CERN TH Seminar
11 August 2010

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Lattice QCD at the Turning Point

My long stays at CERN TH

- September 1978 – August 1979 as a post doc
  - Division Head: Jack Prentki → Maurice Jacob
  - Heyday of perturbative QCD
  - Jet Calculus

    Ken Konishi, Akira Ukawa, Gabriele Veneziano,

    Nucl. Phys. B157, 45 (1979)
- January 1988 – January 1989 as a visitor
  - Division Head: John Ellis
  - LEP construction close to completion
  - CRAY XMP just installed in the Computer Division
    - 4 CPU's with 16MB of memory
    - 200Mflops/CPU
  - Hybrid Monte Carlo simulation with Wilson fermion

    Akira Ukawa, Nucl. Phys B(Proc. Suppl) 9, 463 (1989)

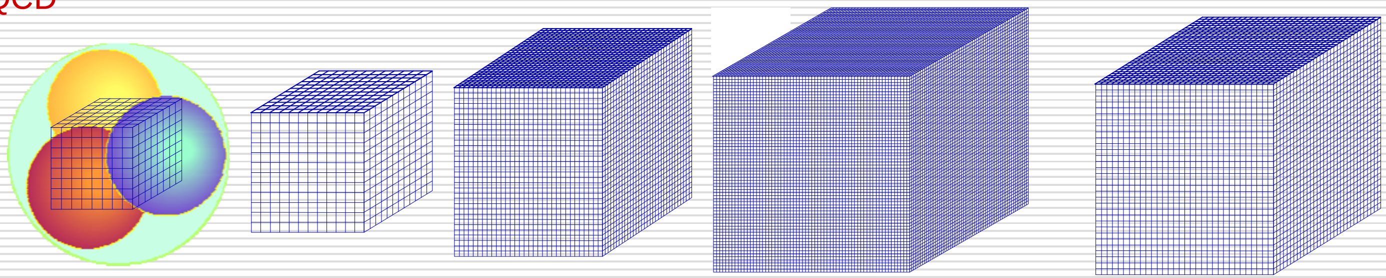
Lattice QCD over the years...

1975 1980 1985 1990 1995 2000 2005 2010

1973 QCD
1974 lattice QCD

Physics

1^{st} spec calculation
1981
Hamber-Parisi
Weingarten



Lattice size L

0.8fm	1.6fm	2.4fm	3.0fm	3.0fm
8^3x16	16^3x32	24^3x48	64^3x118	32^3x64

Algorithms

Nf=0 quenched

Nf=2 u,d

Nf =#sea quarks

Nf=2+1 u,d,s

Machines

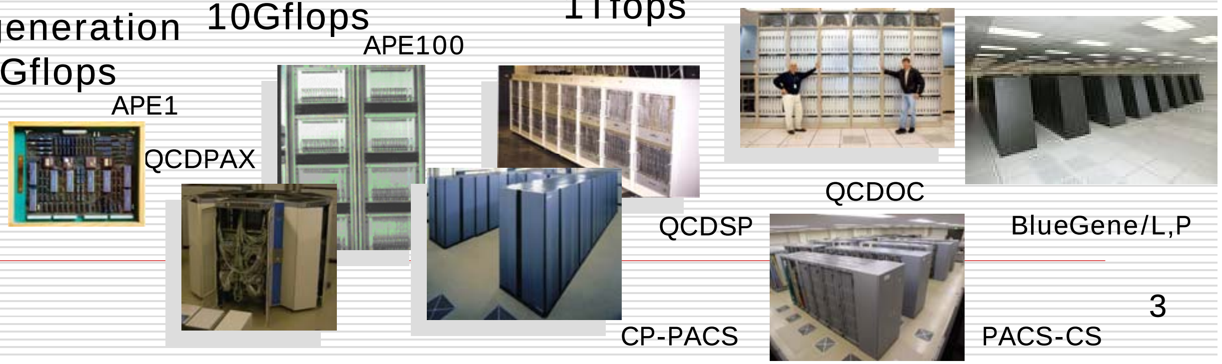
1st generation
1Gflops

2^{nd} generation
10Gflops

3^{rd} generation
1Tfops

4^{th} generation
10Tfops

100Tflops



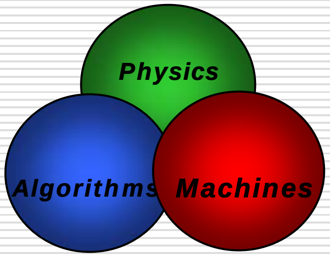
My personal view

- Lattice QCD is turning a corner in the last couple of years.
- Previously, despite the promise, it remained an uncertain method requiring assumptions/extrapolations in a number of ways (quenching, unphysically large quark masses, etc).
- Progress over the years has been removing these restrictions, and it is now becoming a real first principle method *allowing calculations of physical quantities directly at the physical point.*

What I wish to do today

Review recent progress and try to share this view with you

- Algorithmic progress and physical point simulation
- Going beyond particle physics - a trial with Helium nuclei -
- Status of the Japenese 京"Kei" Supercomputer Project
- Conclusions



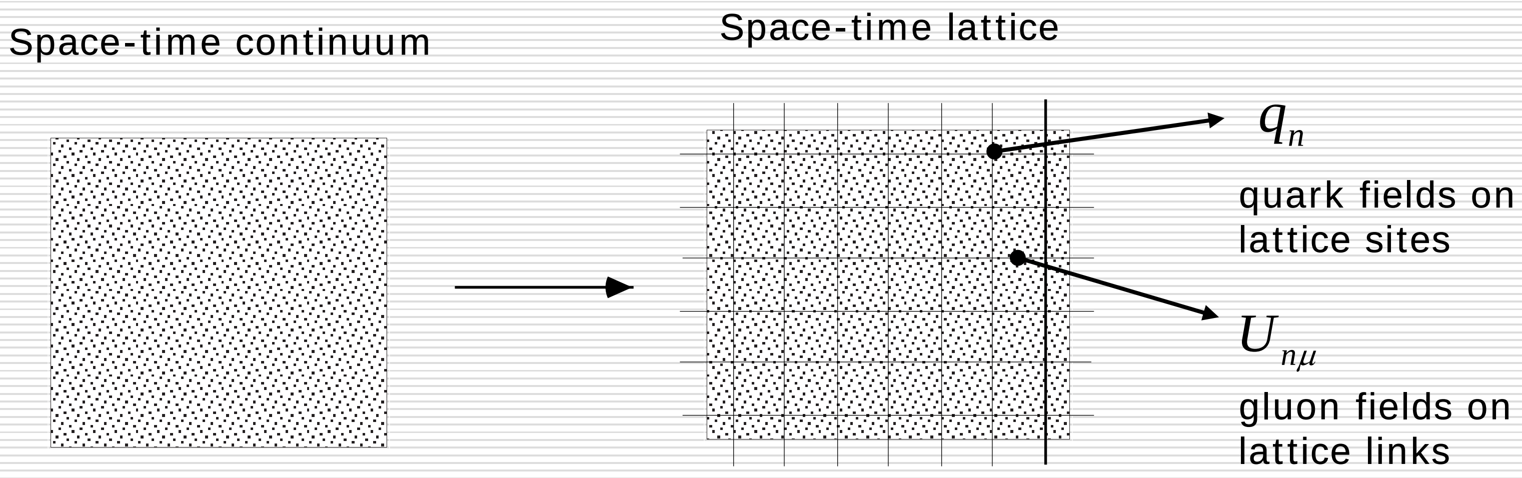
Algorithmic progress and Physical point simulation

Obstacles in lattice QCD calculations

- Using quark action with chiral symmetry
  - Domain-wall/overlap formalism have resolved the issue
- Including quark vacuum polarization effects
  - Quenching(ignore these effects) is a thing of the past, Nf=2+1 calculations (include up, down, strange quark effects) now standard
- Using small enough lattice spacing
  - Improved lattice actions for minimizing lattice spacing errors have been developed and are employed
- Using large enough lattice volume
  - No real remedy other than to use large enough volume
- Using light enough quark masses
  - Relied on chiral perturbation theory to extrapolate from heavy quark masses, a large source of ambiguity in lattice calculations

QCD on a space-time lattice

K. G. Wilson 1974



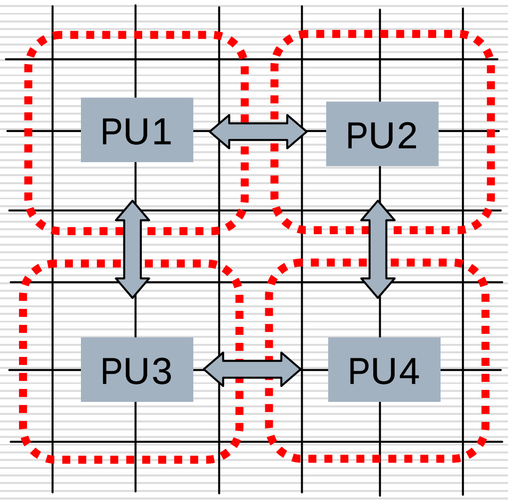
- Feynman path integral
  - Action $S_{QCD} = \frac{1}{g_s^2} \sum_P tr(UUUU) + \sum_f \bar{q}_f (\gamma \cdot U + m_f) q_f$
  - Physical quantities as integral averages ⇒ Monte Carlo calculation of the integral average

$$\langle O(U, \bar{q}, q) \rangle = \frac{1}{Z} \int \prod_{n\mu} dU_{n\mu} \prod_n d\bar{q}_n dq_n \; O(U, (U, \bar{q}, q)) e^{-S_{QCD}}$$

Lattice QCD as computation(I)

- QCD is a local field theory; only nearest neighbor interactions

- Natural mapping of space-time lattice to processor array
  - Each compute node carries a sub-lattice
  - Only nearest neighbor communication needed



→ Highly parallelizable and scalable

Lattice QCD as computation(II)

- Quarks are fermions, so their field, being anti-commuting, needs a special trick

$$\int \prod_n d\bar{q}_n dq_n \, e^{-\sum_{n,m} \bar{q}_n D_{nm}(U) q_m} = \det D(U) = \int \prod_n d\bar{\phi}_n d\phi_n \, e^{-\sum_{n,m} \bar{\phi}_n \left(\frac{1}{D(U)}\right)_{nm} \phi_m}$$

Grassmann rep — Boson rep

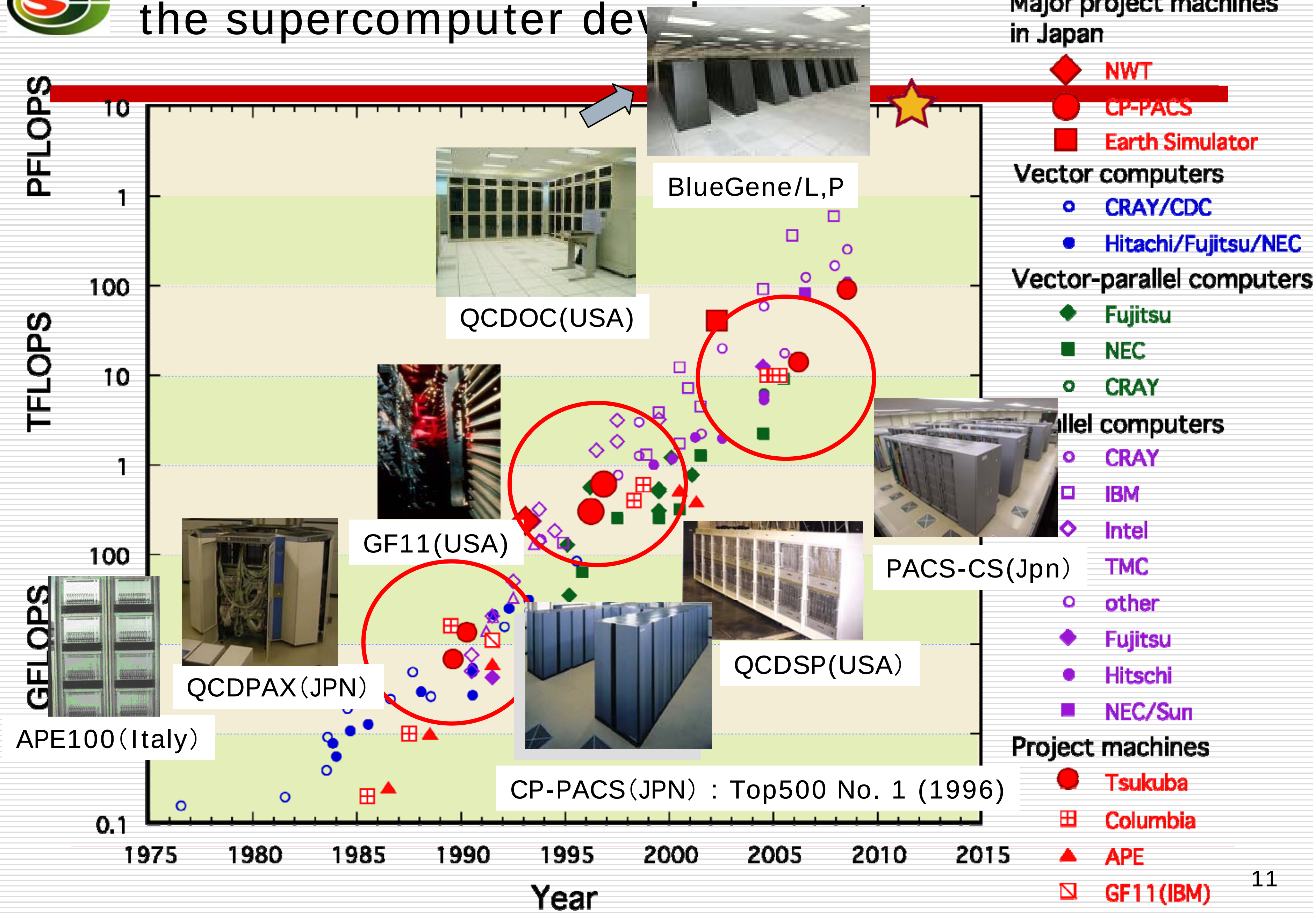
- Need to invert the lattice Dirac operator D(U)
  - Sparse but large matrix
  - Large condition number ∼ $1/m_q$ for light quarks

$$\sum_m D_{nm}(U) x_m = \phi_n \Rightarrow x_n = \left(\frac{1}{D(U)}\right)_{nm} \phi_m$$

Core calculation of QCD

⇒ Computationally very intensive

Impact of lattice QCD machines on the supercomputer dev...



But, of course(?), machine power by itself was not enough

…

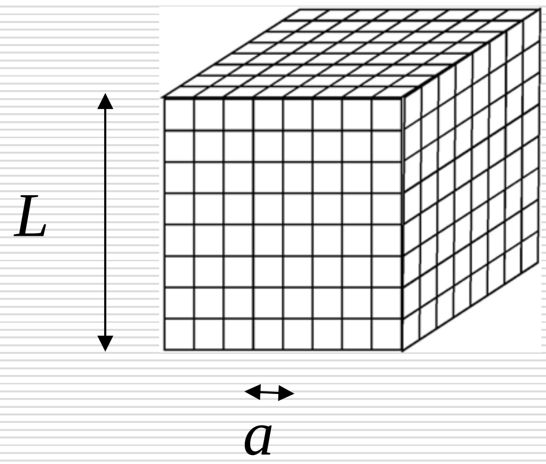
Difficulties with light quark masses

- #arithmetic ops of hybrid Monte Carlo (HMC) algorithm for Nf=2 flavor full QCD(2001)

$$\#FLOP's \approx 1.9 \left[\frac{\#conf}{1000}\right] \cdot \left[\frac{m_\pi}{500MeV}\right]^{-6} \cdot \left[\frac{L}{3\,fm}\right]^{5} \cdot \left[\frac{a}{0.1\,fm}\right]^{-7} Tflops \cdot year$$

