



# Lattice QCD: Looking inside hadrons with computers

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Akira Ukawa  
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University of Tsukuba

- Introduction
- QCD and lattice QCD
- lattice QCD and computers
- current focus :  $N_f=2+1$  full QCD simulations
- future outlook
- summary



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# QCD and lattice QCD

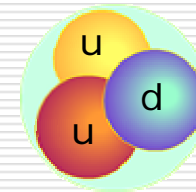


# The Standard Model

## □ Matter particles

- Six quarks  $\begin{pmatrix} u \\ d \end{pmatrix}$   $\begin{pmatrix} s \\ c \end{pmatrix}$   $\begin{pmatrix} t \\ b \end{pmatrix}$
- Six leptons  $\begin{pmatrix} e \\ \nu_e \end{pmatrix}$   $\begin{pmatrix} \mu \\ \nu_\mu \end{pmatrix}$   $\begin{pmatrix} \tau \\ \nu_\tau \end{pmatrix}$

*hadrons* (proton, neutron, pion etc) are bound states or resonances of quarks



proton=uud

## □ Gauge particles mediating interactions

- Photon  $\gamma$  EM interactions
- Weak bosons  $W, Z$  Weak interactions
- Gluons  $g$  Strong interactions

Weinberg-Salam theory

Quantum Chromo-Dynamics (QCD)



# Quantum Chromodynamics

Gross-Wilczek-Politzer 1973

- Quantum field theory of quarks and gluon fields

$$\left. \begin{array}{ll} q_f(x) & \text{Quark field} \\ A_\mu(x) & \text{Gluon field} \end{array} \right\} \text{ defined over 4-dim space time}$$

$$L_{QCD} = \frac{1}{8\pi\alpha_s} \text{Tr}(F_{\mu\nu}F_{\mu\nu}) + \sum_f \bar{q}_f (\gamma_\mu \cdot (\partial_\mu - iA_\mu) + m_f) q_f \quad \text{QCD lagrangian}$$

$$\langle O(A, \bar{\psi}, \psi) \rangle = \frac{1}{Z} \int dA d\bar{q} dq O(A, \bar{q}, q) e^{-\int d^4x L_{QCD}} \quad \text{Physical quantities by Feynman path integral}$$

- Knowing

$$\begin{array}{ll} 1 \text{ coupling constant} & \alpha_s = \frac{g_s^2}{4\pi} \\ \text{and} & \\ 6 \text{ quark masses} & m_u, m_d, m_s, m_c, m_b, m_t \end{array}$$

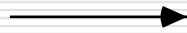
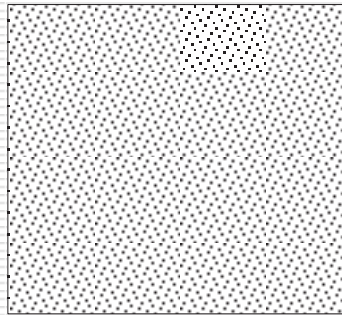
will allow full understanding of hadrons and their strong interactions



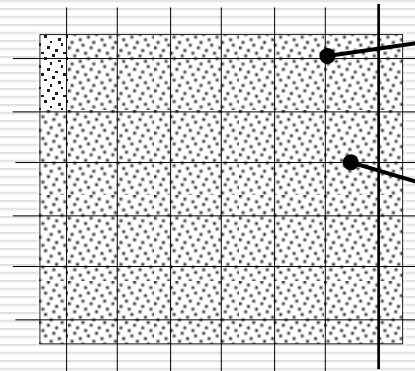
# QCD on a space-time lattice

Wilson 1974

Space-time continuum



Space-time lattice



$q_n$   
quark fields on  
lattice sites

$U_{n\mu}$   
gluon fields on  
lattice links

## □ Feynman path integral

■ Action  $S_{QCD} = \frac{1}{g_s^2} \sum_P \text{tr}(UUUU) + \sum_f \bar{q}_f (\gamma \cdot U + m_f) q_f$

■ Physical quantities as **integral averages**

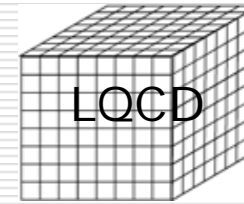


*Monte Carlo  
Evaluation of  
the path integral*

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



# Impact of lattice QCD



## Hadron spectrum and Fundamental constants of QCD

- Strong coupling constant
- Quark masses

$$\alpha_s$$

$$m_u, m_d, m_s, m_c, m_b, m_t$$

*Fundamental natural constants*

## Hadron physics

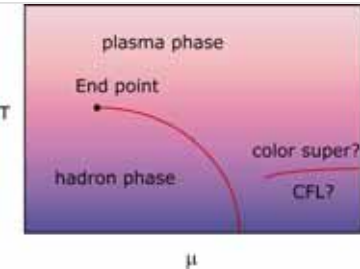
- eta' meson mass and U(1) problem
- exotic states  
glueball, hybrids, penta-quark, ...
- hadronic matrix elements  
proton spin, sigma term, ...
- structure functions/form factors

$$\int_0^1 dx x^{n-1} F(x, q^2) = (\ln q^2)^{-\gamma_n} \langle N | O_n | N \rangle$$

*Long-standing issues of hadron physics*

## Finite-temperature/density behavior

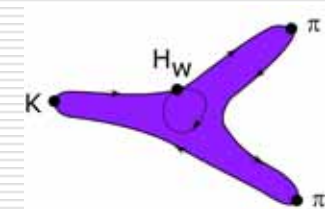
- order of transition
- critical temperature/density
- equation of state



*Physics of quark-gluon plasma*

## Weak interaction matrix elements

- K meson amplitudes  
 $B_K$   
K  $\pi\pi$  decays
- B meson amplitudes  
 $f_B, B_B$  form factors



*CKM matrix and CP violation*



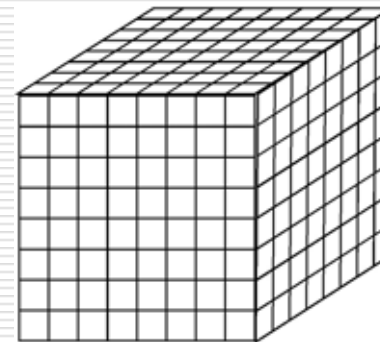
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# Lattice QCD and computers



# Lattice QCD as computation

- Monte Carlo simulations of lattice QCD
  - Powerful and only general method to calculate the QCD Feynman path integral
  
- From computational point of view
  - Relatively simple calculation
    - Uniform mesh *lattice spacing*  $a$
    - Single scale *QCD scale parameter*  $\Lambda_{QCD}$
  - Requires much computing power due to
    - 4-dimensional Problem
    - Fermions (quarks) essential
    - Physics is at lattice spacing  $a=0$
  - Precision required  
( $<a$  few % error in many cases)





## Development of lattice QCD simulations (I)

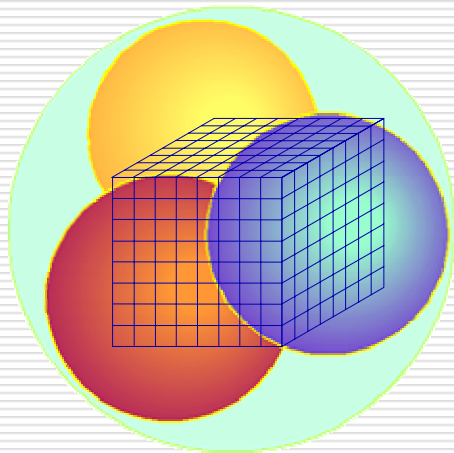
### 1981 First lattice QCD simulation

$4^4 \sim 8^4$  lattice  
quenched approx (no sea quarks)

