Developing supercomputers and computational physics

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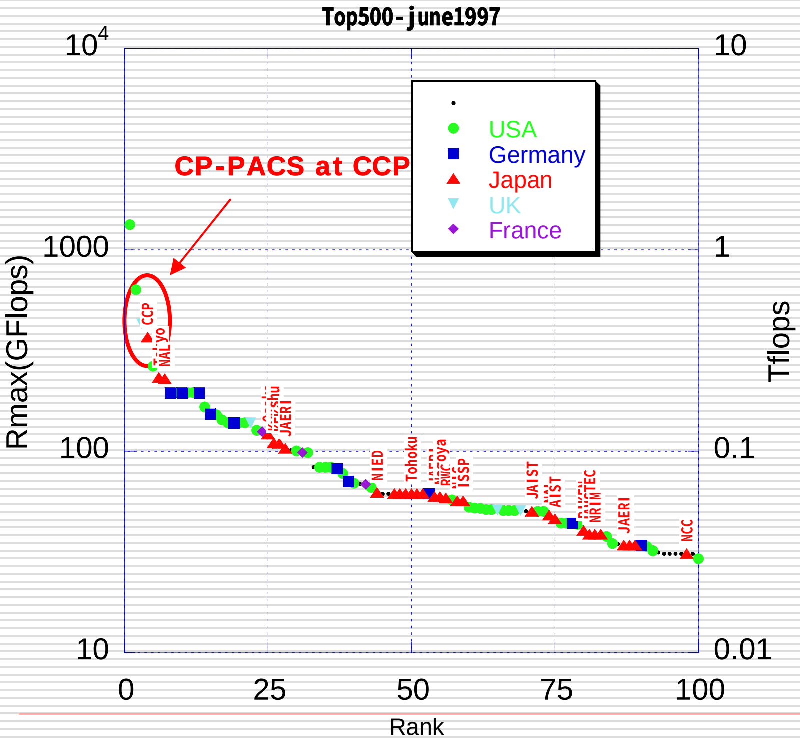
- Academic HPC environment in Japan
- Center for Computational Physics
- lattice QCD on CP-PACS computer
- CP-PACS/GRAPE-6 complex and galaxy formation simulation
- National networks and beyond

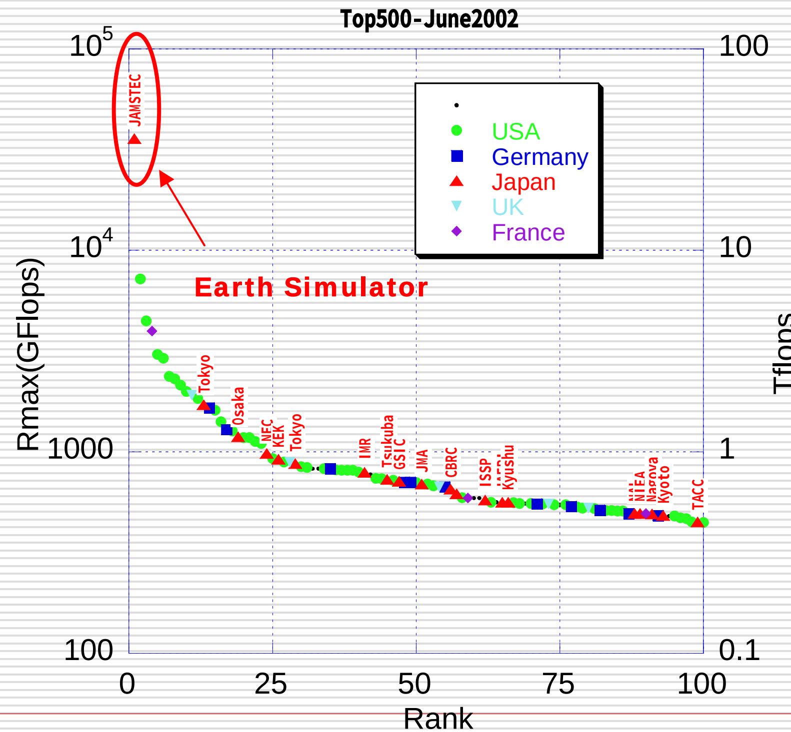
Academic HPC environment in Japan

- Supercomputer resources viewed in the Top 500 list

June 1997
30 systems
23% of total Rmax
in the top 100

June 2002
20 systems
37% of total Rmax
in the top 100



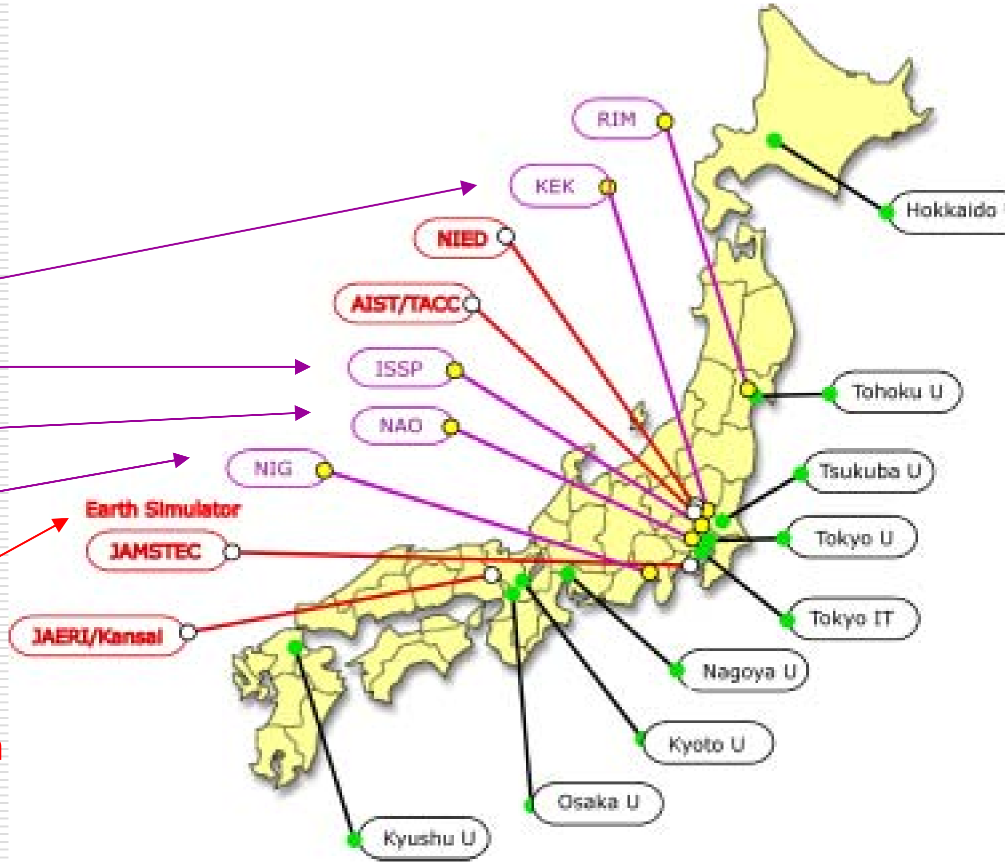


Supercomputers classified by affiliations

- Computer Centers of major universities
- Academic research institutes/organizations

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

    belongs to JAMSTEC (Japan Marine science and Technology Center)



Resource allocation to users

- Computer centers of universities
  - Charged by CPU time and disk usage
  - Special low rates for larg-scale usage
- Academic research institutes/organizations
  - Application by users and selection by peer committee
  - Typical large-scale applications: 1 week of full system

		peak	max allocation	#projects/year
KEK	high energy	1.2Tflops	decide by case	20
NAO	astrophysics	0.6Tflops	1 week of full system	20
ISSP	condensed matter	0.6Tflops	1 week of full system	100

- Government labs
  - Mission-oriented
  - Limited access by outside users
  - Earth Simulator: application and selection
    - 27 projects this year

      Atomosphere/ocean 15; earth 8; computer science 3; others 1

System procurement and upgrade

- Installed under rental contract with vendors
- Contract renewed at every 5-6 years
- Selection of system/vendor by a bidding under strict government regulations
- Rental budget part of annual budget of installation sites

→

- System renewal at every 5-6 years
- successfully provided high level of HPC resources to general scientific users

In Tsukuba,
a somewhat different tradition has been pursued.....

