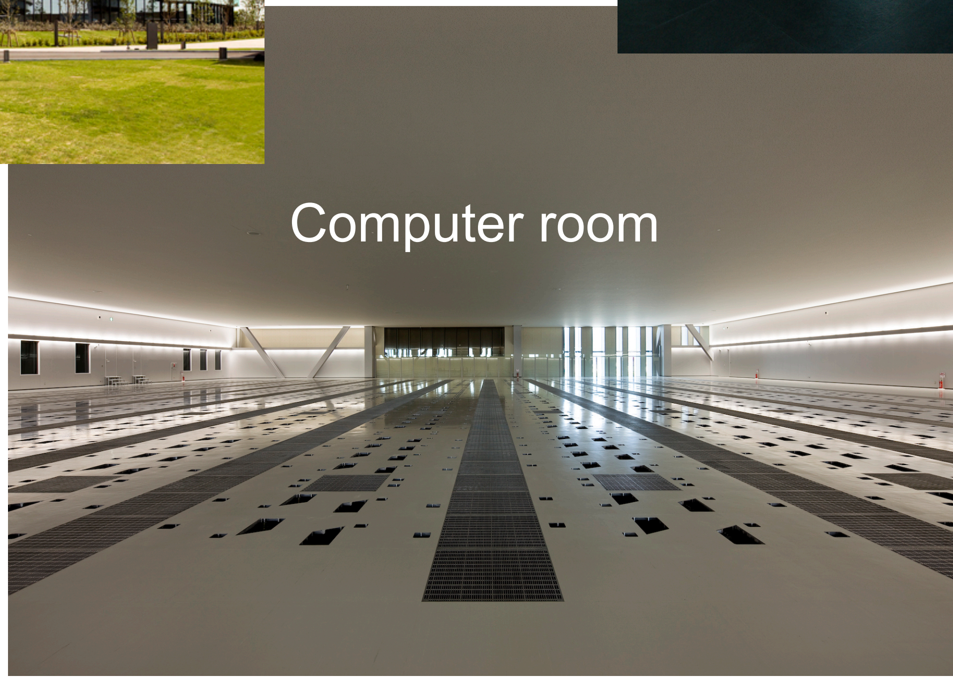
Site for K computer

450km (280miles) west from Tokyo

Some Photo

Building

Logo



Courtesy of RIKEN

Advanced Institute for Computational Science

founded on July 1, 2010

Objectives

- Research and development of computational and computer science
- Operation of K computer
- Lead High Performance Computing (HPC) in Japan

Special emphasis on

- Strong collaboration between computational and computer scientists
- Research on future HPC systems after K computer
- Fostering young scientists with expertise in both computational and computer science

Research Division

launched on October 1, 2010

7 research teams lead by Principal Investigators (PI)

Computational Science	Field theory
	Computational Molecular Science
	Computational Biophysics
	Computational Materials Science
Computer Science	System Software
	Computing Environment
	Processor

Seeking Research Scientists
http://www.riken.go.jp/engn/r-world/info/recruit/k101226_e_aics.html

Strategic Field Program

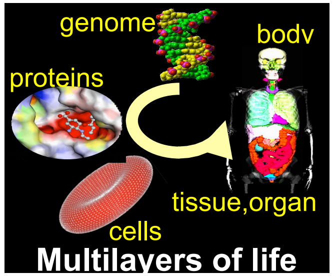
For strategic use of K computer

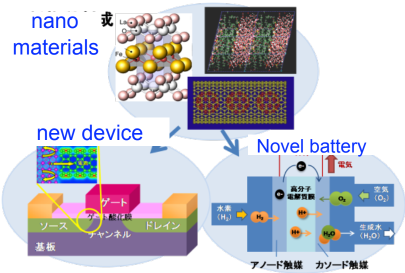
- Government selected 5 strategic fields in science and technology for importance from national view point
- For each field, Government also selected a core institute
- Each core institute is responsible for organizing research and supercomputer resources in the respective field and its community, for which they receive
  - priority allocation of K computer resources
  - funding to achieve the research goals