Creutz-Jacobs-Rebbi  
Creutz  
Wilson  
Weingarten  
Hamber-Parisi

lattice size      lattice spacing

$L = 0.8 \text{ fm}$        $a = 0.1 \text{ fm}$



$size \approx 2 \times 10^{-15} \text{ m}$



VAX

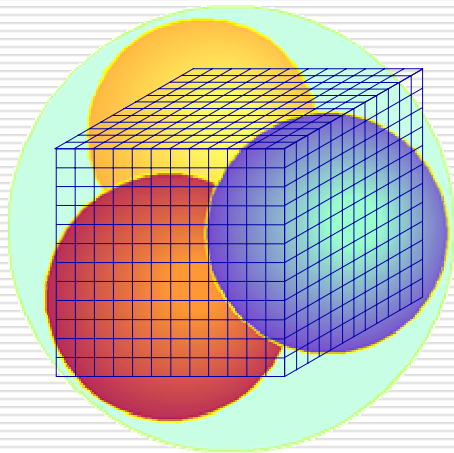
$speed \approx 1 \text{ Mflops}$



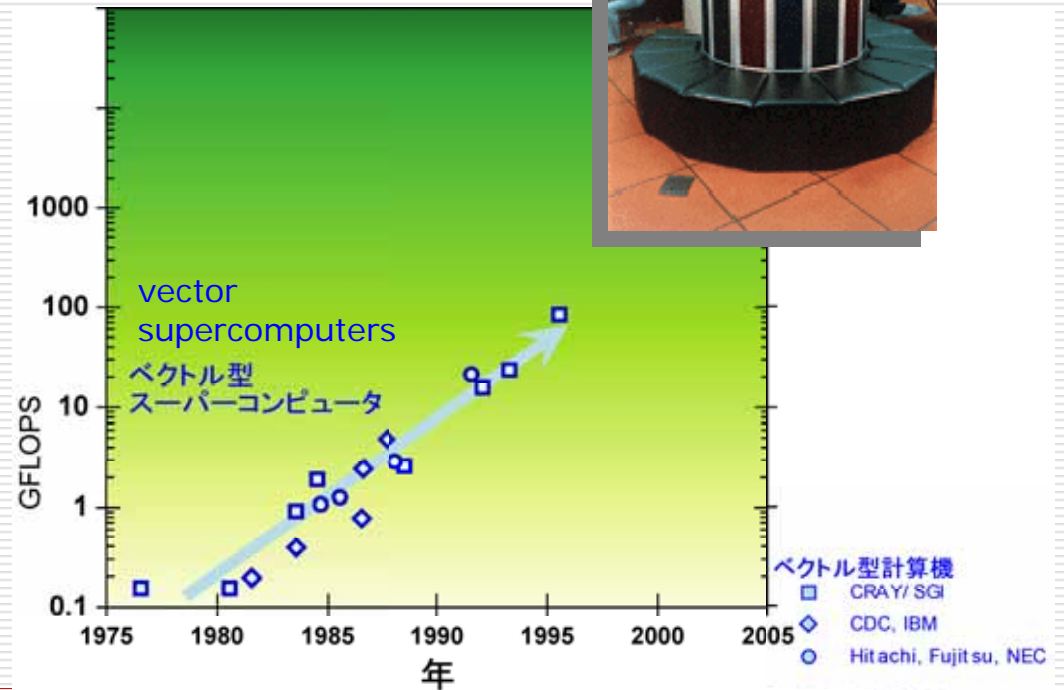
## Development of lattice QCD simulations (II)

### 1980's Taking advantage of vector supercomputers

	L(fm)	a(fm)
1981	0.8	0.1
1985	1.2	0.1
1988	1.6	0.1



CRAY-1



1 GFLOPS = one billion flop/sec



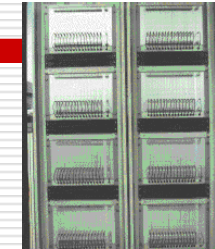
# Development of lattice QCD simulations (III)

## 1990's QCD dedicated parallel computers

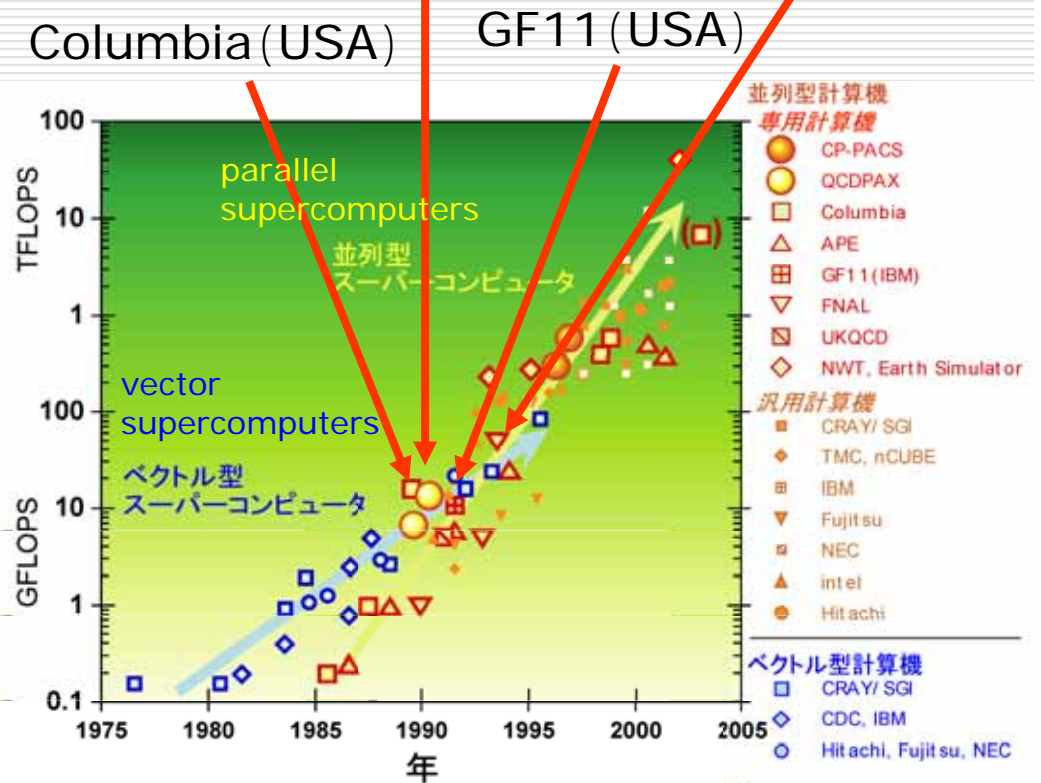
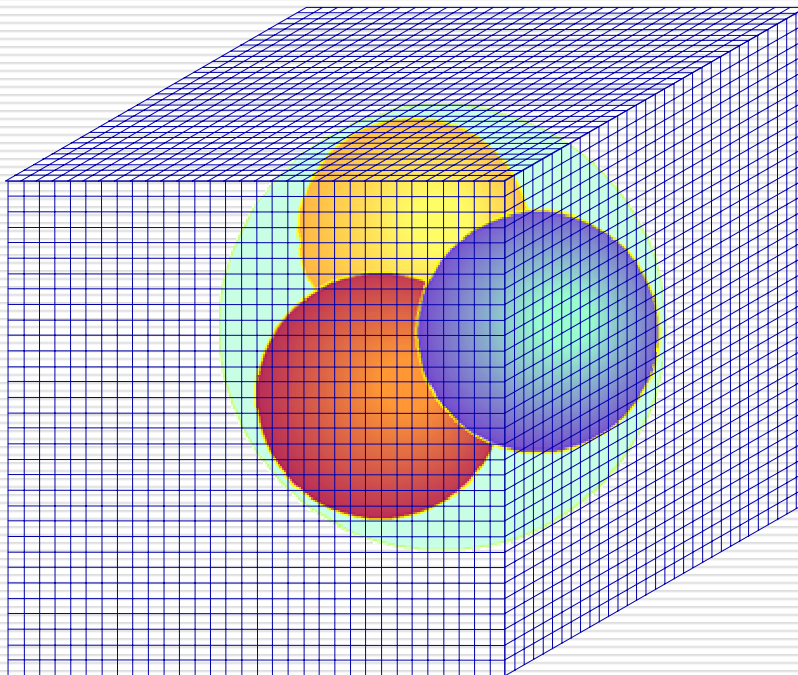
	L(fm)	a(fm)
1993	2.4	0.07



QCDPAX (JPN)



APE (Italy)

