4 October 2011
German-Japanese Workshop
Modern Trends in QCD

Lattice QCD and High Performance Computing in Japan

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Japan

- eastern Japan Great earthquake
- quarks, hadrons, nuclei and lattice QCD
- Japanese “K” computer Project
- summary

Eastern Japan Great Earthquake

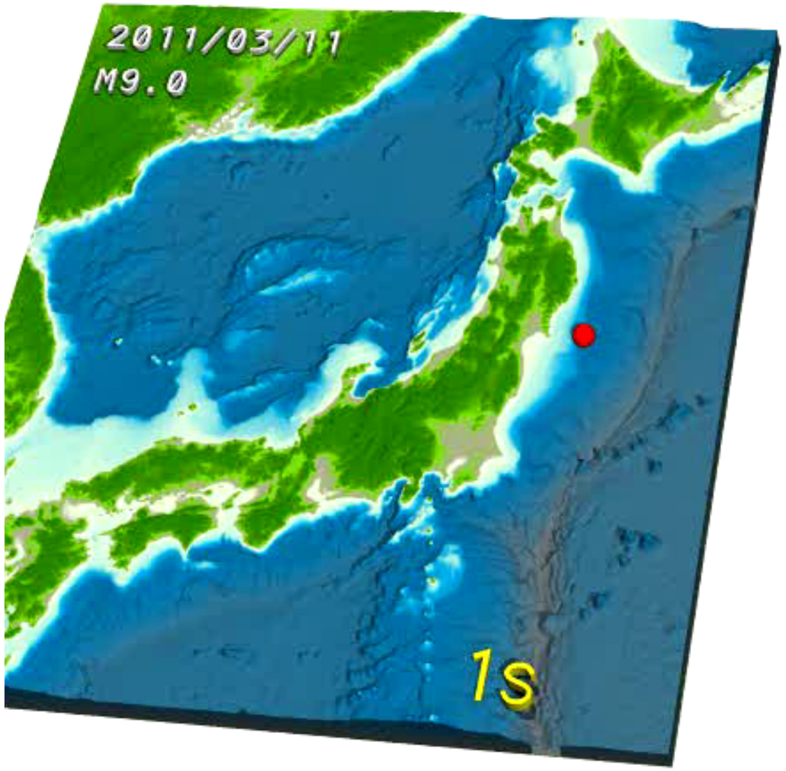
- Triple disasters
  - The earthquake 14:46 JST on 11 March
  - The tsunamis 15:00-16:00 on 11 March
  - The Nuclear Power Plant 11 – 15 March

- Human loss and damages
  - 15,805 died, 4,040 still missing (over 0.2% of the area population), 75,000 still relocated from home
  - 222,905 houses destroyed; 454,711 damaged
  - 22,000 ships lost (80% in the area)/300 sea ports damaged
  - 24,000ha farmland damaged by tsunami (2.6% in the area)
  - Total damage estimated at 300B$

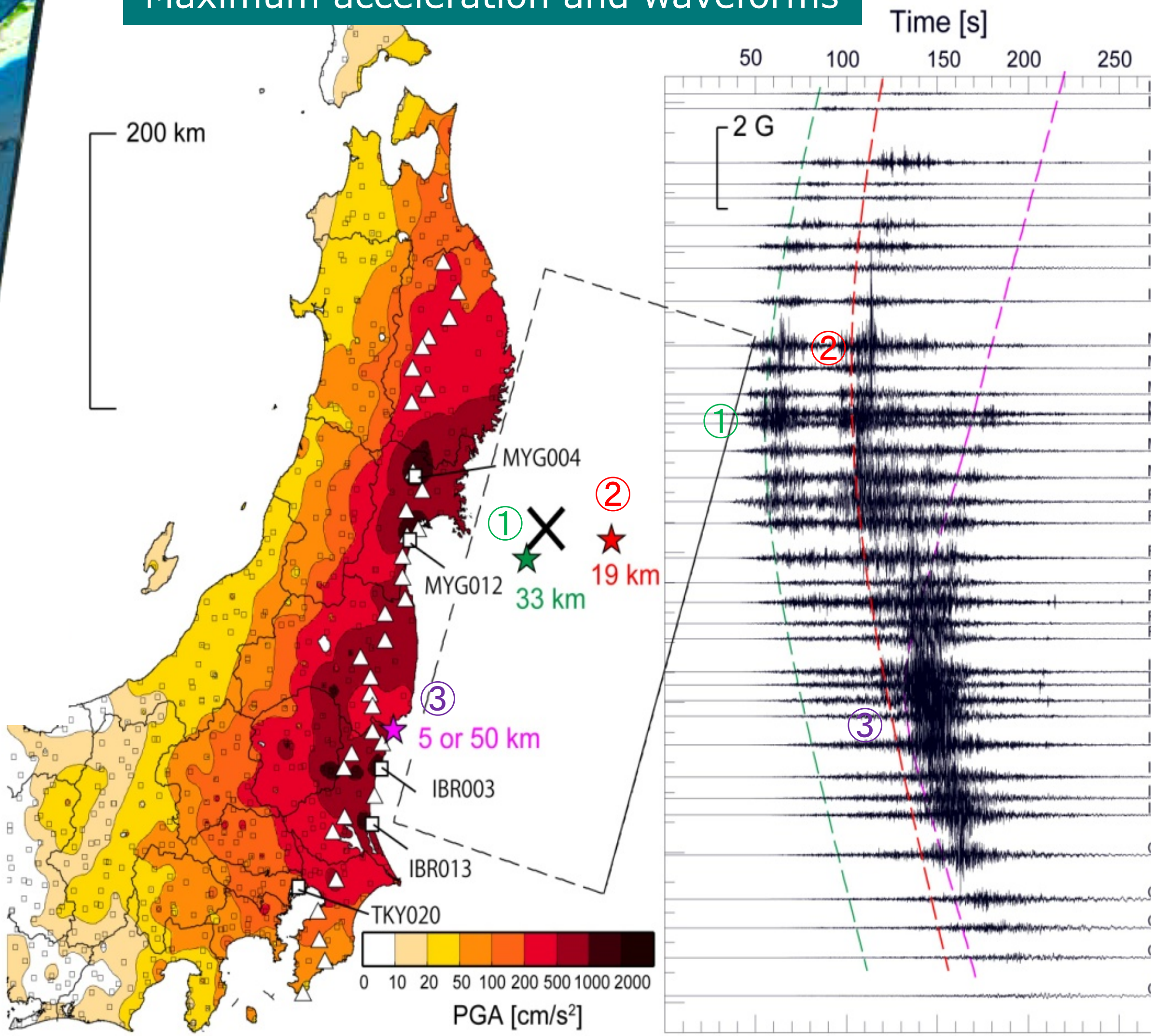
- Wish to provide a snapshot from computational science point of view

The earthquake had a strong and long time shaking

Courtesy: T. Furumura (U. Tokyo)



Maximum acceleration and waveforms



NIED K-NET/KiK-net strong shaking data collected at about 1800 sites

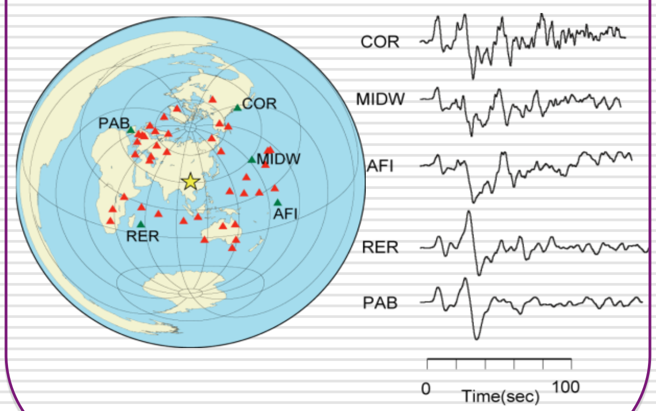
NIED: National Research Institute for Earth Science and Disaster Prevention

Seismic source inversion analysis

Courtesy: Y. Yagi (U. Tsukuba)