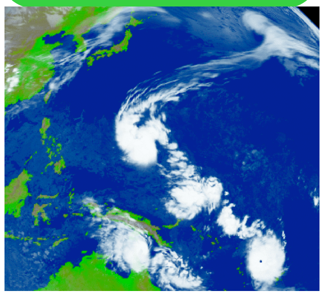
Strategic Fields and Core Institutes

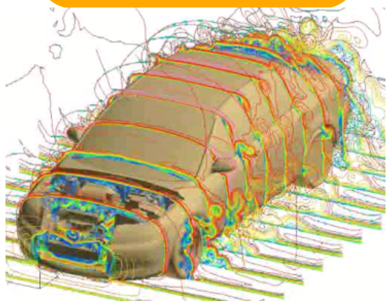
strategic field

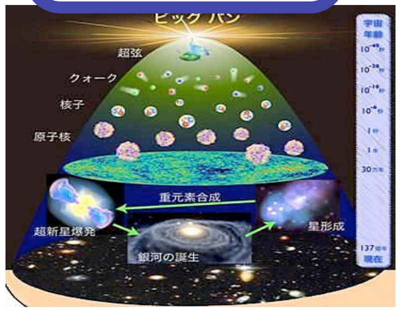
Life Science & Medicine	New materials & Energy	Global change prediction	Next generation Engineering	Matter & Universe











core institute

RIKEN	Institute for Solid State Physics U. Tokyo	Earth Simulator Center JAMSTEC	Institute for Industrial Science U. Tokyo	Center for Comp. Science U. Tsukuba
Life science Community	materials science Community	Earth science Community	Engineering Community Industry	Basic science Community
Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources

Direct Construction of Nuclei on the Lattice

Yamazaki-YK-Ukawa for PACS-CS Collab., PRD81(2010)111504

§1. Introduction

§2. What is the Difficulties?

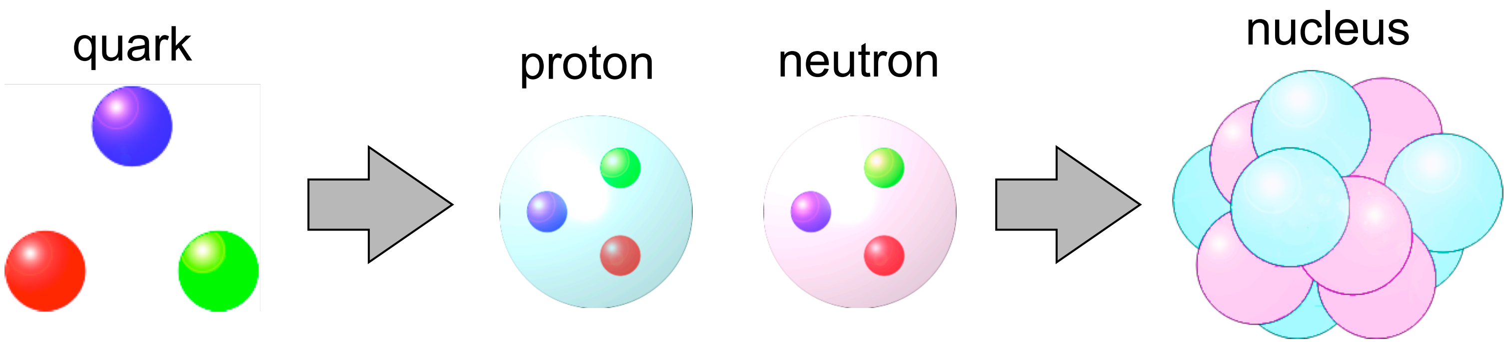
§3. Simulation Details

§4. Results

§5. Summary and Future Plan

§1. Introduction

Multi-scale physics is a real challenge in computational science



Investigate magic numbers, neutron-rich nuclei etc. based on QCD

radius of nuclei $\sim$ (1.1−1.2) $A^{1/3}$ fm
^{12}C: 2.5−2.7 fm

⇒ manageable size, at least, in quenched QCD

Previous Studies

Multi-nucleon system

- $\Lambda\Lambda$ system ⇒ H dibaryon: likely unbound in quenched QCD
  Mackenzie-Thacker 85, Iwasaki et al. 88,
  Negele et al.@lat98, Wetzorke et al.@lat99,
  Wetzorke-Karsch@lat02