Center for computational Physics
University of Tsukuba

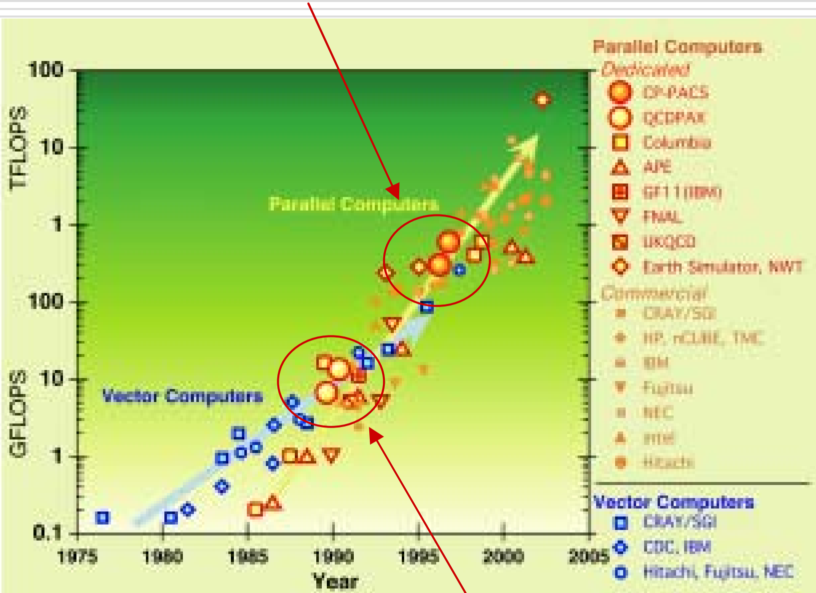
- Founded in 1992
- Emphasis on
  - Development of HPC systems suitable for computational physics
  - Close collaboration of physicists and computer scientists

- Computing facility
  - CP-PACS parallel system
    - MPP with 2048PU/0.6Tflops peak
    - Developed at the Center with Hitachi Ltd.
    - #1 of Top500-November 1996
  - GRAPE-6 system
    - Dedicated to gravity calculations
    - Developed at U. Tokyo
    - 8Tflops equivalent

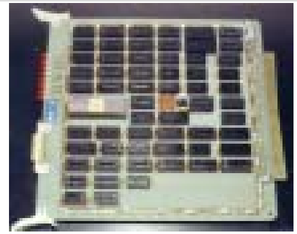
History of PACS/PAX computers at Tsukuba

- Long history (since late ’70s) of developing parallel machines for scientific calculations

CP-PACS/96



QCDPAX/89



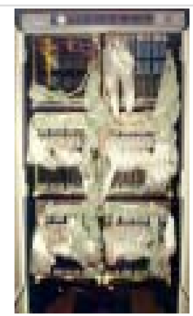
PU board of PACS-9 (1978)

PAX-128 (1983) with control unit

Year	Machine	Performance	#PU	Memory	CPU/MPU
1978	PACS-9	7 KFLOPS	9		M6800
1980	PAX-32	0.5 MFLOPS	32	576 KB	M6800/AM9511
1983	PAX-128	4 MFLOPS	128	3 MB	M68B00/AM9511-4
1984	PAX-32J	3 MFLOPS	32	4 MB	DCJ-11
1989	QCDPAX	14 GFLOPS	480	3 GB	M68020/L64133
1996	CP-PACS	307 GFLOPS	1024	64 GB	extended PA-RISC
1997	CP-PACS	614 GFLOPS	2048	128 GB	1.1

PU array of PAX-32 (1980)

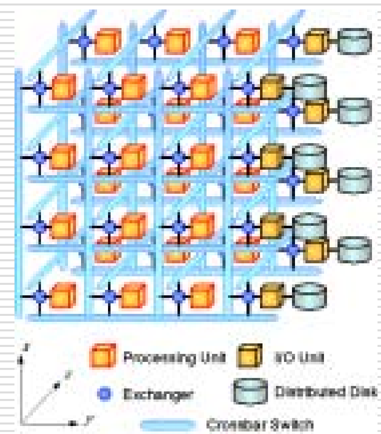
PAX-32J (1984)



A cabinet of QCDPAX (1989)

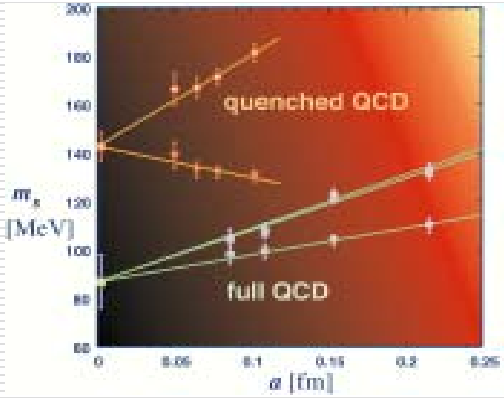
CP-PACS parallel computer

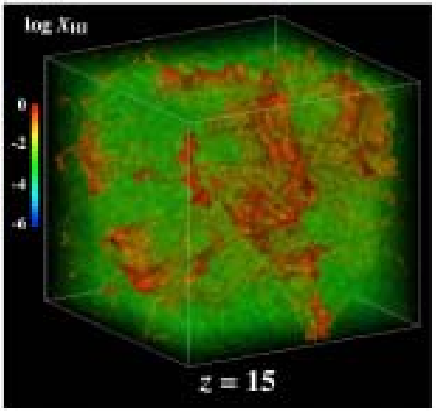
- MPP with 2048 compute nodes and 128 I/O nodes
  - 0.6Tflops peak , 0.3Gflops/node,
  - 16x16x17 node array, 3-dim crossbar network, 0.3GB/sec throughput/link
- Built by a joint effort of
  - Computer scientists (about 15 members)
  - Physicists (about 15 members)
  - Vendor (Hitachi Ltd.)
    - Developed to SR2201/SR8000 series
- Architecture development
  - PVP-SW (vector processing on a RISC processor)
  - Remote-DMA (zero-copy data transfer between nodes)
  - Detailed benchmark on real applications (QCD)



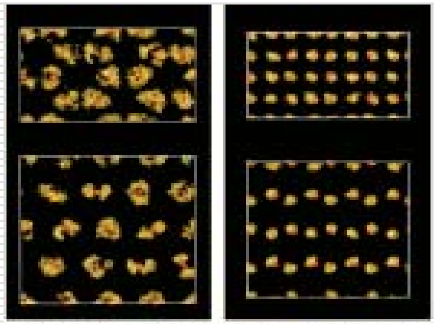
Computational physics with CP-PACS

- Concentrated usage
  on a few fundamental physics problems
  which demands large-scale calculations