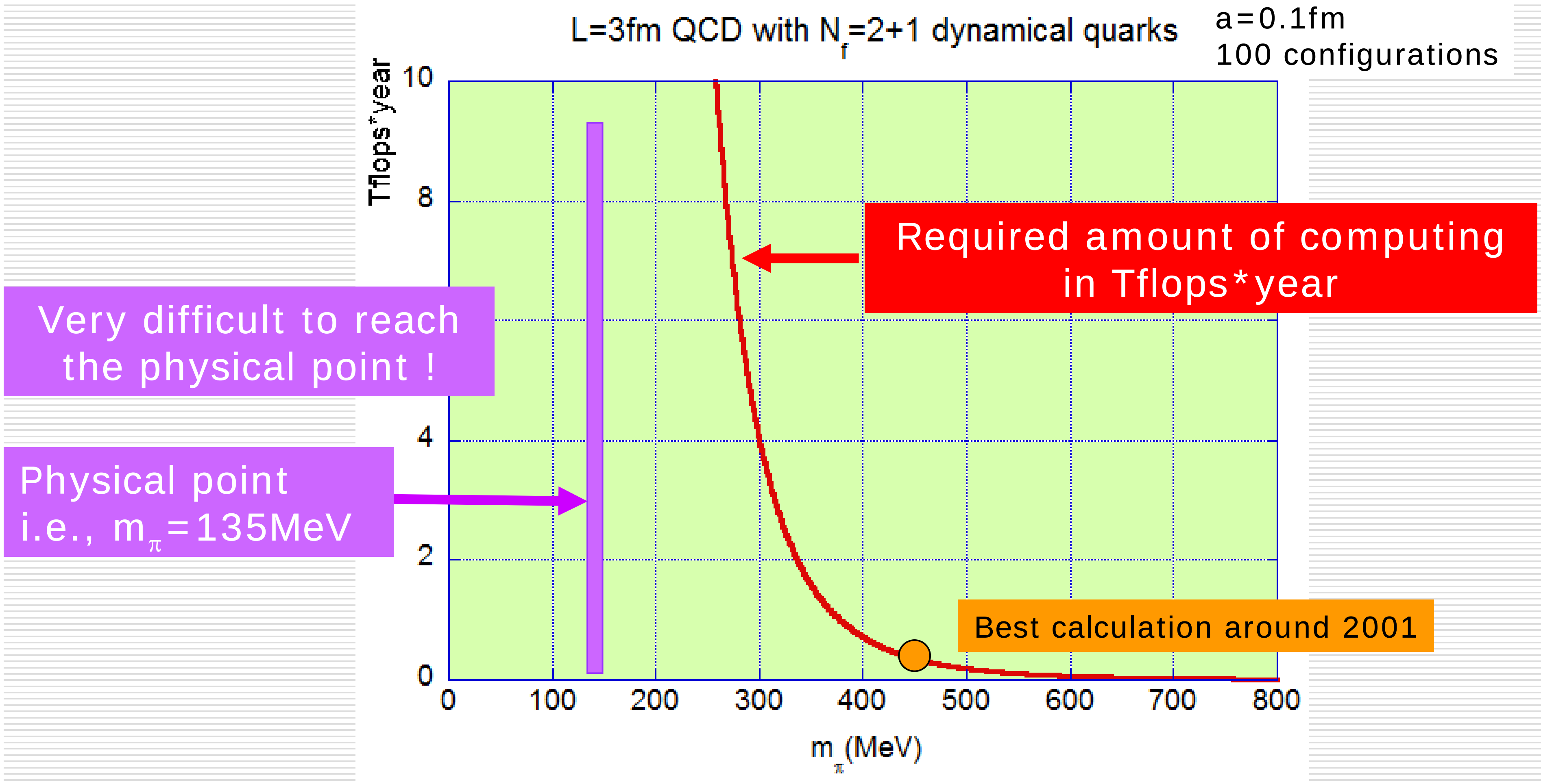
  - Severe scaling toward small pion mass /large volume/small lattice spacing

  - Parameters of lattice QCD simulation:
    - Quark mass $m_q \; or \; m_\pi \propto \sqrt{m_q}$
    - Lattice size $L\,(fm)$
    - Lattice spacing $a\,(fm)$

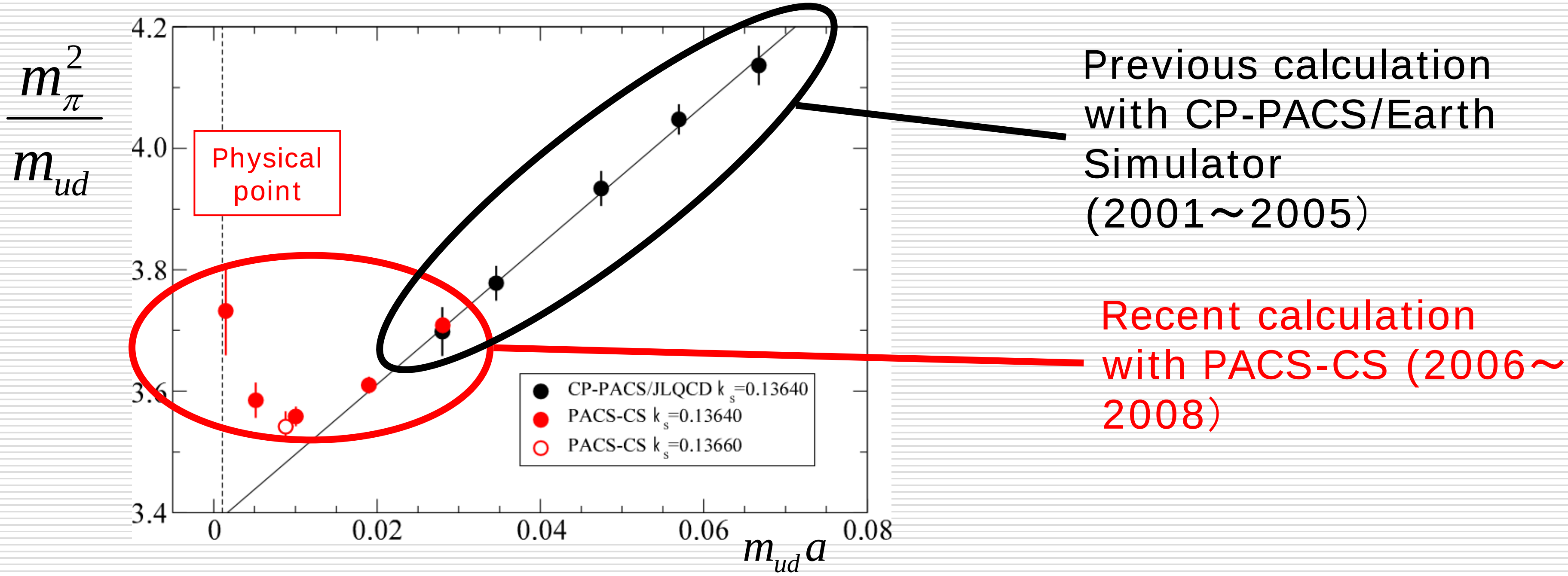


"Berlin wall" at Lattice 2001@Berlin

A. Ukawa for CP-PACS and JLOCD



Why so important to go physical?



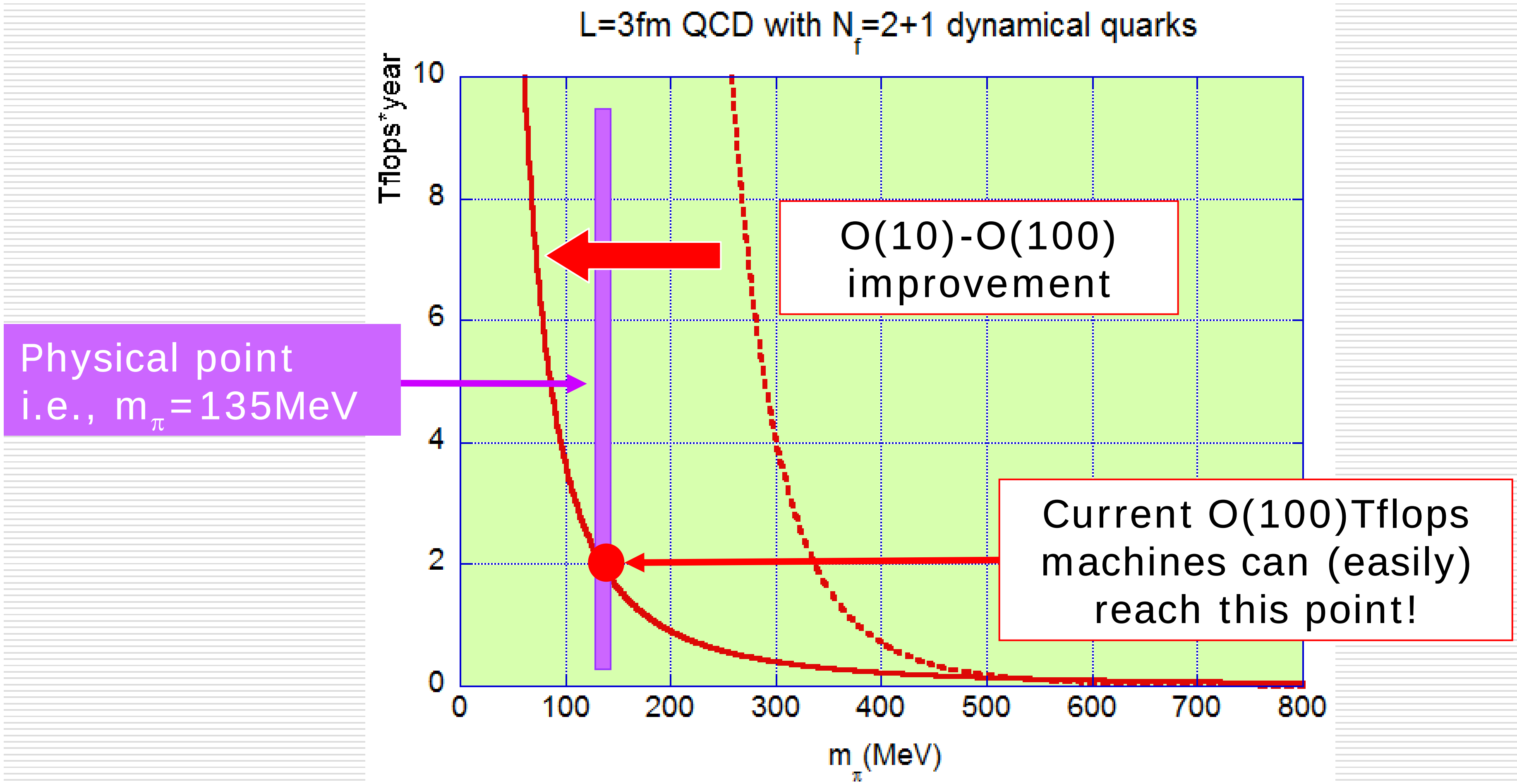
- Anticipated effect of *chiral logarithm* at zero quark mass

$$\frac{m_\pi^2}{m_{ud}} \propto 1 + \frac{2Bm_{ud}}{(4\pi f)^2} \log \frac{2Bm_{ud}}{\mu^2} + \cdots$$

- However, extrapolation difficult to control since
  - Convergence radius a priori not known
  - Have to determine a number of unknown constants

Those technical points aside, I believe that it would be beautiful if one can sit right at the physical point and calculate the physical observables, because *then we are no longer simulating; we will be calculating the strong interactions as they are taking place in Nature itself.*

Revolutionary progress since 2005 ; beating the critical slowing down



Physical Point Simulation has become reality

How that progress came about?

- Molecular dynamics equation of hybrid Monte Carlo algorithm

$$\frac{d}{d\tau}U_{n\mu} = -iU_{n\mu}P_{n\mu}$$

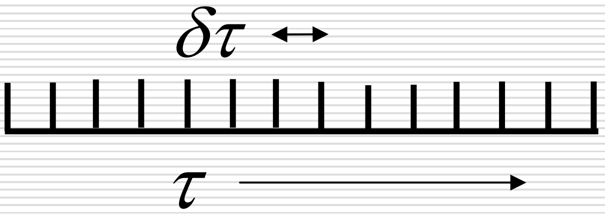
gluon force

quark force

$$\frac{d}{d\tau}P_{n\mu} = F_{n\mu} = \frac{1}{g^2}(UUUU\ )_{n\mu} + \bar{\phi}\left(\frac{1}{D(U)}\right)\frac{\partial D(U)}{\partial U_{n\mu}}\left(\frac{1}{D(U)}\right)\phi$$

Most time-consuming part of computation

- Molecular dynamics equation is integrated in discrete steps, so a larger time step is better!



Key observation

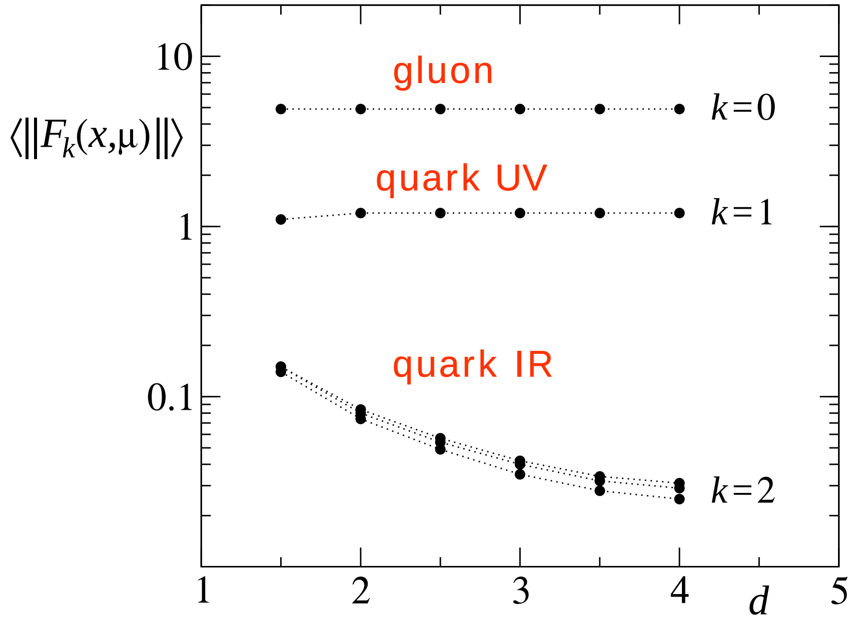
M. Luescher、C

- Separate UV and IR modes of quark fluctuations
- gluon:UV:IR forces are order of magnitude different!

$$F_{gluon} >> F_{quark,UV} >> F_{quark,I}$$

- This invites a multi-time step integration:

$$\delta\tau_{gluon} << \delta\tau_{quark,UV} << \delta\tau_{quark,}$$



i.e., one can enlarge the time step for the most compute intensive IR quark force, *leading to a large reduction in the computing requirement.*

This is physics!

Our conscious effort toward physical pion mass (I)

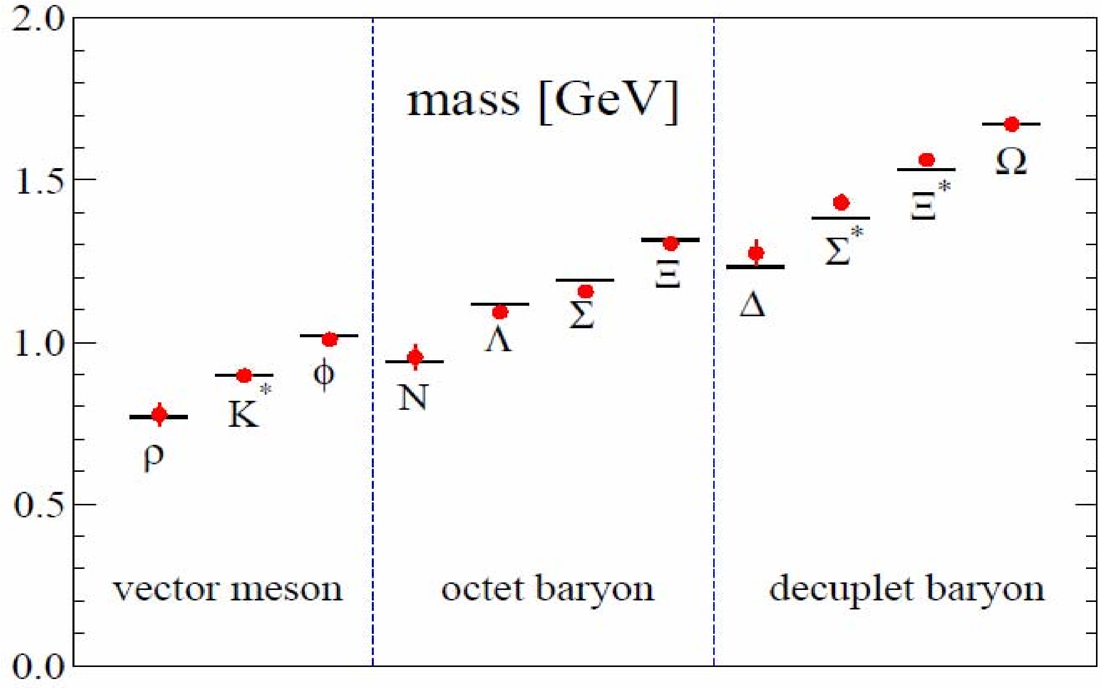
- Development of PACS-CS computer with a view of running the improved HMC algorithm (2005 – 2007)
  - 2560 nodes with Intel Xeon (5.6Gflops) CPU (14.3Tflops)
  - 16x16x10 3d hypercrossbar network(0.75GB/sec/node)
  - 3-year project with US$24M budget
  - Built by Hitachi Ltd.
- Development of domain-decomposed hybrid Monte Carlo code for Wilson-clover action
- Operation
  - Started running June 2006
  - Full production since late 2006

PACS-CS

Our conscious effort toward physical pion mass (II)