- NN system ⇒ Deuteron: no systematic studies
  Fukugita et al. 95, NPLQCD 06 (scattering lengths from ΔE)

- NNN system ⇒ Triton: trial phase
  NPLQCD 09

No one has succeeded in detecting binding energies

§2. What is the Difficulties?

He nucleus correlator in terms of quark fields

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

^{4}He operator consists of two protons (udu) and two neutrons (dud)

⇒ No. of Wick contraction: $N_u!\times N_d! = (2N_p+N_n)!\times(2N_n+N_p)!$

^{4}He: 6!×6!=518400

^{3}He: 5!×4!=2880

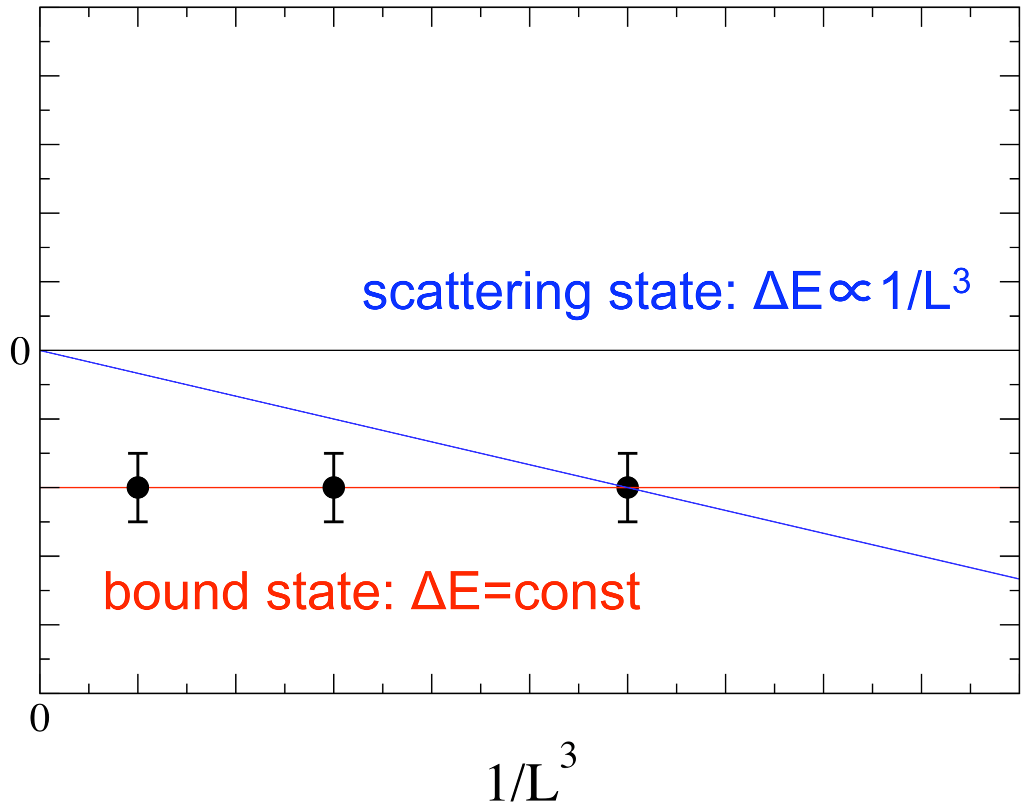
cf. N-N: 3! ×3!=36

^{12}C: 18!×18!∼4×10^{31}

independent quark diagrams are reduced by imposing $m_u=m_d$

Identification of Bound State in a Finite Box

ΔE<0 both for bound state and attractive scattering state



mandatory to check volume dependence of ΔE

§3. Simulation Details

Exploratory study for ^{4}He and ^{3}He nuclei

- large binding energy ΔE_{4He}=28.3 MeV
- ^{4}He has double magic numbers (Z=2,N=2)