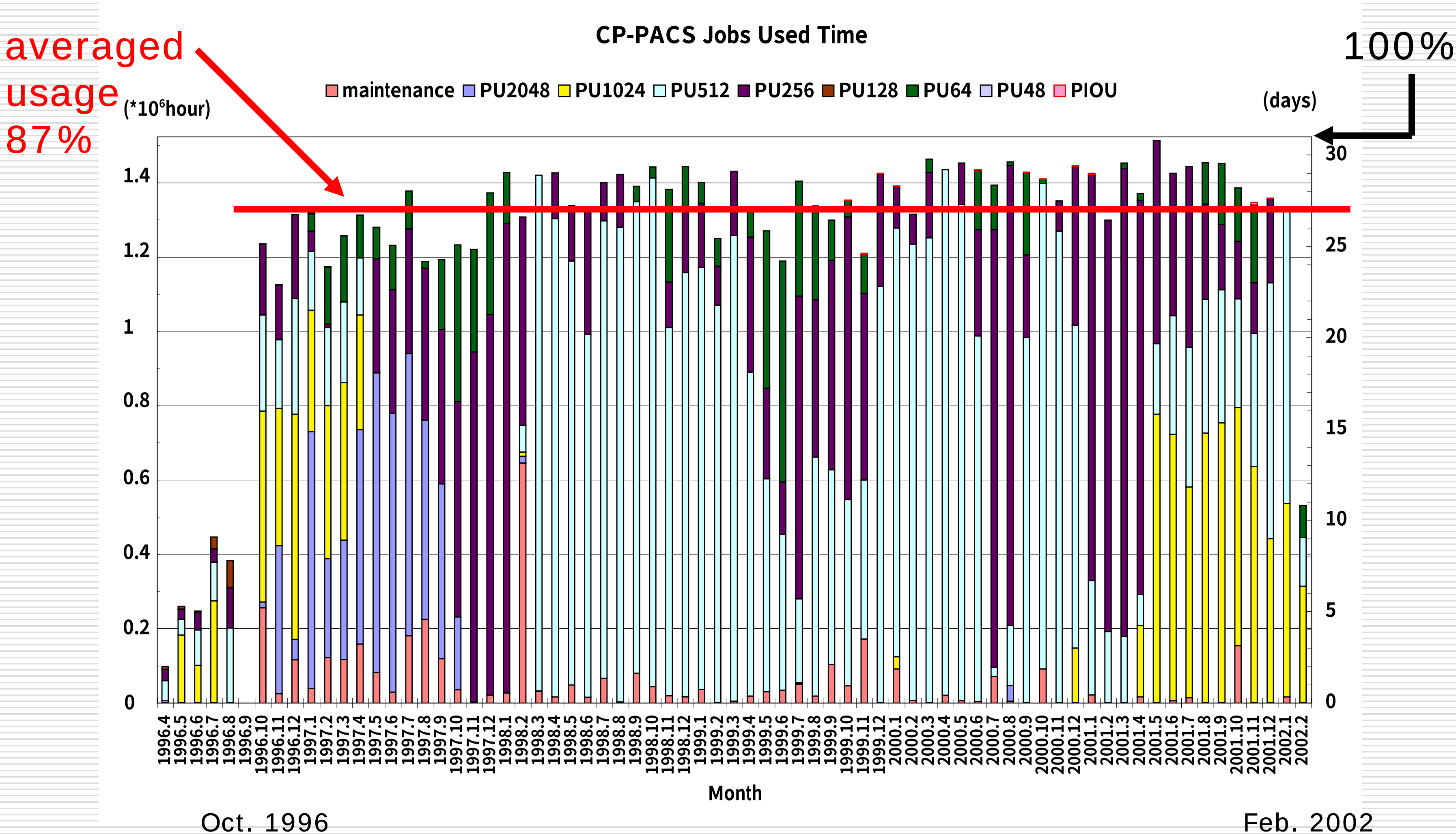


  - High energy physics; QCD
  - Astrophysics; Radiation hydrodynamics
  - Condensed matter; phases of solid hydrogen



CP-PACS run statistics

Oct.96-Feb.02



Lattice QCD on the CP-PACS computer

- Lattice Quantum Chromodynamics (QCD) and its goal
- Physics achievements
  - Quenched light hadron spectrum
  - Light quark masses in two-flavor full QCD
  - $\Delta I=1/2$ rule and CP violation parameter ε'/ε in weak decays of K mesons

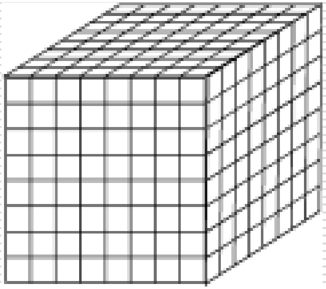
Lattice QCD and its goal

- Quantum Chromodynamics (QCD)
  - Fundamental theory of quarks and gluons and their strong interactions
  - Knowing 1 coupling constant α_s
    and 6 quark masses $m_u, m_d, m_s, m_c, m_b, m_t$
    will allow full understanding of strong interactions (Yukawa's dream)

- From computational point of view
  - Relatively simple calculation
    - Uniform mesh
    - Single scale
  - Requires much computing power due to
    - 4-dim. Problem
    - Fermions essential
    - Physics is at lattice spacing a=0
  - Precision required(<a few % error in many cases)

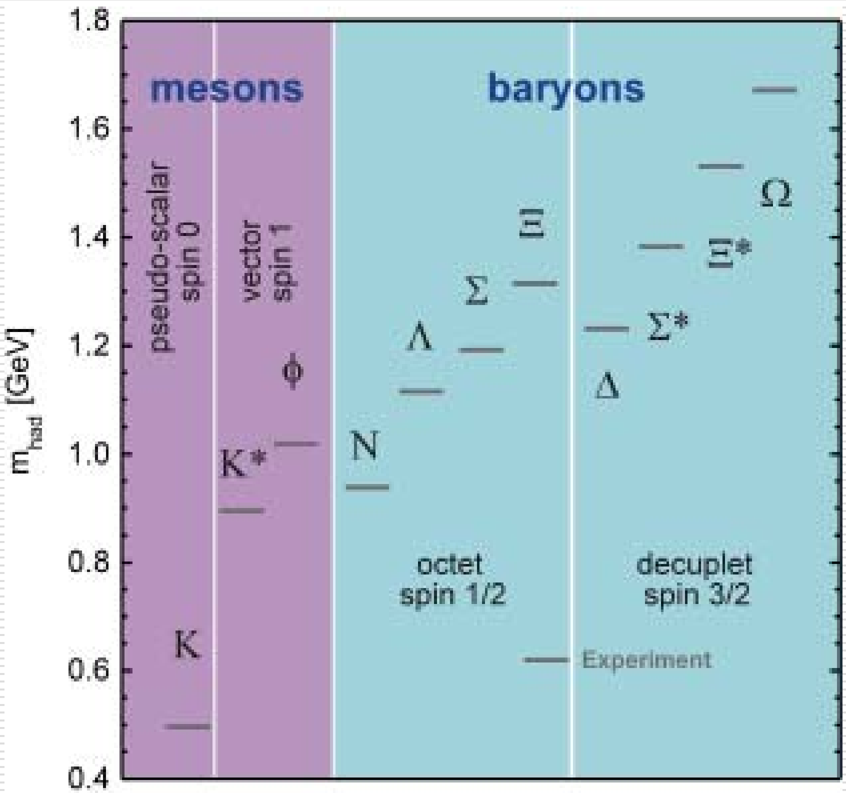
$$S = \frac{1}{\alpha_s}\sum_P tr(UUUU) + \sum \overline{\psi}(\gamma \cdot U + m_q)\psi$$

$$\langle O(U,\overline{\psi},\psi)\rangle = \frac{1}{Z}\int dU d\overline{\psi} d\psi O(U,\overline{\psi},\psi) e^{-S}$$



Quenched hadron mass spectrum

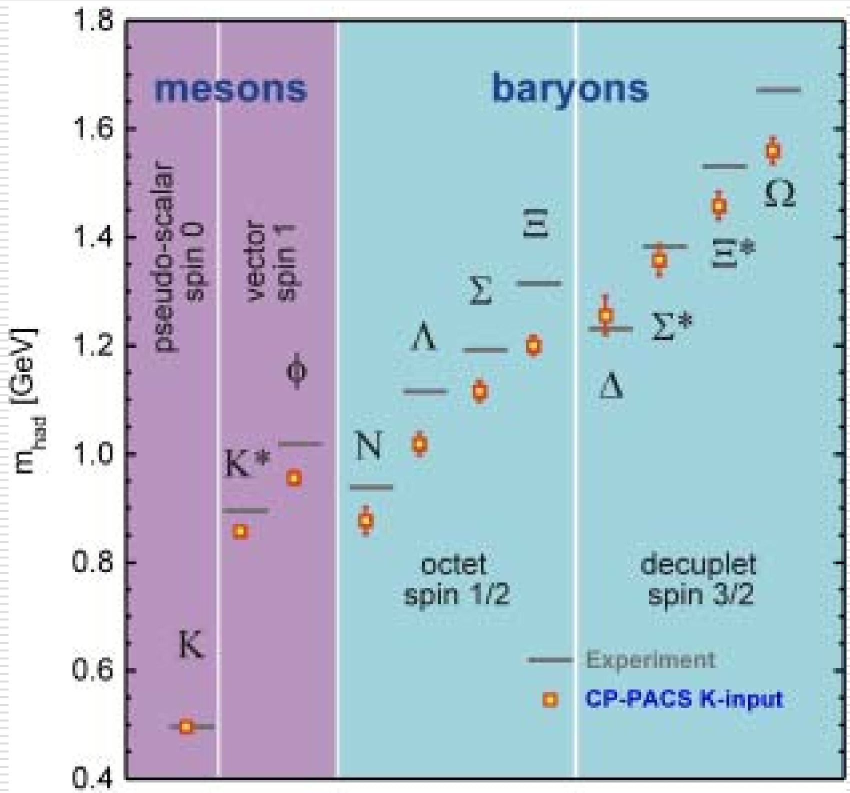
- Benchmark calculation to verify QCD
  - Pursued since 1981 (Weingarten/Hamber-Parisi)
- Quenched: quark-antiquark pair creation/annihilation ignored
- Essential to control various sysmatic errors down to a % level
  - Finite lattice size L>3fm
  - Finite quark mass mq→0
  - Finite lattice spacing a→0



Experimental spectrum

CP-PACS result for the quenched spectrum

- General pattern in good agreement with experiment
- Clear systematic deviation below 10% level
  - Indirect evidence of sea quark effect
- Completes the calculation pursued since 1981



