Research Center for Computational Science

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Research Center for Computational Science, Okazaki Research Facilities, National Institutes of Natural Sciences, provides state-of-the-art computational resources and software to academic researchers in molecular science and related fields. The Center currently has over 600 users in 145 project groups from a wide range of molecular science, *i.e.* quantum chemistry, molecular simulation, chemical reaction dynamics and solid state physics. In order to meet a wide variety of users' demands, the computer systems consist of Fujitsu PRIMEQUEST, SGI Altix4700, and Hitachi SR-16000. These systems are linked to Internet through Science Information Network (SINET3).

The Center provides a number of state-of-the-art application programs, including Gaussian 03, GAMESS, Molpro, AMBER, NAMD, *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 2007, contains 97,718 data of quantum chemical studies. Detailed information on the hardware and software at the Center is available on the web site (http://ccinfo.ims.ac.jp/).

In addition to offering computer resources to 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 10 TFlops. In 2006, the NAREGI project was reformed to join a new national project Development and 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.