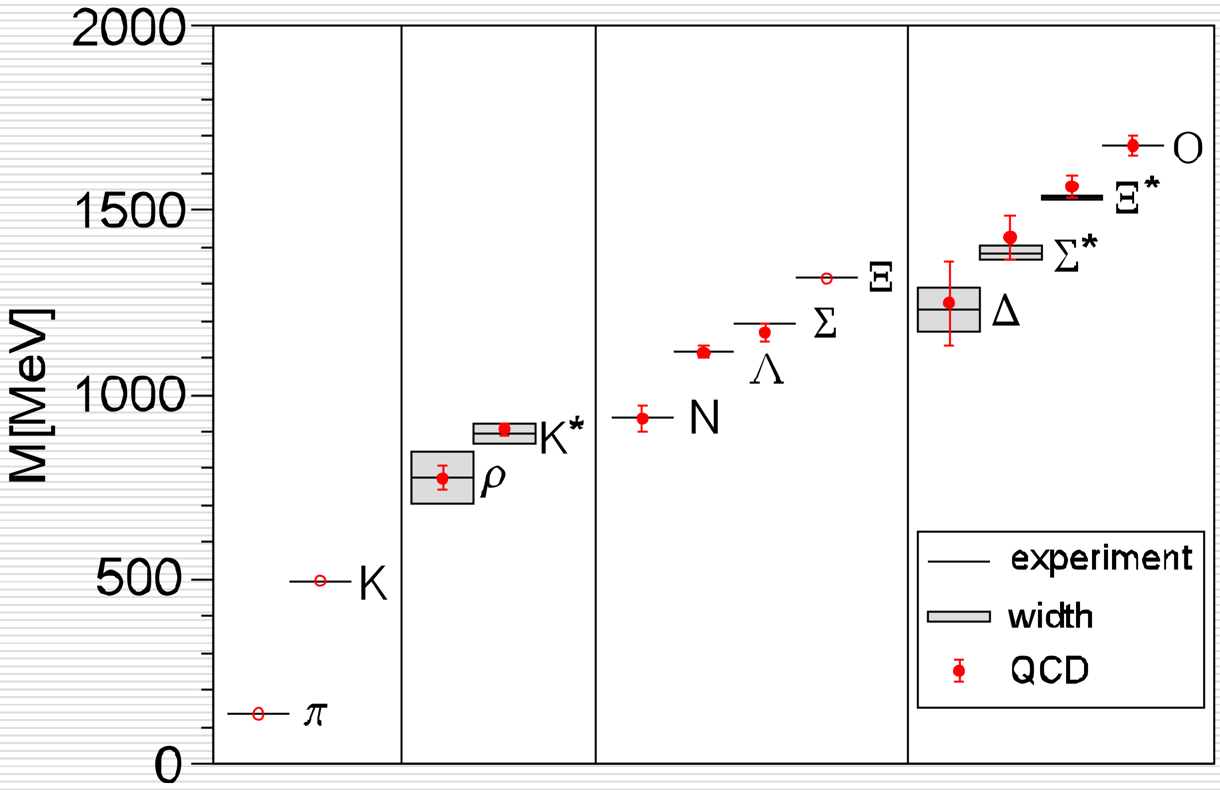
PACS-CS Collaboration Phys. Rev. D79 034504 (2008)

pion mass down to $m_\pi \approx 156 MeV$ $32^3 \times 64, \quad a = 0.907(13)\,fm$



In the mean time,
came along the BMW Collaboration

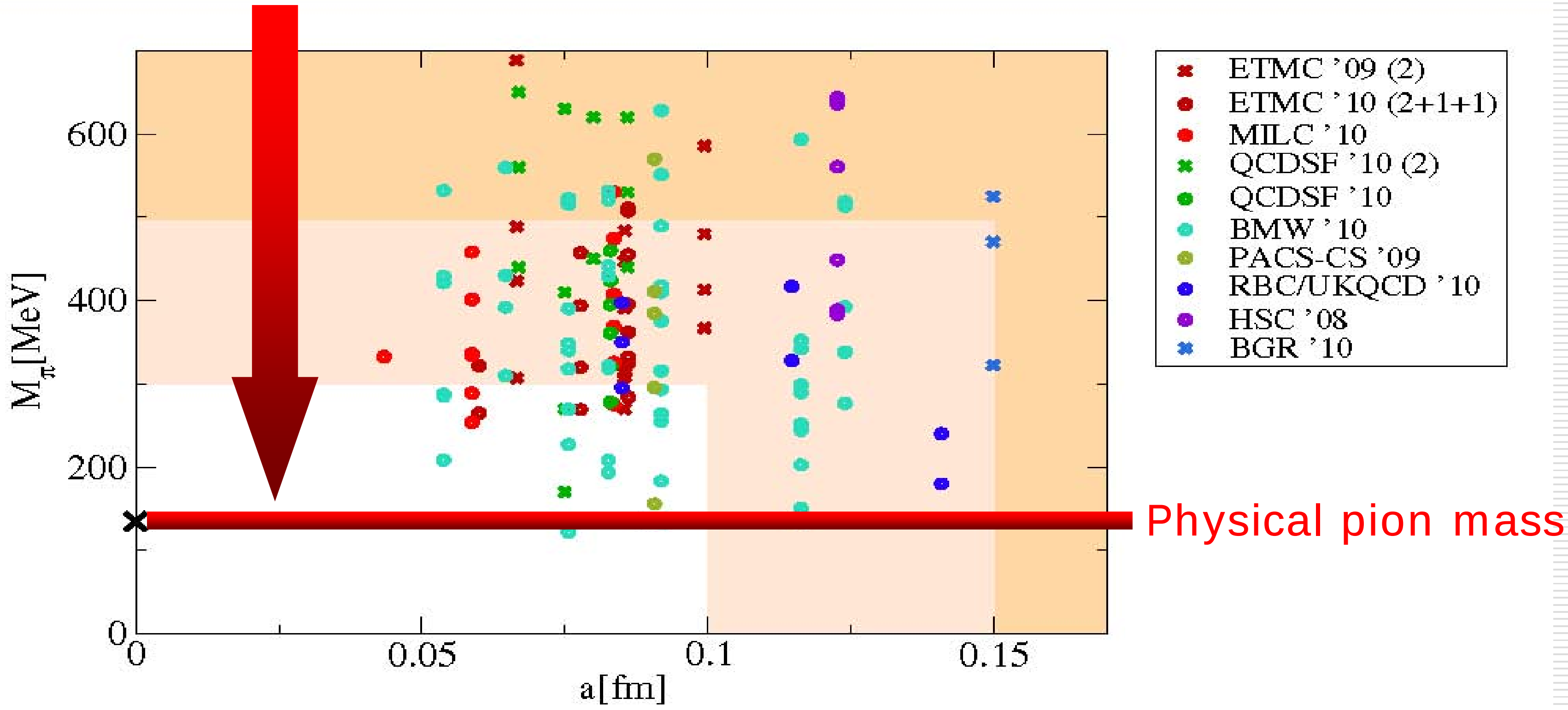
BMW Collaboration (Butapest-Marseille-Wuppertal)
Science 322(2008) 1224
m_π>200MeV but large lattices (m_πL>4) and continuum extrapolated!



Status this year:
pion mass vs lattice spacing

Continuum Landscape

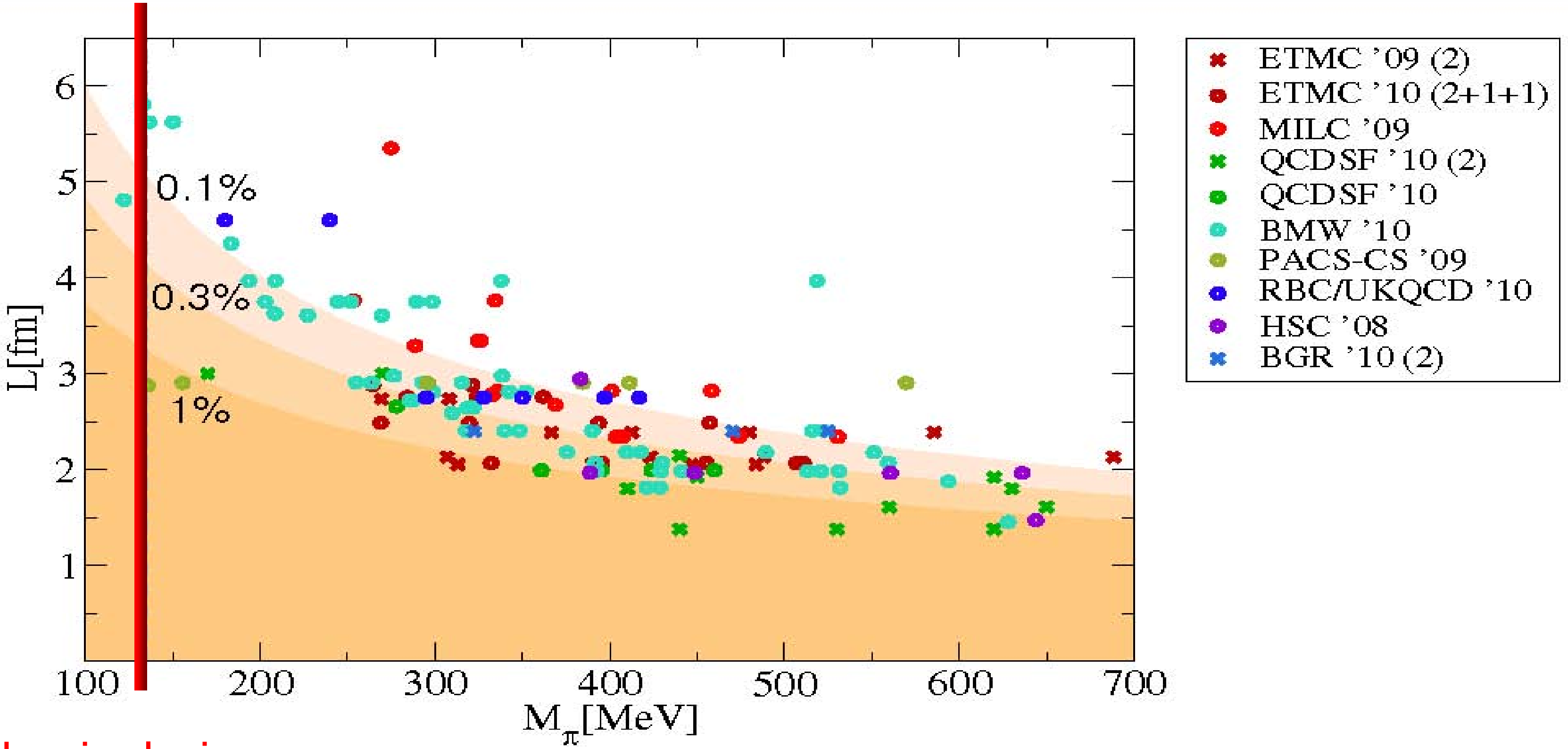
From C. Hoelbling's review at Lattice 2010



Status this year: lattice size vs pion mass

FV Landscape

From C. Hoelbling's review at Lattice 2010



Physical pion mass

Upshot of algorithmic progress

- *Realistic calculation directly at the physical point finally reality*
  - Fruit of continuous effort over 25 years toward:

    Better physics understanding, Better algorithms, and More powerful machines

- *Change of philosophy from "simulation" to "calculation"*
  - No more approximations/extrapolations (other than the continuum extrapolation)

    In particular, no more reliance (other than checks) on ChPT
  - Gluon configuration produced is strong interaction in Nature itself

Impacts

- *Expect fundamental issues of lattice QCD as particle theory make major progress over the next five year range*
  - Single hadron properties and fundamental constants
  - Precision flavor physics (<1%) and resolution of old issues including $K \to \pi \pi$ decays
  - Hot/dense QCD with chiral lattice action on large lattices and physical pion mass
- *Vast area of multi-hadron systems/atomic nuclei lies in wait to be explored*
  - Nuclear force from lattice QCD
  - Exotic nuclei with unusual n/p ratios/strangeness etc

Several (diverse) subjects of personal interest

Can you sit exactly at the physical point?

- *NO*, but this can be resolved by the reweighting technique.
- Reweighting technique
  - An old idea by A. Ferrenberg, R. Swendsen, PRL 61, 2635 (1988), used in many phase transition studies
  - Recently applied to *shift quark mass by a small amount*

See e.g., A. Hasenfratz etal PRD78, 014515 (2008)

$$\int \prod_{\ell} dU_{\ell} \det\left[D(U) + m'_q\right] e^{-S_{gluon}(U)} = \int \prod_{\ell} dU_{\ell} \frac{\det\left[D(U) + m'_q\right]}{\det\left[D(U) + m_q\right]} \det\left[D(U) + m_q\right] e^{-S_{gluon}(U)}$$

$$\left\langle O \right\rangle_{m'_q} = \left\langle O \cdot R \right\rangle_{m_q} \qquad R = \frac{\det\left[D(U) + m_q\right]}{\det\left[D(U) + m'_q\right]} = \det\left[1 + \left(m_q - m'_q\right)\left(D(U) + m'_q\right)^{-1}\right]$$

  - Have to calculate only the determinant ratio instead of a full simulation

An exemplary calculation

PACS-CS Collaboration, PRD81, 074503 (2010)

- Original calculation
  - Nf=2+1 with Wilson-clover action
  - 32^3x64 lattice, 1/a=2GeV
  - hopping parameter $\kappa_{ud} = 0.13778500, \quad \kappa_s = 0.13660000$
  - Misses the physical point by a fair amount, e.g.,

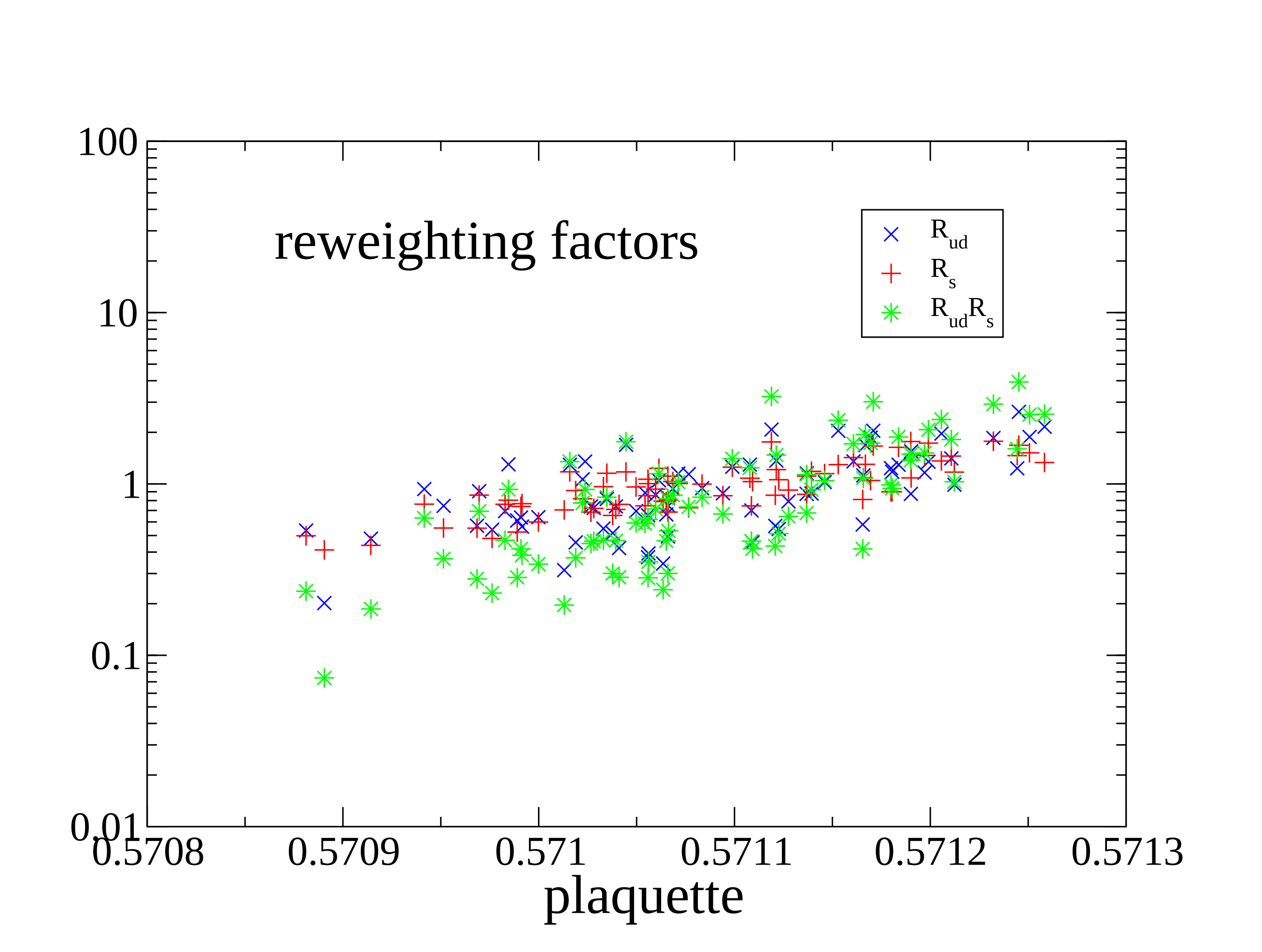
$$m_\pi = 151 \pm 6 MeV \quad cf \quad \exp = 135 MeV$$