- From observed wave form,

Observed waveform at point x



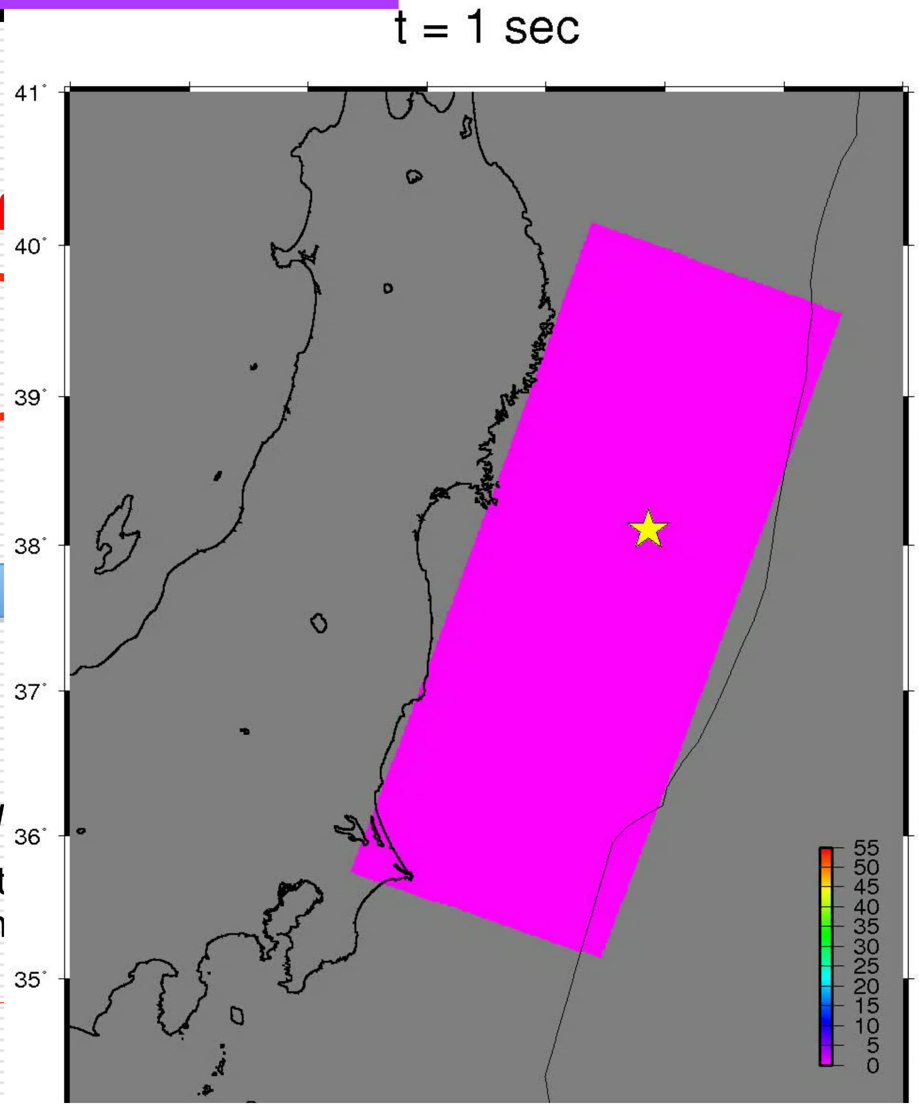
Wave f

$u(x,$

Yagi & Fukahata (2011, *Geophys. J. I*

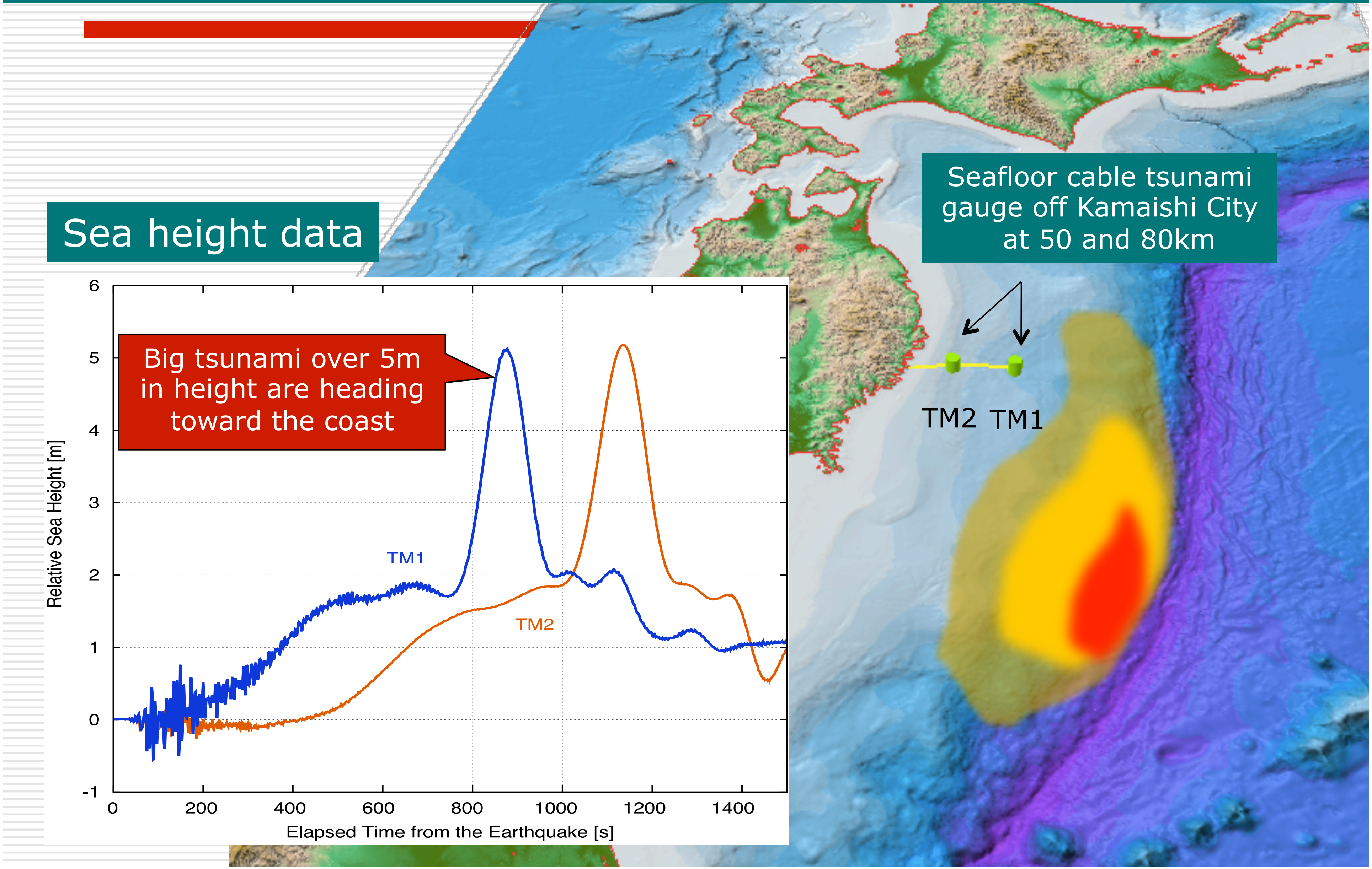
First estimate of M9.0 made on 12 March

Accumulated slip



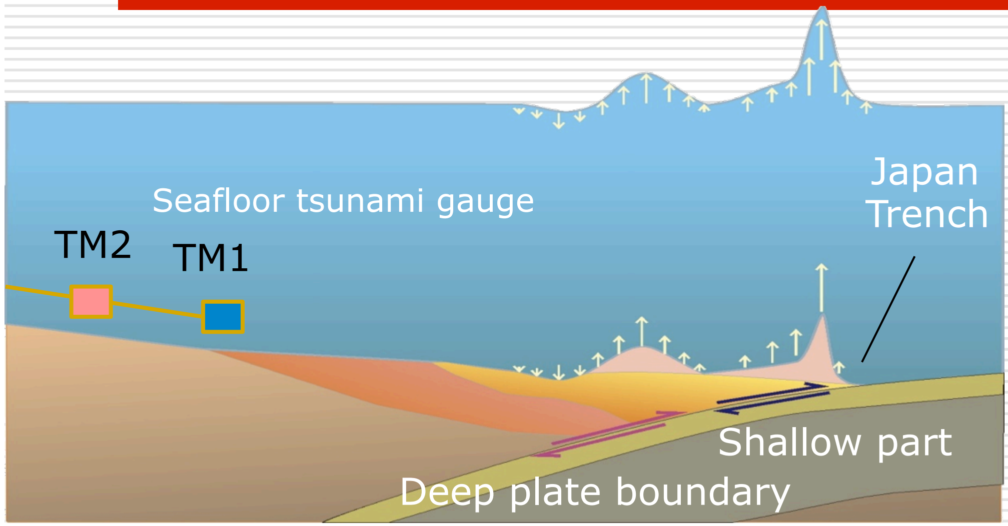
The tsunamis were captured by seafloor pressure gauge

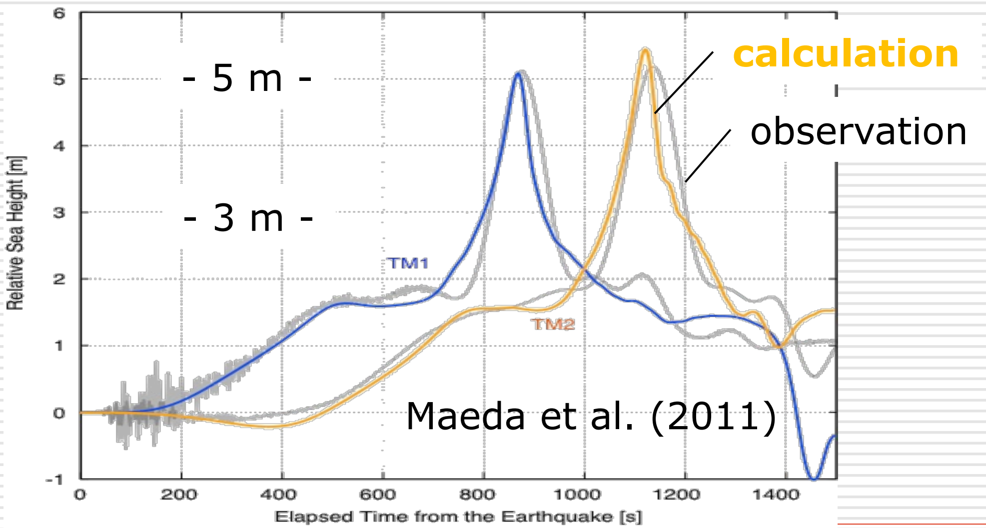
Courtesy: T. Furumura (U. Tokyo)



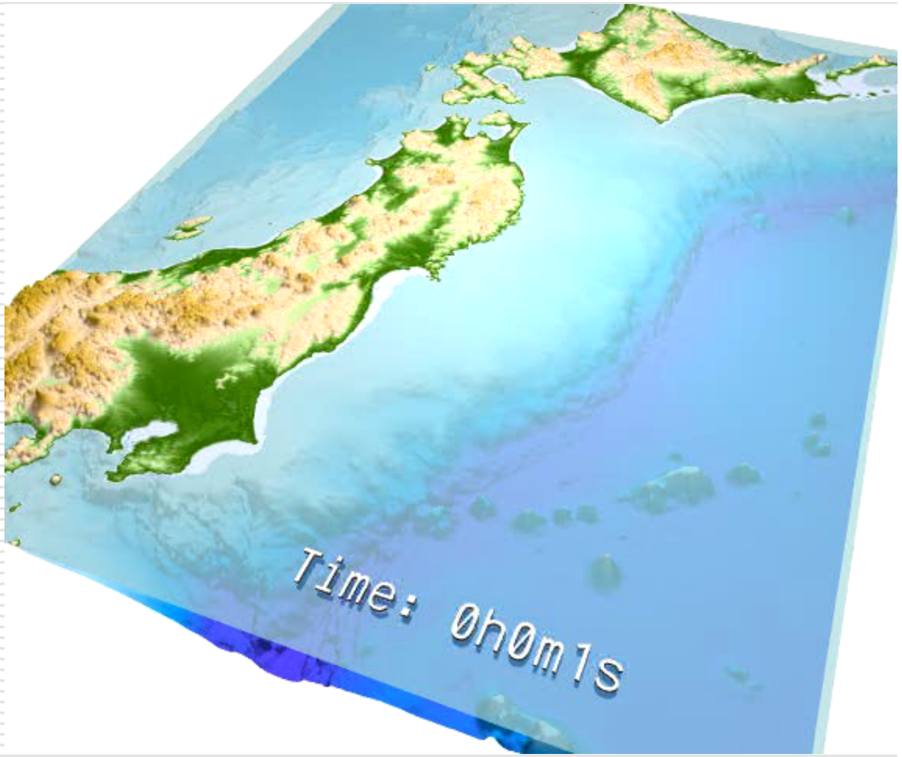
The combination of deep and shallow plate slips generated the big tsunamis

Courtesy:
T. Furumura (U. Tokyo)





Coupled earthquake tsunami simulation



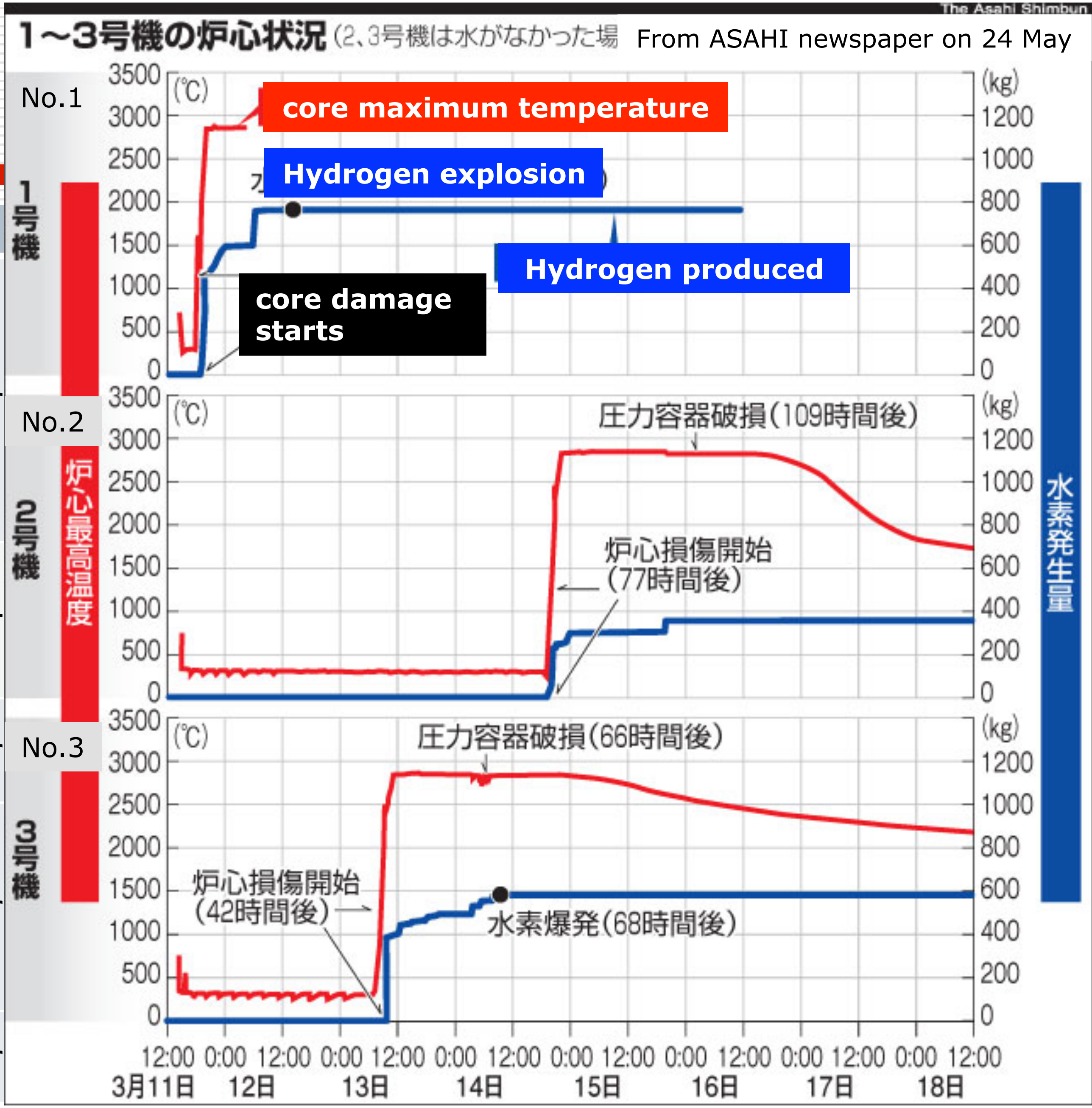
Fukushima Dai-ichi nuclear power plant

- Located on the pacific coast about 220km N of Tokyo
- 6 BWR reactors built from 1971 to 1979 with total output of 4.7GW
- No. 1, 2, 3 reactors running at the time of earthquake; No. 4, 5, 6 shutdown for maintenance
- Hit by 14m high tsunami arou[illegible] 15:30 JST
- Lost all [illegible] JST

Photos made public by TEPCO on 24 May

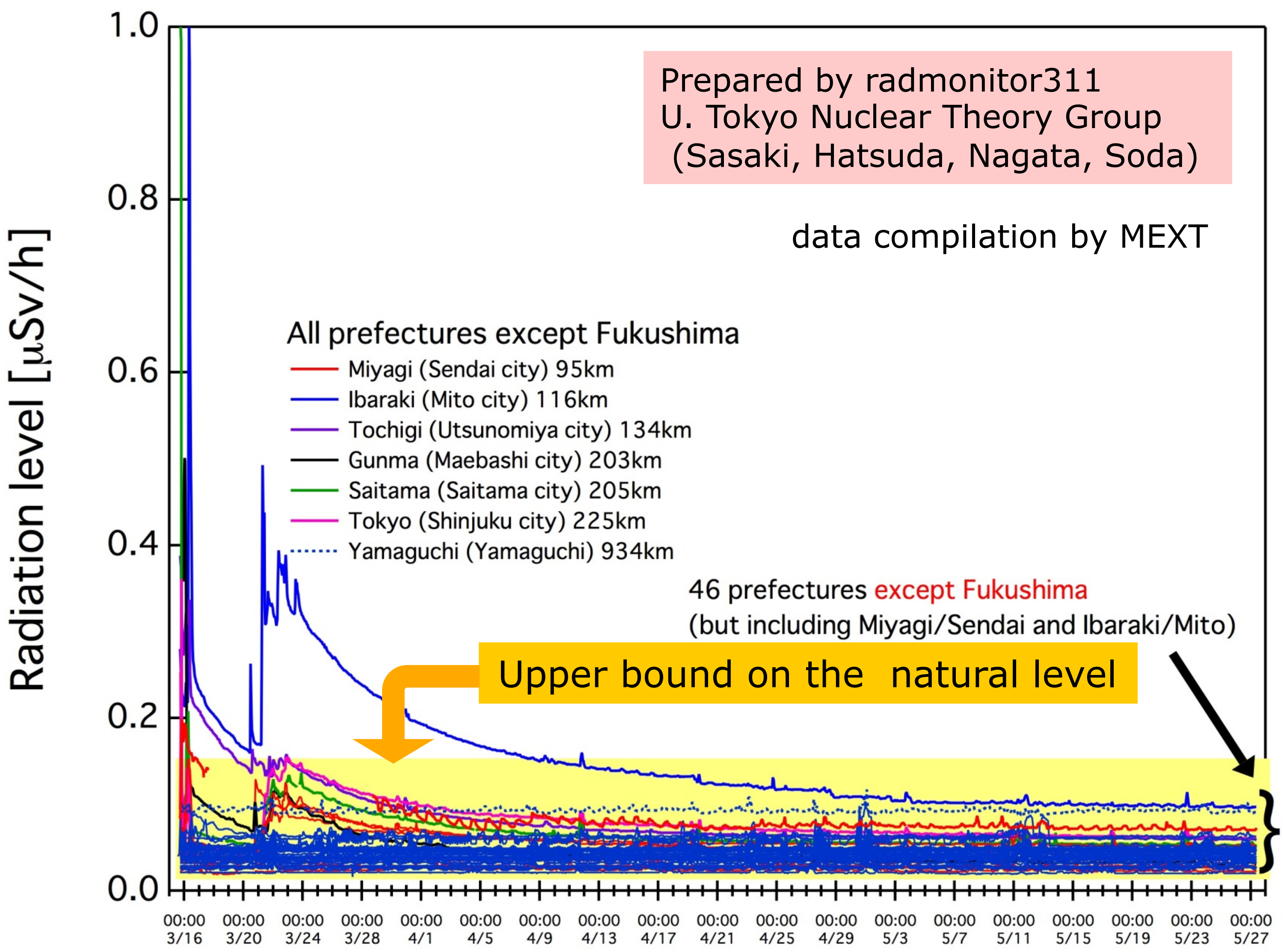
…ents

date		No.3
11 Mar		…ency shutdown
		…ower loss
12 Mar		…system stopped
13 Mar		…ing stopped
		…el exposed
14 Mar		*…/ meltdown*
		…gen explosion
15 Mar		