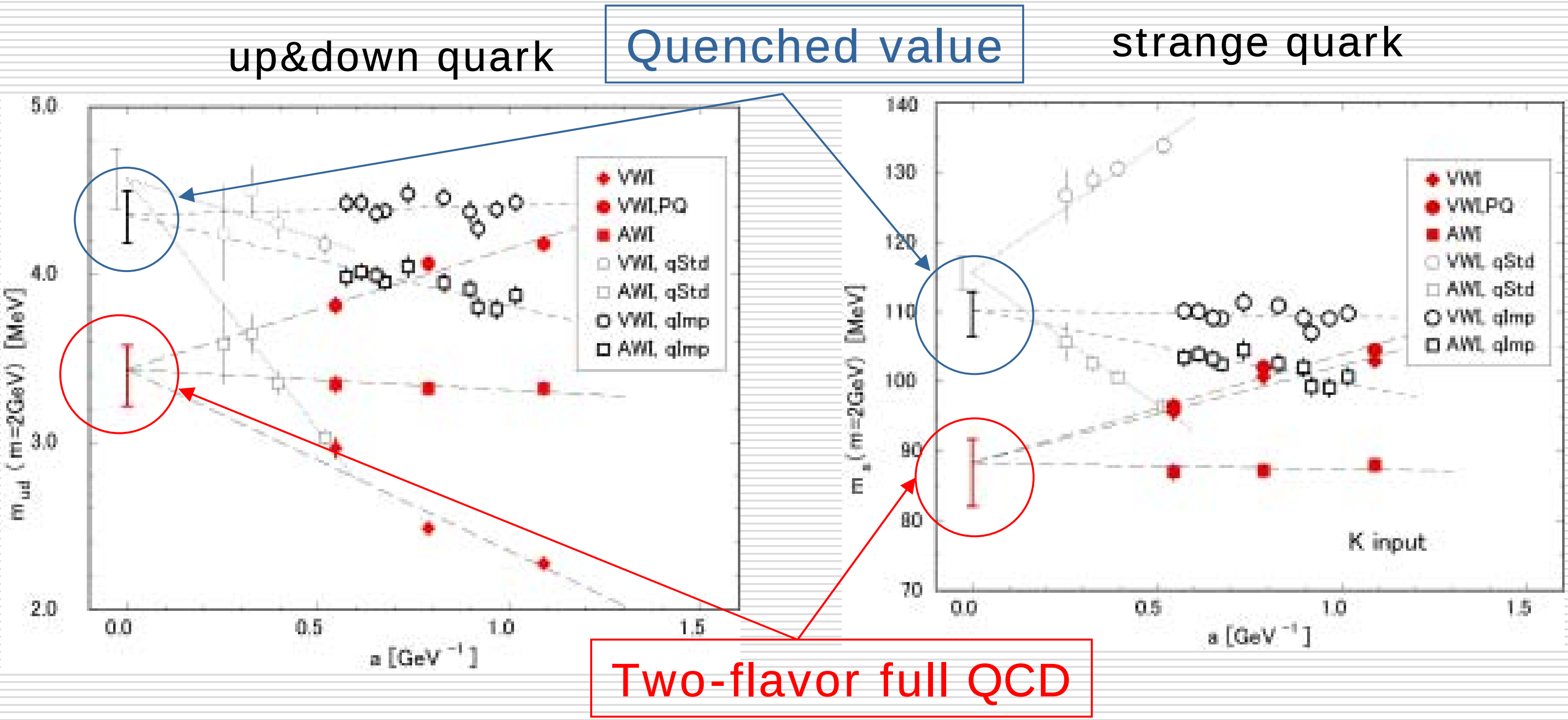
Calculated quenched spectrum

Two-flavor full QCD

- Spectrum of quarks
  - 3 light quarks (u,d,s) m < 1GeV
    - Need dynamical simulation
  - 3 heavy quarks (c,b,t) m >1GeV
    - Quenching sufficient
- Dynamical quark simulation
  - costs 100-1000 times more computing power
  - Algorithm for odd number of quarks still being developed
- First systematic study of two-flavor full QCD
  - u and d quark dynamical simulation
  - s quark quenched approximation

Quark masses from lattice QCD

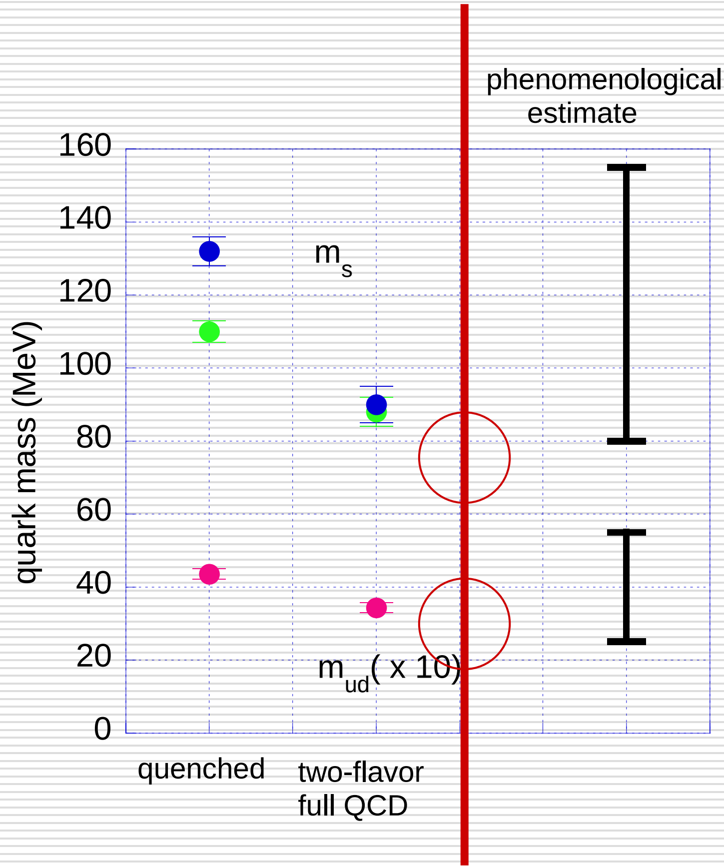
- Continuum extrapolation of light quark masses
  - Several methods yield a unique value in the continuum limit
  - Significant decrease by inclusion of sea quark effects



Summary on quark masses

- Significant sea quark effects
- Lower edge of phenomenological estimates;

  lighter than one believed for a long time
- Nf=3 simulations being pursued to obtain physical values of light quark masses



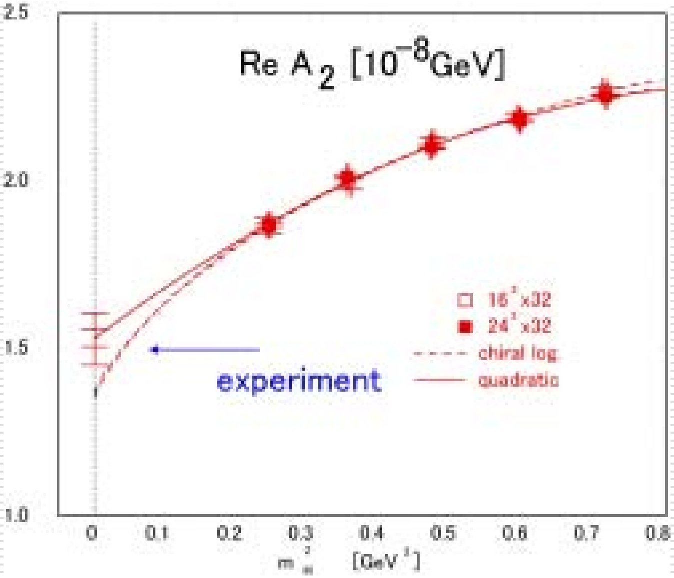
Real world;three flavors

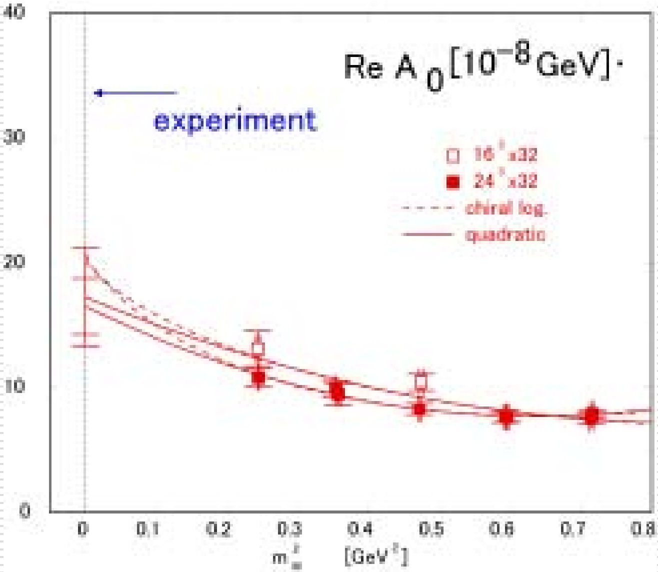
ΔI=1/2 rule and CP violation in K decays

