RIKEN AICS Software Center aims to:

- develop and deploy high quality applications, libraries, programming tools, etc. (called “AICS software”) for many platforms including the K computer and “Post-K”.
- support AICS software users to promote High Performance Computing for various fields of science and engineering.

More than 30 softwares have already been developed and ported by RIKEN AICS and are available for HPC users.

**OACIS**

Organizing Assistant for Comprehensive and Interactive Simulations

OACIS is a job management software for large scale simulations. With a user-friendly interface of OACIS, you can easily submit various jobs to appropriate remote hosts. After these jobs are finished, all the result files are automatically downloaded from the remote hosts and stored in a traceable way together with logs of the date, host, and elapsed time of the jobs. It also provides APIs.

**NTChem**

NTChem is a high-performance software package for the molecular electronic structure calculation for general purpose on the K computer. It is a comprehensive new software of ab initio quantum chemistry made in AICS from scratch. NTChem contains not only standard quantum chemistry approaches but our own original approaches.

**GENESIS**

GENESIS (GENeralized-Ensemble Simulation System) is molecular dynamics and modeling software for biomolecular systems such as proteins, lipids, glycans, and their complexes. GENESIS is open source software distributed under the GPUv2 license.

**SCALE**

SCALE (Scalable Computing for Advanced Library and Environment), which stands for Scalable Computing for Advanced Library and Environment, is a basic library for weather and climate model of the earth and planets aimed to be widely used in various models.

Other softwares:

- Profiling/Analysys tool: 7 softwares
- Job management tool: 2 softwares
- Language: 1 software
- I/O support tool: 3 software
- Numerical library: 4 softwares
- Application/Platform: 2 softwares
- Visualization: 4 softwares
- Misc.: 9 softwares

Software development and enhancement
Research Div. (16 teams & 2 units)

Promotion and user support
Operations and Computer Technologies Div. (2 teams)

Sample User Program (in preparation)

To accelerate the development of the AICS software and encourage new HPC users, we start "Sample User Program":
1. You apply to join the program as a sample user of AICS software (OACIS, NTChem, GENESIS or SCALE).
2. We provide sufficient machine time of the K computer and special user support for 1 year.

- You give us feedback for improvement and enhancement of the software.
- We improve and enhance the software and You experience a world class HPC environment and Apps.

Please contact: aics-ungi-hud@riken.jp
Recently jobs with large power consumption have increased. And total power consumption exceeded the power consumption limit regulated by contract with power provider. If the total power consumption exceed the power limit, we have to pay additional charge as a penalty.

Analysis of correlation with power consumption and application performance was performed. As a result, standby power and memory throughput has a greater impact on the power consumption of the K computer.

\[
\delta_{\text{Power}} = 8.8128 + 1.3659 \times \text{Floating Calc.} + 4.3906 \times \text{Memory Throughput} - 0.0857 \times \text{L2 Throughput} + 2.3299 \times \text{L1D Throughput} + 0.2429 \times \text{Integer Calc.}
\]

We performed the trial of improving of power consumption and system operation. If both the CPU performance and the memory performance improved to field average, NODExTIME can be reduced as below. The performance of each big user's application has estimated how much differs compared to the field average.

When we improve performance about the 10 (or 50) major user application, we can use 25M (or 66M) NODExTIME. When we improve performance about 10 (or 50) major user application, we can achieve energy savings of 2.7GWh (or 7.0GWh).

**HPCG Performance Tuning on the K computer**

**Evaluate Original HPCG on the K**

The original HPCG code evaluation on the K computer gave the following information.

- Linear scalability was obtained, so parallelization tuning is not necessary
- Single CPU performance was low since SYMGS is not multi-thread

Therefore we have aimed the single CPU tuning

**Tune: Coloring for SYMGS**

In the original code, SYMGS is not able to be multi-thread since there are data dependencies between rows. To avoid data dependencies, we employed the colored blocking that divide the mesh into some blocks and do the coloring to blocks.

**Result of ISC2017**

<table>
<thead>
<tr>
<th>Rank</th>
<th>Computer</th>
<th>Country</th>
<th>HPL PFLOPS</th>
<th>HPCG PFLOPS</th>
<th>Ratio to HPL %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>K computer</td>
<td>Japan</td>
<td>10.510</td>
<td>0.6027</td>
<td>5.7%</td>
</tr>
<tr>
<td>2</td>
<td>Tianhe-2</td>
<td>China</td>
<td>33.863</td>
<td>0.5801</td>
<td>1.7%</td>
</tr>
<tr>
<td>3</td>
<td>Sunway TaihuLight</td>
<td>China</td>
<td>93.015</td>
<td>0.4808</td>
<td>0.5%</td>
</tr>
<tr>
<td>4</td>
<td>Piz Daint</td>
<td>Switzerland</td>
<td>19.590</td>
<td>0.4767</td>
<td>2.4%</td>
</tr>
<tr>
<td>5</td>
<td>Oakforest-PACS</td>
<td>Japan</td>
<td>13.555</td>
<td>0.3855</td>
<td>2.8%</td>
</tr>
</tbody>
</table>

We tried these additional ways.