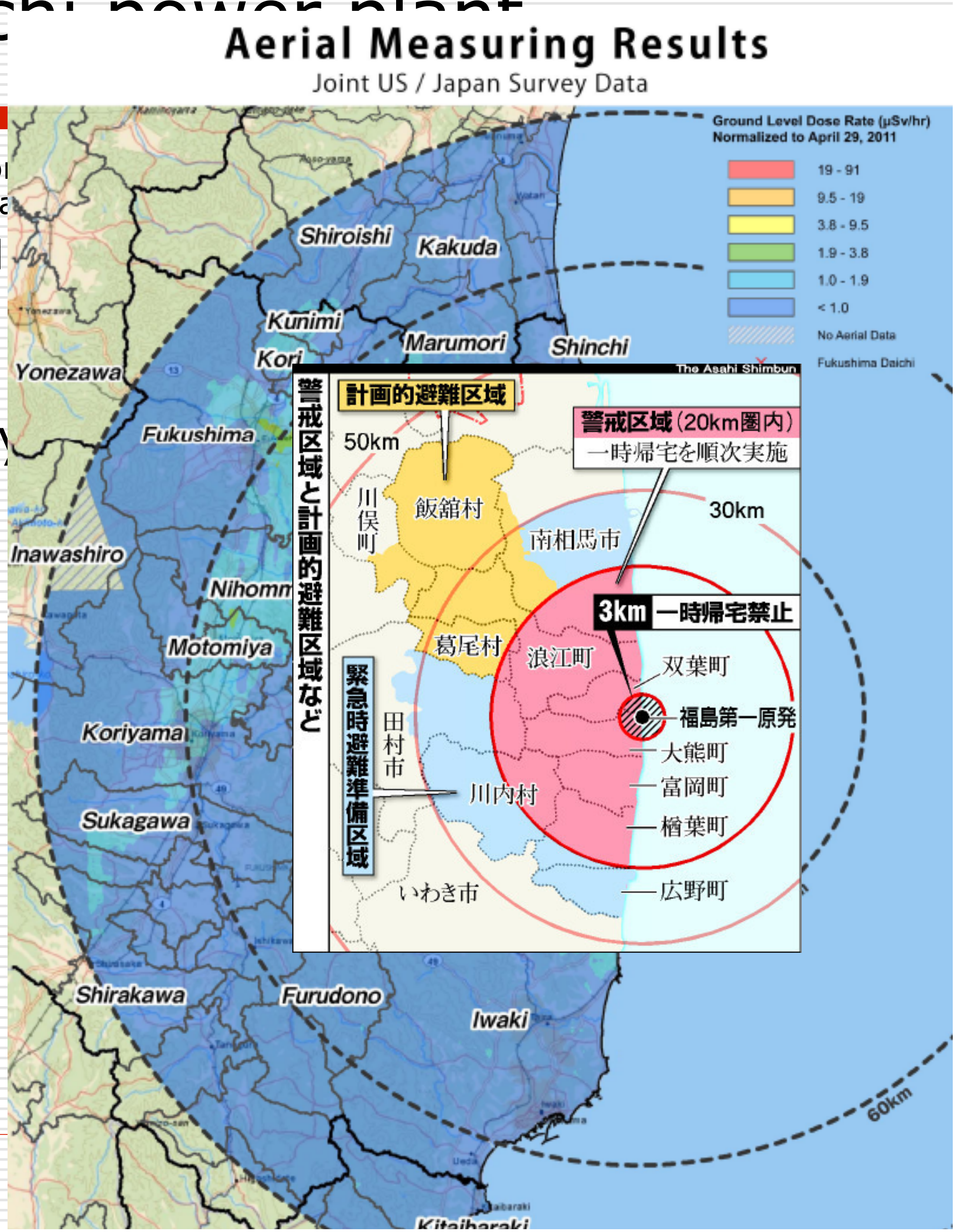
TEPCO report on 16 and 24 May; report by ASAHI newspaper on 25 May

Measured radiation across Japan



Accumulated radiation around Fukushima Dai-Ichi power plant

- Analysis by SPEEDI System for … Informa…
  - 6:00 12 March – 0:00 24 April
  - Released on 3 May
- Joint US/Japan Aerial survey
  - 6 April – 29 April
- Evacuation zone
  - Mandatory
    - 20km radius
    - areas with > 20mSv/year
    - Population 88,000
  - Recommended
    - 30km radius
    - Population 141,000



- Computational science could not foresee the 3.11 earthquake and tsunamis.
- Yet computational science is the key to prevent such disaster to happen again.
- Grave social responsibility of the act of prediction in computational science.
  - Reliability and Openness -

Help from the world LQCD community

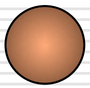
- After the earthquake, and throughout the summer, computing resources in Japan were substantially cut due to severe electricity shortage (15% mandatory cut imposed by the Government)

- Very early (March-April) proposals of help from oversea lattice colleagues
  - UK offered the use of HECTOR supercomputer at Edinburgh; 3 groups in computational science
  - US offered the use of USQCD resources at FNAL, JLAB, BNL up to 10% untill the end of 2011;6 groups in lattice QCD

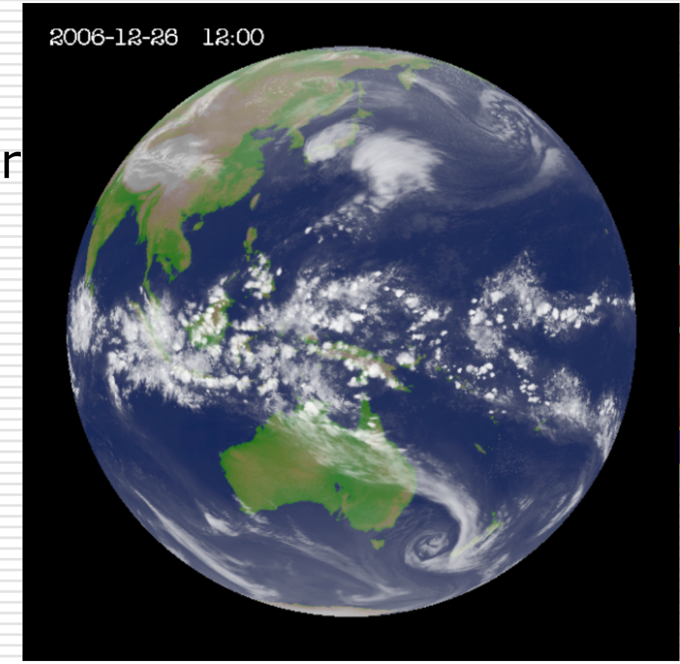
- We imagine that this is not an easy decision, not just because the resource for their own is reduced, but also the funding is given to achieve their own scientific goals.

From Earth

quarks



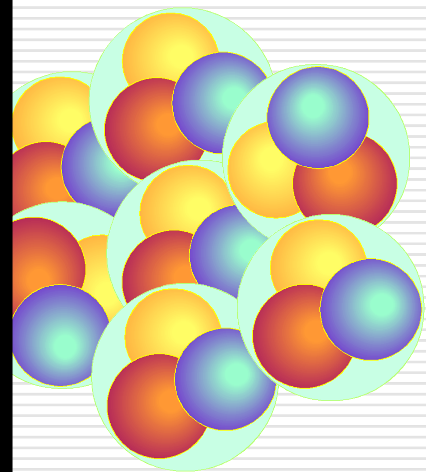
Pr



NICAM 3.5km mesh on ES
Courtesy M. Sato (U. Tokyo)

nuclei

..,C,...,O,...,Fe,...,U,...



To quarks, hadrons, nuclei and lattice QCD

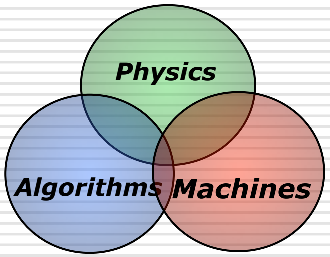
My personal view

- Lattice QCD has turned a corner over the last couple of years.
- Previously, despite the promise, it had 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 has become a real first principle method *allowing precision 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
- Selected topics of personal interest
- Going beyond particle physics - a trial with Helium nuclei –



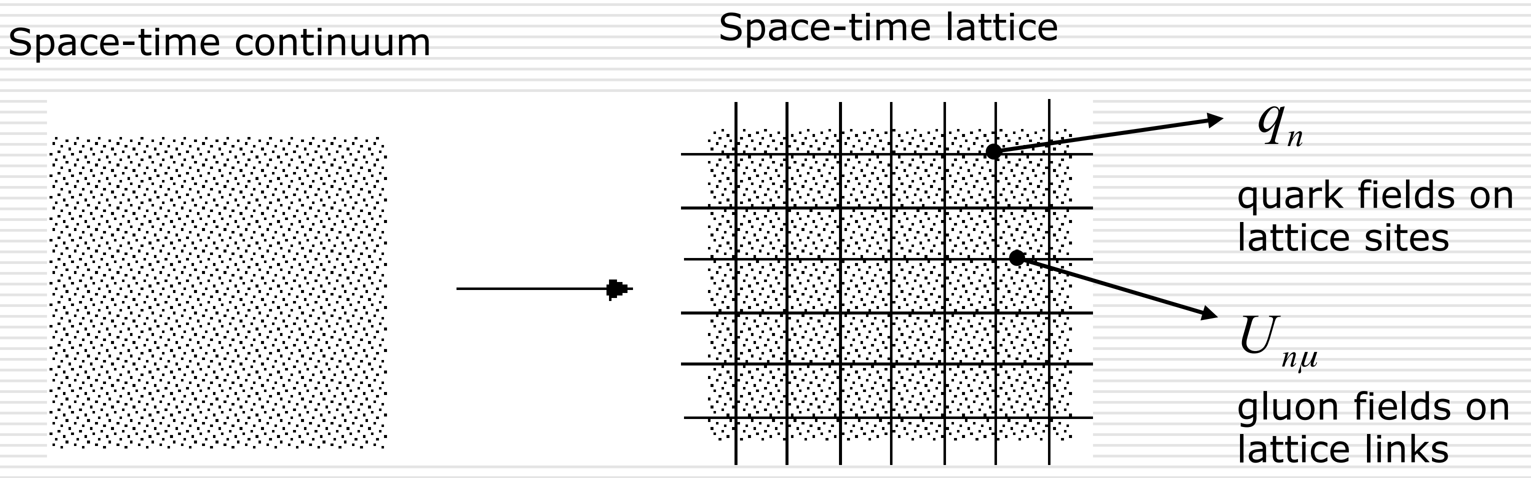
Algorithmic progress and Physical point simulation

Obstacles with 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



- Physical quantities are given by (multi-dimensional)integral averages

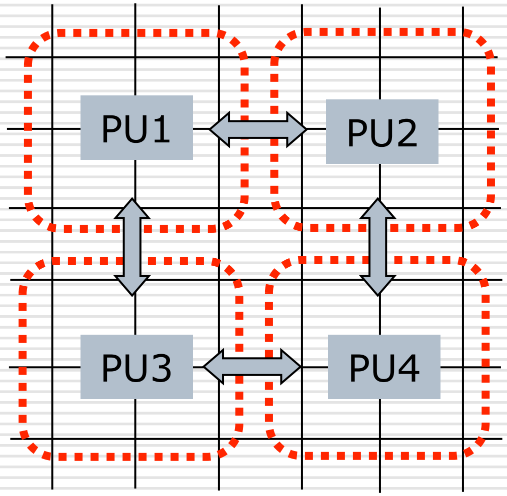
$$\langle O(U,\bar{q},q)\rangle = \frac{1}{Z}\int\prod_{n\mu} dU_{n\mu}\prod_{n} d\bar{q}_n dq_n\, O(U,(U,\bar{q},q))e^{-S_{QCD}}$$

→ Monte Carlo calculation using importance sampling

Lattice QCD as computation(I)