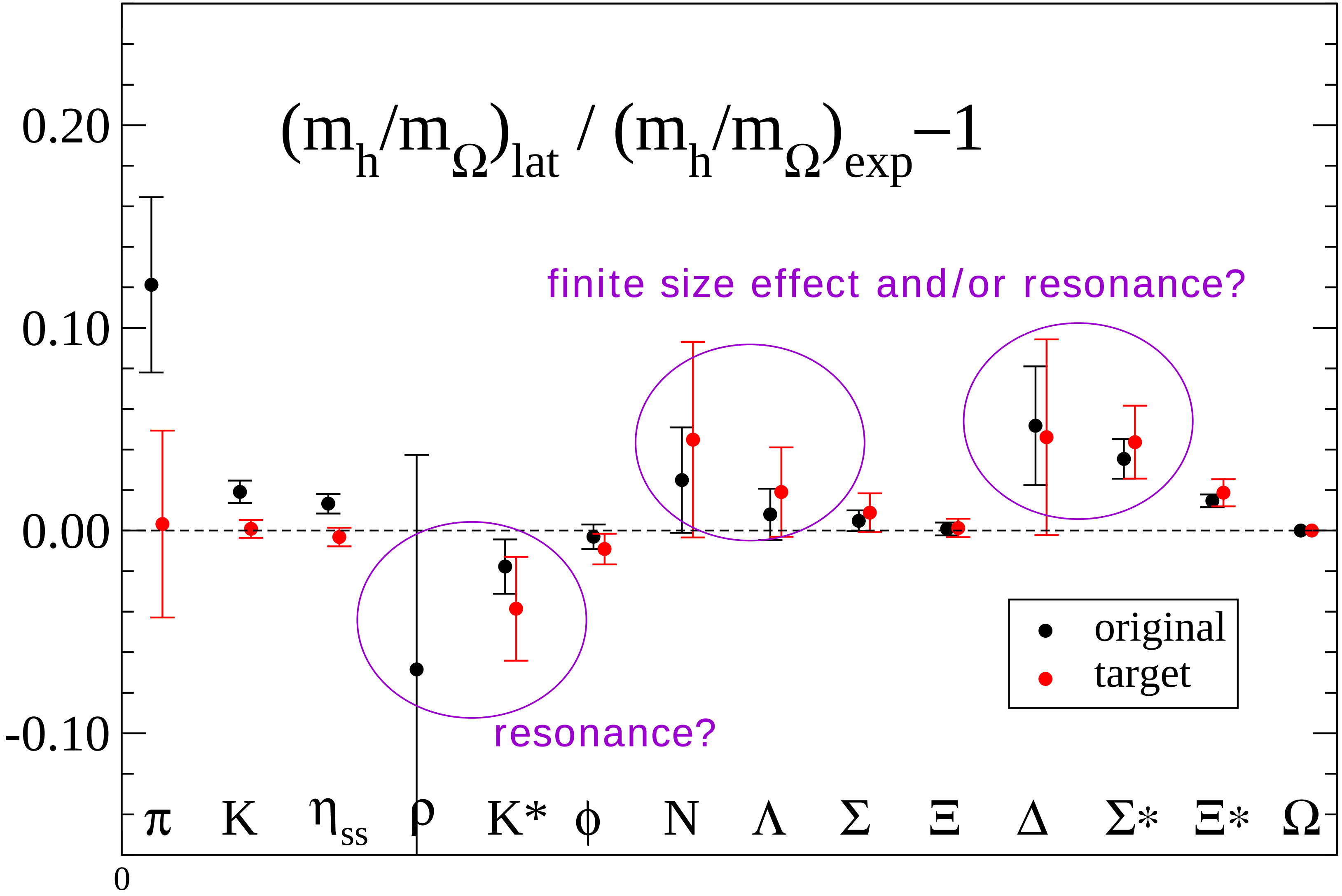
$$m_K = 505 \pm 8 MeV \quad cf \quad \exp = 495 MeV$$

- Target calculation
  - Hopping parameter $\kappa_{ud} = 0.13779625, \quad \kappa_s = 0.13663375$
    estimated from the original calculation

Distribution of the reweighting factor

- Reasonable distribution around R=1; fluctuation is reasonably controlled
- Posit





$(m_h/m_\Omega)_{lat} / (m_h/m_\Omega)_{exp} - 1$
0.20
0.10
0.00
-0.10
0
finite size effect and/or resonance?
resonance?
original
target
π K η_ss ρ K* φ N Λ Σ Ξ Δ Σ* Ξ* Ω

Isospin breaking
– further application of reweighting –

- Isospin breaking in some channels is determined very precisely, e.g.,

$$m_{\pi^\pm} - m_{\pi^0} = 4.5936 \pm 0.0005 MeV$$

$$m_{neutron} - m_{proton} = 1.2933321 \pm 0.0000004 MeV$$

- Very interesting probe to examine
  - up/down quark mass difference, $m_{up} \neq m_{down}$ including the possibility of $m_{up} \approx 0$
  - requires disentangling QED effects $Q_{up} = \frac{2}{3}e, \quad Q_{down} = -\frac{1}{3}e$
- Apply reweighting to
  - Split up and down quark mass
  - Introduce EM coupling

Isospin breaking – first attempt –

- T. Izubuchi et al talk on Friday for details
- Nf=2+1 configuration with domain-wall quark as base configuration
  - 16^3x48, 24^3x48 lattice
- In the initial study, only valence quarks carry
  - up/down quark mass difference $m_{up} \neq m_{down}$
  - EM coupling to non-compact EM field $Q_{up} = \frac{2}{3}e, \quad Q_{down} = -\frac{1}{3}e$
- Partially quenched ChPT for QCD & QED to determine the low energy constants

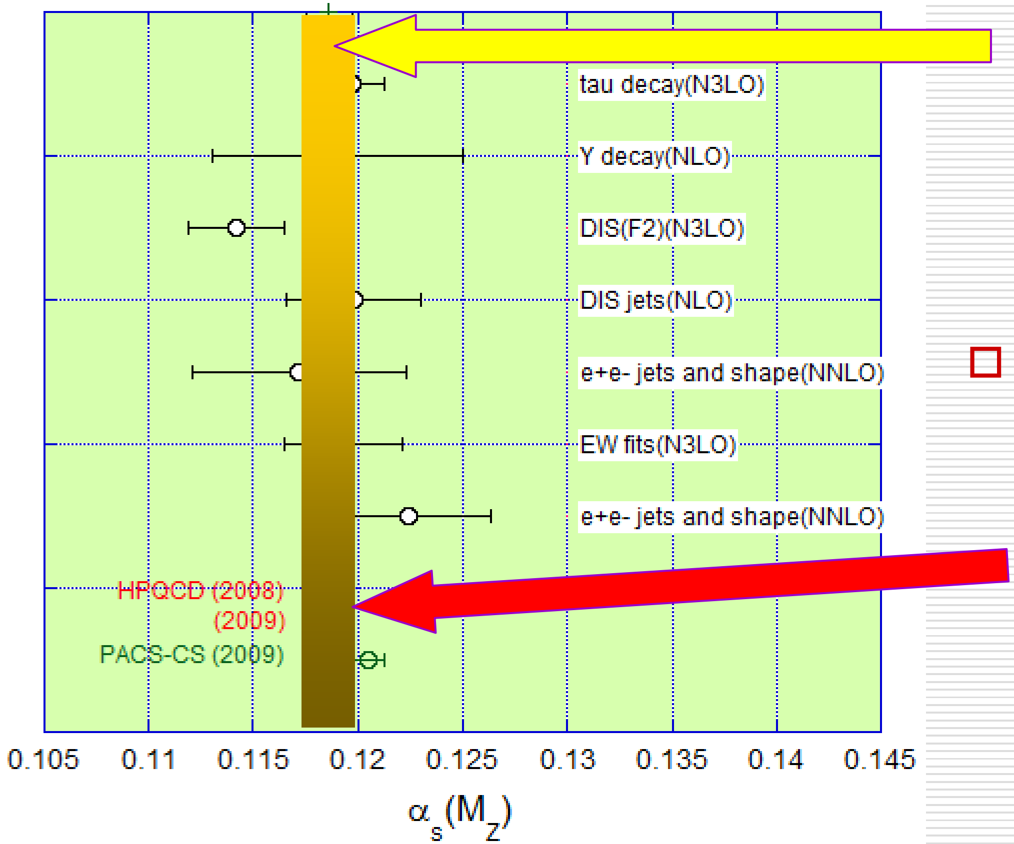
→ Physical predictions, e.g.,

$$m_{up} = 2.37 \pm 0.10 \pm 0.24 MeV$$

$$m_{down} = 4.52 \pm 0.15 \pm 0.26 MeV$$

- Further work in progress to include sea quark effects

Strong coupling constant



- Experimental average

$$\alpha_s^{MS}(M_Z) = 0.1186 \pm 0.0011$$

S. Bethke, ArXiv.0908.1135

- Nf=2+1 Lattice QCD

HPQCD 2009 update

(private communication from C. Davies)

$$\alpha_s^{MS}(M_Z) = 0.1184 \pm 0.0004$$

PACS-CS 2009 Y. Taniguchi et al

JHEP 0910, 053 (2009)

$$\alpha_s^{MS}(M_Z) = 0.1205^{+0.009}_{-0.0027}$$

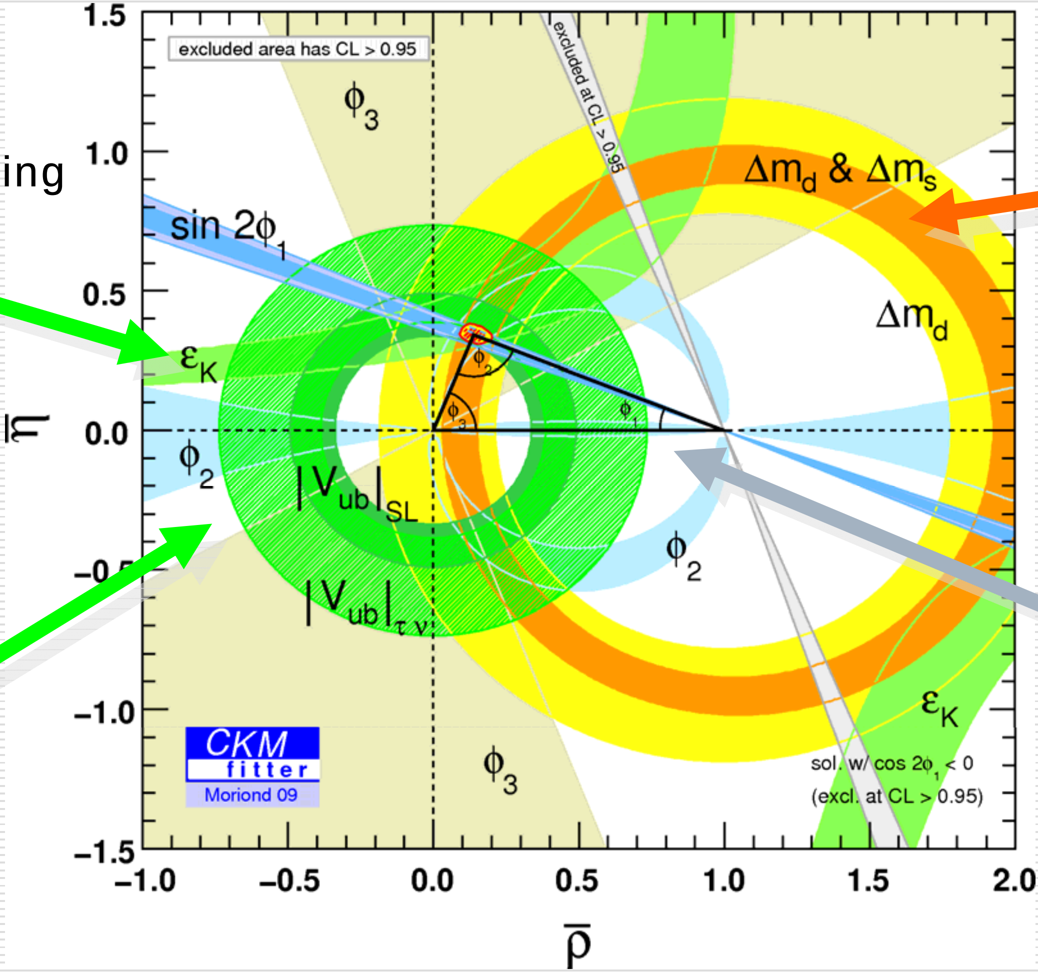
CKM matrix and lattice QCD

Neutral Kaon mixing

B_K

B-meson decays

$f_+(q^2)$



B-meson mixings

f_B, B_B

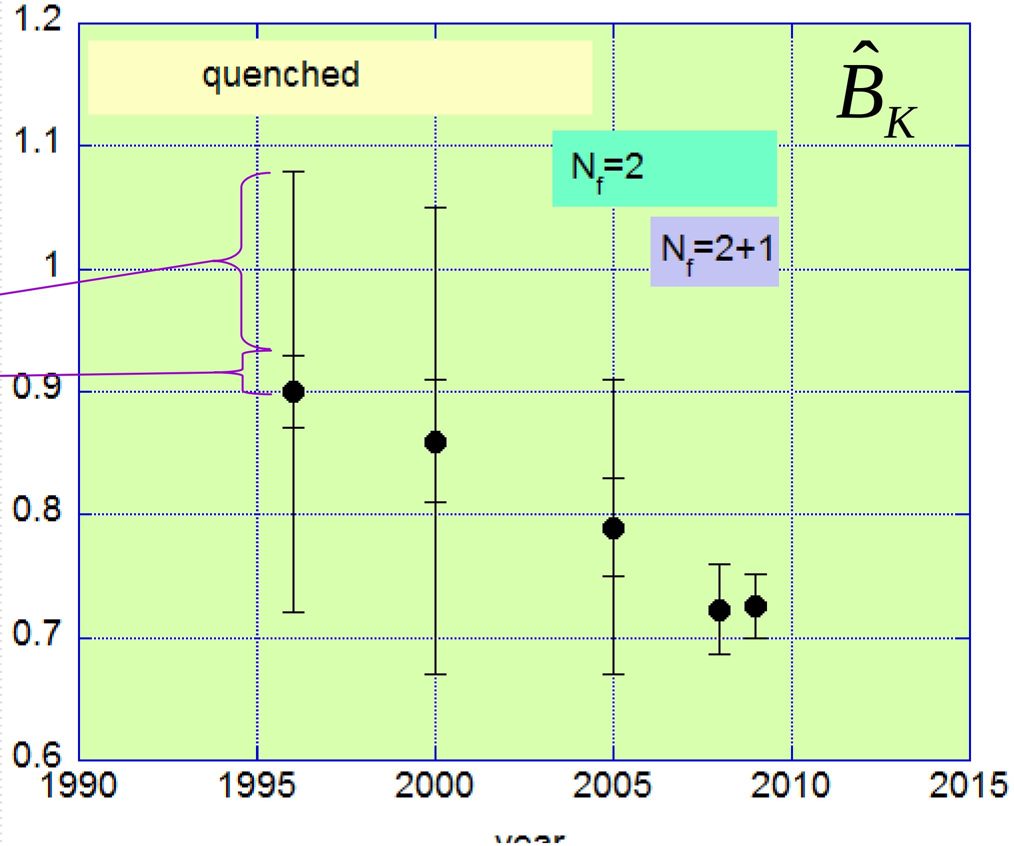
$$\xi = \frac{f_{B_s}\sqrt{B_{B_s}}}{f_{B_d}\sqrt{B_{B_d}}}$$

B->D* decays

$F(1), G(1)$

B_K over the years

- 1996: JLQCD
  - Quenched
  - Continuum extrapolated
- 2008:RBC/UKQCD
  PRL 100,0321001 (2008)
  - Nf=2+1
  - Chiral action
    DWF on DWF sea
  - one lattice spacing
- 2009:Aubin-Laiho-Van de Water
  PRD81, 014507 (2010)
  - Nf=2+1
  - Chiral action
    Overlap on staggered sea (?)
  - Two lattice spacing and Continuum extrapolated



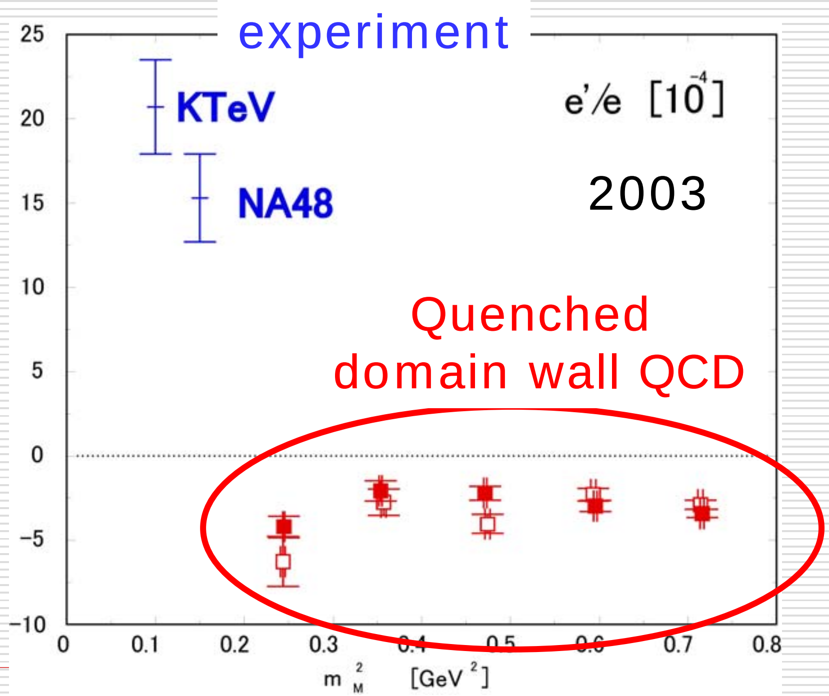
4% error of B_K is now smaller than 10% error due to $|V_{cb}|^4$ in ε_K

ε'/ε

Quenched calculation with domain-wall quark action:
RBC Collaboration, T. Blum et al, PRD68, 114506 (2003)
CP-PACS Collaboration , J. Noaki et al, PRD68, 014501 (2003)

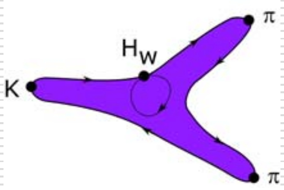
- Failure of the previous lattice calculation (2003) indicates
  - Inadequacies of Quenched approximation
  - Failure of SU(3) chiral perturbation theory
- Steady progress since then

$$\frac{\varepsilon'}{\varepsilon} = \frac{\omega}{\sqrt{2}|\varepsilon|}\left[\frac{\mathrm{Im}\,A_2}{\mathrm{Re}\,A_2} - \frac{\mathrm{Im}\,A_0}{\mathrm{Re}\,A_0}\right]$$



