Research Center for Computational Science (Okazaki Research Facilities)

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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. solid state physics, biophysics, basic biology, and physiology. Our systems consist of HPE Apollo 2000 and Apollo 6500 (since Feb. 2023). The combined system, named "Molecular Simulator," is ranked 196th position in the TOP500 supercomputer list in June 2023. These massive computer resources have been used for various kinds of large-scale calculations, for example accurate electronic structure calculations of molecular systems and conformation searches using generalized ensemble methods. We also provide about 30 application programs to the users: Gaussian, ORCA GAMESS, AMBER, Gromacs, and so on. In particular, we have implemented some original programs developed by researchers in Japan to provide them to the users. From the fiscal year 2024, supercomputer of NIBB was also integrated to the system. The supercomputer systems had been used by 1,737 researchers from 429 groups in the fiscal year 2024. Some of the computational resources are provided to the national projects, Program for Promoting Research on the Supercomputer Fugaku and Program for Data-Driven Material Research and Development.

For fostering young generation, we organize the schools of quantum chemistry and molecular dynamics simulation every year. In the fiscal year 2024, the numbers of registered attendants of these schools were 348 and 365, respectively. We also organize the RCCS supercomputer workshop focusing on the new trends of computational chemistry for the purpose of the research exchange and human resource development. In the fiscal year 2024, we organized the workshop under the title, "Materials Design and Development based on AI/ML: Interplay between Theory and Experiment," which was attended by about 200 researchers.

In cooperation with Institute for Solid State Physics, University of Tokyo, Institute for Materials Research, Tohoku University and R^3 Institute of Newly-Emerging Science Design, University of Osaka, we established the Computational Materials Science Forum (CMSF) to promote the cutting-edge computational materials science technology of Japan, to create world-class results, and to realize the social implementation of simulation technology and materials information science technology.

The center is jointly managed with National Institute for Physiological Sciences and National Institute for Basic Biology (both in the same campus).

Figure 1. HPE Apollo 2000 and Apollo 6500.