- Lattice QCD has 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

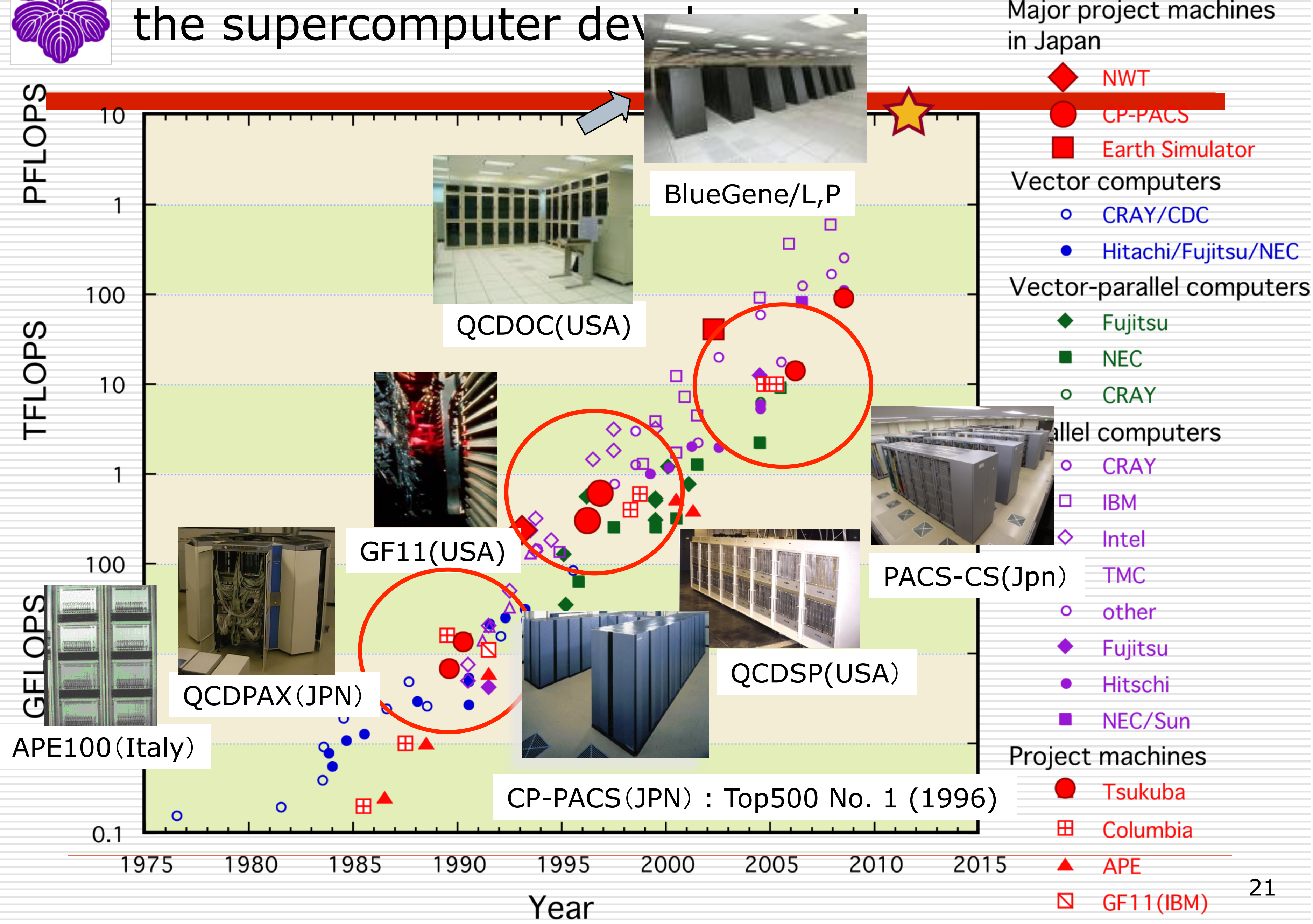
- Need to invert the *lattice Dirac operator D(U)*
  - Sparse but large matrix
  - Large condition number ～ $1/m_q$ for quarks in nature

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

Core calculation of QCD

⇨ Computationally very intensive

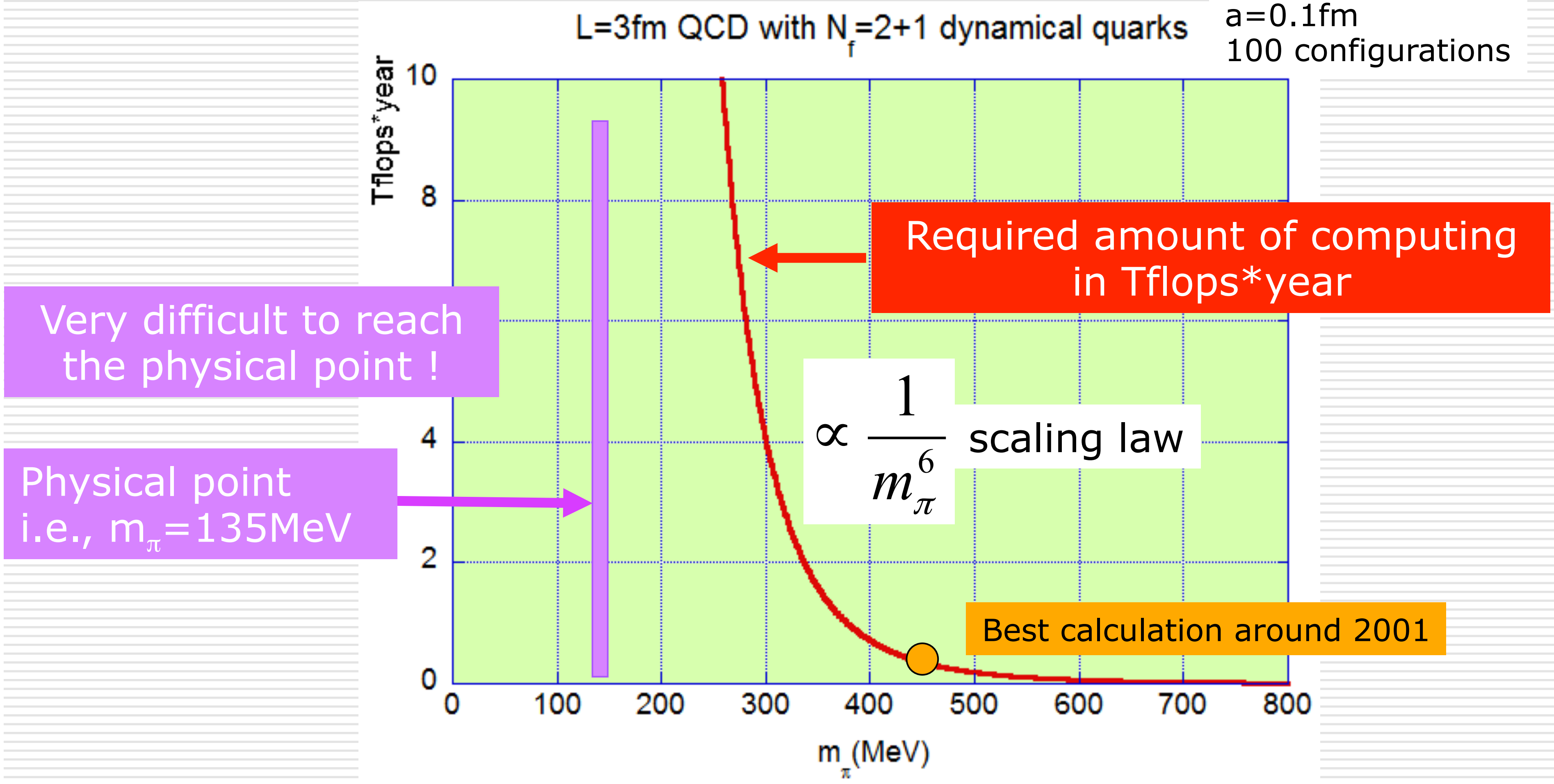
Impact of lattice QCD machines on the supercomputer dev



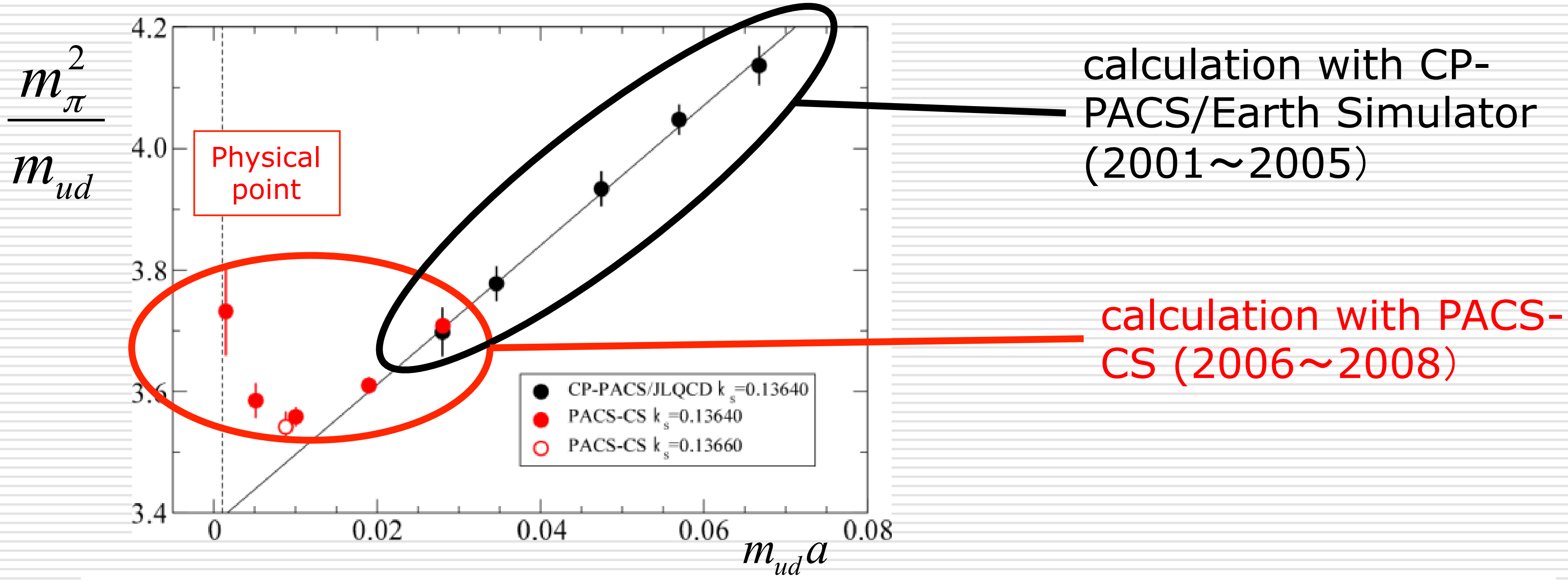
But, of course(?), machine power by itself was not enough …

“Berlin wall” at Lattice 2001@Berlin

A. Ukawa for CP-PACS and JLQCD at Lattice 2001



Why so important to go physical?

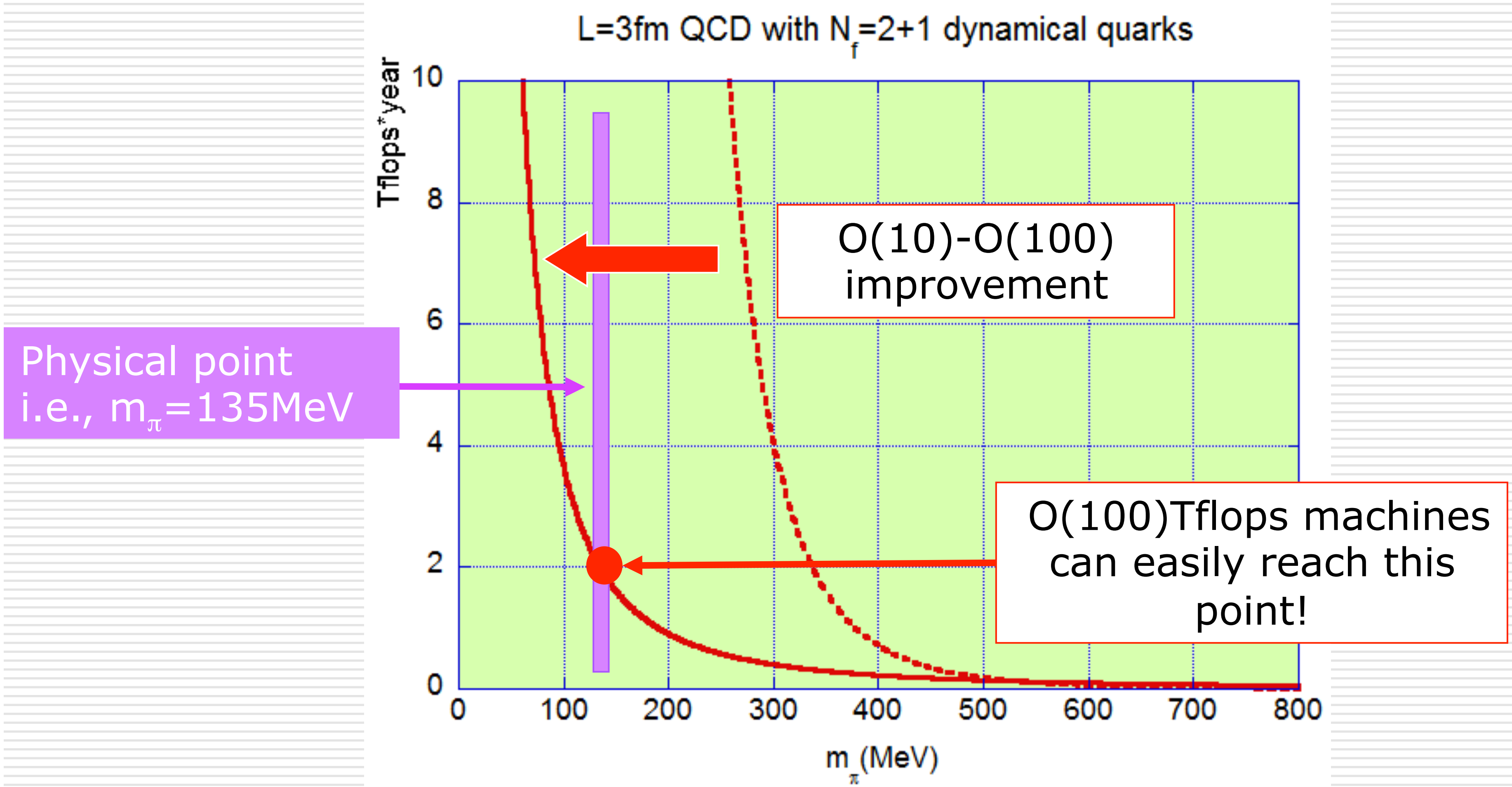


- Anticipated effect of *chiral logarithm* at zero quark mass

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

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

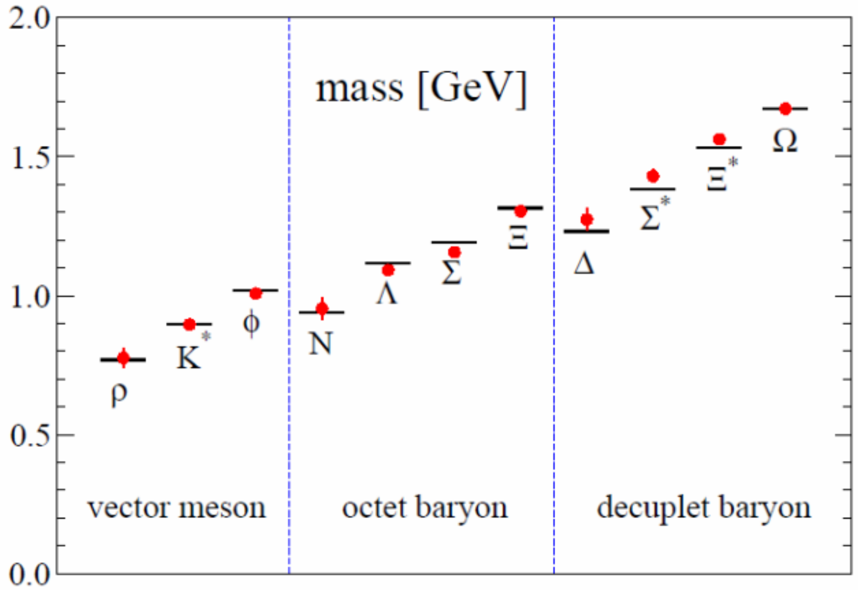
Revolutionary progress around 2005 ; beating the critical slowing down



