Japan’s 10 Peta FLOPS Supercomputer Development Project and its energy saving designs

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2) Deputy Program Director for Computational Science
3) Director of Advance Center for Computer & Communication
1. Self introduction
2. Japan’s next generation supercomputer R&D project:
   1. Before the project started
   2. Introduction and current status
   3. Energy issues
3. Introduction of focused application area
Who am I?
Gyroball
From Wikipedia, the free encyclopedia

For the gyroscopic toy Powerball, see Powerball.

A gyroball is a kind of fastball or the physical phenomenon itself. The name is given to a unique baseball pitch used primarily by players in Japan.

Contents [show]

Overview

The gyroball was developed by a Japanese scientist, Ryutaro Himeno, and a baseball instructor, Jonathan Park, who used computer simulations to create a new style of delivery intended to reduce stress on the pitcher. They published their work in a book, currently available only in Japan, whose title is roughly translated as, The Secret of the Miracle Pitch.

Tezuka got the idea in 1995, when he found an American toy in a Japanese store. The toy is called the X-Zylo Ultra, and its reliance on the gyroscopic effect allows it to fly more than 500 feet when thrown.[1]

Amid many conflicting claims, Tezuka says the gyroball has been misunderstood.

According to Himeno and Tezuka, a gyroball pitch works because the pitcher's arm moves inward towards the body as the pitcher rotates his arm so that it moves away from and toward first base for a left-handed pitcher.

However, the technique to throwing the gyroball is different. Kazushi Tezuka is an instructor at the Jyogaka school and says Tezuka, as he grabs his thigh, "is the key, not doing with the hands."[3]

The unusual method of delivery creates a unique direction of the throw similar to the way an American football is thrown.


Hardware development at RIKEN

- Special purpose computers
  - In 1989, GRAPE developed by U. Tokyo
  - MDM:MD-GRAPE2 develop by RIKEN
  - MDM was integrated in RSCC, 2004
  - MD-GRAPE3 developed in 2004
  - MD-GRAPE-3 will be integrated in RSCC soon.
Current RSCC System installed in 2004 at Riken Advance Center for Computing & Communication

- **HDD**: 20 TB
- **Itanium2 Server**: 2
- **Vector Parallel**: NEC SX-7/32
  - 282.5 GFLOPS
  - 256 GB
- **MD-GRAPE3**: 64 TFLOPS
- **Intel Xeon 3.06 GHz**: 2 GB/Node, Myrinet/IB, 1.56 TFLOPS × 4
- **Tape Storage**: 200 TB
- **POWER4 Server**: 7
  - Tape Drive: 4 (16)
  - Disk Cache: 2 TB
- **Intel Xeon 3.06 GHz**: 4 GB/Node, IB, 6.26 TFLOPS × 4

**Front end Server**

**Cluster**
- 128 Nodes
  - (256 CPUs)
  - Cluster × 4
- **Intel Xeon 3.06 GHz**: 4 GB/Node, IB, 1.56 TFLOPS × 4
Basic concept of RSCC

- Each computer architecture has each advantage and disadvantage
- There is no single architecture which fits wide variety of applications
- RSCC is composed of 3 subsystem, Linux cluster with Xeon, Vector Parallel computer and MD-GRAPE3

We made a proposal of the NGSP based on this concept to MEXT
Our Proposal

Needs of Multi-scale Multi-physic simulation

Integration of multiple computation components

Tightly-coupled heterogeneous computer

Proposing architecture
Policy and Outline of
A Next Generation Supercomputer Project

Purpose of policy:
development, installation and application of an advanced high performance supercomputer system, as one of Japan’s “Key Technologies of National Importance”

Total Budget:
about 115 billion Yen (1.15 billion US dollars)

Period of Project:
FY2006 – FY2012
Formation of the 10 Peta R&D Project

RIKEN: Project HQ
Next-Generation Supercomputer R&D Center
(Ryoji Noyori)

Project Leader: Tadashi Watanabe
R&D G.: Ryutaro Himeno

NII: Grid Middleware and Infrastructure
IMS: Nano Science Simulation
Riken Wako Institute: Life Science Simulation

Visiting Researchers from Univ. & National Labs.

MEXT: Policy & Funding
Office for Supercomputer Development Planning

Project Committee

Industries
Industrial Forum for Promotion of Supercomputing

Evaluation Scheme
(MEXT and CSTP)

Evaluation Committees

Computer Companies

Advisory Board

(Note) NII: National Institute of Informatics,
IMS: Institute for Molecular Science
Goals of the Next Generation Supercomputer Project

1. Development and installation of the most advanced high performance supercomputer system

2. Development and wide use of application software to utilize the supercomputer to the maximum extent

3. Provision of flexible computing environment by sharing the next generation supercomputer through connection with other supercomputers located at universities and research institutes

4. Establishment of “Advanced Computational Science and Technology Center (tentative name)”
Expansion of Highest Computer for Global Usage

Sustained Performance (FLOPS)