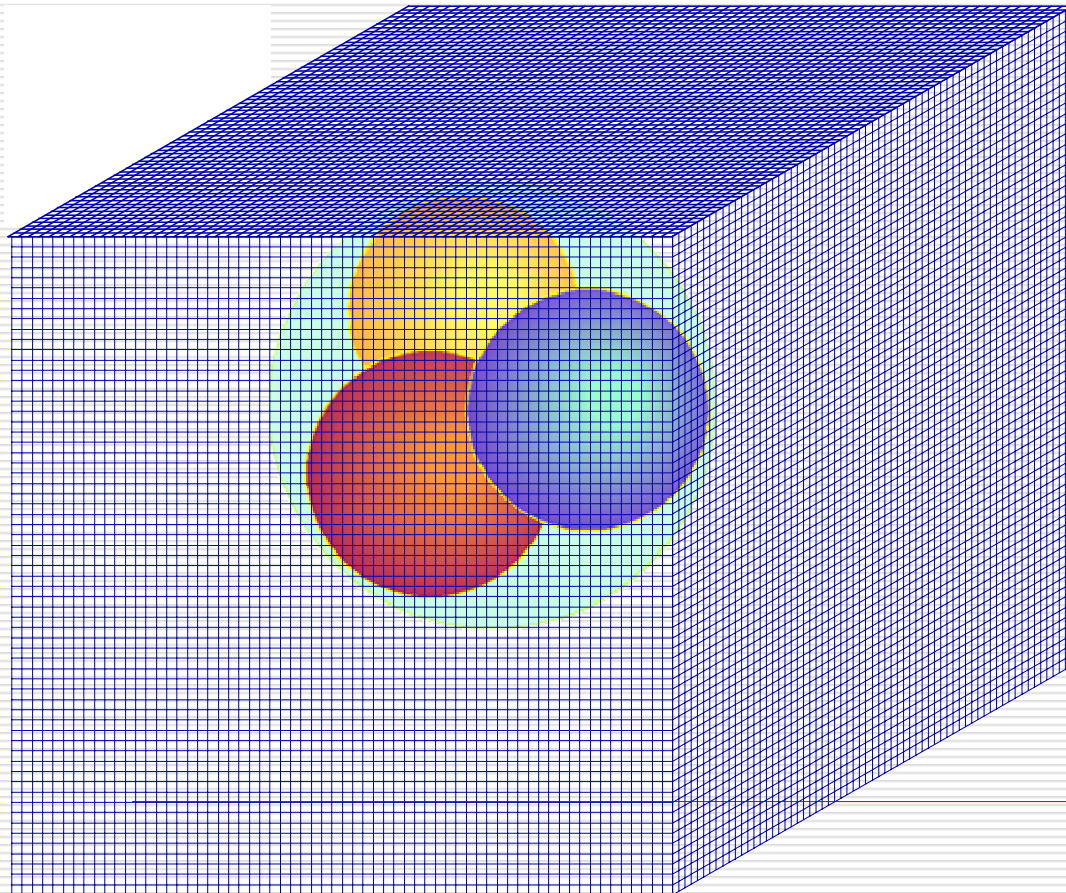




# Development of lattice QCD simulations (IV)

2000s further development of  
QCD dedicated computers

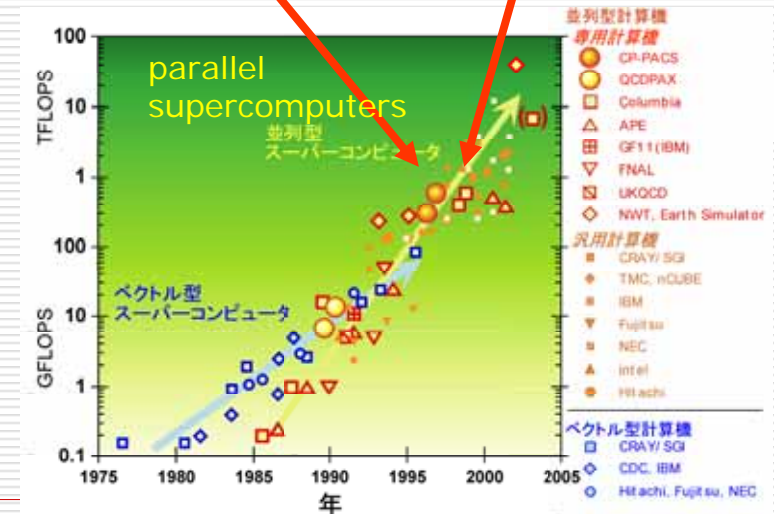
	L(fm)	a(fm)
1998	3.0	0.05



CP-PACS(JPN)



QCDSMP(USA)





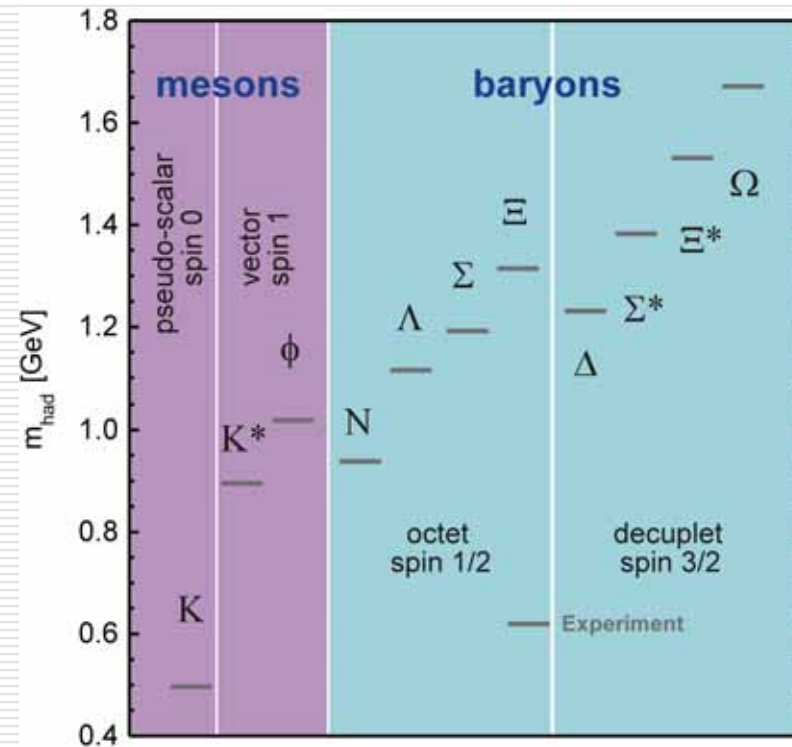
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# Current focus



# Light hadron mass spectrum

- Benchmark calculation to verify QCD
- Indispensable for determination of QCD scale and quark masses
- Essential to control various systematic errors down to a few % level
  - Finite lattice size  $L > 3\text{fm}$
  - Finite quark mass  $m_q \neq 0$
  - Finite lattice spacing  $a \neq 0$



Experimental spectrum

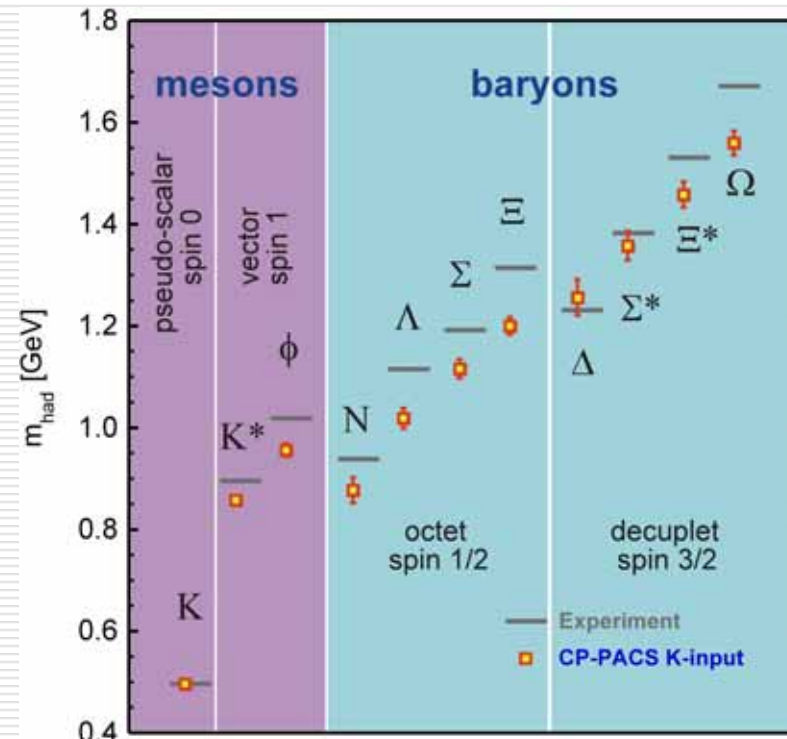


# CP-PACS result for the **quenched** spectrum'98

- Sea quark effects ignored

$$Z = \int \prod_{n\mu} dU_{n\mu} \prod_n d\bar{q}_n dq_n e^{-S_{gluon}(U) - \bar{q}D(U)q}$$
$$= \int \prod_{n\mu} dU_{n\mu} \det D(U) e^{-S_{gluon}(U)}$$

- adopted for computational ease
- General pattern reproduced, but clear systematic deviation beyond 10% precision