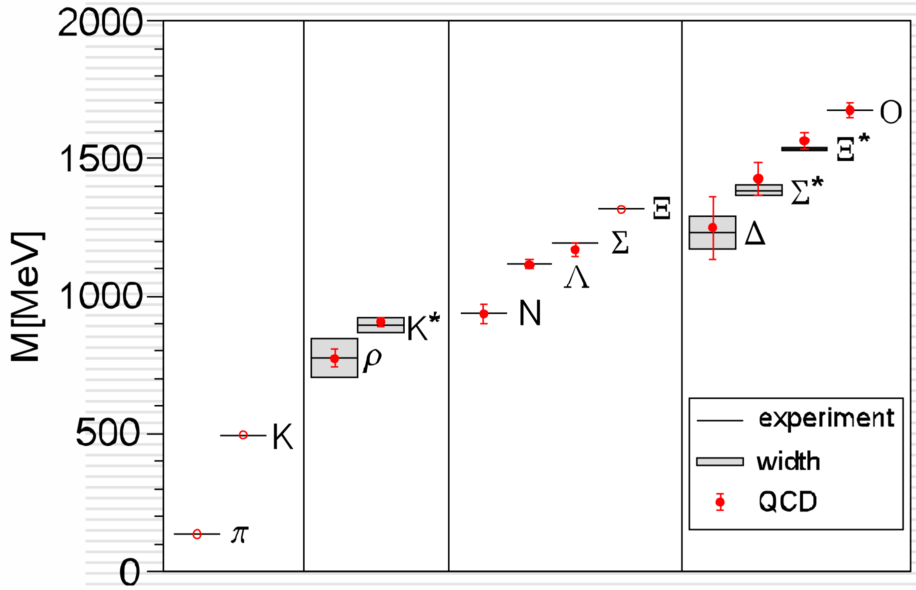
Physical Point Simulation has become reality

Mass spectrum of hadrons 2008

PACS-CS Collaboration
(Tsukuba, Japan)
S. Aoki et al, Phys. Rev. D79 034504 (2008)



BMW Collaboration
(Butapest-Marseille-Wuppertal)
S. Durr et al, Science 322(2008) 1224
Continuum extrapolated



Single hadrons are now (almost) under control!

How that progress came about?

- Molecular dynamics equation of hybrid Monte Carlo algorithm

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

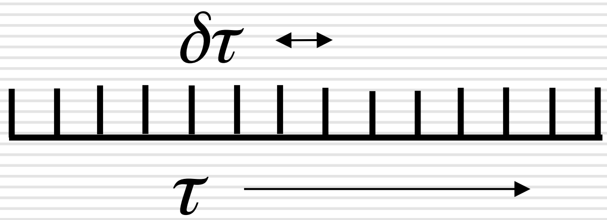
gluon force

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!

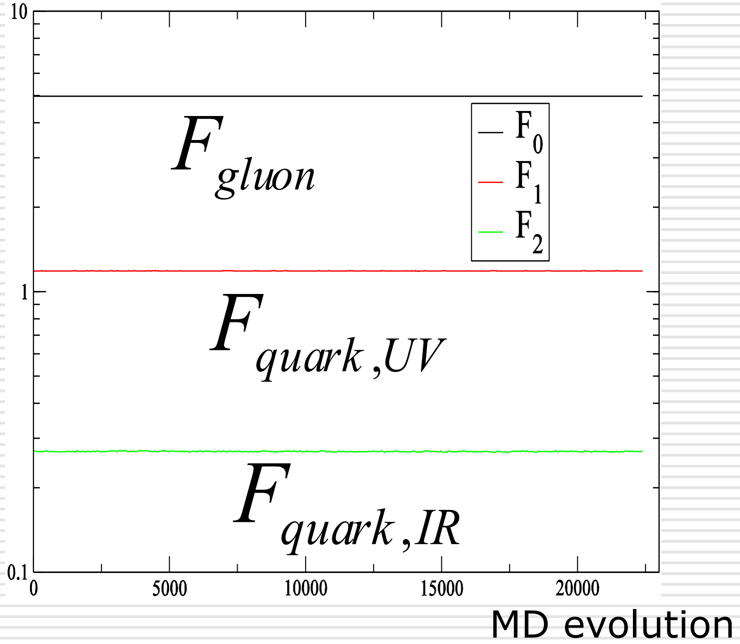


Key observation

M. Luescher (2005)

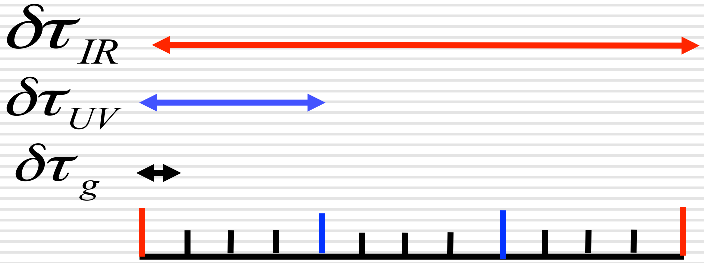
- IR modes of quark force, which is most time consuming to compute, have much weaker force than UV modes

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



- So enlarge the time step for IR modes, gaining a large factor in computation, i.e.,

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



This is an acceleration based on physics!

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→ππdecays
  - 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)

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

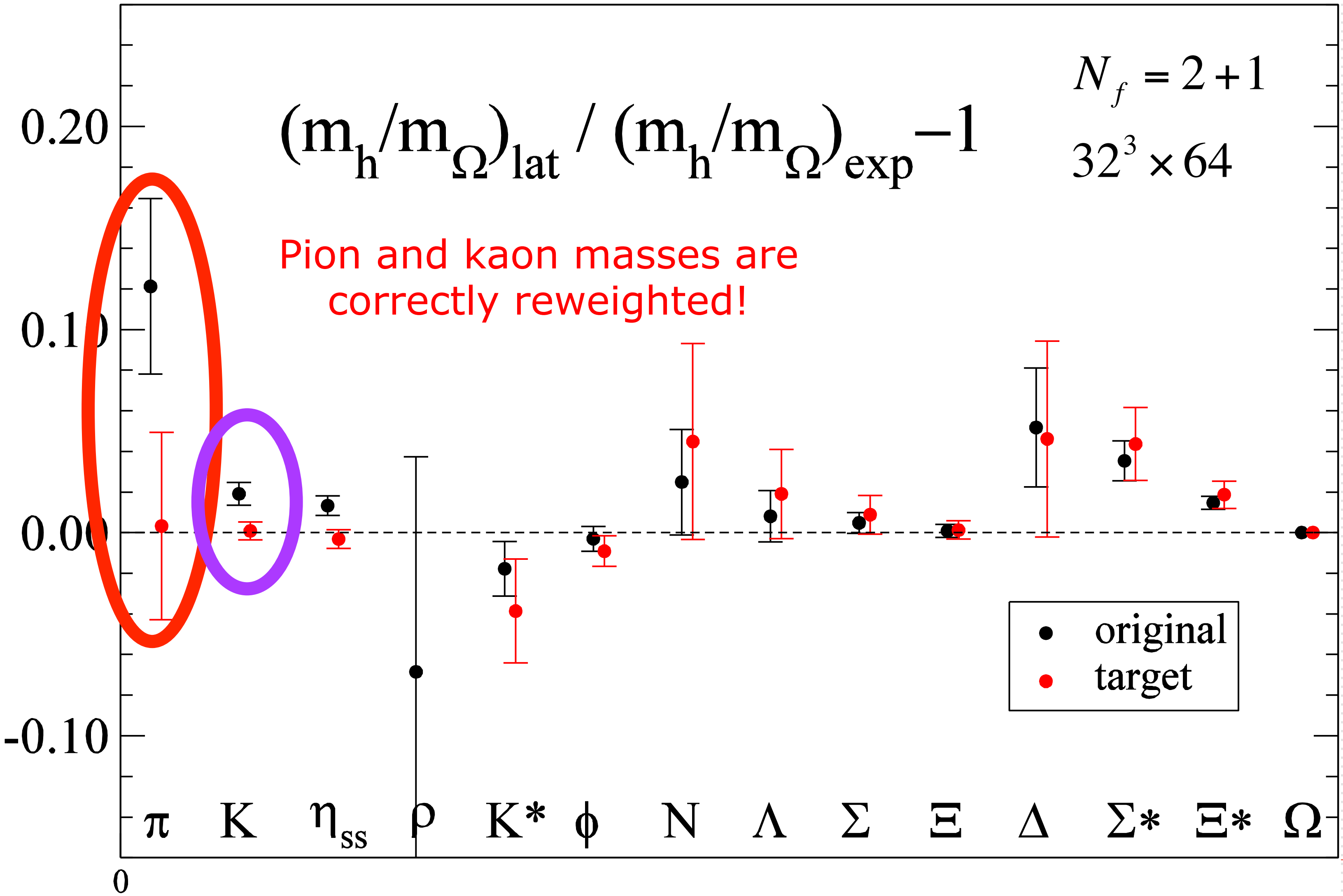
$$\langle O \rangle_{m'_q} = \langle O \cdot R \rangle_{m_q} \qquad R = \frac{\det\left[D(U)+m_q\right]}{\det\left[D(U)+m'_q\right]} = \det\left[1+\left(m_q - m'_q\right)\left(D(U)+m'_q\right)^{-1}\right]$$

  - Have to calculate determinant ratio only
  - Works well to fine-tune to the physical point

PACS-CS Collaboration, PRD81, 074503 (2010)

Hadron mass *before* and *after* reweighting

PACS-CS Collaboration, PRD81, 074503 (2010)



Isospin breaking
– further application of reweighting –

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

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

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

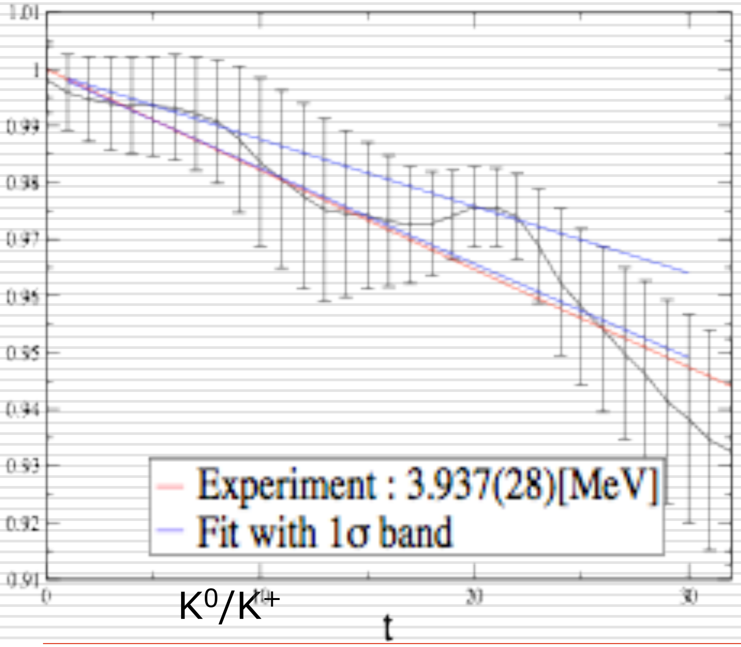
- Very interesting probe to examine
  - up/down quark mass difference, $m_{up} \neq m_{down}$ including the possibility of $m_{up} \approx 0$
  - requires disentangling QED effects $Q_{up} = \frac{2}{3}e, \quad Q_{down} = -\frac{1}{3}e$
- Apply reweighting to
  - Split up and down quark masses
  - Introduce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

