Research Center for Computational Science

OKAZAKI, Susumu	Director, Professor
SAITO, Shinji	Professor
MORITA, Akihiro	Professor
OONO, Hitoshi	Assistant Professor
MIZUTANI, Fumiyasu	Technical Associate
TESHIMA, Fumitsuna	Technical Associate
NAITO, Shigeki	Technical Associate
SAWA, Masataka	Technical Associate
IWAHASHI, Kensuke	Technical Associate
MATSUO, Jun-ichi	Technical Associate
YAZAKI, Toshiko	Secretary
KANO, Seiko	Secretary
TOKUSHI, Hitomi	Secretary

Research Center for Computational Sciences, Okazaki Research Facilities, National Institutes of National Science, provides up-to-date computational resources to academic researchers in molecular science and related fields. In 2006, this facility was used by 555 scientists in 141 project groups.

The computer systems, currently consisting of Fujitsu PRIMEQUEST, SGI Altix4700, NEC SX-7, and NEC TX-7, cover a wide range of computational requests in quantum chemistry, molecular simulation, chemical reaction dynamics and solid state physics. These systems are linked to international networks through Science Information Network (SINET3). Detailed information on the hardware and software of the Center is available on the web site (http://ccinfo.ims.ac.jp/).

The Center provides a number of program suites, including Gaussian 03, GAMESS, Molpro2002, Hondo2003, AMBER, etc, which are installed to the computer systems and kept updated for immediate use of the users. The Center also maintains and offers the Quantum Chemistry Literature Database (QCLDB, http://qcldb2.ims.ac.jp/), which has been developed by the Quantum Chemistry Database Group in collaboration with staff members of the Center. The latest release, QCLDB II Release 2006, contains 89,624 data of quantum chemical studies.

In addition to offering computer resources to wide range of molecular scientists, another vital aspect of the Center is to perform leading computational researches with massive computations. In 2003 the Center joined the National Research Grid Initiative (NAREGI) project, a three-year national project by National Institute of Informatics (NII) and IMS. This joint project aimed at developing grid computing system (NII) and thereby realizing extremely large-scale computational studies in the frontier of nanoscience (IMS). For these purposes, two supercomputer systems, Hitachi SR11000 and HA8000, were introduced to the Center in 2004, with combined performance exceeding 10TFlops. In 2006, the NAREGI project was reformed to join a new national project Development & Application of Advanced High-Performance Supercomputer Project by RIKEN, where IMS plays an important role in the application of the PFlops-scale supercomputer to nanoscience. Further information on next-generation supercomputer project and computer systems at the Center is found on the web site (http://ims.ac.jp/nanogrid/).

Figure 1. Super-High-Performance Molecular Simulator.