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, PRIME HPC FX10 and PRIMERGY CX250 (since March 2013), SGI UV1000 (until March 2013) and UV2000 (since April 2013), and Hitachi SR16000 (until February 2013). Over 730 users in 182 project groups from a wide range of molecular science have used in 2012. Large scale calculations, for example the formation of fullerenes, conformation searches using non-Boltzmann sampling 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 2009, contains 125,646 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 supercomputer 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 next-generation supercomputer. The Center contributes to CMSI by providing up to 20% of its computational resource.

Figure 1. Fujitsu PRIMERGY CX300.

Figure 2. SGI UV2000.