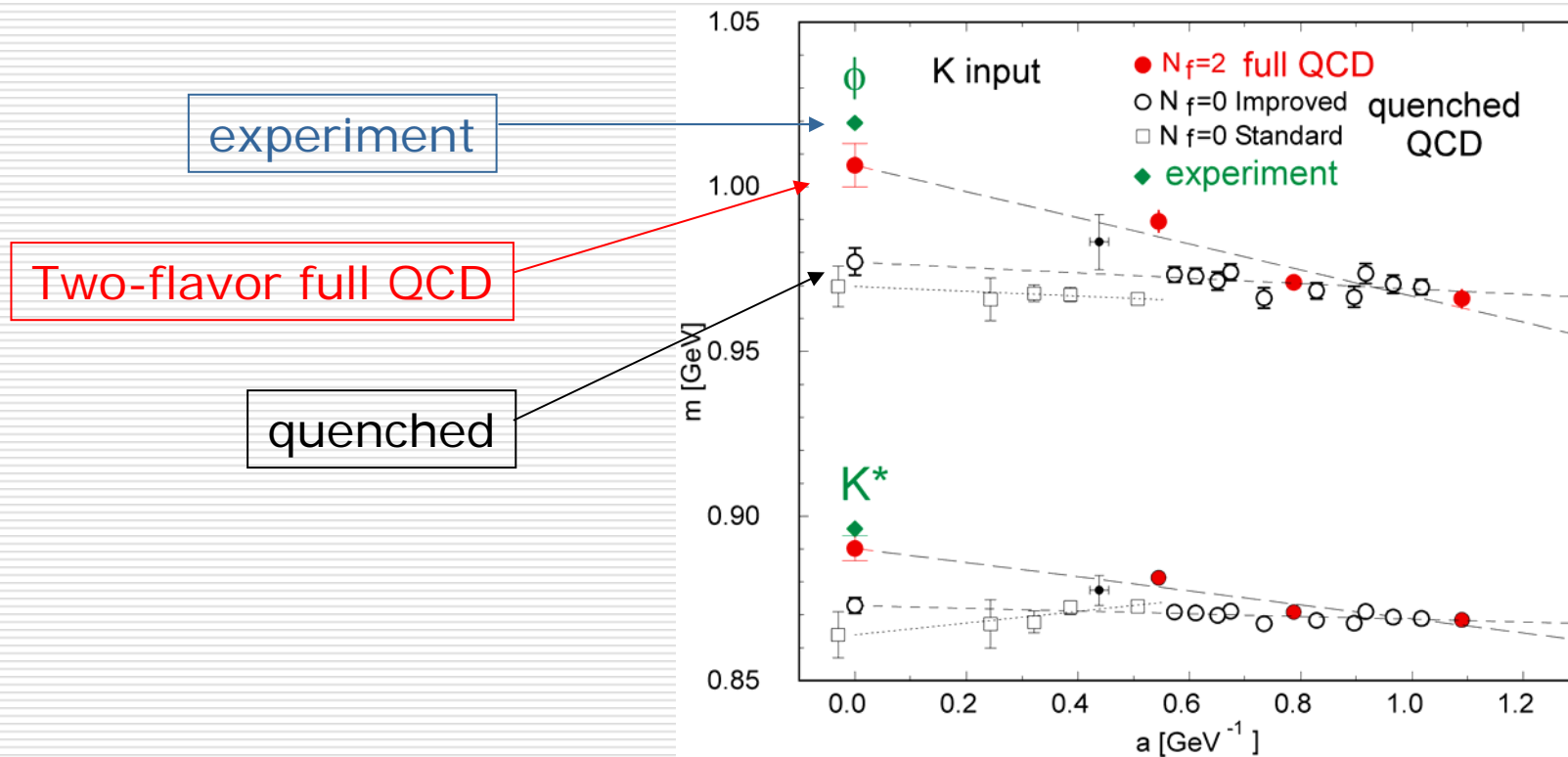


Calculated quenched spectrum



# Sea quark effects in the spectrum

- $K^*-K$  and  $\phi-K$  mass difference (Meson hyperfine splitting)
  - too small in quenched QCD
  - Much closer agreement for two-flavor full QCD





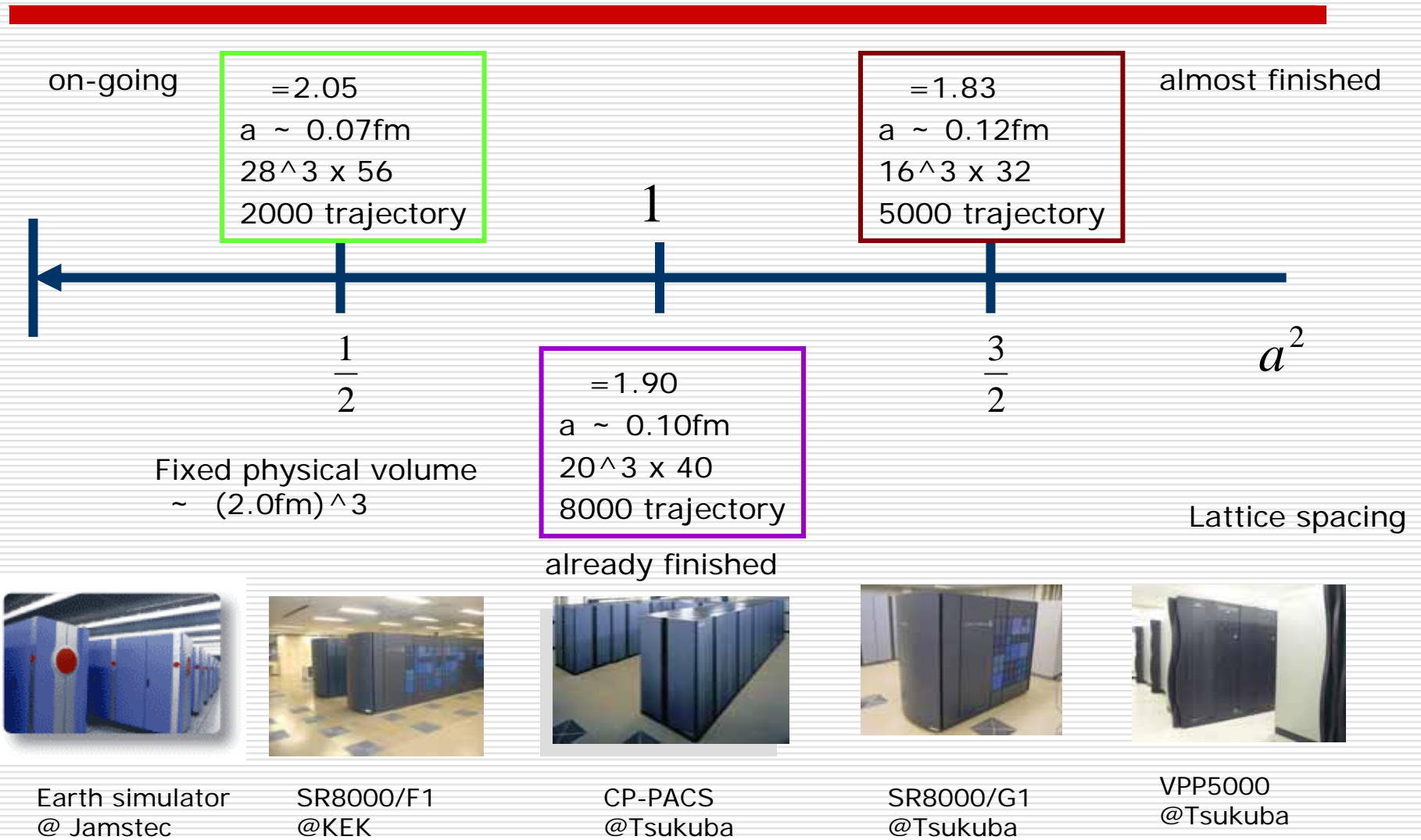
# QCD simulation with dynamical quarks

- Spectrum of quarks
  - *3 light quarks (u,d,s)*  $m < 1\text{GeV}$ 
    - *Need dynamical simulation*
  - 3 heavy quarks (c,b,t)  $m > 1\text{GeV}$ 
    - Quenching sufficient
- Dynamical quark simulation (full QCD)
  - costs 100-1000 times more computing power
  - *Algorithm for odd number of quarks now available*
- *Two-flavor full QCD (since around 1996)*  $N_f = 2$ 
  - u and d quark dynamical simulation
  - s quark quenched approximation
  - Number of studies: SESAM/UKQCD/MILC/CP-PACS/JLQCD
- *Two+One-flavor full QCD (since around 2000)*  $N_f = 2+1$ 
  - s quark also treated dynamically
  - Extensive studies have begun : MILC/CP-PACS-JLQCD