To reduce the computational cost

- quenched approximation
- exact isospin symmetry ($m_u=m_d$)
  - ^{4}He: 6!×6!=518400 ⇒ 1107
  - ^{3}He: 5!×4!=2880 ⇒ 93
- modular construction of nucleus correlator
- rather heavy quark mass m_π = 0.8 GeV, m_N=1.6 GeV
  ⇒ range of pion exchange is reduced

Operator for He Nuclei

Quantum numbers of ^{4}He: $J^P=0^+$ and $I=0$

combination of spin and isospin in L=0 Beam 67

$$\frac{1}{\sqrt{2}}(\bar{\chi}\eta - \chi\bar{\eta})$$

$$\chi = \frac{1}{2}([+-+-]+[-+-+]-[+--+]-[-++-])$$

$$\bar{\chi} = \frac{1}{\sqrt{12}}([+-+-]+[-+-+]+[+--+]+[-++-]$$

$$-2[++--]-2[--++])$$

$$\eta, \bar{\eta} = \chi, \bar{\chi}(+/- \to p/n)$$

Quantum numbers of ^{3}He: $J^P=(1/2)^+$, $I=1/2$ and $I_z=1/2$

Bolsterli-Jezak 64

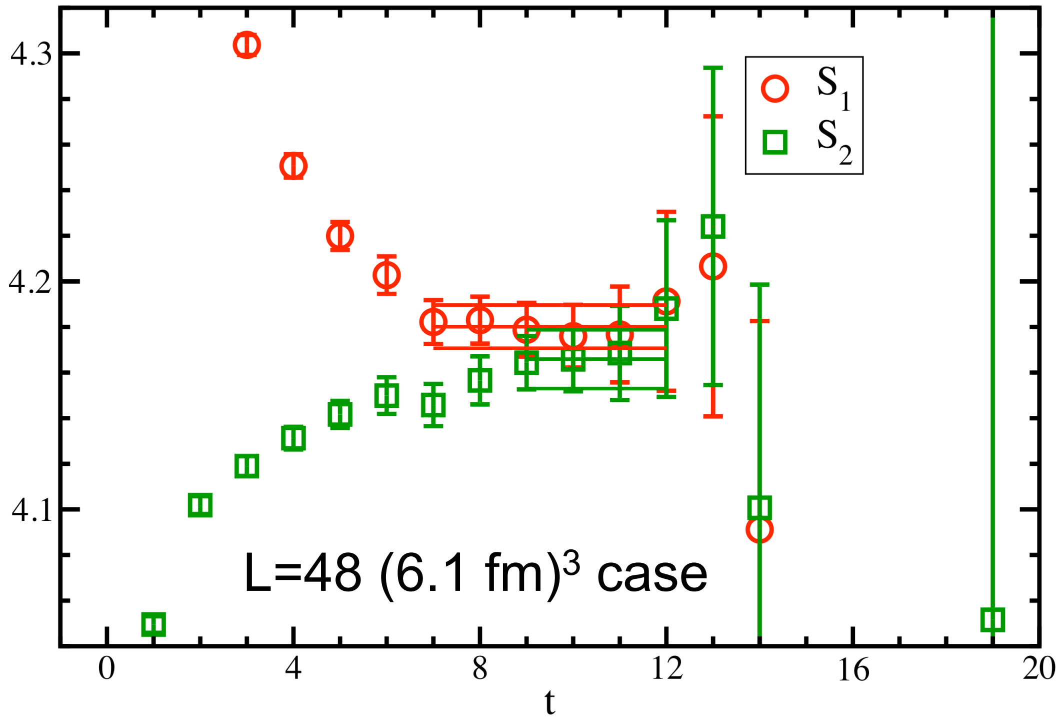
Simulation Parameters

- quenched approximation
- Iwasaki gauge action at β=2.416 ⇒ a=0.128 fm from r_0=0.49 fm
- tadpole-improved Wilson quark action with csw=1.378
- κ=0.13482 ⇒ m_π = 0.8 GeV, m_N=1.6 GeV
- periodic boundary condition
- two sets of exponentially smeared source: Aexp(−Br)