Pioneered by T. Izubuchi et al (RBC Collaboration), Lattice 2010

Preliminary Result : ratio of K^0 to K^+ propagators

N. Ukita et al, PACS-CS Collaboation, Lattice 2011

$$\frac{\langle K^0(t)K^0(0)\rangle}{\langle K^+(t)K^+(0)\rangle} = \frac{C_{K^0}\ \mathrm{e}^{-m_{K^0}t}}{C_{K^+}\ \mathrm{e}^{-m_{K^+}t}} = \frac{C_{K^0}}{C_{K^+}}\left[1-(m_{K^0}-m_{K^+})t+\mathcal{O}\left((m_{K^0}-m_{K^+})^2\right)\right].$$



$$\text{Fit formula} = C(1-\delta m t).$$

$$\delta m|_{\mathrm{Fit}} = 3.21(57)[\mathrm{MeV}]$$

$$\delta m|_{\mathrm{Exp}} = 3.937(28)[\mathrm{MeV}]$$

Preliminary result from 32 configs

N. Ukita et al, PACS-CS Collaboation, Lattice 2011

	Lattice	Experiment
$m_{\pi+}$	139.7(15.5) [MeV]	139.57018(35) [MeV]
m_{K+}	492.4(8.1) [MeV]	493.677(16) [MeV]
m_{K0}	497.6(8.1) [MeV]	497.614(24) [MeV]
$m_{K0} - m_{K+}$	3.21(57) [MeV]	3.937(28) [MeV]
m_u	1.97(67) [MeV]	
m_d	4.31(83) [MeV]	
m_u / m_d	0.457(93)	
$(m_u + m_d)/2$	3.14(72) [MeV]	
m_s	90.32(67) [MeV]	
$2m_s/(m_u + m_d)$	28.8(6.6)	

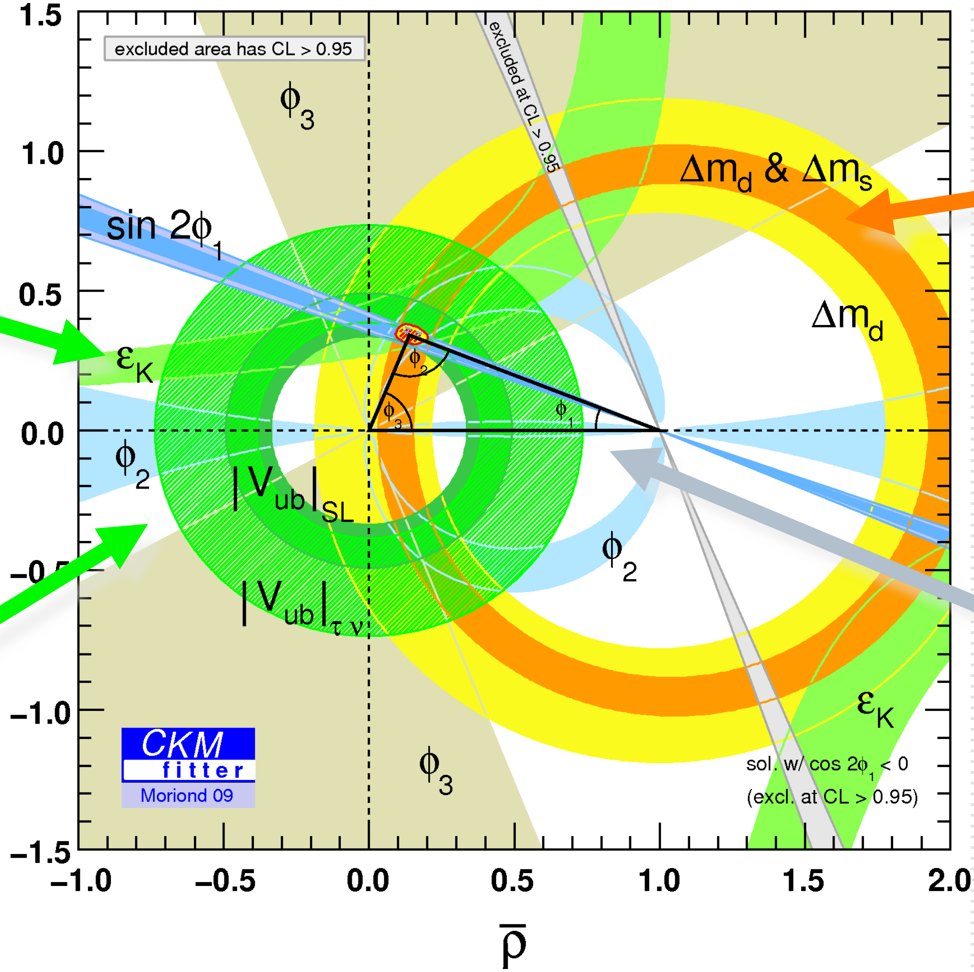
CKM matrix and lattice QCD

Neutral K meson mixing

B_K

B-meson decays

$f_+(q^2)$



B-meson mixings

f_B, B_B

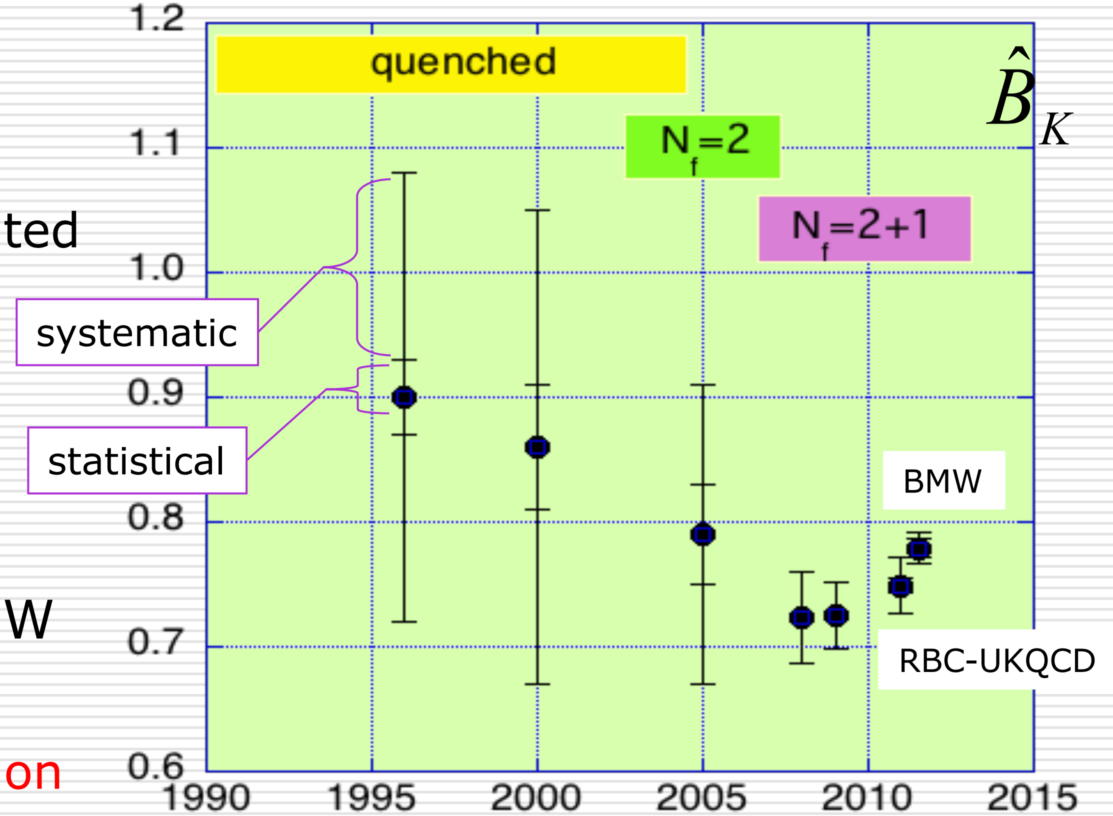
$$\xi = \frac{f_{B_s}\sqrt{B_{B_s}}}{f_{B_d}\sqrt{B_{B_d}}}$$

B->D* decays

$F(1), G(1)$

B_K over the years

- 1996: JLQCD
  - Quenched
  - Continuum extrapolated
- 2008:RBC-UKQCD
  - Nf=2+1
  - Chiral action
  - one lattice spacing
- 2011:RBC-UKQCD/BMW
  - Nf=2+1
  - Chiral/non-chiral action
  - Continuum extrapolated



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

CKM unitarity with lattice inputs 2011

- *First row unitarity* holds to 0.1% accuracy

V_{ud}	V_{us}	V_{ub}	$\sum\left\|V_{ij}^2\right\|-1$
0.97425	0.2254	0.00342	0.0000
±0.00022	±0.0009	±0.00037	±0.0006
Nuclear transitions Hardy-Towner ArXiv 0812.12.02	K-> pi reviewed by Lubic at LP11	B->pi HFAG + Nf=2+1 lattice QCD FNAL/MILC, HPQCD Lattice' 08	

- *Second row unitarity* still requires much improvement

V_{cd}	V_{cs}	V_{cb}	$\sum\left\|V_{ij}^2\right\|-1$
0.234	0.961	0.039	–0.020
±0.013	±0.026	±0.001	±0.050
HPQCD 2011	HPQCD 2011	B->D,D* HFAV + Nf=2+1 lattice QCD FNAL/MILC, Lattice' 08	

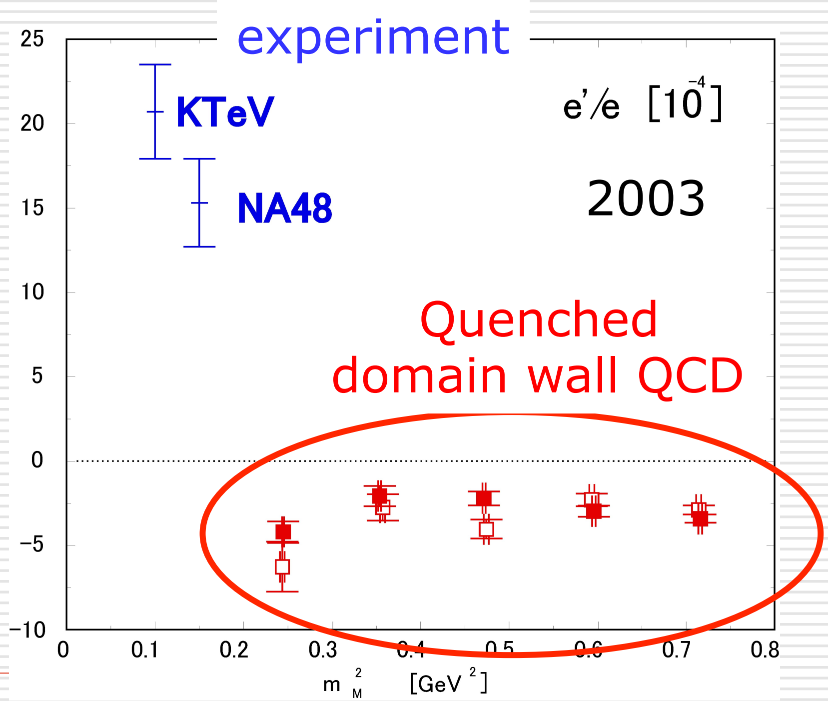
Reviewed by C. Davies Lat2011

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)

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

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

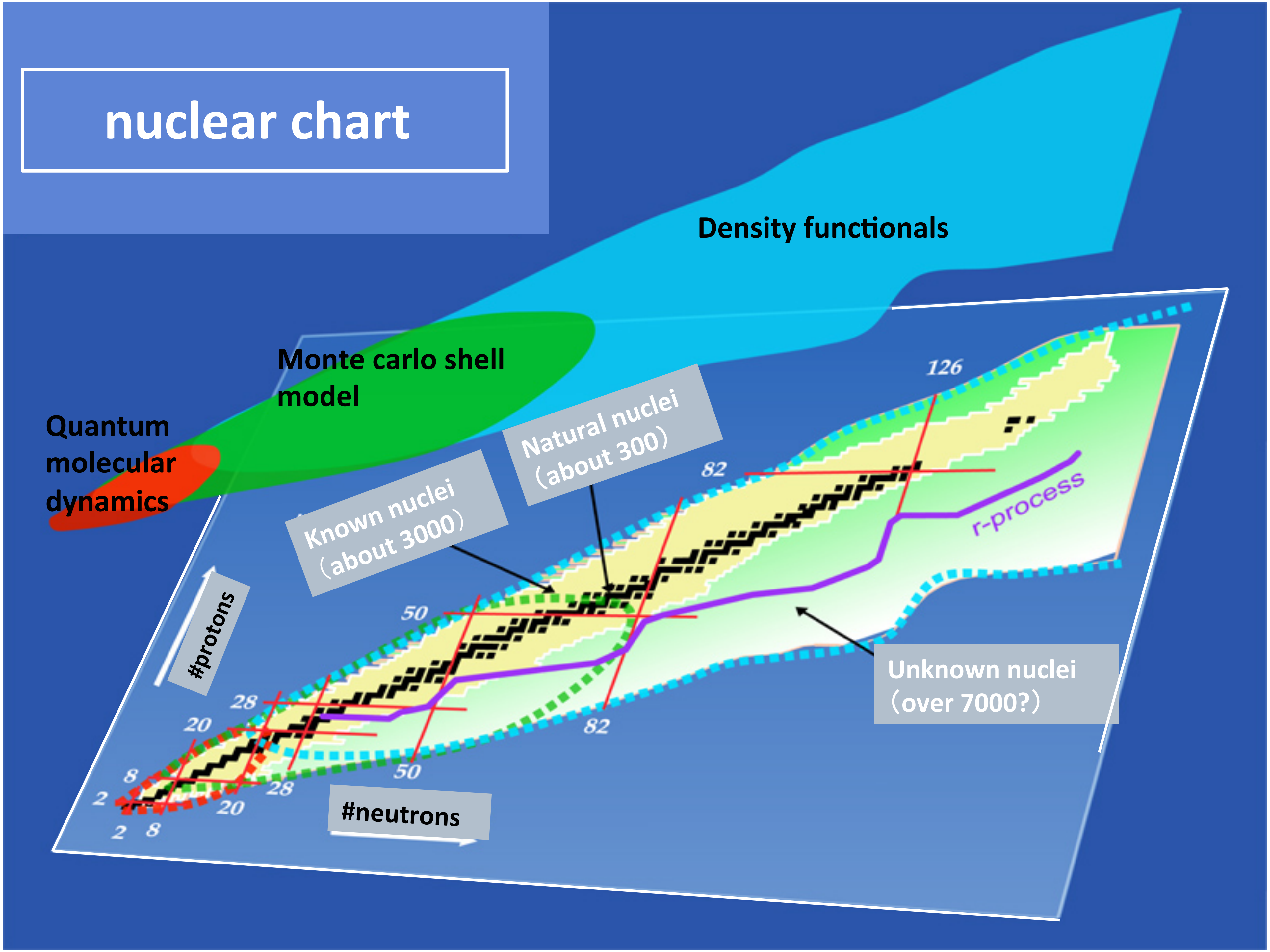


- Steady progress since then due to heroic effort by RBC

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

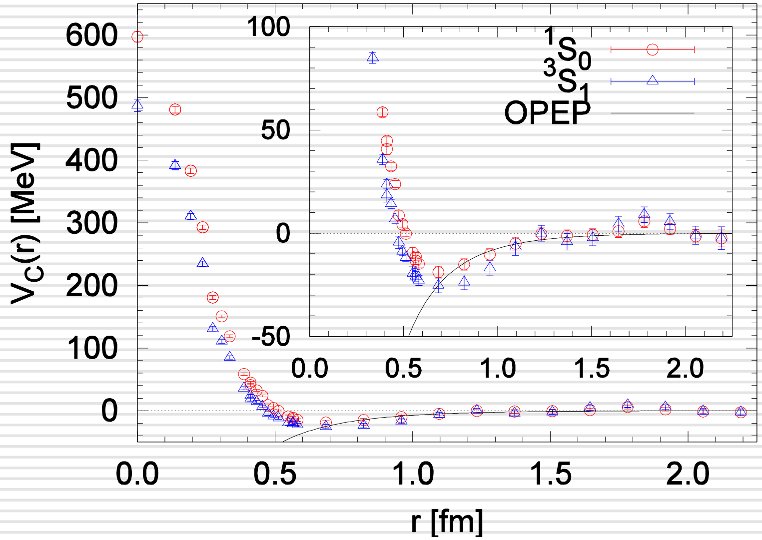
  1949 shell model of nuclei Jansen-Meyer