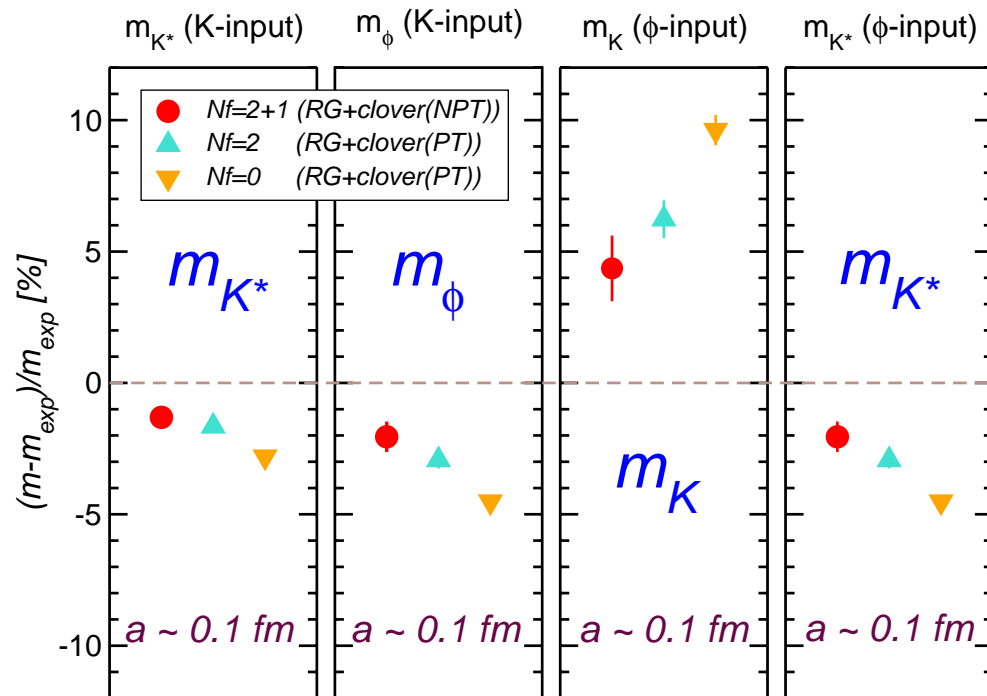
# Tsukuba/KEK joint effort toward $N_f=2+1$

A three year project 2003-2005





# Hyperfine splitting at $a \sim 0.1\text{fm}$



Increasingly closer  
agreement with  
experiment:

$N_f=0$

quenched approx

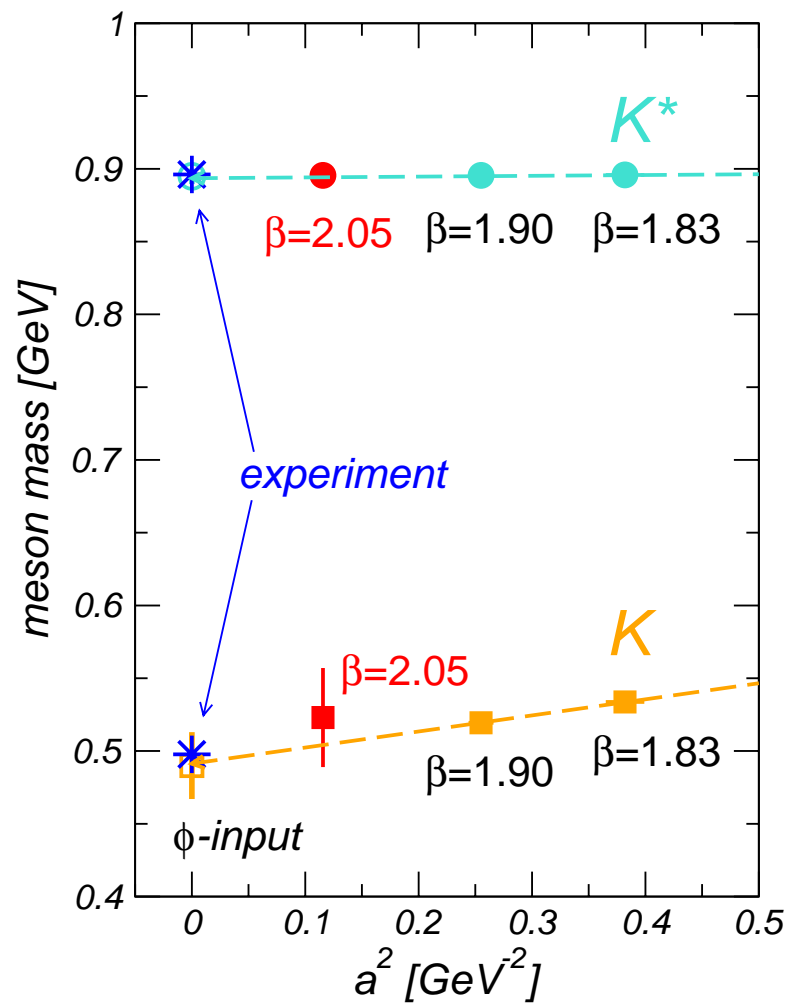
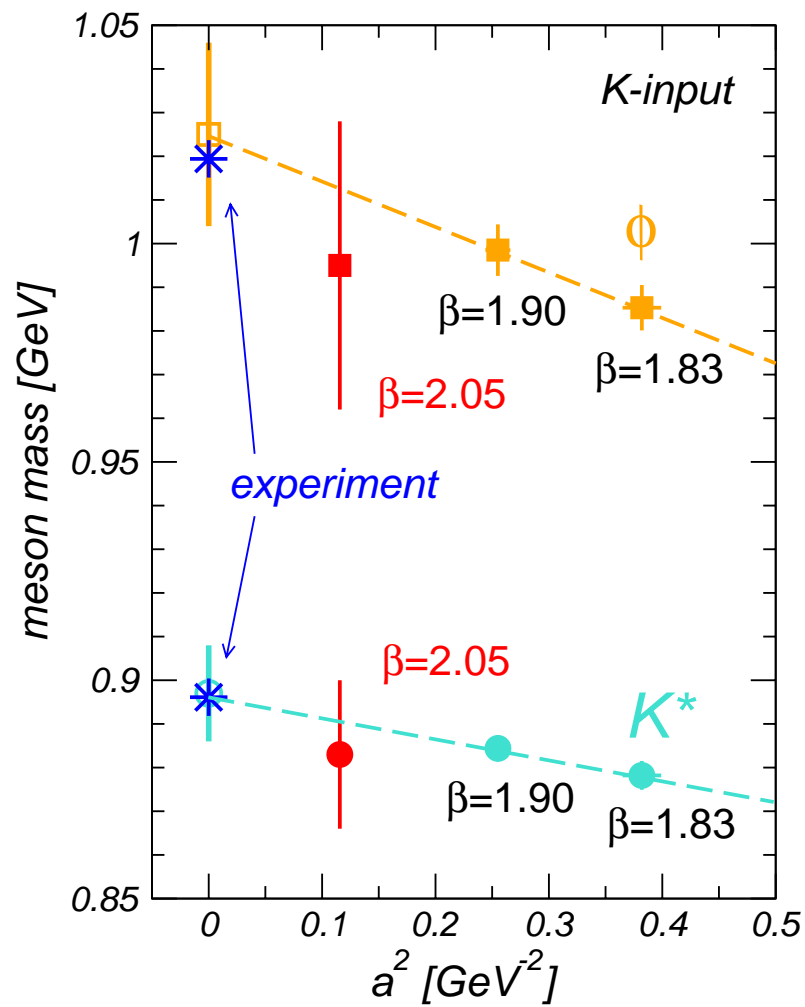
$N_f=2$  u&d quarks  
dynamical

$N_f=2+1$  u,d,s quarks  
dynamical

Remaining difference due  
to finite lattice spacing?