Finite volume framework for K→π π amplitude

C. Lellouche and M. Luescher (2001)



- Finite-size formula for direct K→π π amplitude

$$\left|A_{physical}(K\to\pi\pi)\right|^2 = 8\pi\left(\frac{E_{\pi\pi}}{p}\right)^3\left\{p\frac{\partial\delta(p)}{\partial p}+q\frac{\partial\phi(q)}{\partial q}\right\}\left|\langle K|H_W|\pi\pi\rangle_{lattice}\right|^2$$

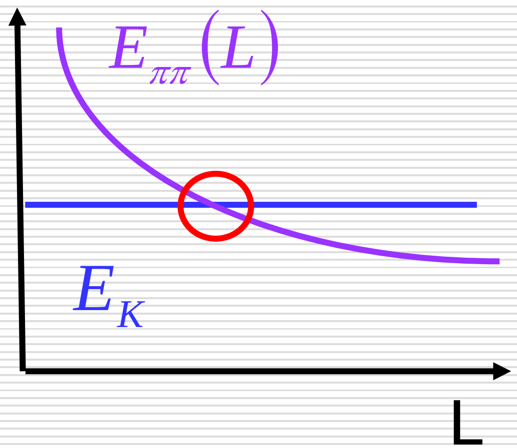
Physical amplitude — Finite volume lattice amplitude

$$p^2 = E_{\pi\pi}^2/4 - m_\pi^2,\quad q^2 = (pL/2\pi)^2$$

$$\tan\phi(q) = -\frac{q\pi^{3/2}}{Z_{00}(1;q^2)},\quad Z_{00}(1;q^2) = \frac{1}{\sqrt{4\pi}}\sum_{\vec{n}\in Z^3}\frac{1}{\vec{n}^2-q^2}$$

$$\delta(p) = n\pi - \phi(q)$$ Phase shift

Requires $E_K = E_{\pi\pi}(L)$



RBC/UKQCD attack with domain wall QCD

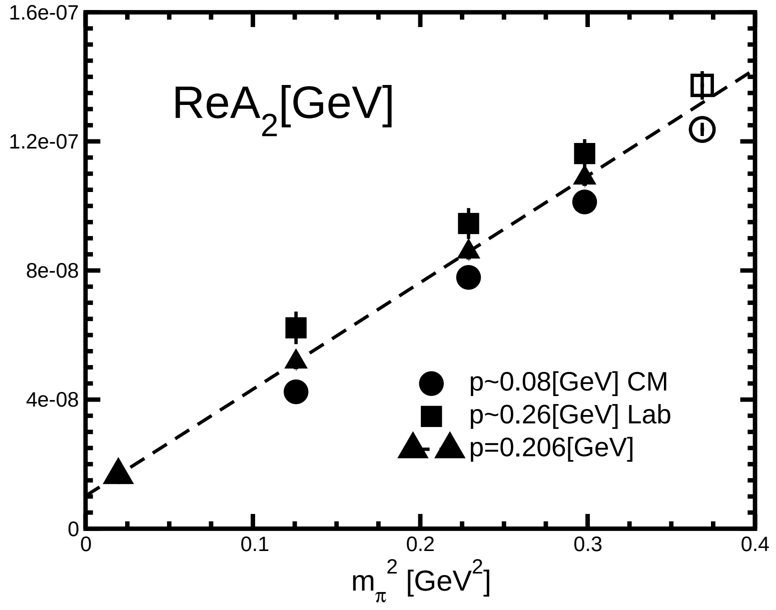
- I=2 channel analyzed in 2008

  T. Yamazaki, PRD79, 094506 (2008)

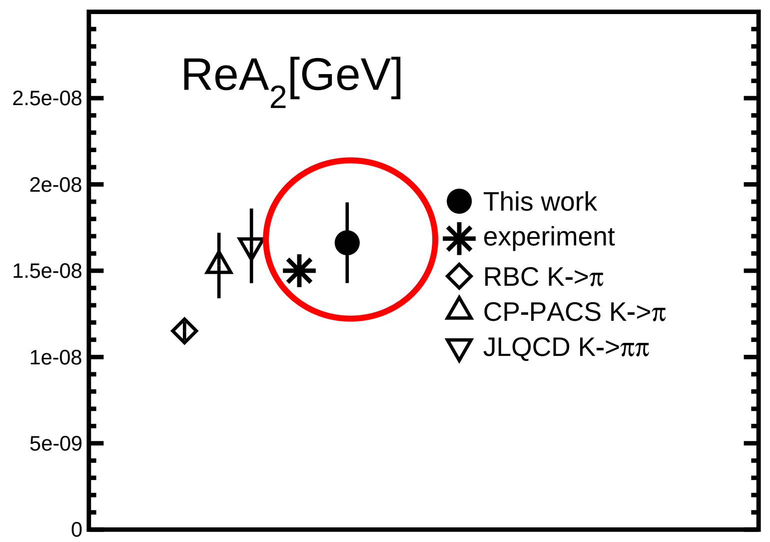
- Further work in progress to look at the amplitudes in I=2 AND I=0 channels

Talk by C. Sachrajda and Q. Liu at this Summer Institute

Pion mass dependence



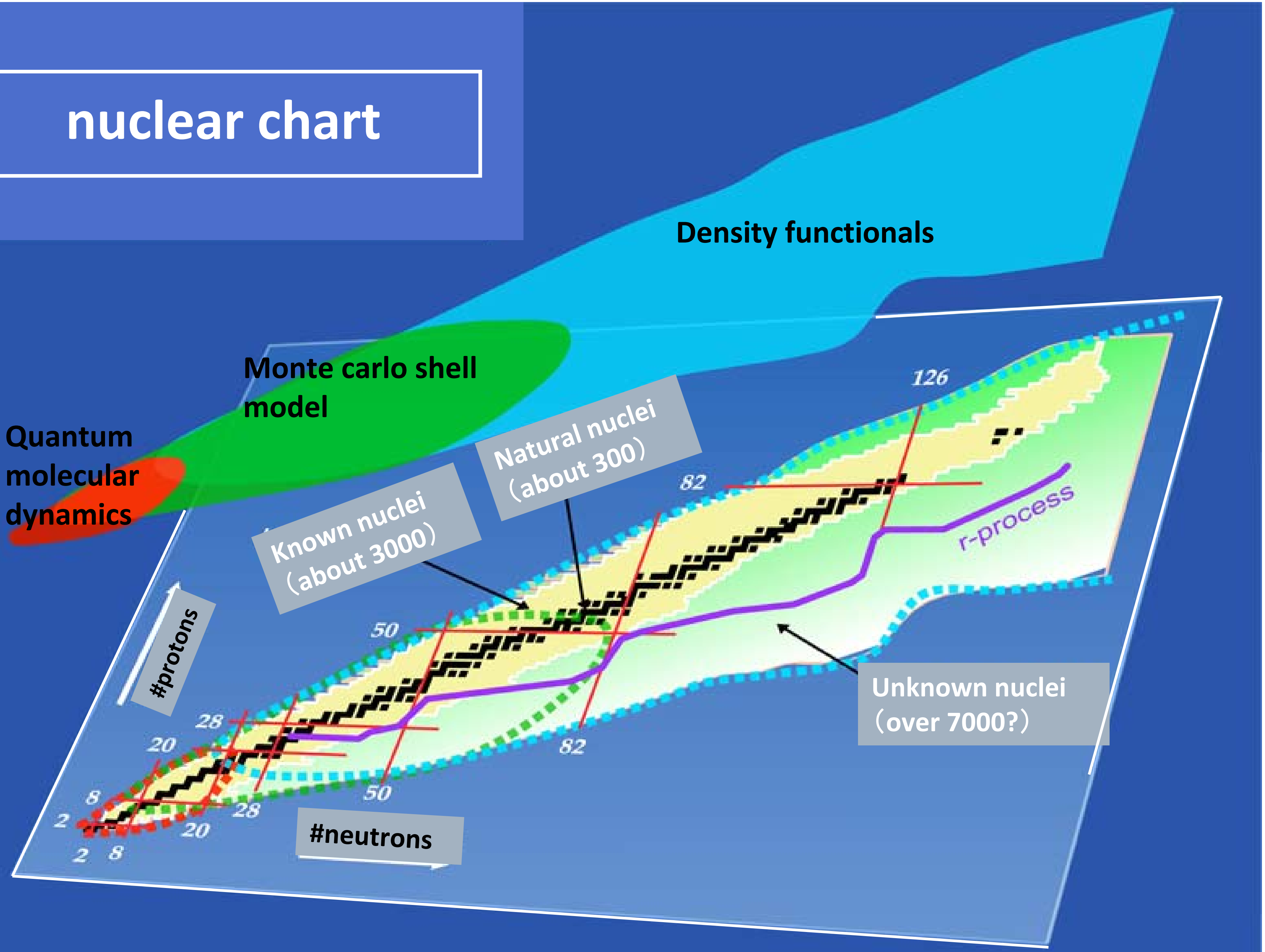
Result for I=2



Going beyond particle physics

– a trial with Helium nuclei –

nuclear chart



What should be the focus?

- Over half a century of nuclear physics has been based on effective theory of nucleons and mesons adapted to natural nuclei

  1934 Pion as origin of nuclear force H. Yukawa

  1949 shell model of nuclei Jansen-Meyer

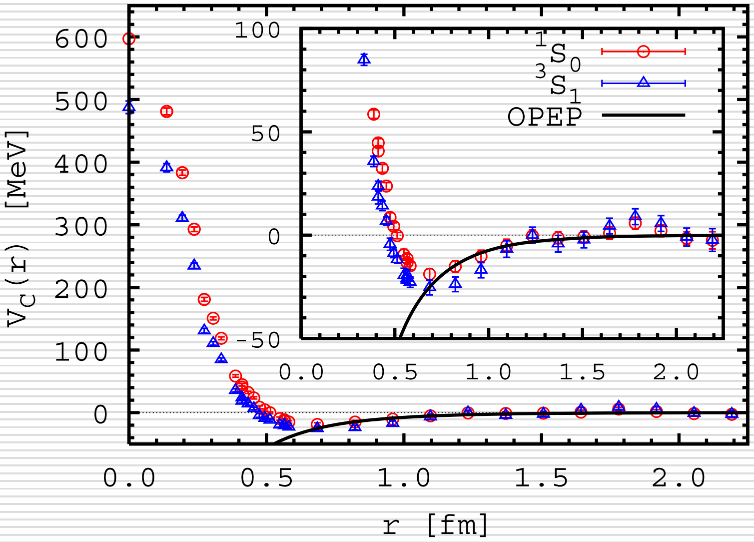
- Limitations of this approach manifest themselves in a number of ways;
  - Purely phenomenological nuclear potentials describe, but do not explain, data, e.g., hard core
  - Uncertain reliability to discuss unnatural nuclei with large/small neutron/proton ratio
  - Impossible to explore what will happen if QCD parameters are different from what they are...

Two appoaches to Nuclear physics from lattice QCD

- Nuclear properties from nuclear potentials extracted from lattice QCD

N. Ishii, S. Aoki, T. Hatsuda, PRL 99, 022001 (2007)

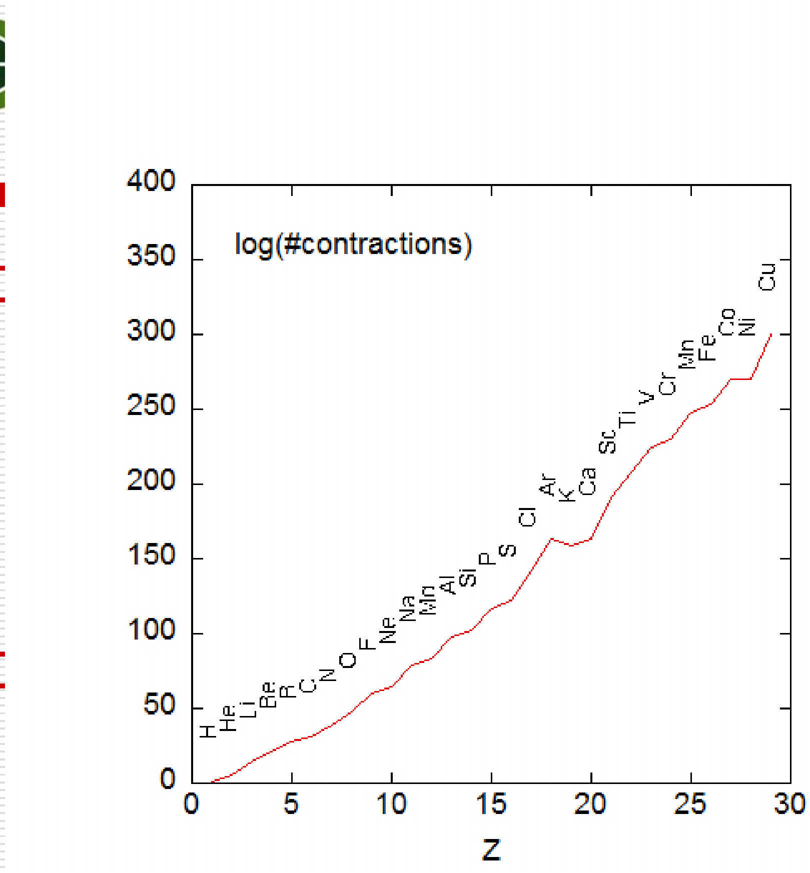
Talk by S. Aoki at this Summer Institute

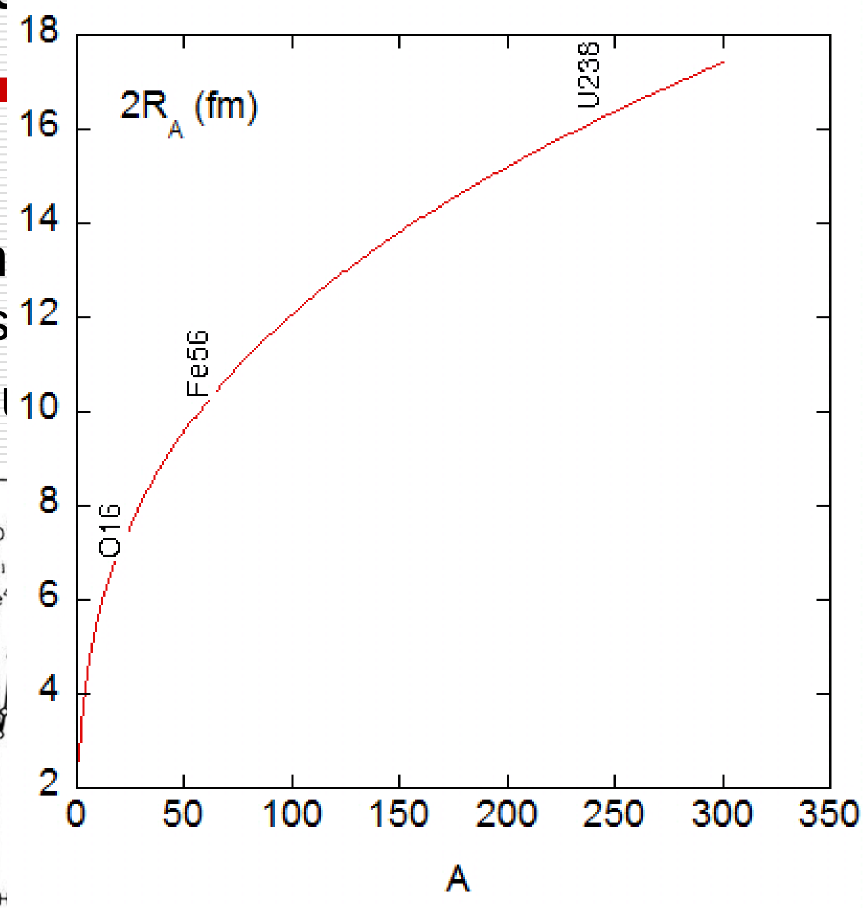


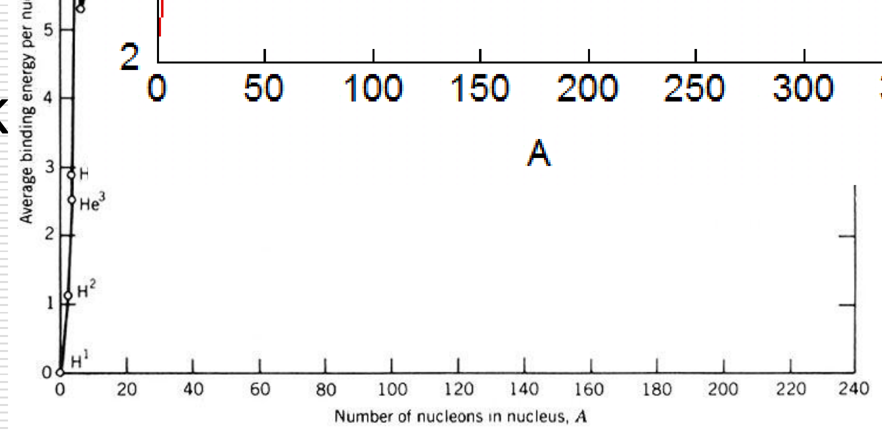
- Direct calculation of nuclear properties from quarks and gluons