- Weak interaction decays of K mesons
  - ΔI=1/2 rule $$\frac{\mathrm{Re}\,A_0\left(K\to\pi\pi(I=0)\right)}{\mathrm{Re}\,A_2\left(K\to\pi\pi(I=2)\right)}\approx 22$$
  - CP violation $$\frac{\varepsilon'}{\varepsilon}=\frac{\omega}{\sqrt{2}|\varepsilon|}\left[\frac{\mathrm{Im}\,A_2}{\mathrm{Re}\,A_2}-\frac{\mathrm{Im}\,A_0}{\mathrm{Re}\,A_0}\right]$$ $$=\begin{cases}(20.7\pm 2.8)\times 10^{-3} & KTeV\ \mathrm{exp}eriment\ (FNAL)\\ (15.3\pm 2.6)\times 10^{-3} & NA48\,\mathrm{exp}eriment\,(CERN)\end{cases}$$
- Crucial numbers to verify the Standard Model understanding of CP violation (matter-antimatter asymmetry)
- Two large-scale calculations using domain-wall QCD
  - RIKEN-BNL-Columbia by QCDSP
  - CP-PACS

ΔI=1/2 rule

- Reasonable agreement with experiment for I=2
- About half of experiment for I=0
- RIKEN-BNL-Columbia obtains a somewhat different result (smaller I=2 and larger I=0)





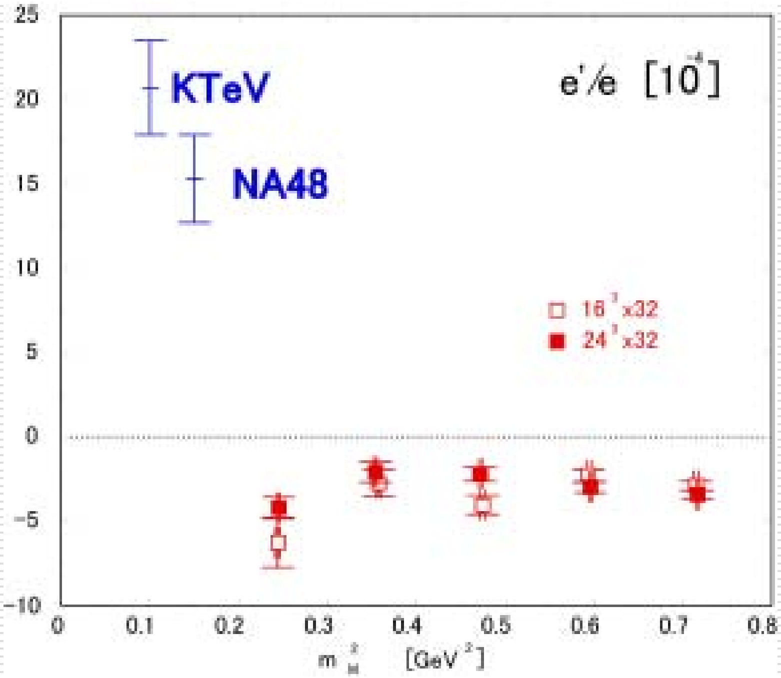
CP violation parameter ε'/ε

- Small and negative in disagreement with experiment
- Similar result from RIKEN-BNL-Columbia

- Possible reasons
  - connected with insufficient enhancement of ΔI=1/2 rule
  - Method of calculation (K→π reduction) may have problems

- Still a big problem requiring further work

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



Scale of QCD simulations

- Sustained speed
  - Quenched QCD — 64^3x112 — 53% of peak
  - Full QCD — 24^3x32 — 34% of peak
- Total CPU time with CP-PACS (0.6Tflops peak)
  - Quenched QCD — 199 days of full machine
  - Two-flavor full QCD — 415 days of full machine
  - K decay — 180 days of full machine
- Scaling law

$$\#FLOP's = C \cdot \left[\frac{\#conf}{1000}\right] \cdot \left[\frac{m_\pi / m_\rho}{0.6}\right]^{-6} \cdot \left[\frac{L}{3\,fm}\right]^{5} \cdot \left[\frac{1/a}{2GeV}\right]^{7} Tflops \cdot year$$

$$C \approx 2.8$$

→ O(10) Tflops machine needed for next progress

QCDOC (Mawhinney)/ApeNEXT(Jansen)

Astrophysics simulation with CP-PACS/GRAPE-6 complex

- Concept of HMCS (heterogeneous multi-computer system)
- Prototype HMCS with CP-PACS/GRAPE-6
- Galaxy formation in the Early Universe

Concept of HMCS

- Two interaction types of physical systems

Short-ranged	long-ranged
Complex and manifold	universal (gravity, Coulomb)
O(N) calculations	O(N^2) calculations
but complex	but simple

- A hybrid approach:
  - General purpose MPP to deal with short-ranged interactions
  - Special-purpose MPP to accelerate calculations of long-ranged interactions
  - Coupling of the two systems by a parallel network

CP-PACS/GRAPE-6 as a prototype HMCS

- GRAPE-6:
  - Developed by Makino et al (U. Tokyo);
    Gordon Bell winner of 2001
  - Gravity calculation accelerator
  - 32Gflops/chip x 32chip/board =1Tflops/board

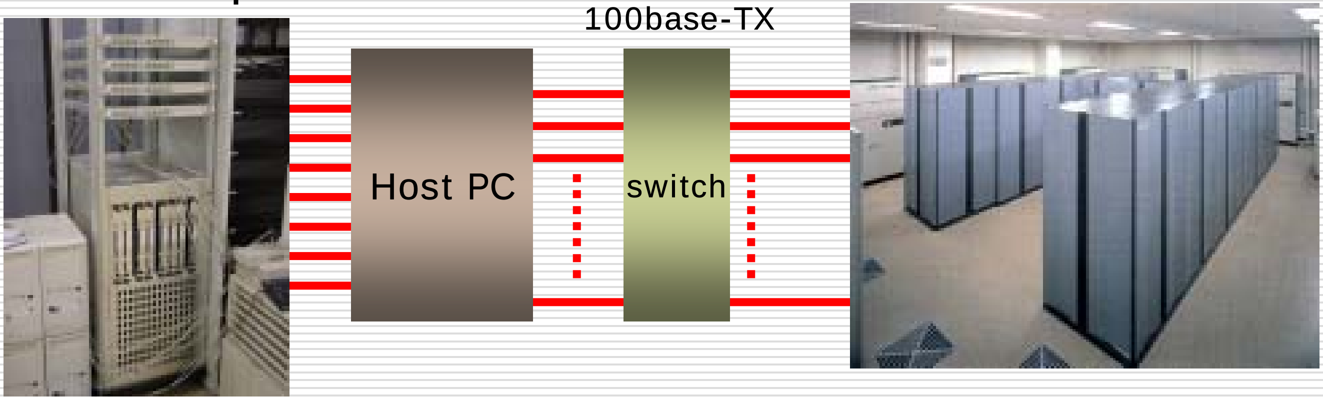
$$-G\sum_{j=1}^{N}\frac{m_i m_j}{r_{ij}^2}, \quad i=1,\cdots,N$$