*examine a dependence*



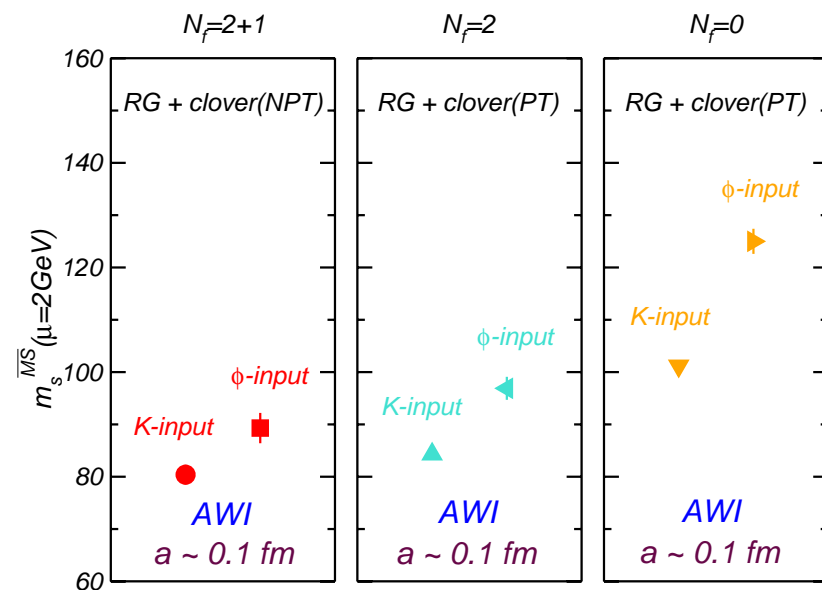
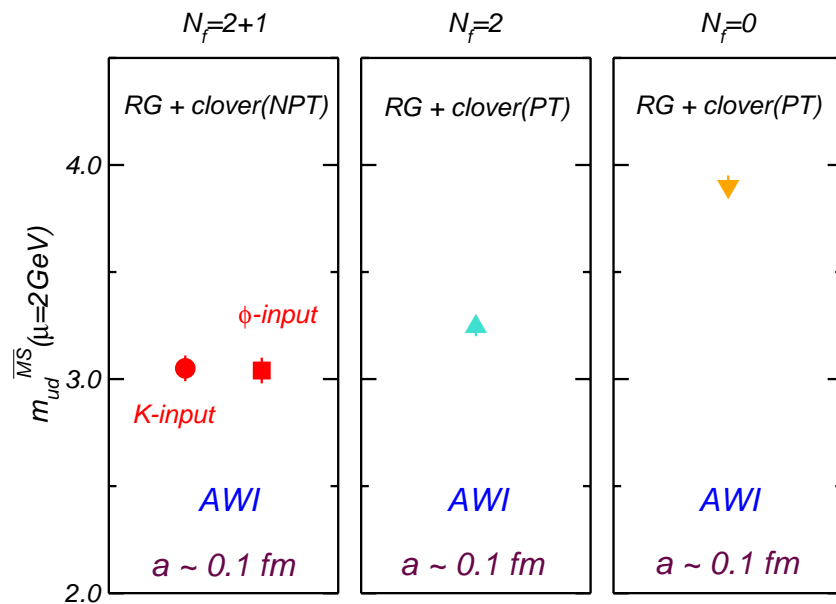


# Light quark mass results at $a \sim 0.1\text{fm}$

$$\overline{m}^{MS}(\mu = 2\text{GeV}) = \frac{m_u + m_d}{2} = 3.05 \pm 0.06\text{MeV}$$

$$m_s^{MS}(\mu = 2\text{GeV}) = 85 \pm 3\text{MeV}$$

Sizably small compared to folklore, e.g.  $m_{ud} \sim 5\text{MeV}$ ,  $m_s \sim 150\text{MeV}$





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# Future perspective



# Next generation of computers

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- 10 TFLOPS class machines for QCD
  - USA
    - *QCDOC (USA)* 2004-2005
      - Riken-BNL and BNL in 2005
    - Large clusters (FNAL and JLAB)
  - Europe
    - *QCDOC at Edinburgh*
    - *ApeNEXT (Italy)* 2005-2006
      - Large installation in Italy and possibly Germany
  - Japan
    - *CP-PACS successor* 2006
      - Development to start in fiscal 2005
      - 2/3 installation in early 2006, completion in 2007
    - KEK supercomputer upgrade in 2006



# 25 years of R&D of parallel computers at Tsukuba

CP-PACS



1978



1980

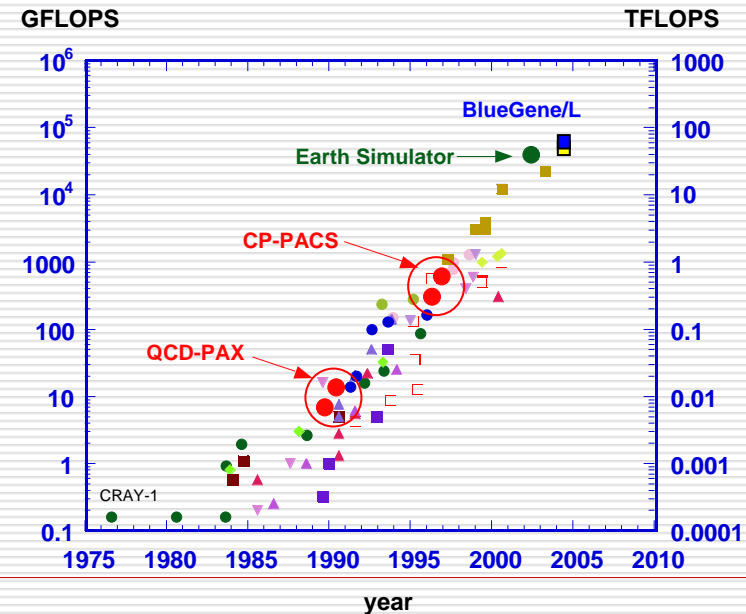


1989



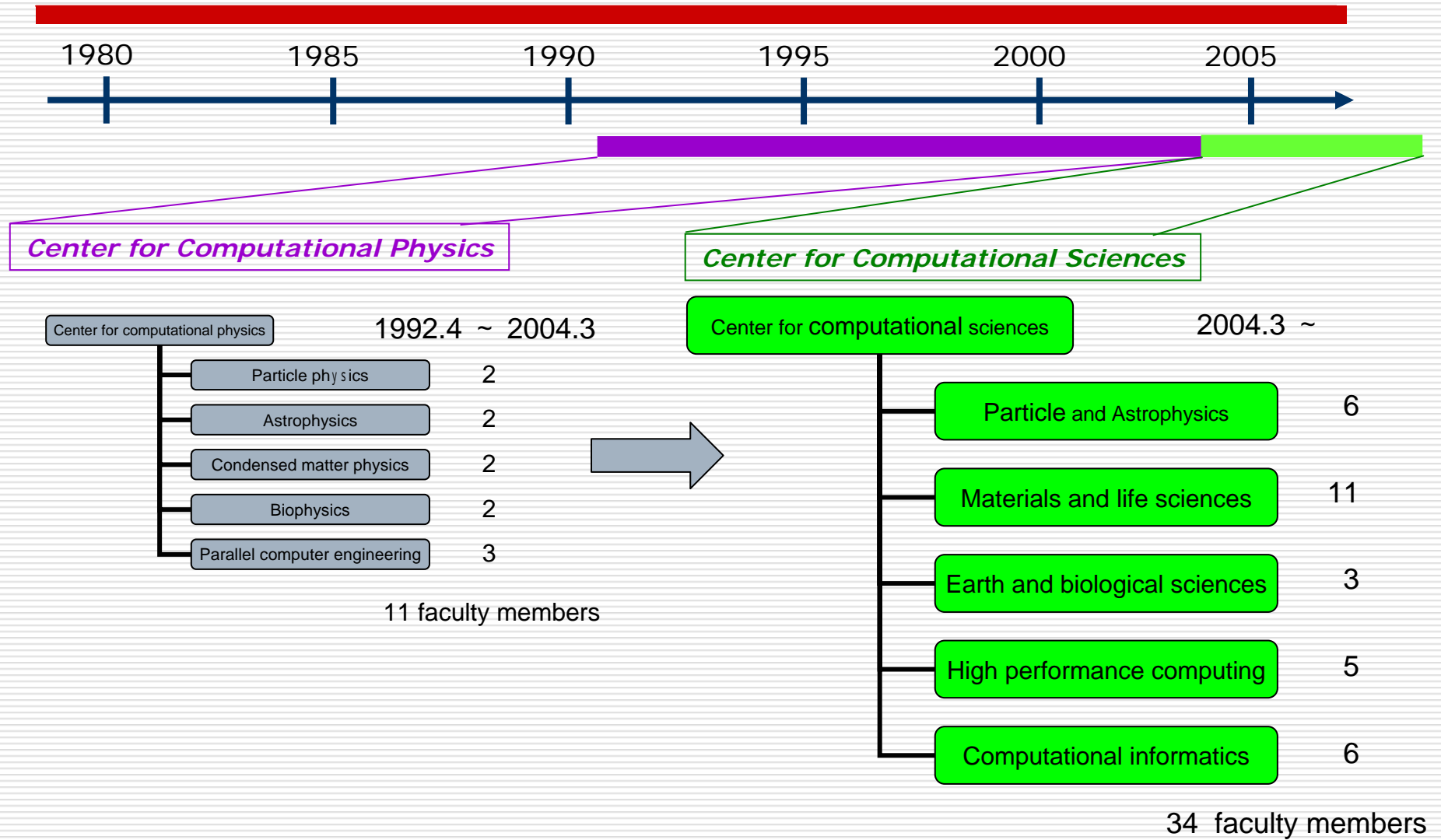
1996

year	name	speed
1978	PACS-9	7kflops
1980	PAXS-32	500kflops
1983	PAX-128	4Mflops
1984	PAX-32J	3Mflops
1989	QCDPAX	14Gflops
1996	CP-PACS	614Gflops