T. Yamazaki, Y. Kuramashi, A. ukawa, PRD81, 111504 (2010)

e direct approach







ndin

ass

natu

- Large number of quark

$$N_{up}! \times N_{down}!$$

A trial with Helium nuclei

- First "real" nuclei and a large binding energy (easiest of the lot?)
- First and foremost issue to address:

  "Is the system of 2 protons and 2 neutrons a bound state?"
- Use standard lattice methods
  - Extraction of energy difference from helium correlation function

$$\frac{\langle He(t)\cdot He(0)\rangle}{\langle p(t)\cdot \bar{p}(0)\rangle^2 \langle n(t)\cdot \bar{n}(0)\rangle^2} \xrightarrow{t\to\infty} \exp\left(-\underbrace{\left(m_{He} - 2m_p - 2m_n\right)}_{\Delta E} t\right)$$

  - Finite volume studies to distinguish if bound state or scattering state

Issue of fermion contractions

- #contractions counted naively

$$N_u! \times N_d!$$

$$He \quad 6! \times 6! = 512{,}000 \quad \rightarrow \quad 1{,}107$$

$$He^3 \quad 5! \times 4! = 2{,}880 \quad \rightarrow \quad 93$$

- Reduction using
  - symmetries
    - neutron ⇔proton, neutron ⇔ neutron in He operator
    - Ispspin: all proton ⇔ all neutron
  - Calculate two contractions simultaneously
    - up ⇔ up in proton or down ⇔ down in neuron
  - Further reduction using blocks of three quark propagators

Simulations and results

- Quenched calculation with heavy pion mass

$$a = 0.13\,fm \quad m_\pi = 0.8\,GeV \quad m_N = 1.6\,GeV$$

- Three volumes to examine size dependence

L	$L(fm)$	N_{conf}	$N_{meas}/conf$
24	3.1	2,500	2
48	6.1	400	12
96	12.3	200	12

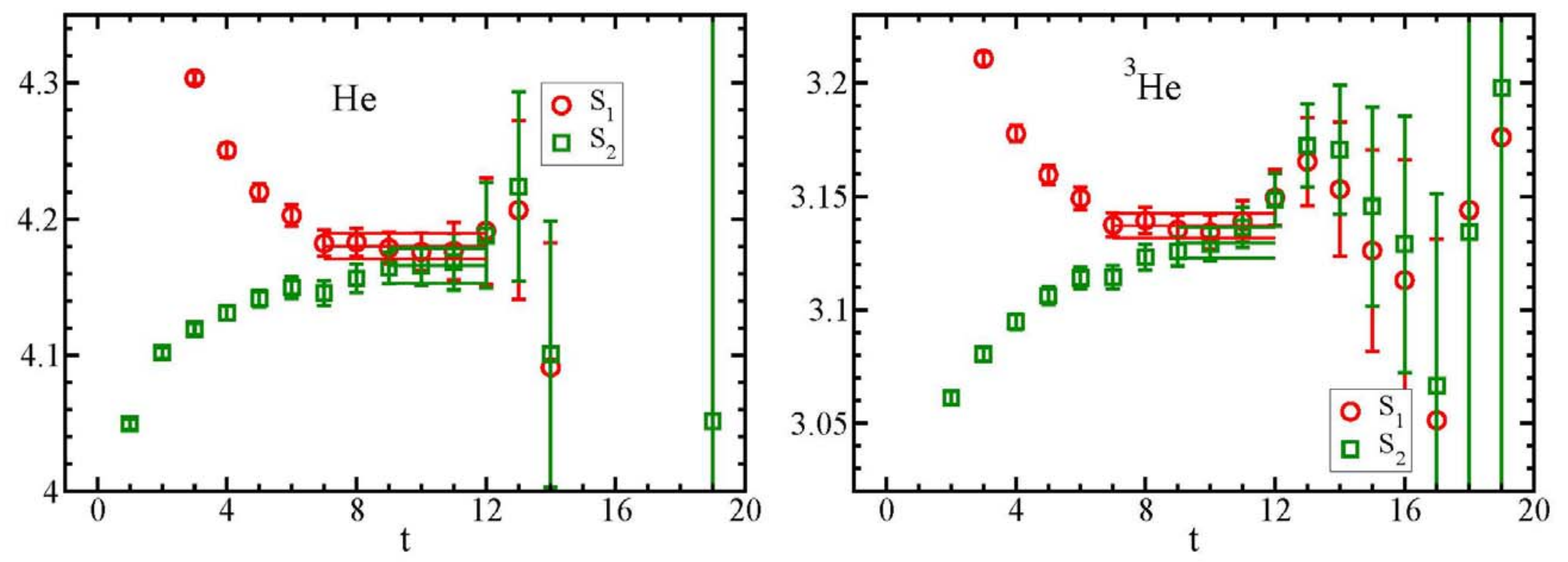
- Two expontially smeared sources

$$q(\vec{x}) = A \cdot \exp(-Br)$$

	S_1	S_2	L
(A,B)	$(0.5,0.5)$	$(0.5,0.1)$	24
(A,B)	$(0.5,0.5)$	$(1.0,0.4)$	48,96

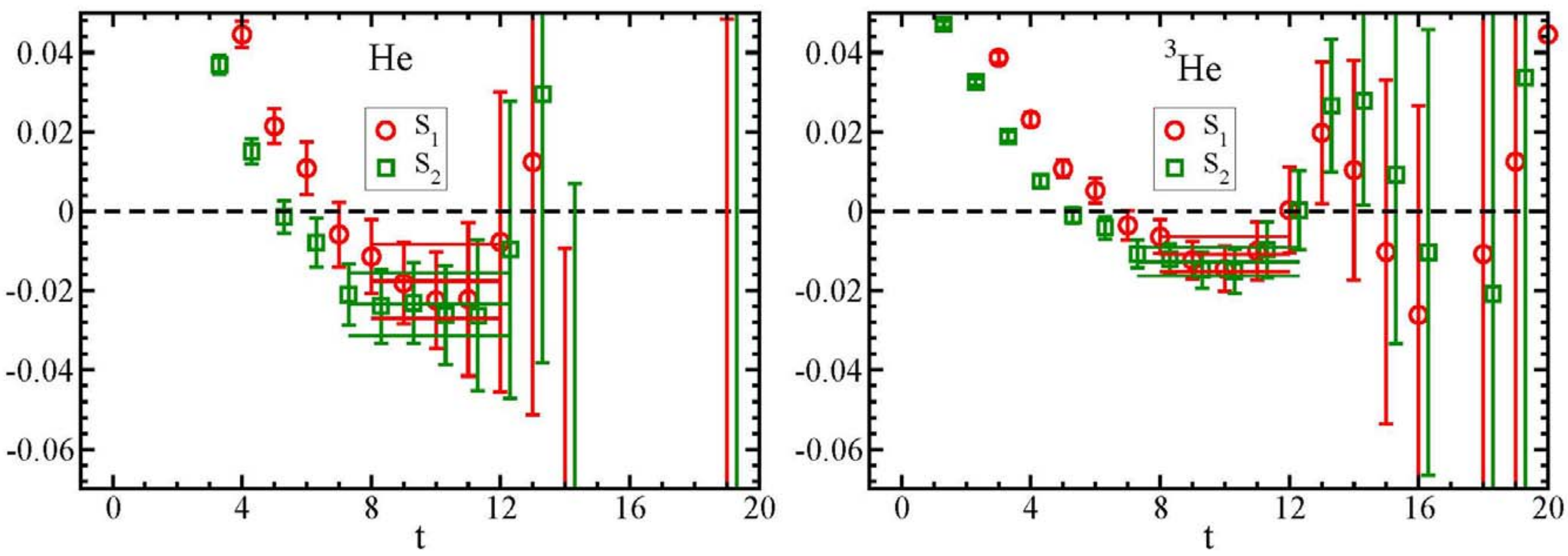
Effective mass plot for He and He^3 for L=24

$$\Delta m_L(t) = \log\left(\frac{C(t)}{C(t+1)}\right), \quad C_{He}(t) = \left\langle He(t)\overline{He}(0)\right\rangle, \quad C_{He^3}(t) = \left\langle He^3(t)\overline{He}^3(0)\right\rangle$$



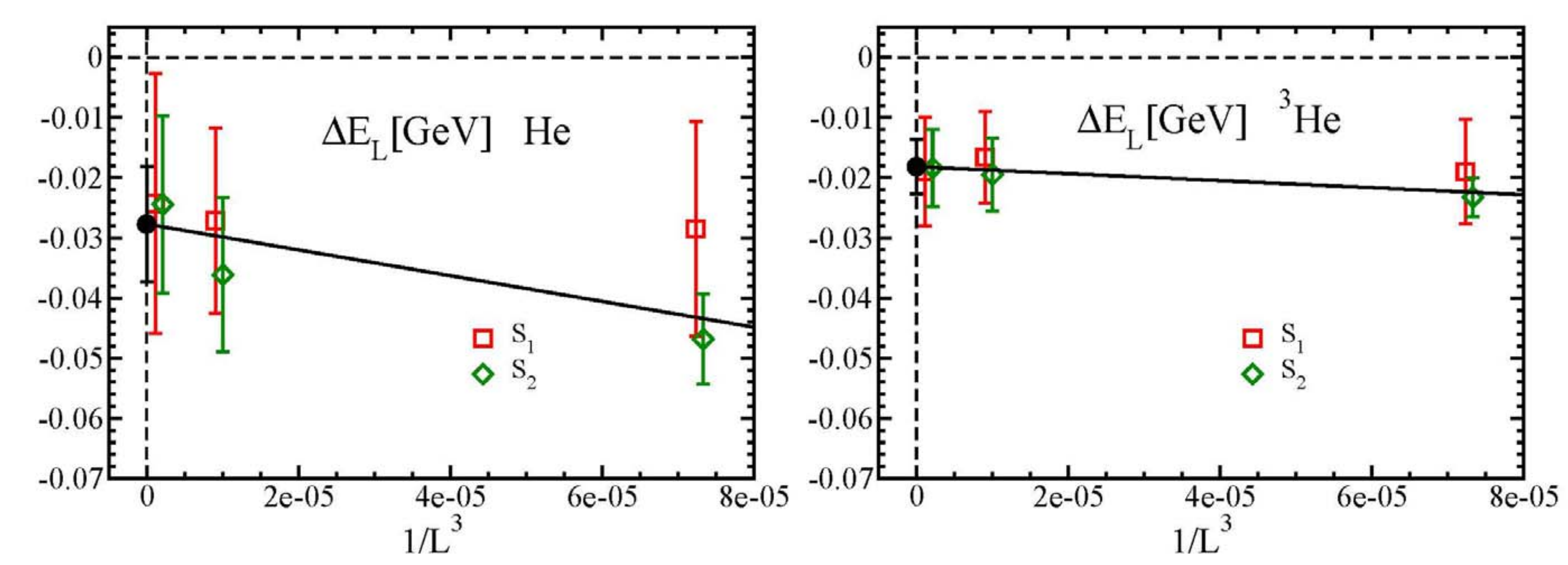
Effective energy difference for L=48

$$\Delta E_L(t) = \log\left(\frac{R(t)}{R(t+1)}\right), \quad R_{He}(t) = \frac{C_{He}(t)}{C_N(t)^4}, \quad R_{He^3}(t) = \frac{C_{He}(t)}{C_N(t)^3}$$



Size dependence of energy difference

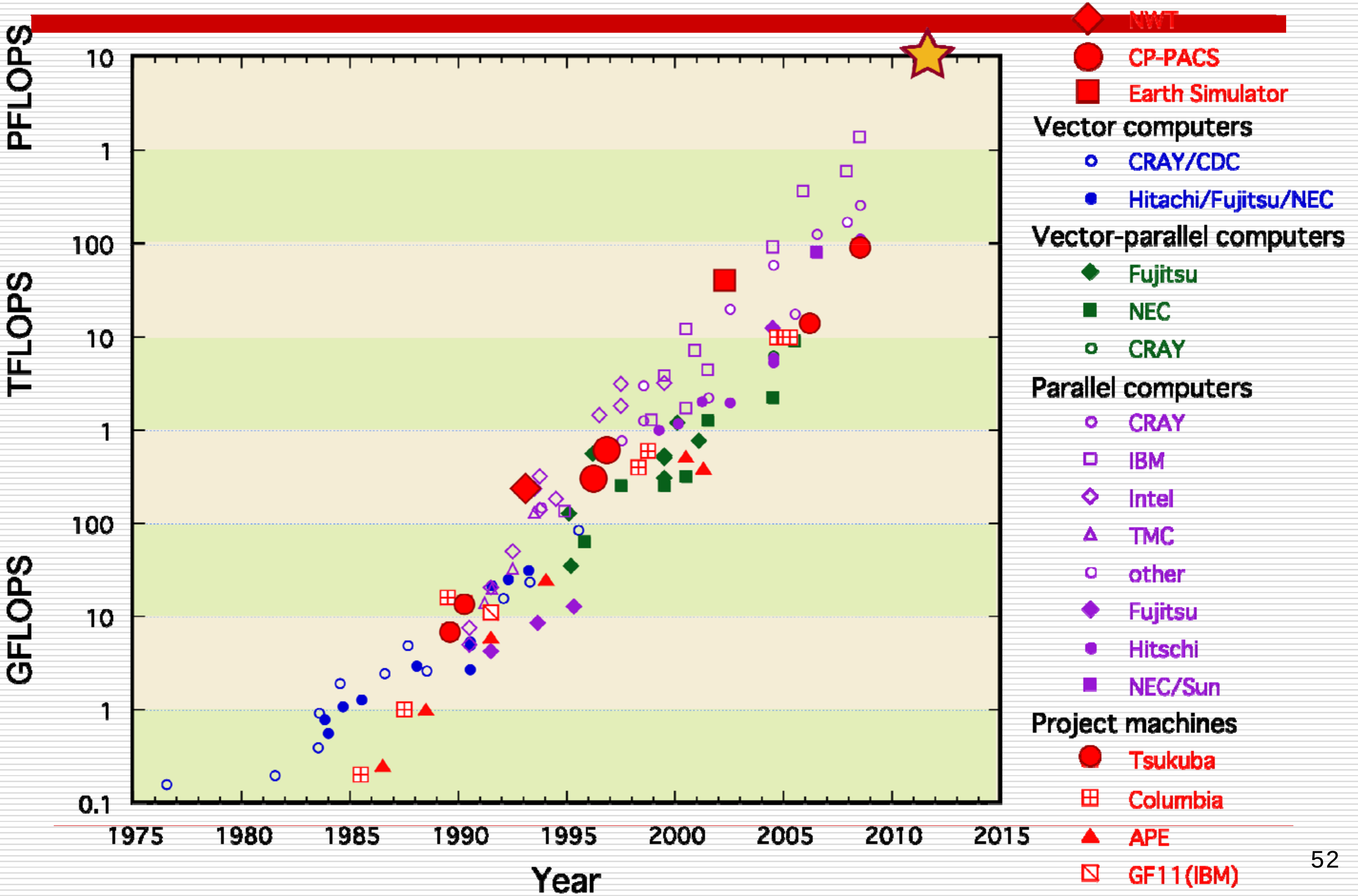
- Negative energy difference in three volumes
- Small volume dependence
- Non-zero intercept at 1/L^3=0 suggests a bound state



Status of the Japanese 京"Kei" Supercomputer Project

1京=10 Peta in the Japanese counting system

Supercomputers trends



Background: our government plan

- 3rd Science and Technology Basic Plan FY2006-2010

  "Next-generation supercomputing technology" was selected as one of *the key technologies of national importance*

  → Development of the 京"Kei" Supercomputer

  Cf. other key technologies:

  Free electron laser, ocean and earth observation and exploration, rapid breeder reactor, space technologies

- 4th Science and Technology Basic Plan FY2011-2015 (now under discussion)
  - Exaflops class HPC Technology

    New chip device, software, hardware...

京"Kei" Project outline

- Goals:
  1. Development of 10 Pflops-class system
  2. Development of grand challenge applications in nano science and life science
  3. Buildup of a research center in computational science
- Project period
  - Japanese FY 2006 to 2012
- Project budget
  - 115.4 B¥ (about 1B Euro)
- Institution responsible for the computer R&D
  - RIKEN

Original schedule of the Project

Big jolt in November 2009

		JFY2006	JFY2007	JFY2008	JFY2009	JFY2010	JFY2011	JFY2012
System R&D		Conceptual design	Detailed design (JFY2007–JFY2008)		Prototyping/evaluation/production (JFY2009–JFY2011)			Tuning
Grand Challenge Applications	Nano applications	R&D and evaluation (JFY2006–JFY2010)					verification	
	Life applications	R&D and evaluation (JFY2006–JFY2010)					verification (JFY2011–JFY2012)	
Building	Computer building	Design (JFY2006–JFY2007)	Construction (JFY2007–JFY2009)					
	Research building		Design (JFY2007–JFY2008)	Construction (JFY2008–JFY2009)				

Political turmoil in Japan since last summer

31 August 2009

Landslide victory by People’s Democratic Party (first real change of power since 1951)

18 September:

“Government Revitalization Unit (GRU) ” is set up; starts reexamination of FY2010 budget

13 November:

GRU Working Group, after an 1-hour public hearing, recommends ***freezing of the Supercomputer Project*** ; many science & technology budget also recommended cut.