GRAPE-6
Special-purpose MPP
8Tflops

Parallel I/O system
PAVEMENT/PIO

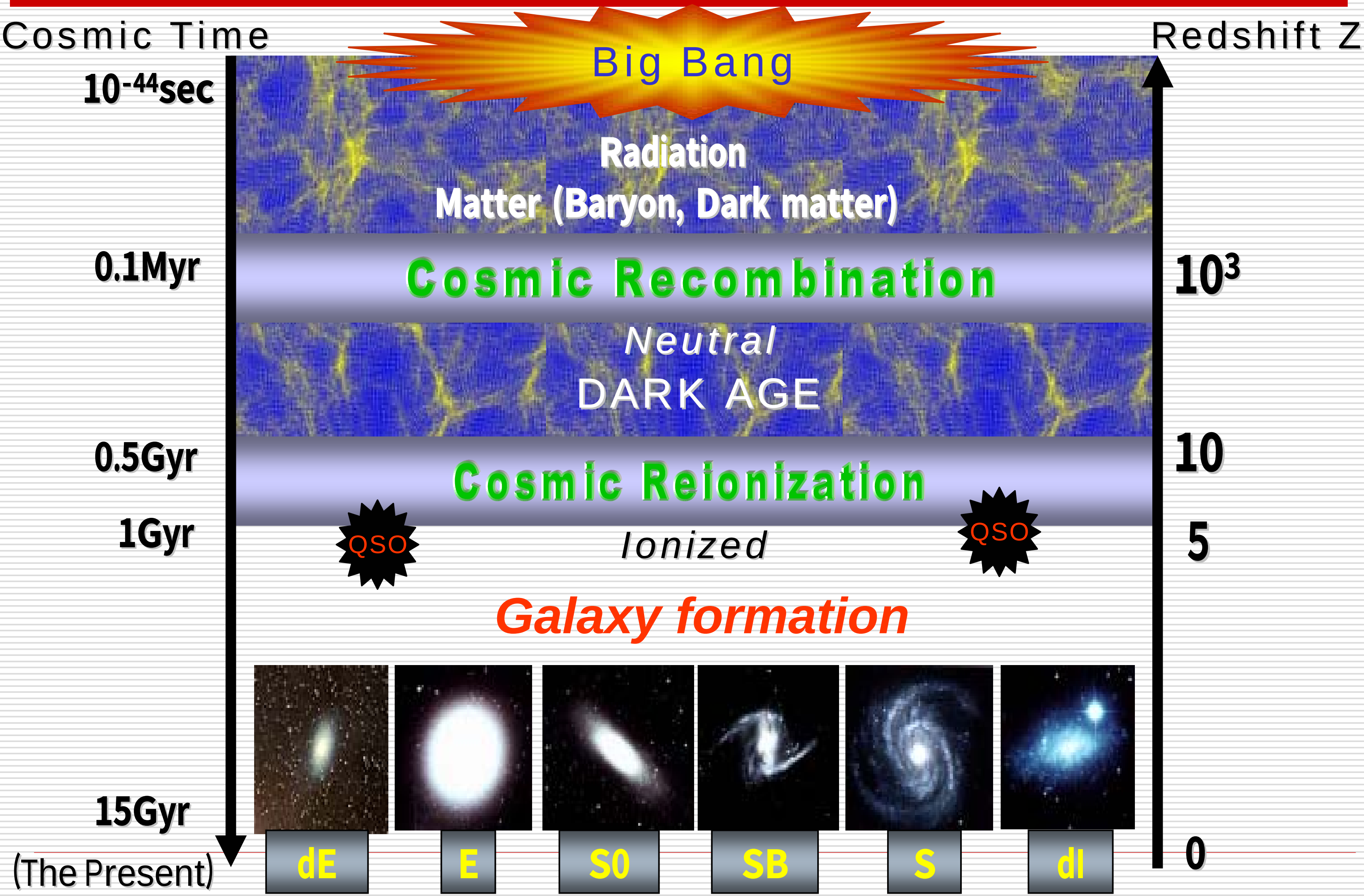
CP-PACS
General-purpose MPP
0.6Tflops

100base-TX



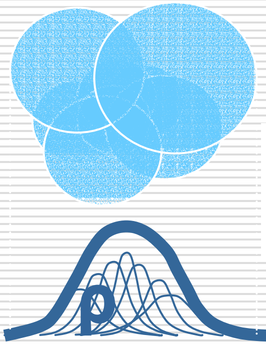
Galaxy formation simulation on HMCS

M. Umemura & H. Susa



Structure of the calculation

- Hydrodynamic motion of matter;
  - Smoothed Particle Hydrodynamics (SPH)
  - Represents matter density as collection of particles



$$\rho(\mathbf{r}_i) = \sum_j \rho_{j0} W(|\mathbf{r}_i - \mathbf{r}_j|)$$

W : kernel function

- Self-gravity acting on matter:
  - Direct calculation by GRAPE-6.

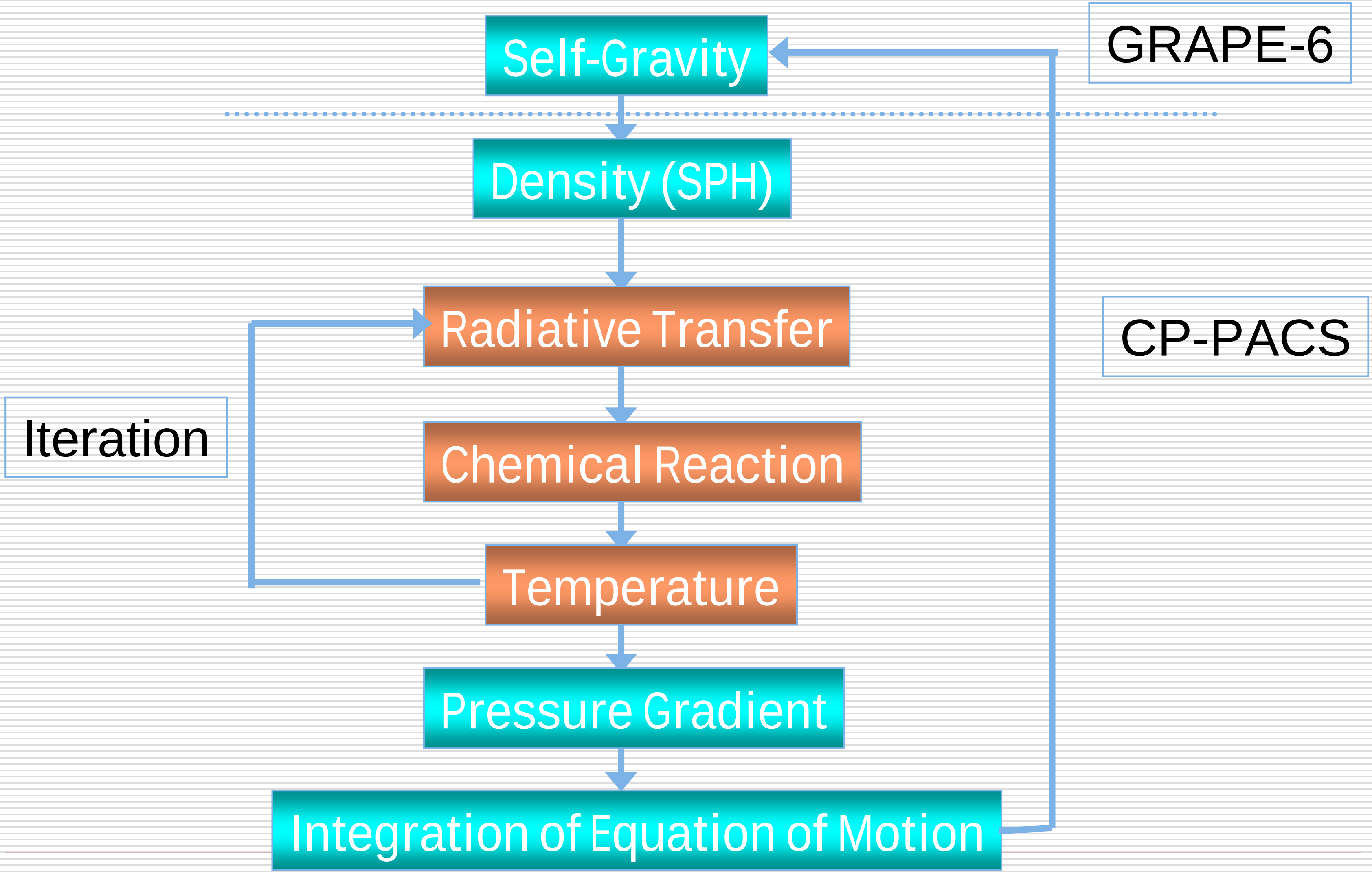
$$-G\sum_{j=1}^{N}\frac{m_i m_j}{r_{ij}^2}, \quad i = 1, \cdots, N$$

- Radiative transfer;
  - Interaction of photon with matter is solved

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \mathbf{n}\cdot\nabla I_\nu = \chi_\nu (S_\nu - I_\nu)$$