- Memory serialize for matrix
- Data access ordering improvement for SYMGS
- Loop optimization for SPMV and SYMGS
- Parameter adjustment
- Improvement of miscellaneous routines

Then, 19 times speed up was obtained finally.

K Computer
Hardware and Operations

System Configuration

The K computer
Compute nodes
Number of CPUs: 82,944
Total memory capacity: 1227PB
Tofu interconnect
(6D mesh/torus network)

IO Nodes
Pre/Post Processing Servers
K computer Front-end Servers

Image of 3D torus

Global IO NW

Global file system
(40PB-)

Local-file system
(11PB-)

User

Internet

Tofu (Torus Fusion) interconnect
- High communication performance and fault-tolerant network
- Network topology: 6D mesh / torus network
  - 10 links (5 GiB/s x 2 bandwidth / link) on each node
  - Axes: X, Y, Z, a, b, c
    - X Z: torus (Z:0: 1O node), Y, a, c: Mesh
  - Network size: (X, Y, Z, a, b, c) = (24, 18, 17, 2, 3, 2)
  - 1, 2 or 3D torus network configurable from user’s programming point of view

SPARC64 VIIIfx
Superscalar Multi-core processor

<table>
<thead>
<tr>
<th>Specification</th>
<th>Performance (peak) 128 GFLOPS (16 GFLOPS x 8 cores)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Core</td>
<td>8</td>
</tr>
<tr>
<td>Clock</td>
<td>2.0 GHz</td>
</tr>
<tr>
<td>Floatingpoint Execution units (Core spec)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Floating-point register (64-bit) : 256</td>
</tr>
<tr>
<td></td>
<td>General purpose register (64-bit) : 188</td>
</tr>
<tr>
<td>Cache</td>
<td>L1S : 32 KB (2way)</td>
</tr>
<tr>
<td></td>
<td>L1DS : 32 KB (2way)</td>
</tr>
<tr>
<td></td>
<td>L2S : Shared 6 MB (12way)</td>
</tr>
<tr>
<td>Memory throughput</td>
<td>64 GB/s (0.58/f)</td>
</tr>
</tbody>
</table>


Computing Resource Allocation (FY2017)

Job Size (# of nodes)

Number of executed jobs of each month (left) and a breakdown of jobs classified by research areas (right) between October 2012 and March 2017.

Amount of used computing resources (product of number of used nodes and elapsed time) and system usage of each month (left) and a breakdown of used resources classified by research areas (right) between October 2012 and March 2017.
K Computer Hybrid Cooling System

- High-efficiency
  - Efficient Power generation and eco-system (CGS)
  - PUE~1.34
- Safety
  - Earthquake preparedness
  - Countermeasures to power interruptions and voltage dips without using a UPS

Chillers & Power Generator
- Chillers: 10,500 USRT (~37MW)
- CGS: 6MW (peak)=2
- Area: 1,900 m²

Substation Supply
- Commercial Power Supply: 11.4MW / 77,000V
- Area: 200 m²

Computer Building
- Six stories above ground and one below
  - Area: 1,800 m²

Research Building
- Three stories above ground and one below
  - Area: 4,800 m²

Data Storage Room
- Global File System

Air-Handling Unit Room
- Air-Handling Unit & Water-Handling Unit

Earthquake preparedness
- Laminated-rubber seismic isolation device
- Lead damper
- Steel damper

Protected area from power interruptions and voltage dips

Chillers & Power Generator
- CGS: Co-Generation System
- Energy efficiency 75%
- Energy 100%

Electric power 40%
- Steam

Absorption Refrigerating Chiller
- Water-cooling 45%
- Exhaust 25%

Substation Supply
- 11.4MW (average) (77,000V=6,600V)

Chillers & Power Generator
- CGS x2: 6MW (peak), 6600 V
- Absorption Refrigerating Chillers x4
- Centrifugal Water Chillers x3

Computer Building
- Air Outlet ~23°C
- Power consumption/rack: Peak ~14.6 kW (210 V)
- 2nd Coolant Loop
- Water outlet ~15°C
- 1st Coolant Loop
- Water inlet ~15°C

System Board
- Air flow
- Water flow
- Power consumption / CPU: 38W (ICC, 29W)
- CPU temperature: keep range: 17~21°C
- Cold water circulate about 20 times per minute

Air-Handling Unit ~50

System-separation Circuit Breaker
- Protect from
  - Power interruptions
  - Voltage dips
  - Protected Area
  - Data Storage room
  - Research Building

Voltage Converter
- 446 over / min / tuck

Protected Area from power interruptions and voltage dips

- High-efficiency air/water hybrid cooling system
- CPU temperature: 17~21°C
- Room temperature: 24°C (peak)
- High reliability
- MTBF (All SBs): 2~3 days