

Research Center for Computational Science

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Research Center for Computational Science provides state-of-the-art computational resources to academic researchers in molecular science and related fields, *e.g.* quantum chemistry, molecular simulations, and solid state physics. The computer systems consist of Fujitsu PRIMERGY RX300 and PRIME HPC FX10, SGI UV1000, and Hitachi SR16000. Over 650 users, 190 project groups, in molecular science have used in 2011. The large scale calculations, for example the formation of fullerenes, conformation searches using non-Boltzmann ensemble methods, and nonlinear spectroscopy of liquids, have been performed with the systems. The Center also provides a number of application programs, for example including Gaussian 09, GAMESS, Molpro, AMBER, and NAMD. The Center offers the Quantum Chemistry Literature Database, which has been developed by the Quantum Chemistry Database

Group in collaboration with staff members of the Center. The latest release, QCLDB II Release 2008, contains 118,989 data of quantum chemical studies. Detailed information on the hardware and software at the Center is available on the web site (<http://ccportal.ims.ac.jp/>).

In addition to the provision of computational resources, the Center contributes to the so-called next-generation super-computer project which is conducted by the government. In 2010, Computational Material Science Initiative (CMSI) was established, after the research field which consists of molecular science, solid state physics, and material science was selected as one of the research fields which scientific breakthroughs are expected by using the supercomputer. The Center contributes to CMSI by providing approximately 20% of its computational resource.



Figure 1. Fujitsu PRIMERGY RX300.



Figure 2. SGI UV1000.