# Center for Computational Sciences, University of Tsukuba





# Our lattice QCD collaboration

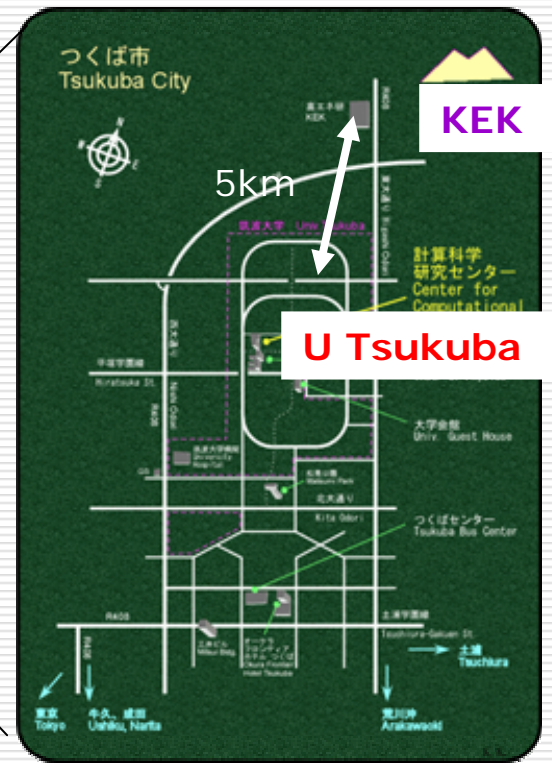
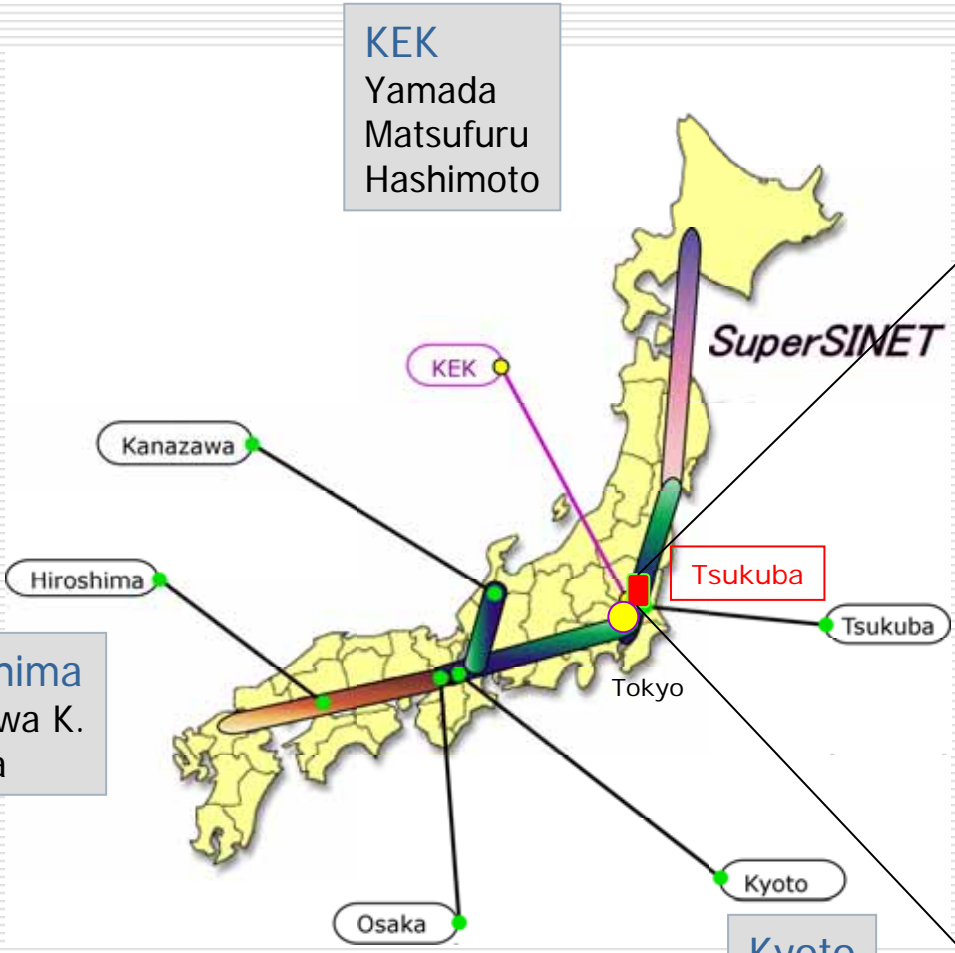
Now elsewhere  
 Okamoto(FNAL)  
 Lesk(Imp. Coll.)  
 Noaki(Southampton)  
 Ejiri(Bielefeld)  
 Nagai(Zeuthen)  
 Aoki Y.(Wuppertal)  
 Izubuchi(Kanazawa)  
 Ali Khan(Berlin)  
 Manke  
 Shanahan(London)  
 Burkhalter(Zurich)

**Tsukuba**  
 Ishikawa T.  
 Baer  
 Taniguchi  
 Kuramashi  
 Ishizuka  
 Aoki  
 Yoshie  
 Kanaya  
 Ukawa  
 Iwasaki

**KEK**  
 Yamada  
 Matsufuru  
 Hashimoto

**Hiroshima**  
 Ishikawa K.  
 Okawa

**Kyoto**  
 Onogi



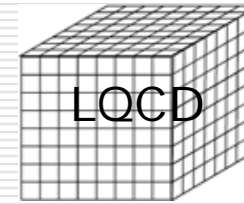


## CP-PACS successor outline

- Strategy: MPP in terms of commodity components
  - Node
    - Single CPU (Xeon 3GHz )
    - 2GB PC3200 memory with FSB800  
i.e., 6.4GB/s peak memory bandwidth to each CPU
    - 200GB disk (Raid0 mirror)
  - Network
    - 3-dimensional hyper-crossbar, i.e., crossbar switch in each direction
    - Dual GbEthernet for each direction,  
i.e., 0.25GB/s/link and an aggregate 0.75GB/s/node
  - System size
    - At least 2048 CPU (16x16x8, 12Tflops/4TB), and hopefully up to 3072 CPU (16x16x12, 18Tflops/6TB)



# Impact of lattice QCD



## Hadron spectrum and Fundamental constants of QCD

- Strong coupling constant
- Quark masses

$$\alpha_s$$

$$m_u, m_d, m_s, m_c, m_b, m_t$$

*Fundamental natural constants*

## Hadron physics

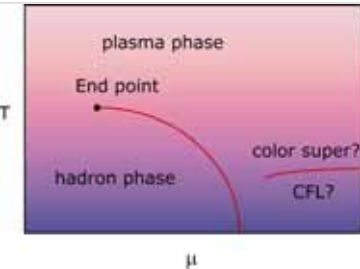
- eta' meson mass and U(1) problem
- exotic states  
glueball, hybrids, penta-quark, ...
- hadronic matrix elements  
proton spin, sigma term, ...
- structure functions/form factors

$$\int_0^1 dx x^{n-1} F(x, q^2) = (\ln q^2)^{-\gamma_n} \langle N | O_n | N \rangle$$

*Long-standing issues of hadron physics*

## Finite-temperature/density behavior

- order of transition
- critical temperature/density
- equation of state



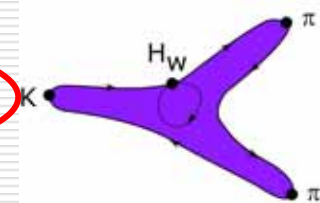
*Physics of quark-gluon plasma*

## Weak interaction matrix elements

- K meson amplitudes

$$B_K$$

$$K \rightarrow \pi\pi \text{ decays}$$



- B meson amplitudes  
 $f_B, B_B$  form factors

*CKM matrix and CP violation*



## I = 1/2 rule and CP violation in K decays

- Weak interaction decays of K mesons

- I = 1/2 rule 
$$\frac{\text{Re } A_0(K \rightarrow \pi\pi(I=0))}{\text{Re } A_2(K \rightarrow \pi\pi(I=2))} \approx 22$$

- CP violation 
$$\frac{\varepsilon'}{\varepsilon} = \begin{cases} (20.7 \pm 2.8) \times 10^{-4} & \text{KTeV experiment (FNAL)} \\ (15.3 \pm 2.6) \times 10^{-4} & \text{NA48 experiment (CERN)} \end{cases}$$