Late November-early December:

appeals by many academic communities against the GRU’s reccomendation

16 December:

Government decides to proceed with the Project

Bitter lessons from the incident

- Revolutionary change of the Japanese political landscape
  - With the old Democratic Party, science and technology was an uncontested budget area
  - This is no more with the People's Democratic Party; it puts priority on policies closer to people, e.g, healthcare, subsidies to child care etc
- Hard times lie ahead for basic science
  - New science and technology policy is geared heavily towards environment ("green") and life related policies
  - Severe financial situation makes big projects a liability in policy making
- Strong support from "people" is becoming overridingly important and essential.

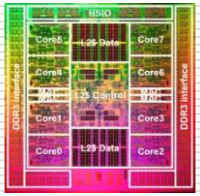
京"Kei" computer

System Configuration

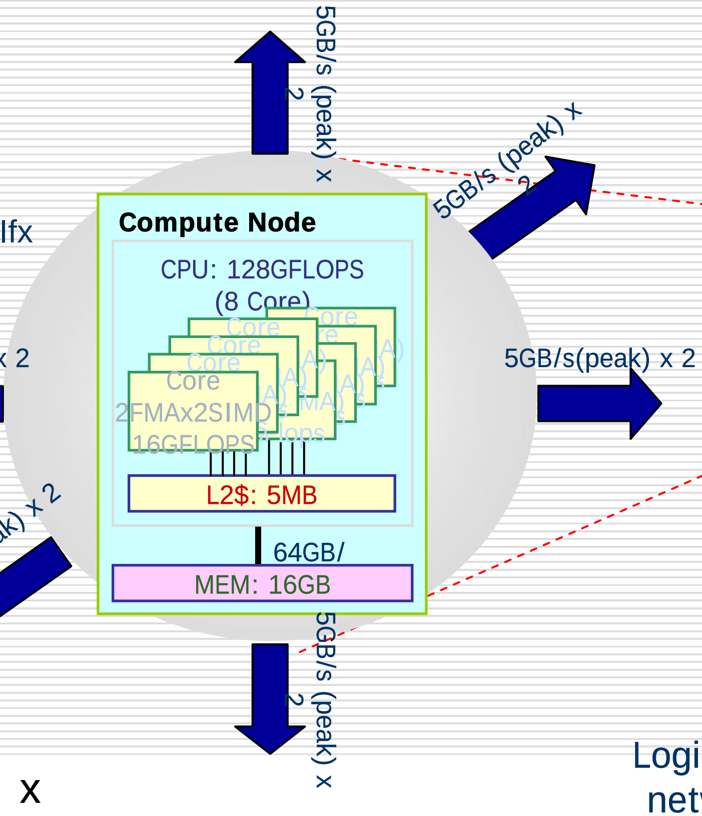
Compute Nodes and network

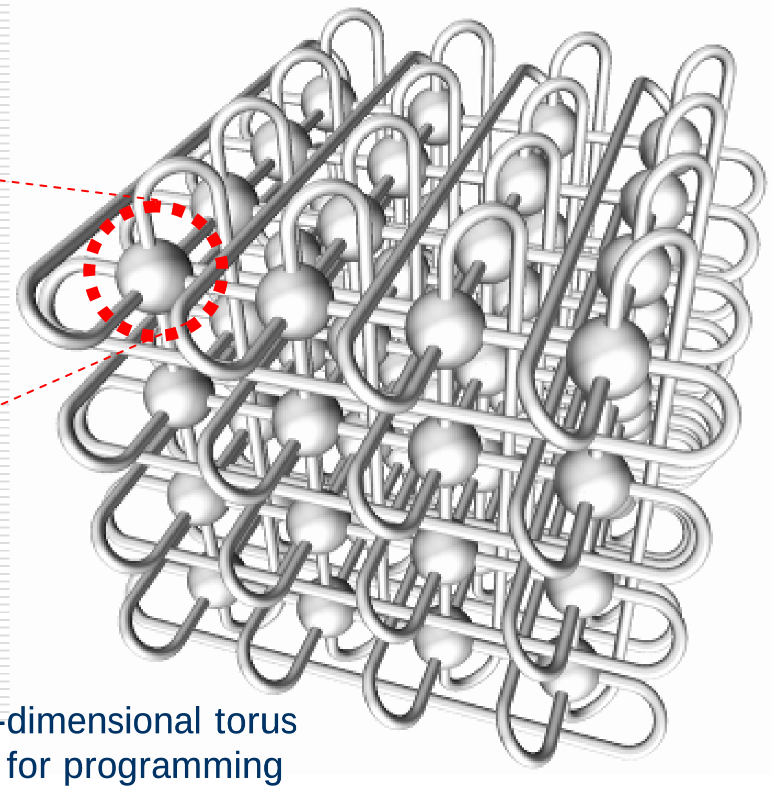
- #compute nodes (CPUs): > 80,000
  - #cores: > 640,000
- Peak performance: > 10PFLOPS
- Memory: > 1PB (16GB/node)

- Logical 3-dimensional torus network
- Peak bandwidth: 5GB/s x 2 for each direction of logical 3-dimensional torus network
- bi-section bandwidth: > 30TB/s



SPARC64[TM] VIIIfx





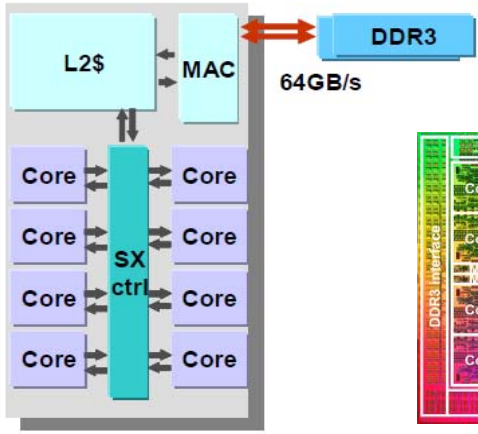
Logical 3-dimensional torus network for programming

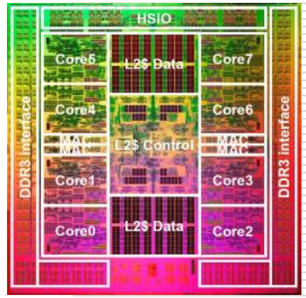
Courtesy of FUJITSU Ltd.

CPU Features (Fujitsu SPARC64™ VIIIfx)

16GF/core(2*4*2G)

- 8 cores
- 2 SIMD operation circuit
  - 2 Multiply&Add floating-point operations (SP or DP) are executed in one SIMD instruction
- 256 FP registers (double precision)
- Shared 5MB L2 Cache (10way)
  - Hardware barrier
  - Prefetch instruction
  - Software controllable cache
    - Sectored cache
- Performance
  - 16GFLOPS/core, 128GFLOPS/CPU





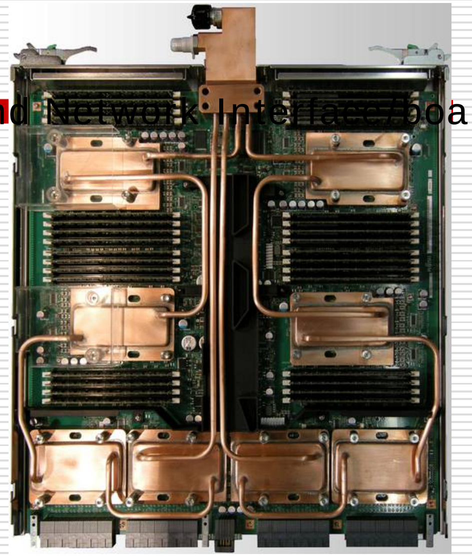
45nm CMOS process, 2GHz
22.7mm x 22.6mm
760 M transisters
58W(at 30℃ by water cooling)

Reference: SPARC64™ VIIIfx Extensions
http://img.jp.fujitsu.com/downloads/jp/jhpc/sparc64viiifx-extensions.pdf

System board and rack

- 4 CPU and 4 ICC (network chip)/board
  467x554mm
- 24 boards (96 CPU's)/rack
  796mm×750mm×2060mm

4 CPU and Network Interface board



System Board

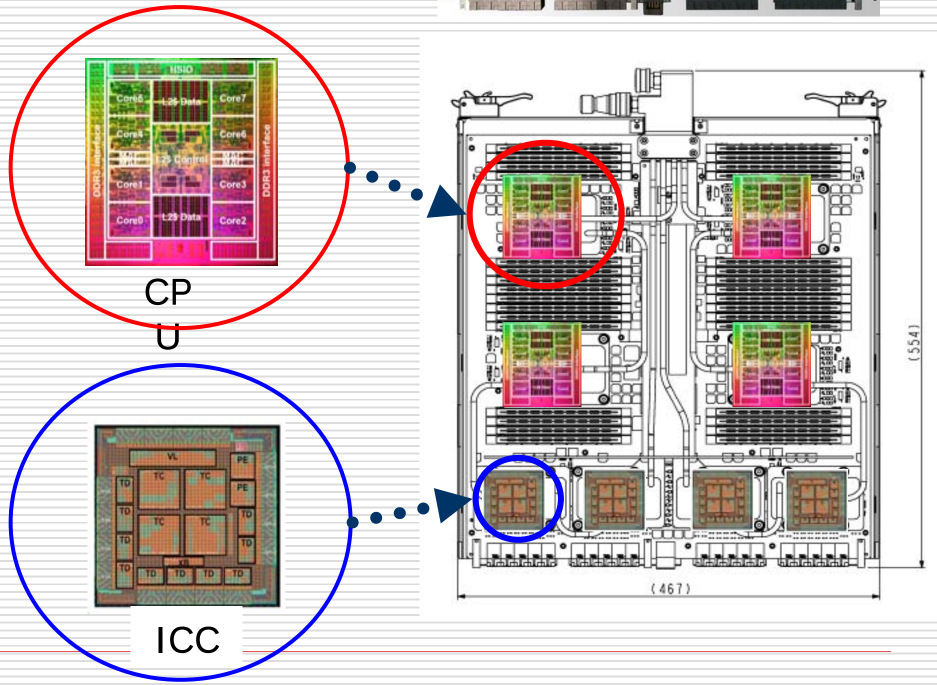
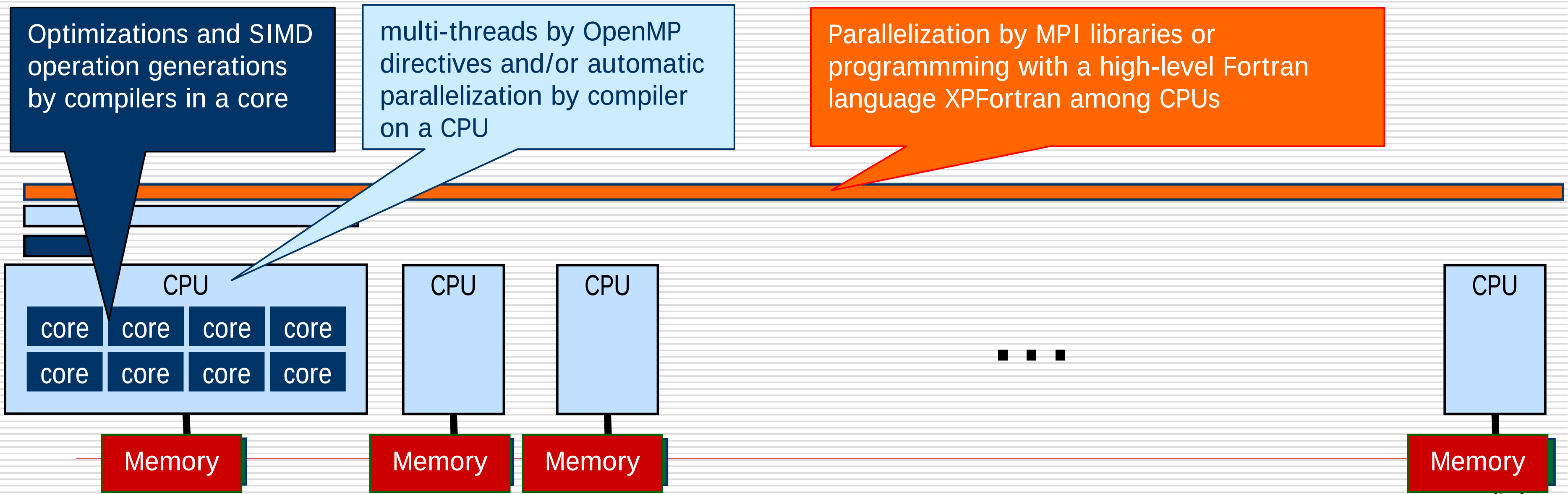


Photo courtesy FUJITSU Limited

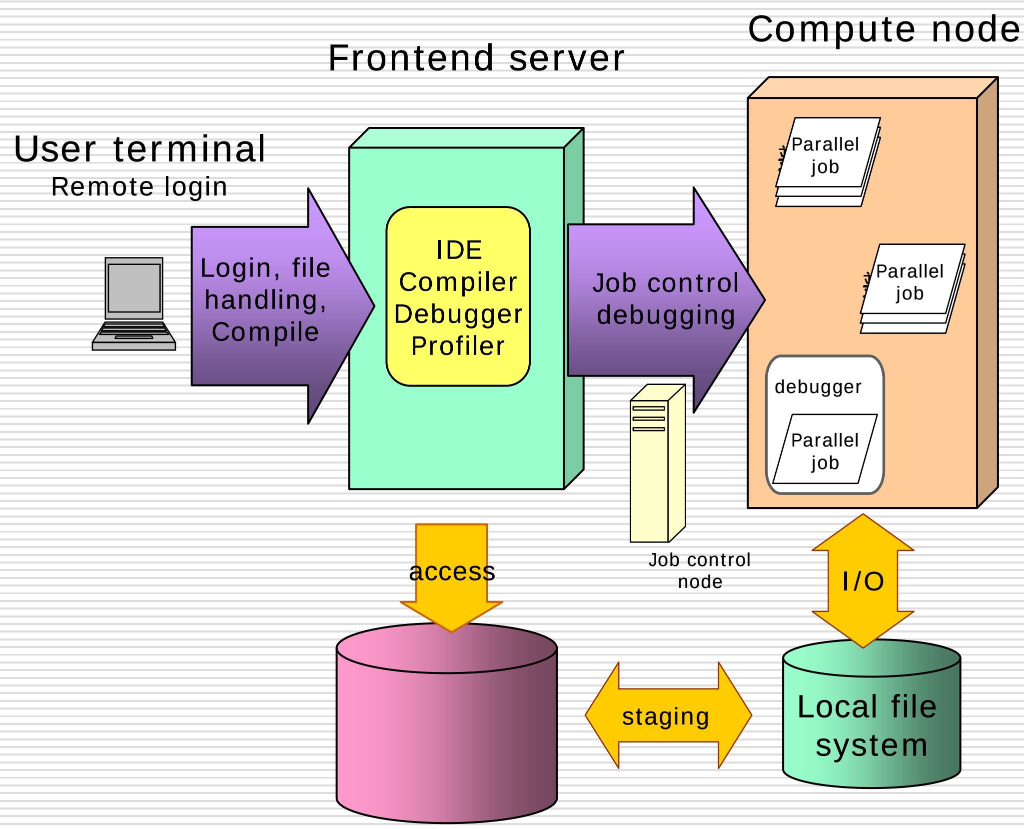
Programming features

- Hybrid programming model with multi-threads and MPI
- Fortran 2003, XPFortran , C, C++
- Optimized compiler (SIMD/256 FP registers/sector cache)
- MPI based on MPI-2.1 specification
- Numerical libraries (BLAS, LAPACK, FFTW, SSL-II (Fujitsu Library)
- Debugger and Profiler

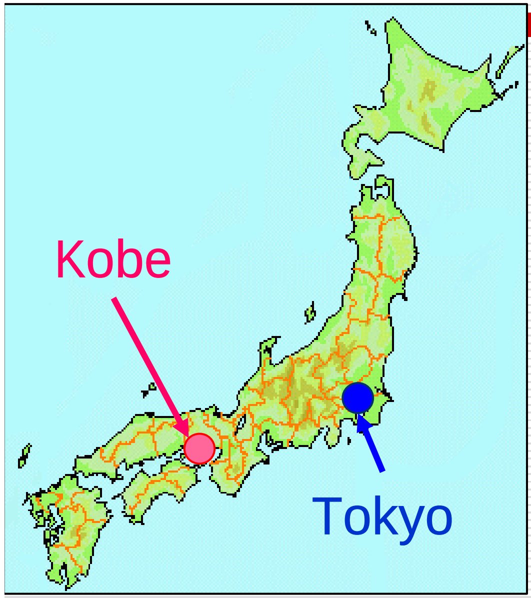


System environment

- OS: Linux-based OS on compute nodes
- File system: 2-level (local/global) system
  - Permanent user files on the global system
  - directly accessible via NSF-like system from frontend server
  - Staged in/out to local system for job execution