- Chemical reaction & radiative cooling

Algorithm



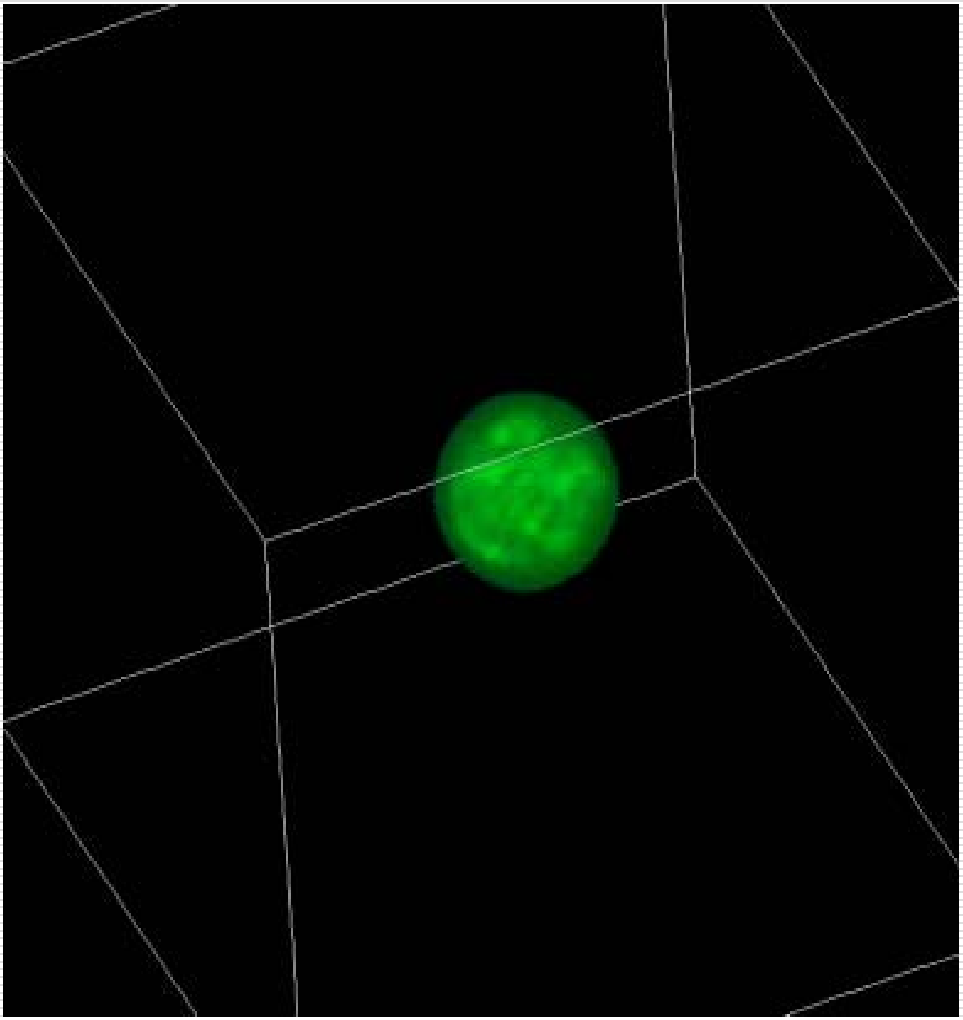
Self-Gravity
GRAPE-6
Density (SPH)
Radiative Transfer
CP-PACS
Iteration
Chemical Reaction
Temperature
Pressure Gradient
Integration of Equation of Motion

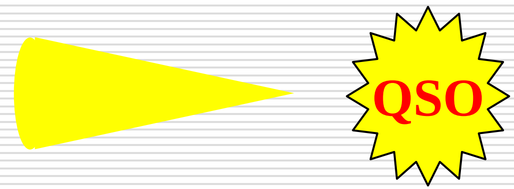
Calculation parameters

- Processors
  - 1024PU of CP-PACS 0.3TFLOPS
  - 4 boards of GRAPE-6 4TFLOPS
- Particle numbers
  - 64K baryonic matter particles
  - 64K dark matter particles
- calculation time/step
  - 4 sec for calculation on CP-PACS
  - 3 sec for communication to/from GRAPE-6
  - 0.1 sec for calculation on GRAPE-6

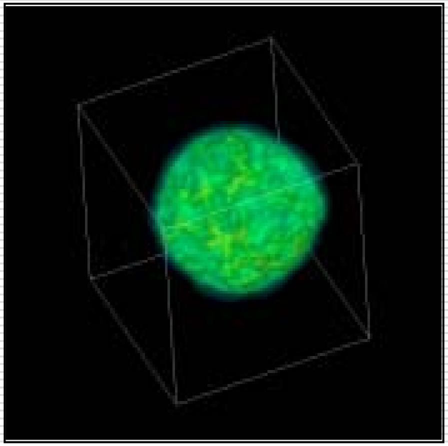
total 7.1 sec/time step

Galaxy Formation under UV Background

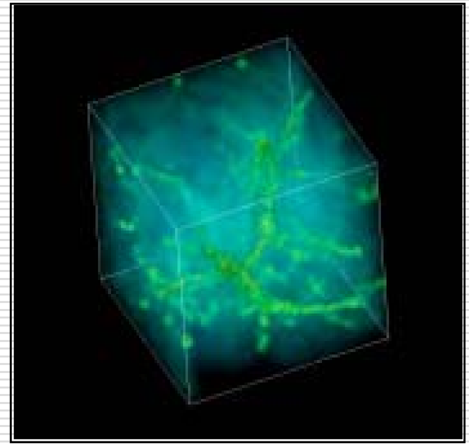




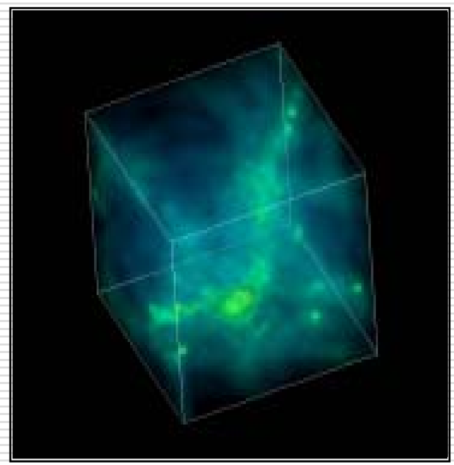
0.3 Gyr



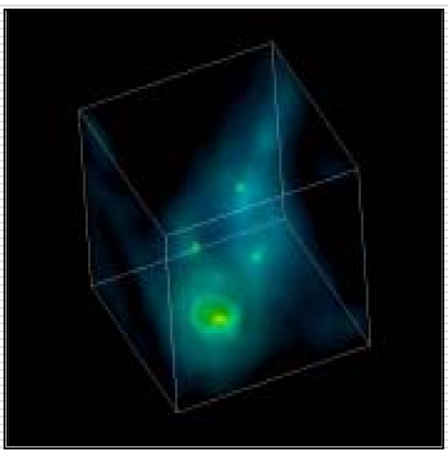
0.5 Gyr



0.7 Gyr



1 Gyr



National network and beyond

- TsukubaWAN
- SuperSINET

Tsukuba Science City

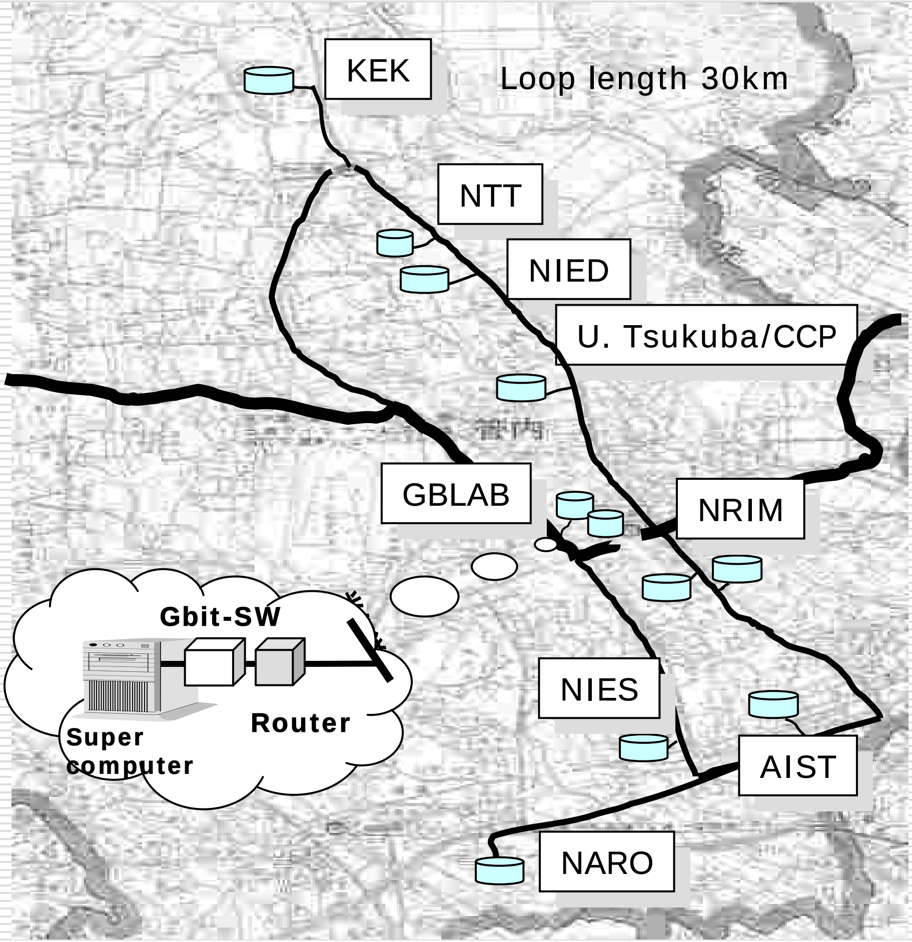
- High density of HPC-related research organizations
  - High energy physics KEK/U of Tsukuba/…
  - Matierial science AIST/NRIM/U of Tsukuba/…
  - Life science RIKEN/AIST/…
  - Computer science AIST/RWCP/…
- High density of supercomputers
  - 12 systems in the Top500 (june/2002)

rank	organization	vendor	model	Gflops	year
26	KEK	Hitachi	SR8000-F1/100	917.00	2000
45	U of Tsukuba	Fujitsu	VPP5000/80	730.00	2001
56	AIST/CBRC	NEC	Magi Cluster PIII	654.00	2001
57	RWCP/Tsuku	elf-mad	SCore III/PIII 93	618.30	2001
89	NIES	NEC	SX-6/64M8	495.20	2002
99	AIST/TACC	Hitachi	SR8000/64	449.00	1999
125	U of Tsukuba	Hitachi	CP-PACS/2048	368.20	1996
160	NIED	SGI	ORIGIN 3000 500	306.30	2002
187	MRI	Hitachi	SR8000/36	255.00	1999
228	NRIM	NEC	SX-5/32H2	241.40	2000
426	U of Tsukuba	Hitachi	SR8000-G1/12	150.10	2002