- 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)

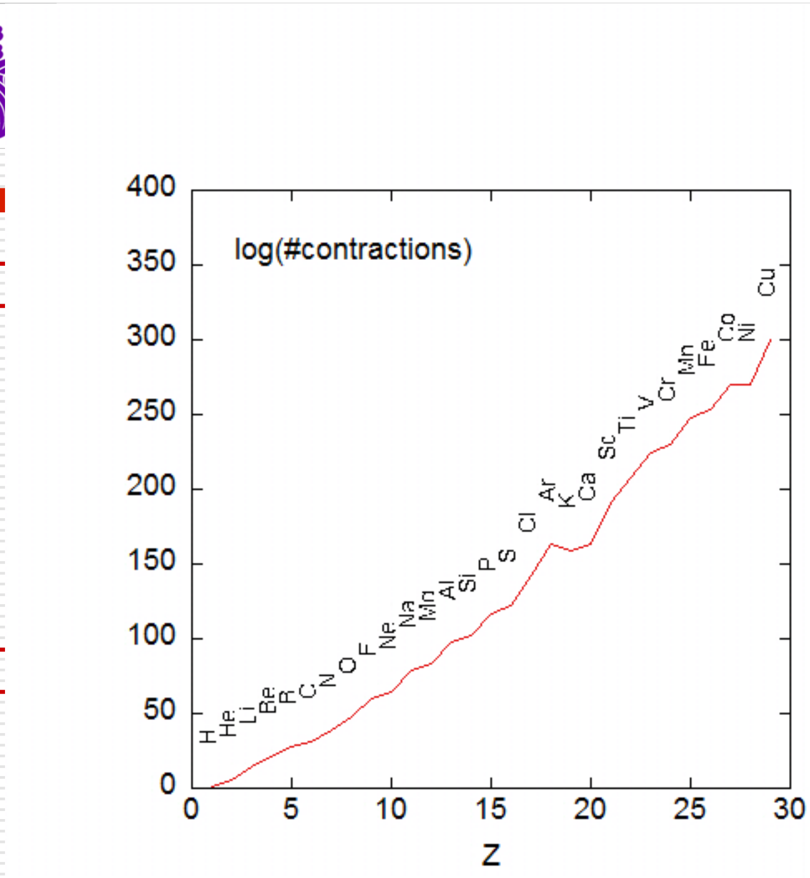


- Direct calculation of nuclear properties from quarks and gluons

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

… e direct approach

- [illegible]



- …ndin…
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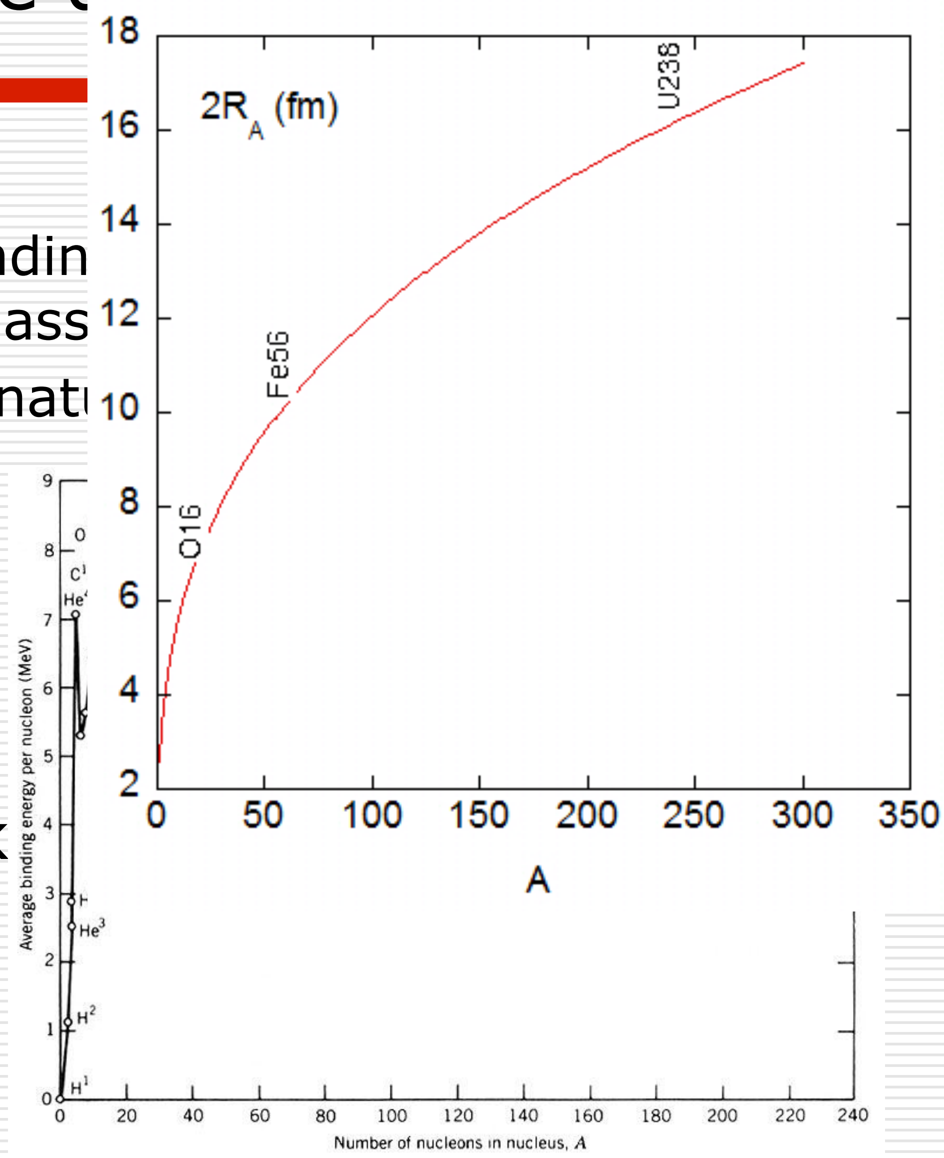


- [illegible]

- 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	$6! \times 6! = 512{,}000$	→	$1{,}107$
He^3	$5! \times 4! = 2{,}880$		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