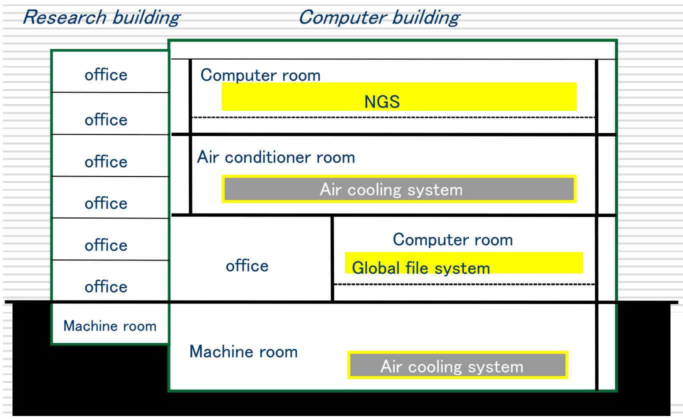


Cite for the 京"Kei" Supercomputer

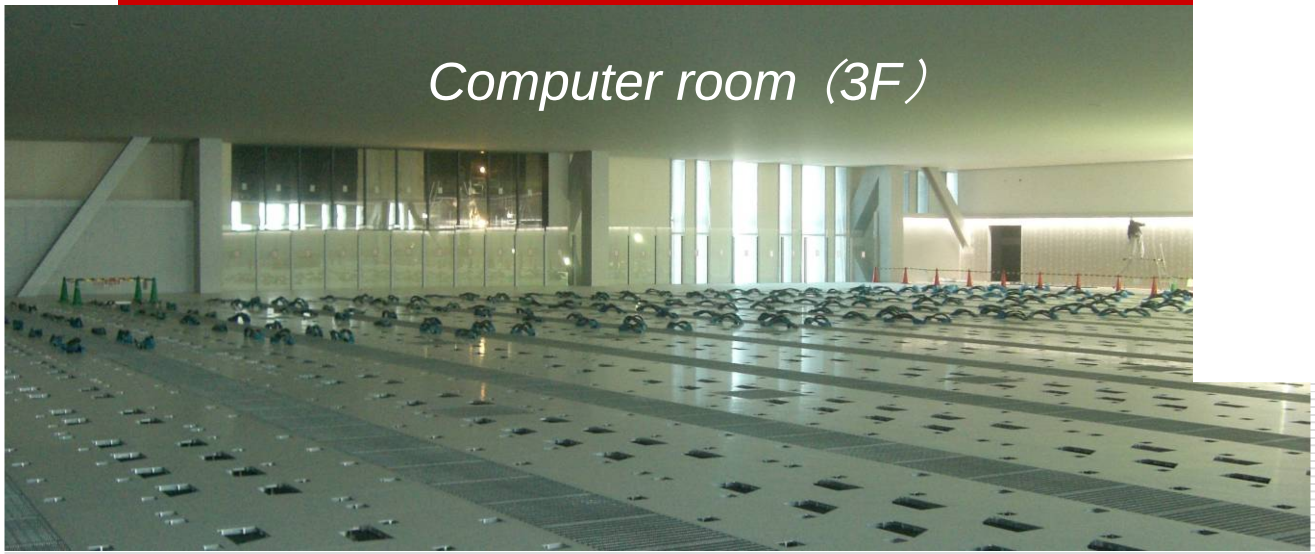


450km (280miles)
west from Tokyo

Photo of building (completed May 2010)



Inside the building



Computer room（3F）

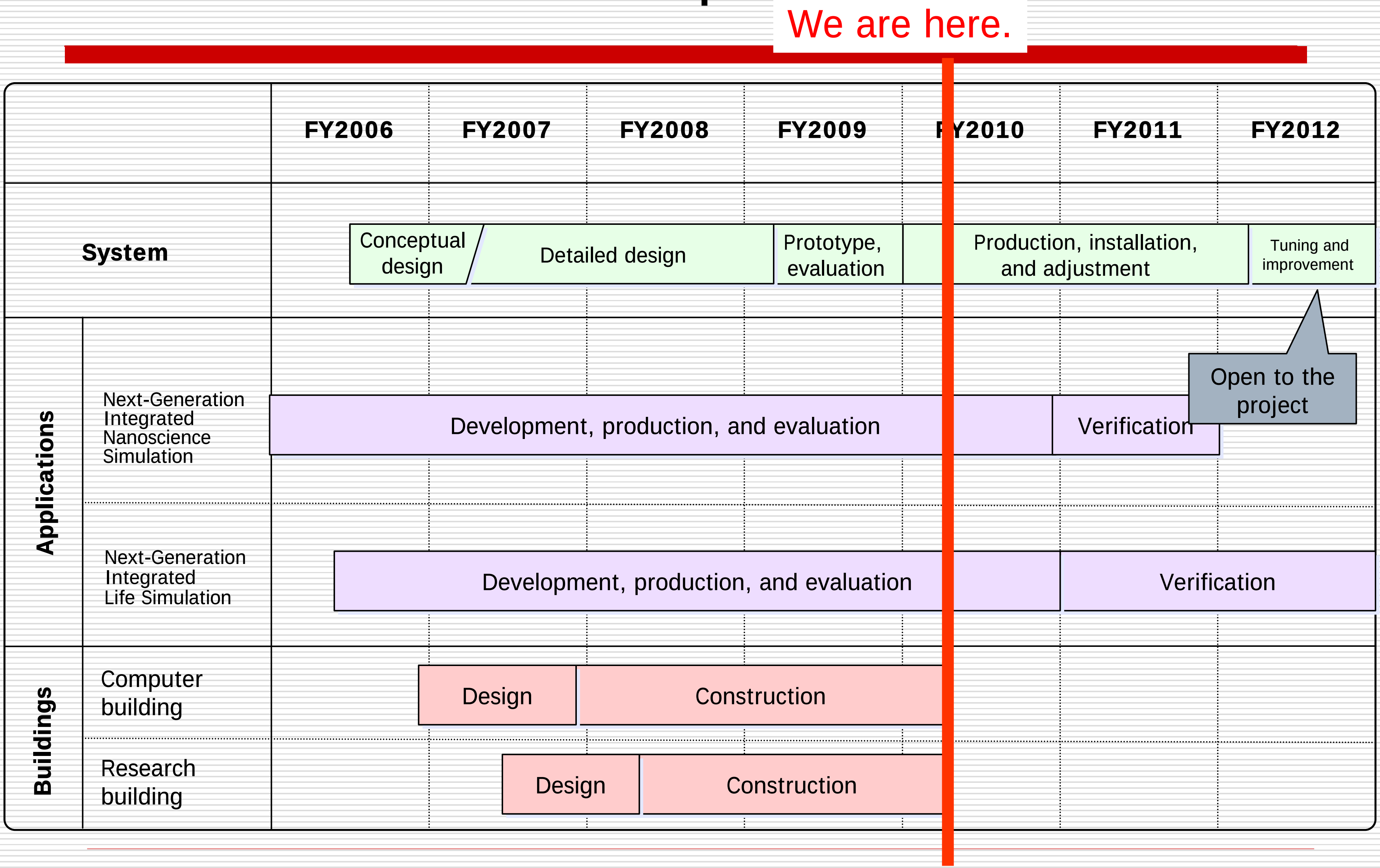
Making a double floor

Research building

Chillers

Solar panels on the top

Schedule of the project



Related developments

- New Institute for Computational Science in Kobe
- Strategic Field Program for 京"Kei" computer

  - Strategic Usage of 京"Kei" -

New Institute in Kobe

“Advanced Institute for Computational Science”

- Size and emphasis
  - About 100 researchers
    - 2/3 in various areas of computational science
    - 1/3 in computer science
    - basic science (particle physics) will be one of the core groups
  - Strong collaboration between computational and computer science
- Location
  - Kobe on site of the 京”Kei” computer
- Schedule
  - Official foundation date : June 2010
  - Research groups to start in October 2010

"Strategic Field Program" for 京"Kei"

In order to put 京"Kei" computer to strategic use,

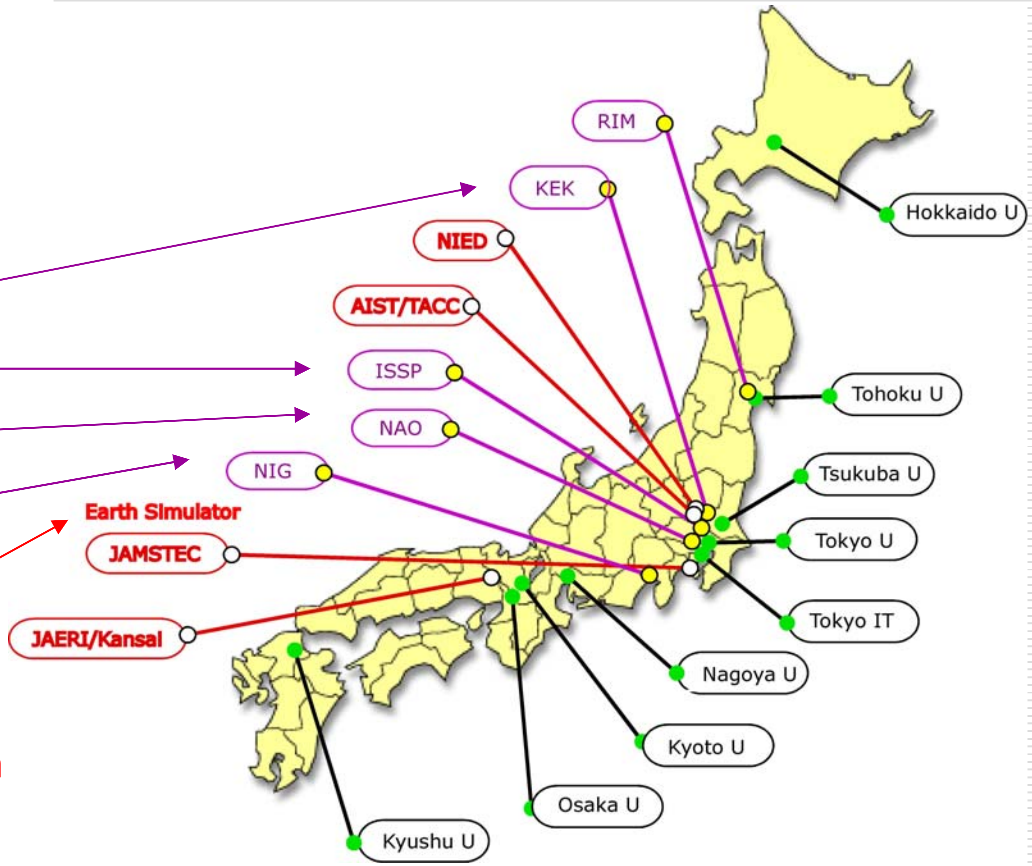
- Government selected *5 strategic fields* in science and technology
- For each field, Government selected a *core institute.*
- Each core institute is responsible for organizing *research and supercomputer resources in the respective field and its community*, for which they receive
  - priority allocation of 京"Kei" resources
  - funding to achieve the research goals
- Project period : JPF2011～2015

Supercomputer installation in Japan

- **Computer Centers of major universities**
- Academic research institutions/organizations

  Each major field has its own supercomputer facility e.g.,
  - High energy physics
  - Condensed matter physics
  - Astrophysics
  - Genetics/bioinformatics
- Government labs
  - AIST/JAEA/NIMS....
  - Earth Simulator

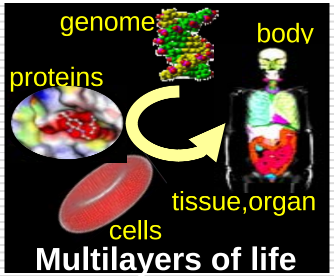
    belongs to JAMSTEC (Japan Marine science and Technology Center)

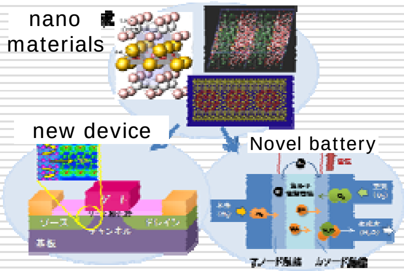


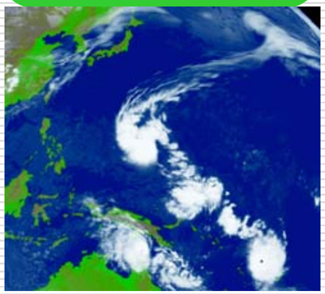
“Strategic Fields” and “core institutes”

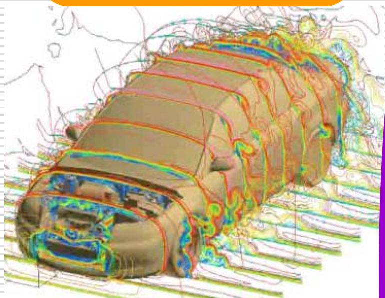
strategic field

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 Insdutry	Basic science Community
Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources

Strategic field "Matter and Universe"

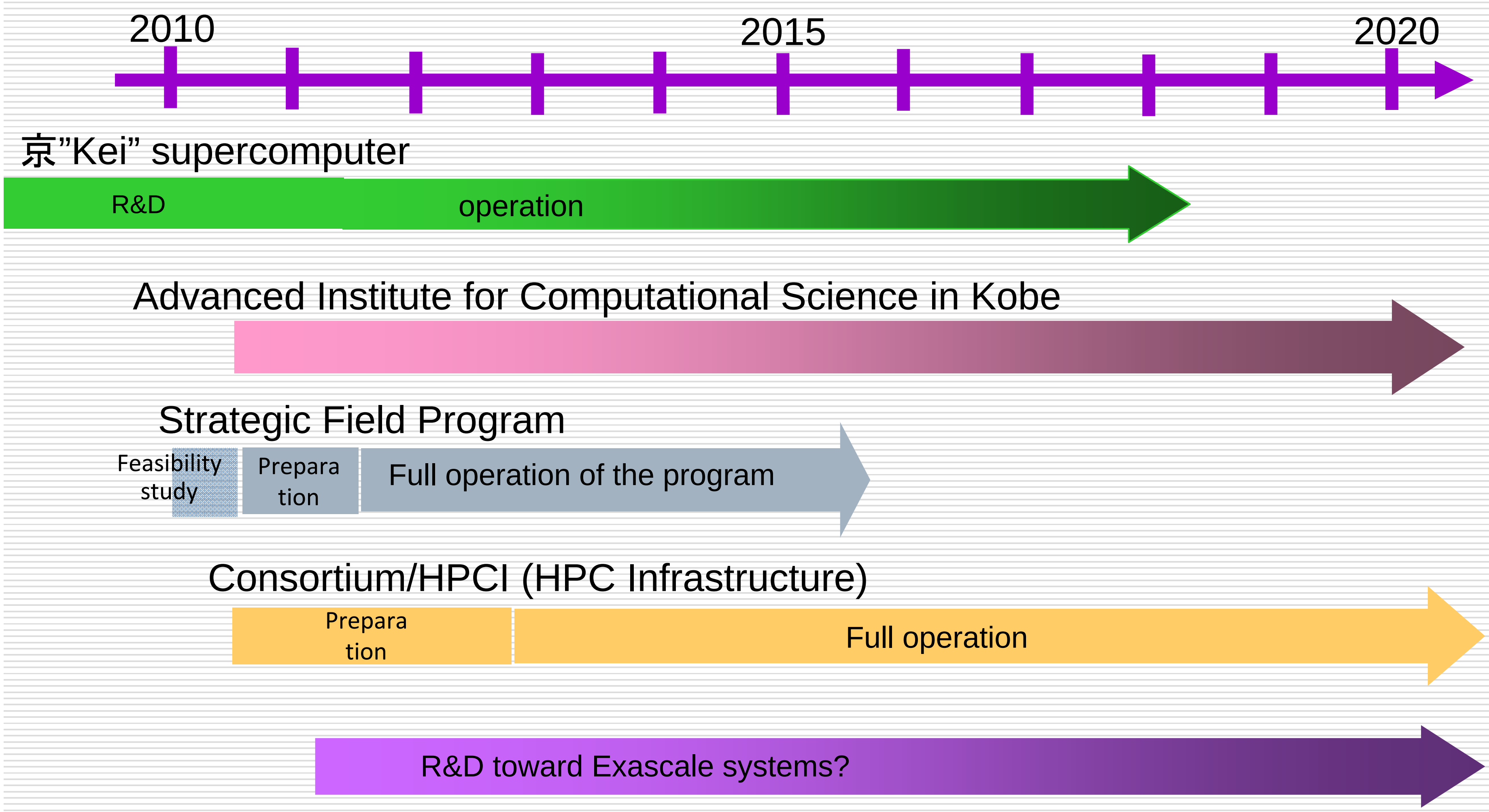
- Unified field of particle physics, nuclear physics and astrophysics
- Core institute

  "Federation for computational fundamental science" :
  virtual federation of
  - Center for Computational Science, Univ. of Tsukuba
  - High Energy Accelerator Research Organization (KEK)
  - National Astronomical Observatory (NAO)
- Leadership: next-generation is taking the lead
  - Leader Sinya Aoki(Tsukuba)
  - Subleaders

    Jun-ichiro Makino (NAO) research planning

    Shoji Hashimoto (KEK) organization
- Lattice QCD is a main emphasis of the field

Next 10 years in Japan



Conclusions

Lattice QCD perspective

- *Realistic calculation directly at the physical point is finally reality; change of philosophy from "simulation" to "calculation"*
- *There are still a number of difficulties, but we expect fundamental issues of lattice QCD as particle theory make major progress over the next five year range*
- *And the vast area of multi-hadron systems/atomic nuclei lies in wait for exploration*

Computational science perspective

- *Lattice QCD is a theory endeavor, but it has aspects distinct from "pencil and paper" theoretical research:*
  - Need of involvement in R&D of supercomputers and related HPC infrastructure such as data grid
  - Need of communal planning and collaboration for efficient use of those expensive HPC resources
- *I expect these aspects to become increasingly important to pursue advancement of our field*
- *Non-science issues including public understanding will also become more and more important, as we in Japan learned with a big jolt last December.*