TsukubaWAN

- City-wide network to connect research institutions
  - 13 sites at present
- Optical ring
  - 10Gbps backbone
  - OADM/ADM node
- Operating since March 2002
- Wil be connected to SuperSINET at U of Tsukuba

TsukubaWAN schematic view

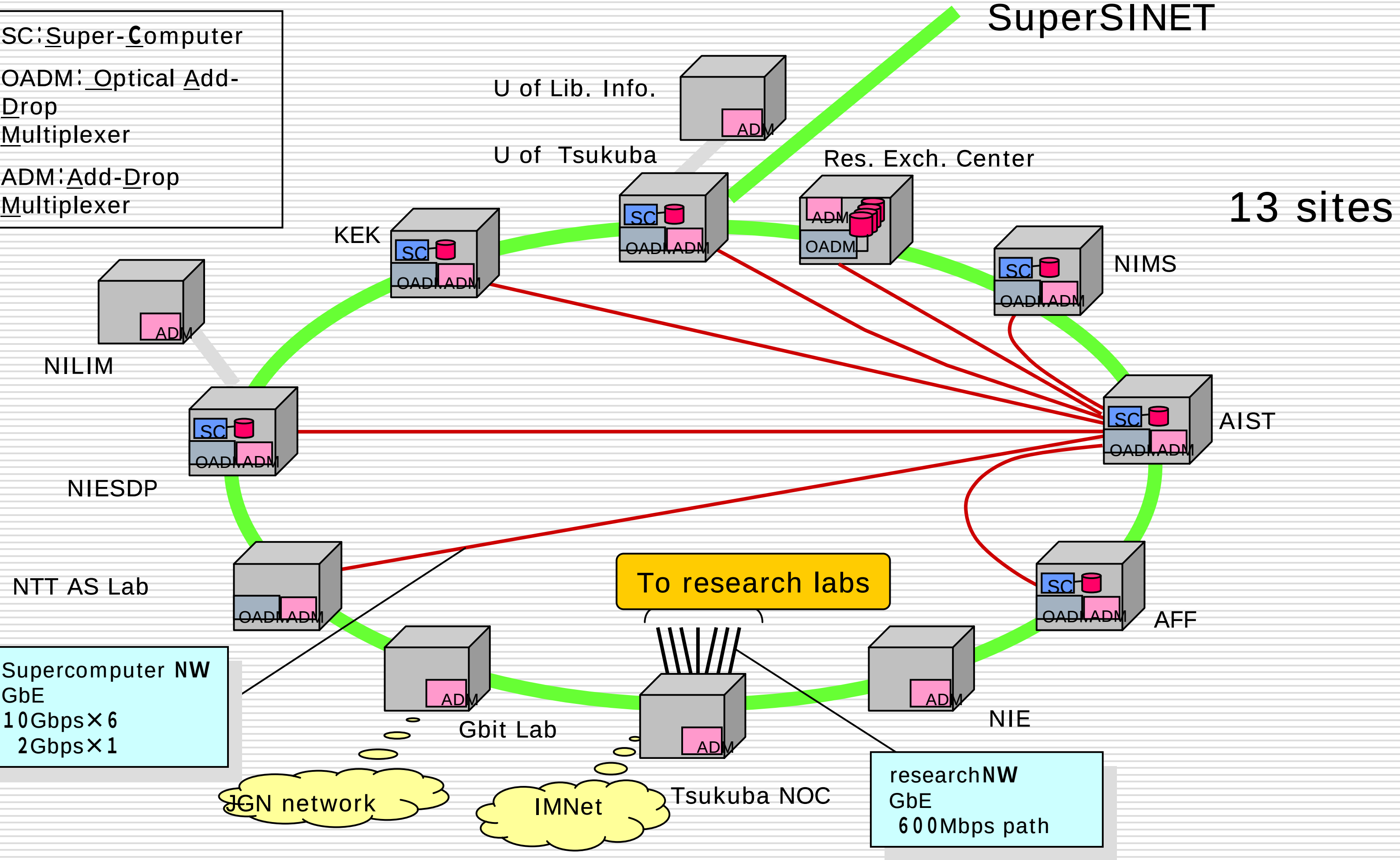


TsukubaWan configuration

SC：Super-Computer

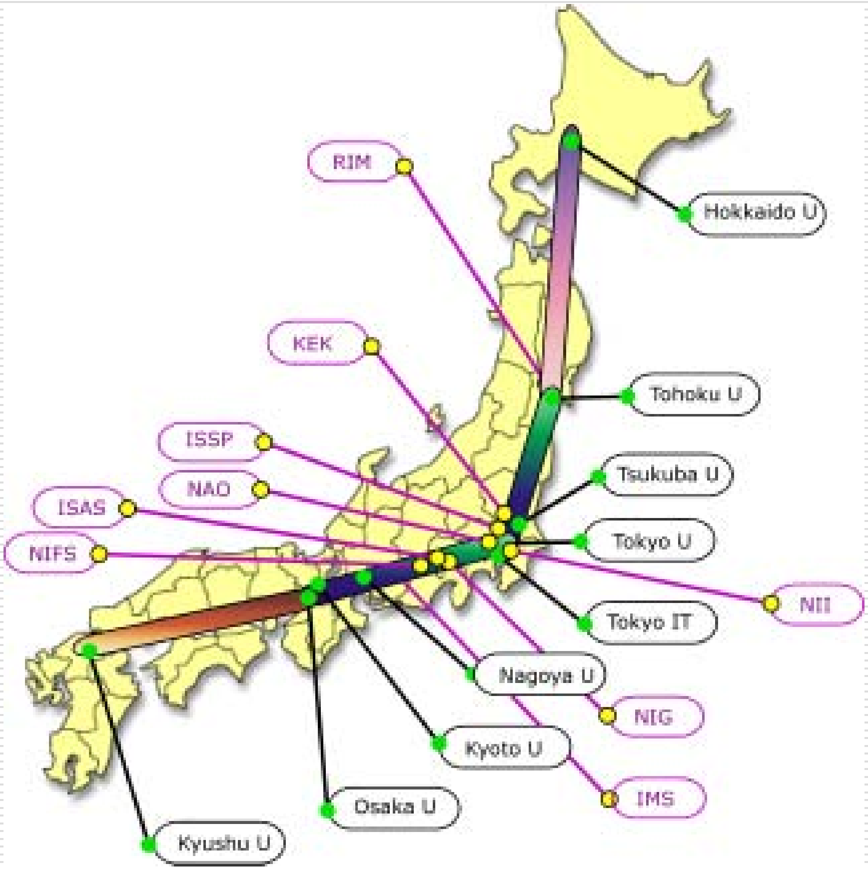
OADM：Optical Add-Drop Multiplexer

ADM：Add-Drop Multiplexer



SuperSINET

- Nationwide research network connecting
  - Major universities
  - Research institutes/organizations
  - Government labs
- Optical network with
  - Optical cross connect
  - 10Gbps WDM backbone
  - 1Gbps point-to-point connection
- Operating since Jan. 2002



SuperSINET research projects

- High-energy and fusion research
  - KEK/BELLE and LHC/ATLAS experiment data analysis
  - Fusion data analysis
  - Lattice QCD
- Space and astronomical science
  - On-line VLBI
  - GRAPE net etc
- Genome information analysis
  - Genome analysis
  - Genome database
- GRID
  - Supercomputer network
- Nanotechnology
  - Material simulation
  - Grid-based large-scale simulations

Conclusions

- Supercomputer Centers in Japan
  - Important component of science and engineering research in Japan
  - Have worked well in providing HPC resources
- Direction pursued at CCP
  - physicist/computer scientist collaboration
  - academia/vendor collaboration
  - concentration on key problems
  - Successfully attacked several fundamental issues in physics
- With emerging high speed network
  - Closer collaboration among centers in Japan
  - Closer collaboration world-wide