The Next Generation Supercomputer Project

Next-next Generation Project

National Leadership (Earth Simulator)

National Leadership (The Next Generation Supercomputer)

Enterprise Company, Laboratory

Personal Entertainment PC, Home Server Workstation, Game Machine, Digital TV

Government Investment

100P

1P

10T

100G

1990

2000

2010

2015

2020

2025
## Schedule of Project

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<td>Processing unit</td>
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<td>Shared file system</td>
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<td><strong>Applications</strong></td>
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<td>Next-Generation Integrated Nanoscience Simulation</td>
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<td>Next-Generation Integrated Life Simulation</td>
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<td>Computer building</td>
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<tr>
<td>Research building</td>
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**present**
Optimization of Computer Design

Requirement from Grand Challenges
- Nano Sci.
- Life Sci.
- Others (Engineering etc)

Requirement from Computer Centers
- Power, Space
- Reliability, operability
- Cost (development, manufacturing, maintenance)

Popular numerical scheme
- FMO
- MO
- RISM
- Fast transform
- Monte Carlo
- Linear Solver
- FEM
- FVM
- Other Project Watch
- Technology Survey

Optimum system
Fastest in the world

21 Selected Target applications
- Nano Science (6)
- Life Science (6)
- Env./ Desaster (3)
- Engineering (4)
- Physics, Astro. prev. (2)

Operation & Utilization
- Essential Element technologies
- LSI process
- Power saving
- SOI
- Low-k
- High-k
- Light transmission tech.
- Software OS, compiler

Spin off to the consumer electronics

Technology Limit
Target applications and BM suit

The application software committee started selecting target applications for making a benchmark suit in January, 2006.

21 codes were selected in March and NextBMT suit was developed.
<table>
<thead>
<tr>
<th>Fields</th>
<th>Program name</th>
<th>Description</th>
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<tbody>
<tr>
<td>Life (6)</td>
<td>SimFold</td>
<td>Prediction of Protein Structure</td>
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<tr>
<td>Life (6)</td>
<td>GNISC</td>
<td>Inference of Genetic Networks from Experimental Data of Gene Expression</td>
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<tr>
<td>Life (6)</td>
<td>MLTest</td>
<td>Validation of statistical significance for development of individualized medicine</td>
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<tr>
<td>Life (6)</td>
<td>MC-Bflow</td>
<td>Simulation for blood-flow analysis</td>
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<tr>
<td>Life (6)</td>
<td>sievgene/myPresto</td>
<td>Docking simulation of protein and drug</td>
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<tr>
<td>Life (6)</td>
<td>ProteinDF</td>
<td>Ab-initio Molecular Dynamics Calculation in Large-Scale Protein Systems</td>
</tr>
<tr>
<td>Nono (6)</td>
<td>GAMESS/FMO</td>
<td>FMO Molecular Orbital Calculation</td>
</tr>
<tr>
<td>Nono (6)</td>
<td>Modylas</td>
<td>Massively-parallel multipurpose software for molecular dynamics calculation</td>
</tr>
<tr>
<td>Nono (6)</td>
<td>RSDFT</td>
<td>Ab-initio Molecular Dynamics Calculation in Real Space</td>
</tr>
<tr>
<td>Nono (6)</td>
<td>RISM/3D-RISM</td>
<td>Analysis of Electron States of Proteins in Solution with the 3D-RISM/FMO Method</td>
</tr>
<tr>
<td>Nono (6)</td>
<td>PHASE</td>
<td>First-Principles Molecular Dynamics Simulation within the Plane-Wave Pseudopotential formalism</td>
</tr>
<tr>
<td>Nono (6)</td>
<td>Octa</td>
<td>Coarse-Grained Molecular Dynamics Calculation</td>
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</tbody>
</table>
## NextBMT and Peta-scale BMT (2/2)

<table>
<thead>
<tr>
<th>Physics Astronomy (2)</th>
<th>LatticeQCD</th>
<th>Study of elementary particle and nuclear physics based on Lattice QCD simulation</th>
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<tbody>
<tr>
<td></td>
<td>NINJA/ASURA</td>
<td>Super large-scale gravitational many-body simulation for finding the celestial origin</td>
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<tr>
<td>Geophysics (3)</td>
<td>NICAM</td>
<td>Nonhydrostatic ICosahedral Atmospheric Model (NICAM) for Global-Cloud Resolving Simulations</td>
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<td>Seism3D</td>
<td>Simulation of Seismic-Wave Propagation and Strong Ground Motions</td>
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<td>COCO</td>
<td>Super-resolution Ocean General Circulation Model</td>
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<tr>
<td>Engineering (4)</td>
<td>Cavitation</td>
<td>Computation of Unsteady Cavitation Flow by the Finite Difference Method</td>
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<td>LANS</td>
<td>Computation of compressible fluid in aircraft and spacecraft analysis</td>
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<td>FrontSTR</td>
<td>Structural Calculation by Finite Element Method (FEM)</td>
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<td>FrontFlow/Blue</td>
<td>Unsteady Flow Analysis based on Large Eddy Simulation (LES)</td>
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</tbody>
</table>
System Configuration

The Next-Generation Supercomputer is designed as hybrid general-purpose supercomputer that provides the optimum computing environment for a wide range of simulations.