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

- 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

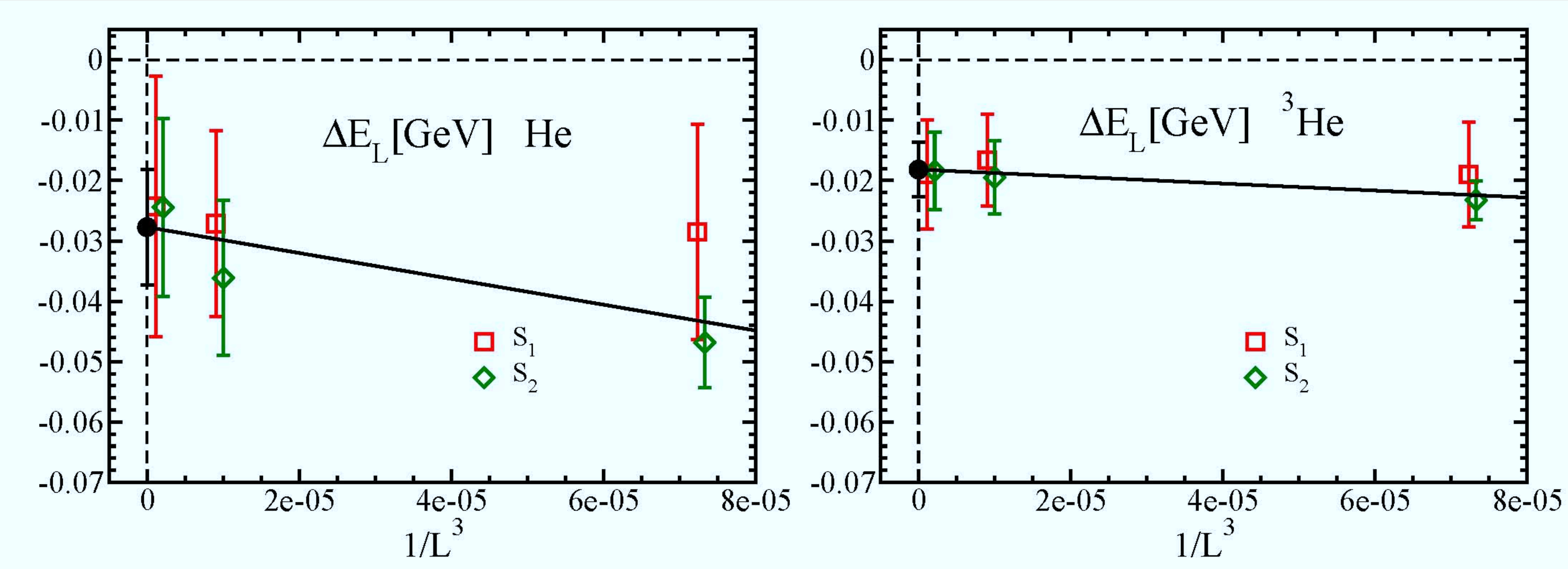
- Two expontially smeared sources

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

	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

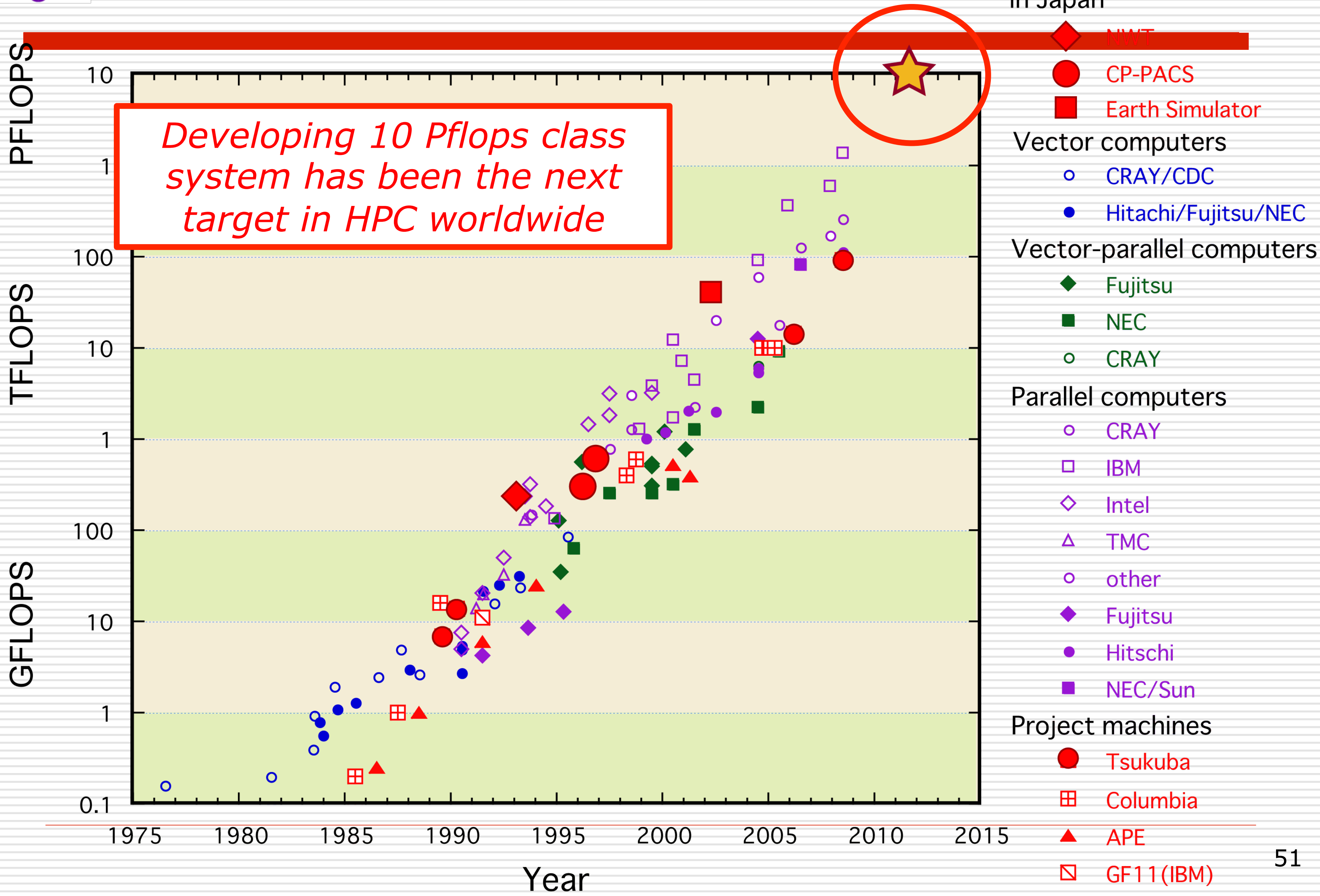
Size dependence of energy difference

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



The Japanese 京"K" Supercomputer Project

Supercomputers trends



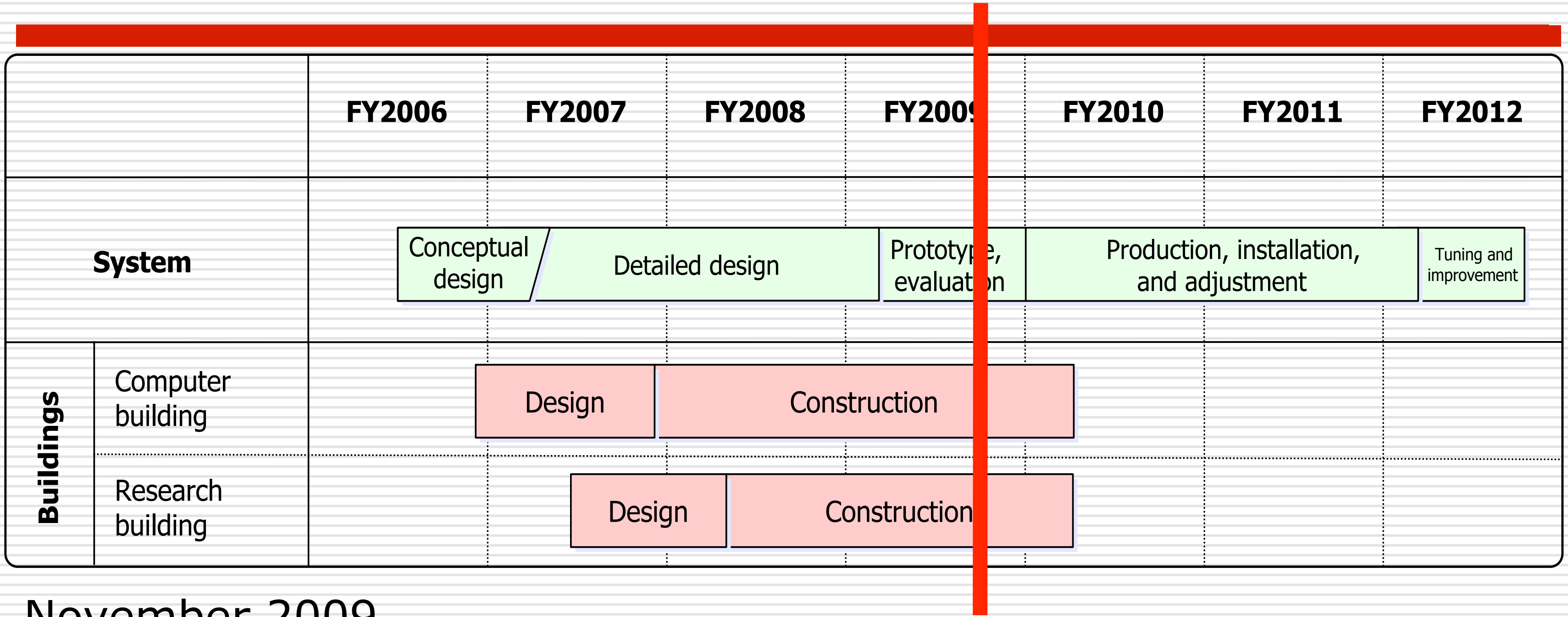
"K" supercomputer project

- Japanese national project to develop a 10 Pflops system
  - 1京=10 Peta in the Japanese counting system
- Project period
  - Japanese FY 2006 to 2012
- Project budget
  - 115.4 B¥ (about 1B Euro)
- Institution responsible for the computer R&D
  - RIKEN

K computer

Schedule of the Project

Big jolt in November 2009



November 2009

reexamination of FY2010 budget by People's Democratic Party recommends ***freezing of the Supercomputer Project*** ; many science & technology budget also recommended cut.

Late November-early December:

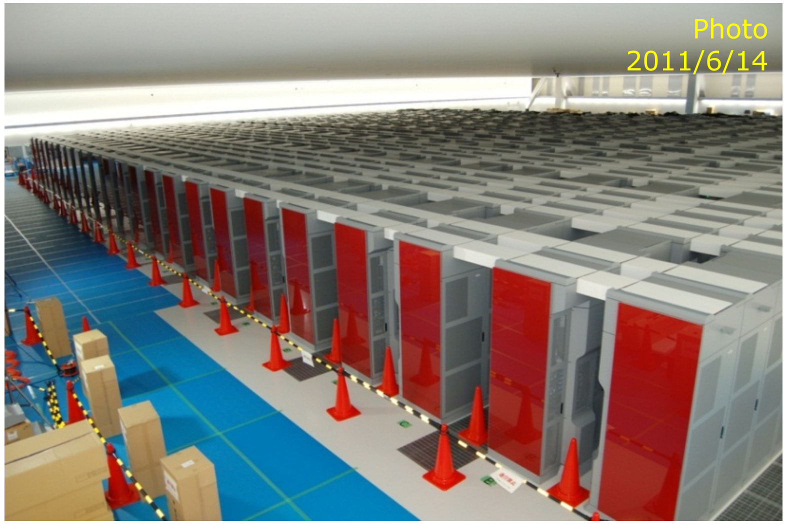
appeals by many academic communities against the reccomendation

16 December

Government decides to proceed with the Project

A happy news! "K" computer was No. 1 in June 2011 Top500 supercomputer list

- Announced on 20 June at ICCS2011 at Hamburg, Germany

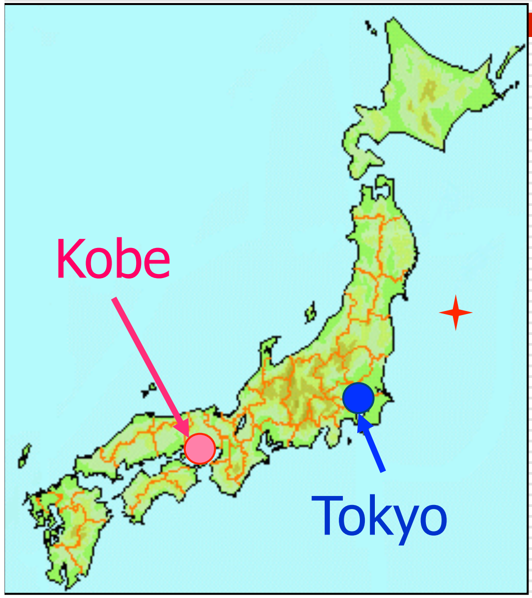


- System parameters at the time
  - #nodes 64,512 nodes (about 80% of full system)
  - Peak speed 8.774 Pflops

- Linpack performance
  - sustained 8.162 Pflops (93.0% of peak)
  - Problem size 10,725,120
  - Execution time 28.0 hours
  - Power performance 825MFLOPS/W

Courtesy: RIKEN AICS

Cite for the 京"K" Supercomputer



450km (280miles)
west from Tokyo

"Advanced Institute for Computational Science" (AICS) in Kobe

- New institute founded in June 2010
- Operates the "K" computer
- Carries out research across computer science and computational science

“Strategic Field Program” for 京”K”

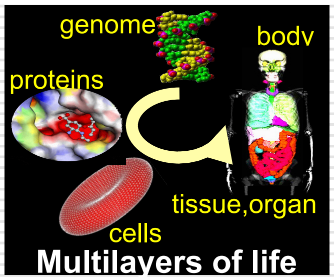
In order to put 京”K” computer to strategic use,

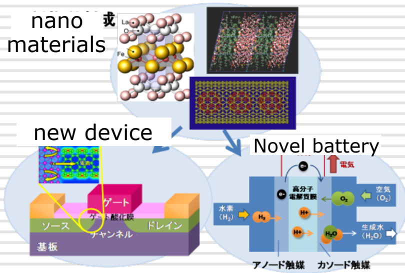
- Government selected *5 strategic fields* in science and technology
- For each field, Government selected a *core institute*.
- Each core institute is responsible for organizing *research and supercomputer resources in the respective field and its community*, for which they receive
  - priority allocation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

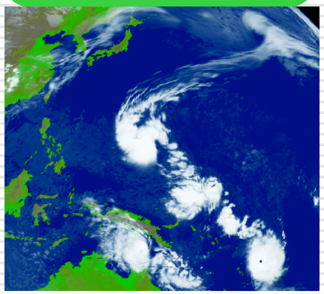
"Strategic Fields" and *"core institutes"*

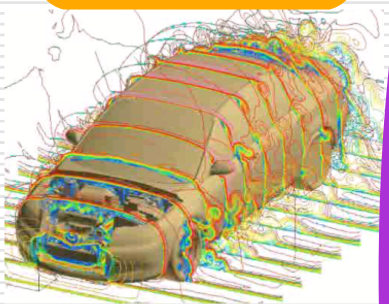
strategic field

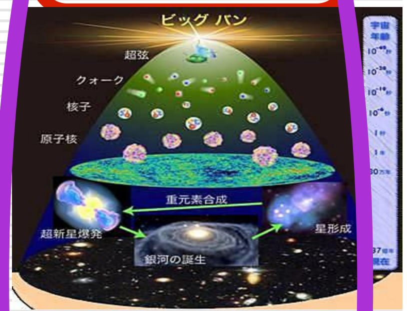
Life Science & Medicine	New materials & Energy	Global change prediction	Next generation Engineering	Matter & Universe











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

JOINT INSTITUTE FOR COMPUTATIONAL FUNDAMENTAL SCIENCE

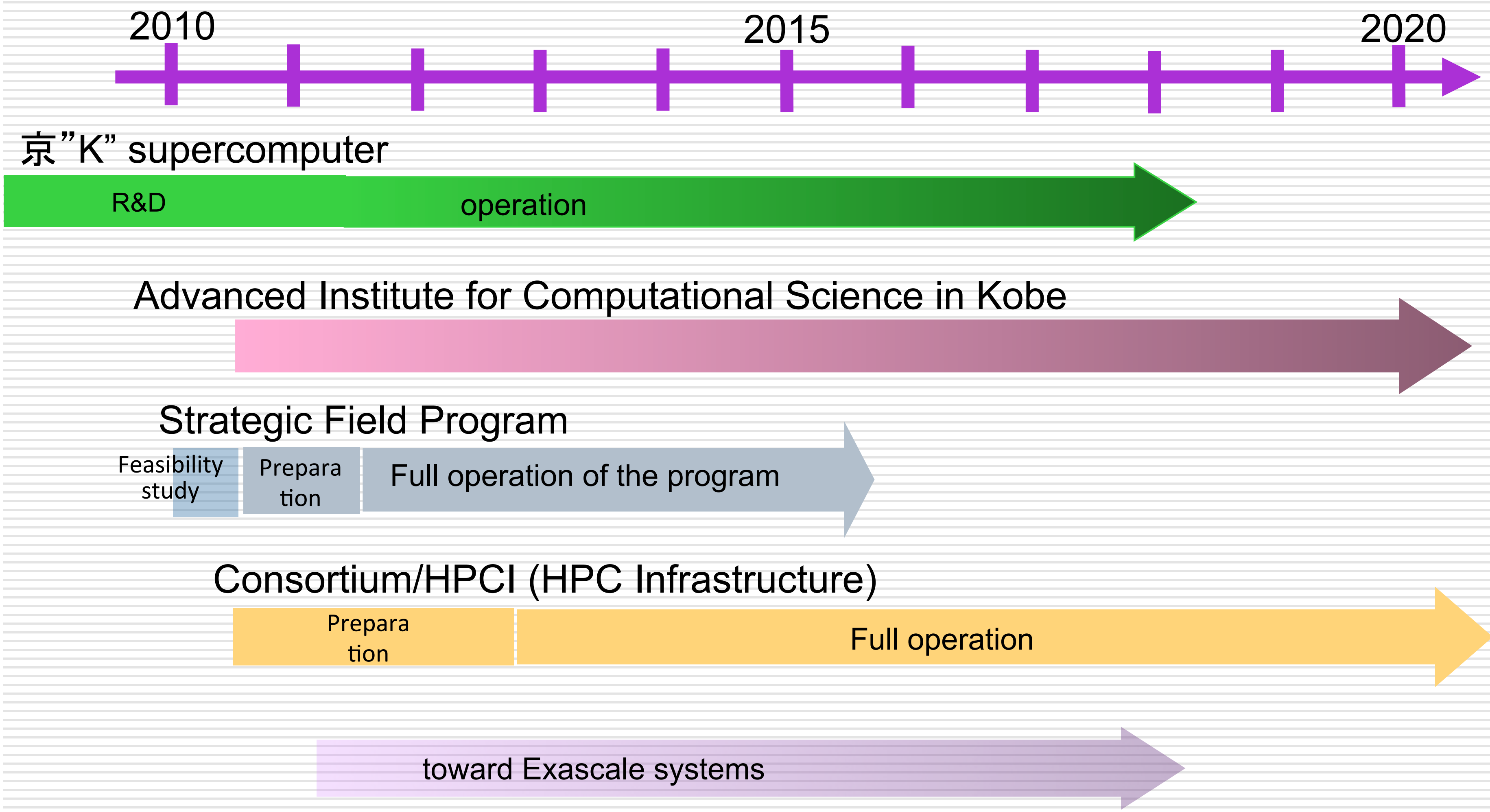
- Core institute

  “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

HPC in Japan over the Next 10 years



CONCLUSIONS

Eastern Japan Great Earthquake and computational science; somber realization and grave responsibility

- *Lattice QCD as a precision vehicle to understand hadrons and nuclei*
- *Japanese status toward Peta and post-Peta scale computational science with lattice QCD as an important comonent*