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RIKEN
Intel K.K.
SGI Japan, Ltd.

Completion of a one-petaflops computer system for simulation of molecular dynamics

New ultra-fast computer will dramatically accelerate the development of new medicines

RIKEN (The Institute of Physical and Chemical Research; Ryoji NOYORI, President), Intel K.K., and SGI Japan, Ltd. today announced that they have succeeded in building a high-speed computer system, named "MDGRAPE-3"*[1], for carrying out molecular dynamics simulations at a theoretical speed of one petaflops*[2] (one thousand trillion calculations per second).

According to the TOP500 list, as of June 16, 2006 the world's fastest supercomputer is the IBM BlueGene/L, owned by Lawrence Livermore National Laboratory, which has a theoretical peak performance of 360 teraflops (360 trillion calculations per second). The MDGRAPE-3 system cannot run the Linpack benchmark, which is the basis for the TOP500 ranking. However, its performance of one petaflops means that it is approximately three times faster than BlueGene/L.

The MDGRAPE-3 computer system consists of 201 units of 24 specially designed MDGRAPE-3 chips (a total of 4808 chips*[3]), plus 64 servers each with 256 of the new Dual-Core Intel® Xeon® Processor 5000 series processors (codename "Dempsey"), and 37 servers each containing 74 Intel Xeon Processor 3.2GHz (2MB L2 cache) processors. The MDGRAPE-3 chips were developed by RIKEN and provide the world's fastest molecular dynamics simulation. The reliable large-scale cluster system based on the latest dual-core processors has made it possible to build a high-performance computer more efficiently.

MDGRAPE-3 was developed through collaboration by RIKEN, SGI Japan, Ltd, and Intel K.K. Within RIKEN, the development was carried out by the RIKEN Yokohama Institute

(Tomoya OGAWA, Director), and the Genomic Sciences Center (Yoshiyuki SAKAKI, Director), and by Makoto Taiji (Team Leader), Tetsu Narumi (Research Scientist), and Yosuke Ohno (Research Scientist), of the High-Performance Molecular Simulation Team in the Computational and Experimental Systems Biology Group*4. SGI Japan is renowned for developing and building large-scale systems in the HPC field, and Intel K.K. provided its latest microprocessors and technological assistance.

Advances in molecular biology are making it possible to study biological mechanisms at the atomic level and to research life processes through computer simulation. In R&D on new medicines, it is believed that computer simulations will enable the rapid and precise measurement of the ease of binding medicine candidate substances to proteins. In this way, molecular dynamics simulation technology is becoming more and more important. RIKEN is a leader in high-performance molecular simulation R&D, and it began development of a petaflops-class computer system for molecular dynamics in 2002. In August 2004 it produced the MDGRAPE-3 chip, a 230GB FLOPS LSI chip with the world's highest calculation performance. The new MDGRAPE-3 computer system is expected to reduce the time taken to develop new medicines. It will also be extremely useful for studying how proteins work by simulation, and for the development of biological nanomachines.

Dual-Core Intel® Xeon® Processor

MDGRAPE-3 is based on Intel's new Dual-Core Xeon processor 5000 series. Manufactured using 65-nanometer process technology, this series features numerous technological innovations, such as a dual core, Intel Virtualization Technology, FB-DIMM memory, and a high-speed system bus (1066MHz). For further performance improvement, MDGRAPE-3 is currently undergoing validation for migration to the Dual-Core Intel Xeon processor 5100 series (codename "Woodcrest"), which is based on the next-generation Intel Core™ Microarchitecture. The Intel Compiler is also being used to optimize RIKEN's program code for the Intel Core Microarchitecture.

Applications of molecular dynamics simulations

The MDGRAPE-3 system is part of the Japanese Ministry of Education, Culture, Sports, Science and Technology's National Project on Protein Structural and Functional Analyses (also called "Protein 3000")*5. After the structures of proteins are worked out, MDGRAPE-3 will make it easier to conduct large-scale simulations during the development of new drugs.

MDGRAPE-3 will also enable accurate estimates of how easy it is for drug candidate substances to bond with proteins - a process that is expected to help accelerate the development of new drugs. It will also make it possible to analyze the structures of proteins, helping to solve the causes of protein-induced diseases on the atomic level. It is expected to be a powerful tool for nanolevel research.

Further information

MDGRAPE-3 will be shown to the public at the RIKEN Yokohama Institute (http://www.yokohama.riken.jp/indexE.html) on June 24, 2006. For information about research using MDGRAPE-3, see the research team's site at http://mdgrape.gsc.riken.jp/.

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*1 : MDGRAPE: The University of Tokyo developed GRAPE (GRAvity PipE), a special-purpose computer for astrophysical simulations, in 1989. RIKEN later developed MDGRAPE-2 (MDM), a special-purpose molecular dynamics system based on GRAPE. It developed the MDGRAPE-3 chip in August 2004.

*2 : FLOPS = floating-point operations per second. MDGRAPE-3 can calculate the force between pairs of particles 27.8 trillion times per second. Assuming the system has 36 times the computing capacity needed to calculate the Coulomb force for one pair, it has the capability to perform one quadrillion (one thousand trillion) floating-point operations per second (one petaflops). The system consists of 3,804 300MHz MDGRAPE-3 chips and 996 250MHz MDGRAPE-3 chips, and each chip calculates the force for 20 pairs per cycle. This results in 27.8 trillion calculations per second.

*3 : In total there are 4824 MDGRAPE-3 chips, but the current number of chips is 4808, because 16 chips are malfunctioning. However, the system is designed to calculate exactly without using these malfunctioning chips.

*4 : The following laboratories in RIKEN contributed the development of the MDGRAPE-3 system: Advanced Center for Computing and Communication (Ryutaro Himeno, Director); Center for Intellectual Property Strategies (Eiichi Maruyama, Director), Innovative Nanopatterning Laboratory (Jun-ichi Onodera, Team Leader; and Shigenori Fujikawa, Associate Team Leader); and Computational Astrophysics Laboratory (Toshikazu Ebisuzaki, Chief Scientist).

*5 : National Project on Protein Structural and Functional Analyses (Protein 3000): Part of Japan's national Research Revolution 2002 (RR2002) project, launched by MEXT (the Ministry of Education, Culture, Sports, Science and Technology) in April 2002. Protein 3000 is a major "post-genome" project to solve the structures and functions of proteins.

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RIKEN (http://www.riken.jp/engn/index.html)

The mission of RIKEN is to conduct comprehensive research in science and technology (excluding only the humanities and social sciences) as provided for under the "RIKEN Law," and to publicly disseminate the results of its scientific research and technological developments. RIKEN carries out high level experimental and research work in a wide range of fields, including physics, chemistry, medical science, biology, and engineering, covering the entire range from basic research to practical application. RIKEN was first organized in 1917 as a private research foundation, and reorganized in 2003 as an independent administrative institution under the Ministry of Education, Culture, Sports, Science and Technology.

Intel

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SGI Japan, Ltd.

SGI Japan has abundant experience and technology of building large-scale parallel system in HPC field including the advanced scientific technology research institutes.
In July 2005, SGI Japan expanded into the molecular dynamics simulation market, which is our part of research & science solutions business field, and is selling molecular dynamics simulation systems jointly with RIKEN.