- Calculations will be performed in processing units that are suitable for the particular simulation.
- Parallel processing in a hybrid configuration of scalar and vector units will make larger and more complex simulations possible.
Hybrid Supercomputer System composed of Scalar and Vector Units

Vector unit is suitable for continuum physics simulation
Scalar unit is suitable for Data Base application, particle-based simulation
Hybrid system has both strong points for users to choose better units for different applications

Scalar Unit
Data base, homology search
Similarity with PC
• high speed low power CPU
• New strong network for enormous parallelism

Vector Unit
Vector processor based on the Earth Simulator
strong for continuum physics simulation
• New generation low-power vector processor with optical network

Characteristics
For Energy Saving,

- Cogeneration system: gas turbine power generator & steam generator using natural gas
  - Generates electric power and steam
  - Steam is used in cooling system which makes child water
  - Child water is used in two ways
    - Water-air heat exchanger
    - Directly provided to computer
- Clock frequency is decided from energy saving point of view
Cogeneration system: 2 points of Saving Energy

- Total energy efficiency of cogeneration system is better than ordinary commercial electric power plant
  - Using natural gas as fuel, CO$_2$ will be reduced at the same time
- Direct water cooled computer system can save pumping loss of air blowing for cooling
  - Full water cooled system has difficulty in maintenance
  - We will use partial water cooling system
Photographs of the facilities

2009/02/06

2009/03/04

2009/04/25
Major Applications of Next Generation Supercomputer

- Manufacturing
  - Designing safe cars
  - Faster development of products

- Nanotechnology
  - Designing new materials
  - Studying enzyme and catalytic reactions

- Disaster prevention
  - Predicting seismic waves
  - Predicting tsunami damage

- Aerospace
  - Designing rocket engines
  - Aircraft development

- Life sciences
  - Drug development
  - New technologies for medical treatment and diagnosis

- The environment
  - Predicting climate change
  - Predicting effects of the El Nino phenomenon

- Nuclear power
  - Analyzing whole nuclear power plants
  - Developing nuclear fusion reactors

- Astronomy and astrophysics
  - Research on the origin of the universe
  - Studying the formation of planets and galaxies

Targeted as grand challenges
To create **next-generation nano-materials**
(new semiconductor materials, etc.) by integrating
- theories (such as **quantum chemistry, statistical dynamics and solid electron theory**)
- and - simulation techniques in the fields of new-generation information functions/materials, nano-biomaterials, and energy
To provide new tools for breakthroughs against various problems in life science by means of petaflops-class simulation technology, leading to comprehensive understanding of biological phenomena and the development of new drugs/medical devices and diagnostic/therapeutic methods.
Total Simulation of Living Matter

Goal
Understand the life phenomena: reproducing life program on computer
Develop new medicine and medical equipment

Approach
combination of analytical approach and Data-driven approach on Peta-scale computer

- Analytical approach
- Data-Based approach to analysis
- Peta scale simulation

- Molecular scale
- Cell scale
- Organ/Whole body scale

- Fusion of Data based approach and Analytical approach

- Basic principal (Equations)
- Experimental data

- New methodology

- Understand the life phenomena: reproducing life program on computer
- Develop new medicine and medical equipment
Cyber Science Infrastructure Plan

VOs (Virtual Organizations)

University/inter-university research institutes VO

Next Generation Supercomputer

Project VO

Virtual research environment for various fields

Industrial project VO

Infrastructural middleware (GRID, Infrastructure for certification, etc.)

Operated by National Institute of Informatics (NII)

(Note) VO: Virtual Organization
CACST: Center for Advanced Computational Science and Technology (tentative name)

- Computer science and Computational science
- Both researchers will gather and expect to develop new research fields and methodologies
- Currently, we are designing the center and operation policy of the supercomputer
  - The users will be chosen by a new committee independent from RIKEN to pick up valuable subjects

Kobe Port-Island

Kobe Airport

Shinkansen-Line
Shin-Kobe Station

Mt. Rokko
Ashiya

Kobe Medical Industry Development Project
Core Facilities

Kobe Sky Bridge

Port Island

To Osaka

To Notoh / Awaji Island

Photo: June 2009

Next-Generation Supercomputer
Tentative Plan of the computer center

- Hub of the Computer Science and Computational Science in Japan and Asia.
  - Cross point of various sciences and technologies using HPC
  - Operation of 10-Peta FLOPS Supercomputer
  - User support and spreading the usage in various field
  - Development of the next-next supercomputer
  - Research on computational science
  - Education
Summary

- From energy saving point of view, gas cogeneration system is adopted
- For saving pumping loss of air handling, water cooling system is partially adopted
- We are focusing on application development in Nano science and Life science
- Currently all development of hardware and software are on schedule