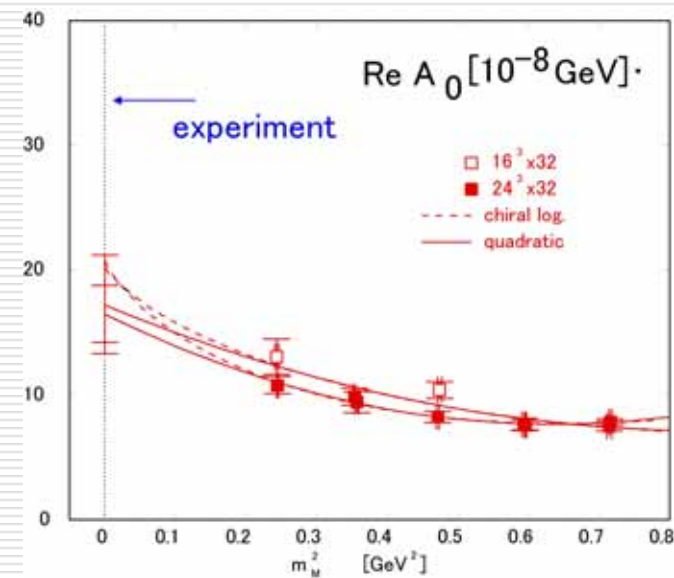
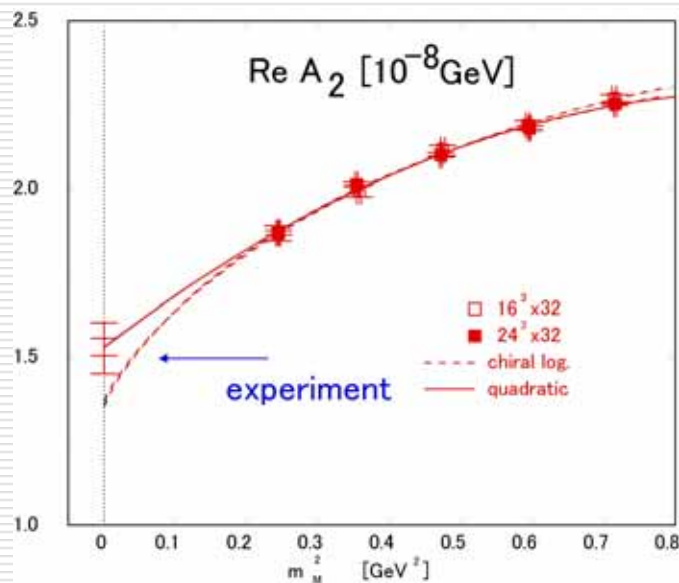
- Crucial numbers to verify the Standard Model understanding of CP violation
- Long-standing issue of particle physics since 1960's



# $I=1/2$ rule

CP-PACS Collaboration, Phys.Rev. D68 (2003) 014501  
RBC Collaboration, Phys.Rev. D68 (2003) 114506

- Reasonable agreement with experiment for  $I=2$
- About half of experiment for  $I=0$





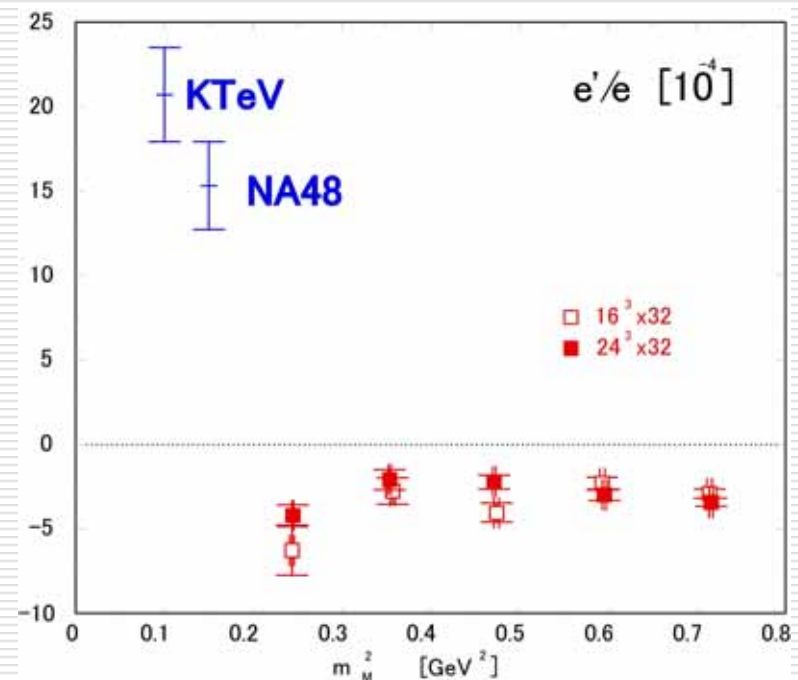
# CP violation parameter $\epsilon'/\epsilon$

- Small and negative in disagreement with experiment

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

- Possible reasons
  - connected with insufficient enhancement of  $I=1/2$  rule
  - Method of calculation (K reduction) may have serious problems

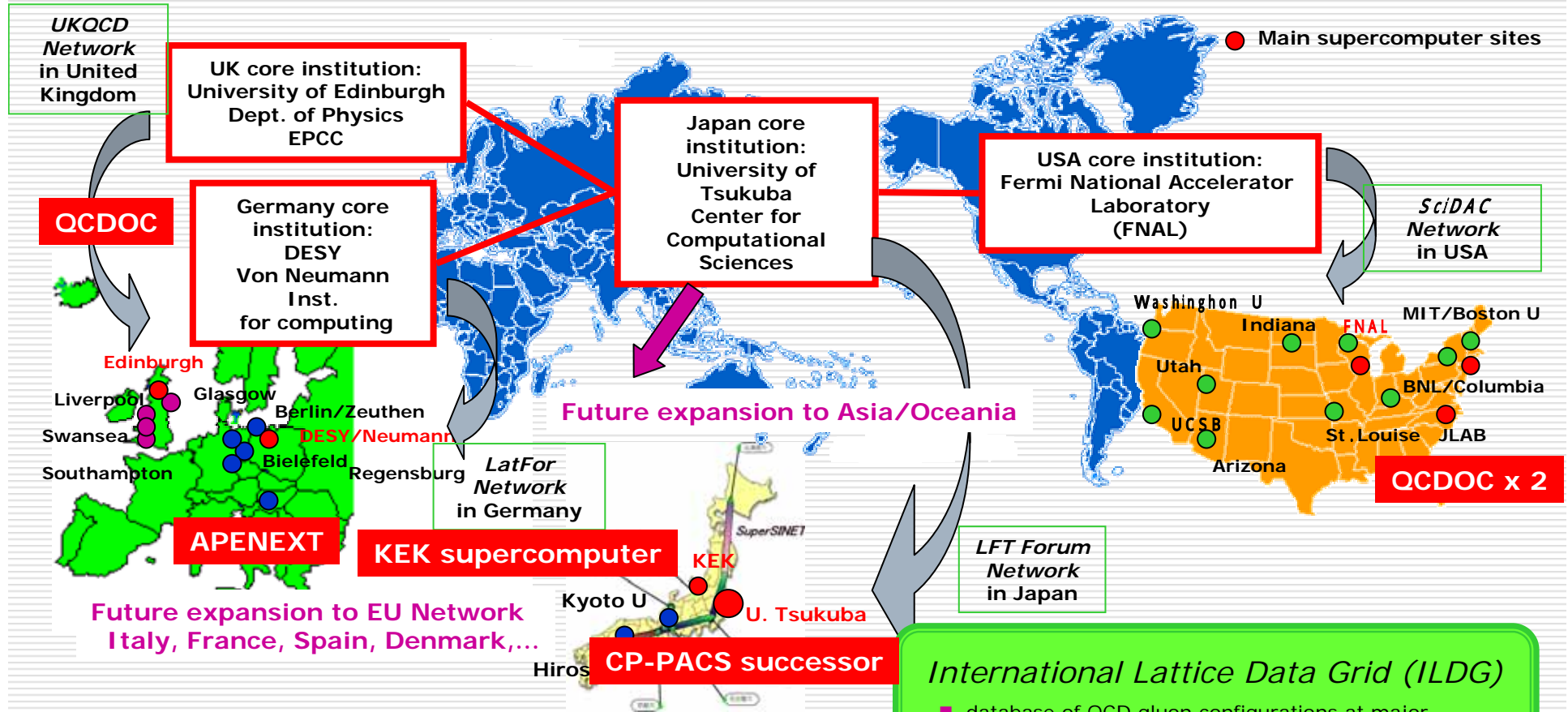
*A major challenge  
awaiting further work*





# International Research Network for Computational Particle Physics

JSPS core-to-core program



- database of QCD gluon configurations at major supercomputer facilities
- acceleration of research via mutual usage of QCD gluon configurations via fast internet
- future international sharing of supercomputing and data storage resources

<http://www.lqcd.org/ildg/tiki-index.php>



# Summary

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- *Lattice QCD as a physical theory*
  - *One of the fundamental areas of particle physics research requiring high performance computing*
  - *Welcome prospect toward precision predictions with realistic quark spectrum in sight*
- *Lattice QCD as computational physics*
  - *One of most compute- and network-intensive applications*
  - *Prototype in which theory and instrument making has developed hand in hand*
- *Lattice QCD as world discipline*
  - *Rapid move toward international collaboration and coordination for enhancing development*