L [a]	[fm]	**#conf**	**#src**	**S_1** **(A_1,B_1)**	**S_2** **(A_2,B_2)**
24	3.1	2500	2	(0.5,0.5)	(0.5,0.1)
48	6.1	400	12	(0.5,0.5)	(1.0,0.4)
96	12.3	200	12	(0.5,0.5)	(1.0,0.4)

§4. Results

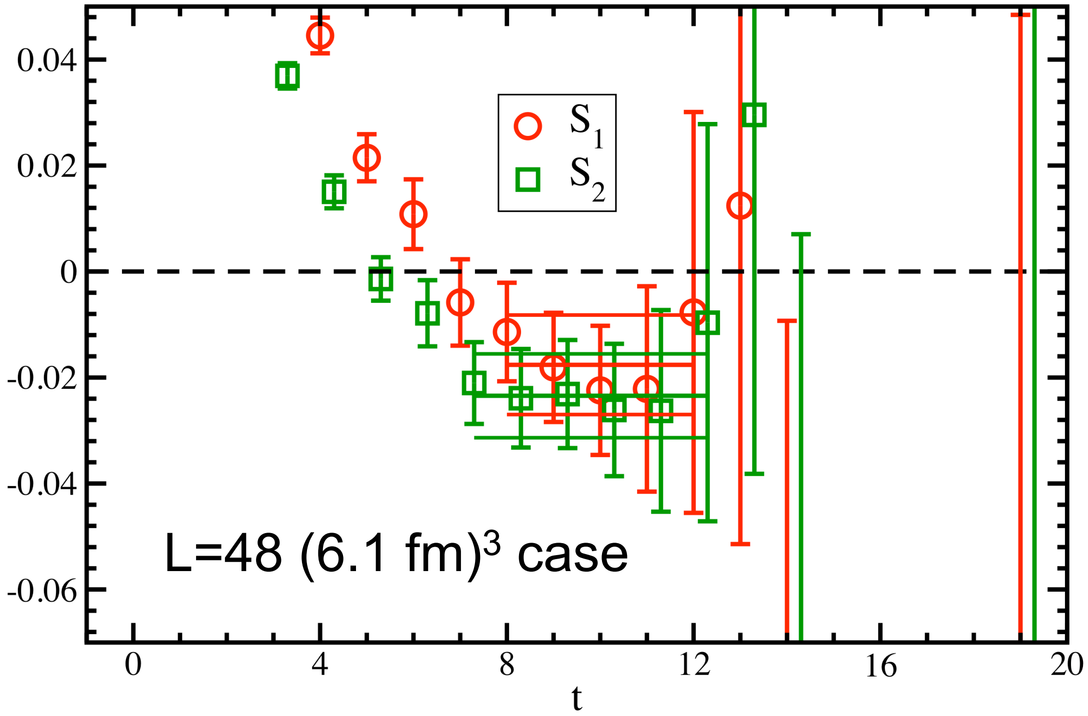
effective mass for ^{4}He nucleus



reasonable agreement between S_1 and S_2

Effective Energy Shift of ^{4}He nucleus

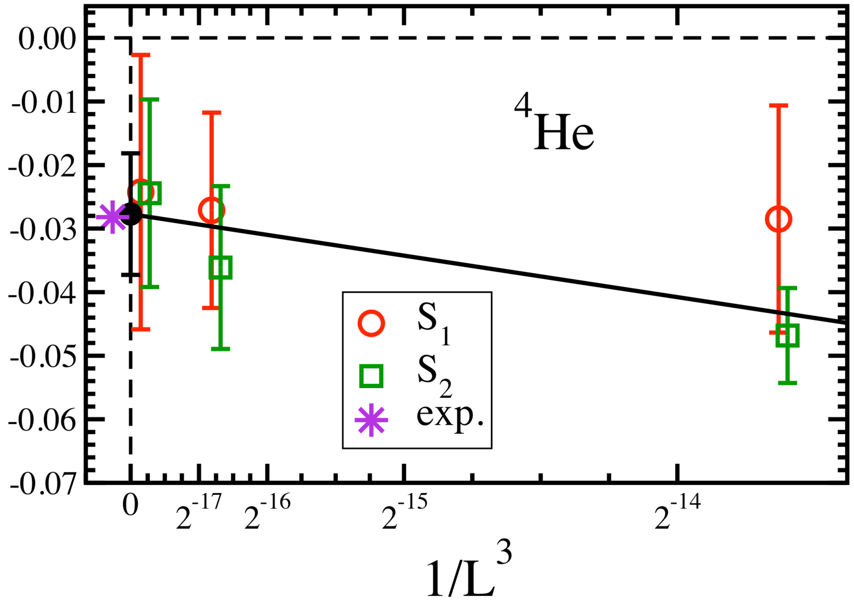
$$R(t) = G_{^4\mathrm{He}}(t)/(G_N(t))^4 \quad \Rightarrow \quad \Delta E_L^{\mathrm{eff}} = \ln(R(t+1)/R(t))$$

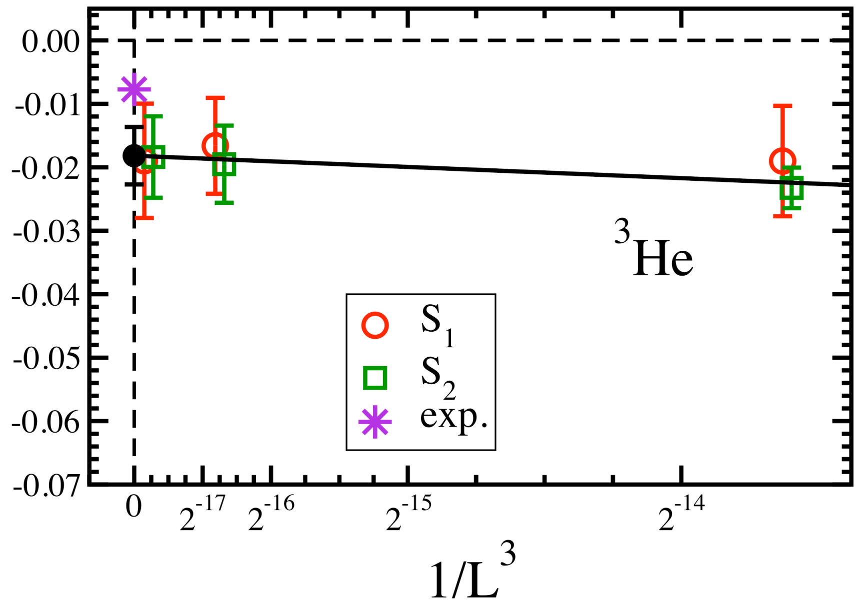


negative energy shift both for S_1 and S_2

Volume Dependence of ΔE_{He}

fit with $\Delta E_{\infty}+C/L^3$ due to possible contaminations by scattering state





ΔE_{∞}=27.7(9.6) MeV
ΔE_{exp}=28.3 MeV

ΔE_{∞}=18.2(4.5) MeV
ΔE_{exp}=7.72 MeV

same order to experimental values

§5. Summary and Future Plan

Helium nuclei are directly constructed in lattice QCD

− quenched approximation

− rather heavy quark mass

Future plan

- reduction of quark mass
- construction of nuclei with larger atomic/mass numbers
- application to full QCD