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 large-scale usage

- Academic research institutes/organizations
  - Application by users and selection by peer committee
  - Typical large-scale applications: 1 week of full system

<table>
<thead>
<tr>
<th></th>
<th>Peak Allocation</th>
<th>Max Allocation</th>
<th>#Projects/Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>KEK high energy</td>
<td>1.2Tflops</td>
<td>decide by case</td>
<td>20</td>
</tr>
<tr>
<td>NAO astrophysics</td>
<td>0.6Tflops</td>
<td>1 week of full system</td>
<td>20</td>
</tr>
<tr>
<td>ISSP condensed matter</td>
<td>0.6Tflops</td>
<td>1 week of full system</td>
<td>100</td>
</tr>
</tbody>
</table>

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

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

PU board of PACS-9 (1978)  
PAX-128 (1983) with control unit

CP-PACS/96

QCDPAX/89

PU array of PAX-32 (1980)  
A cabinet of QCDPAX (1989)
CP-PACS parallel computer

- MPP with 2048 compute nodes and 128 I/O nodes
  - 0.6 Tflops peak, 0.3 Gflops/node,
  - 16x16x17 node array, 3-dim crossbar network, 0.3 GB/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

100% averaged usage 87%
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
  - $I=1/2$ rule and CP violation parameter 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 $\alpha_s$ 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)
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 systematic errors down to a % level
  - Finite lattice size \( L > 3\text{fm} \)
  - Finite quark mass \( m_q < 0 \)
  - 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) \( m < 1\text{GeV} \)
    - Need dynamical simulation
  - 3 heavy quarks (c,b,t) \( m > 1\text{GeV} \)
    - 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

![Graph showing quark masses with two flavors of QCD and a quenched value highlighted.]
Summary on quark masses

- Significant sea quark effects

- Lower edge of phenomenological estimates; lighter than one believed for a long time

- $N_f=3$ simulations being pursued to obtain physical values of light quark masses

Real world; three flavors
I=1/2 rule and CP violation in K decays

- Weak interaction decays of K mesons
  - \( \frac{\text{Re } A_0(K \rightarrow \pi\pi(I = 0))}{\text{Re } A_2(K \rightarrow \pi\pi(I = 2))} \approx 22 \)
  - CP violation
    \[ \frac{\varepsilon'}{\varepsilon} = \frac{\omega}{\sqrt{2}} \left| \left[ \frac{\text{Im } A_2}{\text{Re } A_2} - \frac{\text{Im } A_0}{\text{Re } A_0} \right] \right| \]
    \[ = \begin{cases} 
      (20.7 \pm 2.8) \times 10^{-3} & \text{KTeV experiment (FNAL)} \\
      (15.3 \pm 2.6) \times 10^{-3} & \text{NA48 experiment (CERN)} 
    \end{cases} \]

- 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
I=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 $\varepsilon'/\varepsilon$

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

Possible reasons:
- Connected with insufficient enhancement of $I=1/2$ rule
- Method of calculation (K $\rightarrow \pi$ reduction) may have problems

Still a big problem requiring further work

\[ \frac{\varepsilon'}{\varepsilon} = \frac{\omega}{\sqrt{2} |\varepsilon|} \left[ \frac{\text{Im} A_2}{\text{Re} A_2} - \frac{\text{Im} A_0}{\text{Re} A_0} \right] \]
Scale of QCD simulations

- Sustained speed
  - Quenched QCD \(64^3 \times 112\) 53% of peak
  - Full QCD \(24^3 \times 32\) 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

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

\[C \approx 2.8\]

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

<table>
<thead>
<tr>
<th>Short-ranged</th>
<th>long-ranged</th>
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</thead>
<tbody>
<tr>
<td>Complex and manifold</td>
<td>universal (gravity, Coulomb)</td>
</tr>
<tr>
<td>O(N) calculations</td>
<td>O(N^2) calculations</td>
</tr>
<tr>
<td>but complex</td>
<td>but simple</td>
</tr>
</tbody>
</table>

- 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

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

**CP-PACS**
- General-purpose MPP
- 0.6Tflops

**GRAPE-6**
- Special-purpose MPP
- 8Tflops

**Parallel I/O system**
- PAVEMENT/PIO

**100base-TX**
- Host PC
- switch

![Diagram of CP-PACS/GRAPE-6 system architecture]
Galaxy formation simulation on HMCS
M. Umemura & H. Susa

Cosmic Time

Redshift Z

Big Bang

Cosmic Recombination

Neutral
DARK AGE

Cosmic Reionization

Ionized

QSO

Galaxy formation simulation on HMCS

Galaxy formation

(The Present)
Structure of the calculation

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

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

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

- Chemical reaction & radiative cooling

\[ \rho(r) = \sum_{j} \rho_{j} \delta(r - r_{j}) \]

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

- Self-Gravity
- Density (SPH)
- Radiative Transfer
- Chemical Reaction
- Temperature
- Pressure Gradient
- Integration of Equation of Motion

Iteration

GRAPE-6
CP-PACS
Calculation parameters

- Processors
  - 1024PU of CP-PACS 0.3 TFLOPS
  - 4 boards of GRAPE-6 4 TFLOPS

- 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

QSO
National network and beyond

- TsukubaWAN
- SuperSINET
Tsukuba Science City

- High density of HPC-related research organizations
  - High energy physics: KEK/U of Tsukuba/…
  - Material 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)

<table>
<thead>
<tr>
<th>rank</th>
<th>organization</th>
<th>vendor</th>
<th>model</th>
<th>Gflops</th>
<th>year</th>
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<tbody>
<tr>
<td>26</td>
<td>KEK</td>
<td>Hitachi</td>
<td>SR8000-F1/100</td>
<td>917.00</td>
<td>2000</td>
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<tr>
<td>45</td>
<td>U of Tsukuba</td>
<td>Fujitsu</td>
<td>VPP5000/80</td>
<td>730.00</td>
<td>2001</td>
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<tr>
<td>56</td>
<td>AIST/CBRC</td>
<td>NEC</td>
<td>Magi Cluster PIII</td>
<td>654.00</td>
<td>2001</td>
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<td>57</td>
<td>RWCP/Tsukuba</td>
<td>NEC</td>
<td>Score III/PIII 93</td>
<td>618.30</td>
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<td>89</td>
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<td>99</td>
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<td>125</td>
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<td>160</td>
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<td>2002</td>
</tr>
</tbody>
</table>
TsukubaWAN

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

TsukubaWAN schematic view

Loop length 30km
TsukubaWan configuration

SC: Super-Computer
OADM: Optical Add-Drop Multiplexer
ADM: Add-Drop Multiplexer

To research labs

Supercomputer NW
GbE
10Gbps ⊕ 6
2Gbps ⊕ 1
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