**Supercomputer Center**

The Supercomputer Center (SCC) is a part of the Materials Design and Characterization Laboratory (MDCL) of ISSP. Its mission is to serve the whole community of computational condensed-matter physics of Japan, providing it with high performance computing environment. In particular, the SCC selectively promotes and supports large-scale computations. For this purpose, the SCC invites proposals for supercomputer-aided research projects and hosts the Steering Committee, as mentioned below, that evaluates the proposals.

The ISSP supercomputer system consists of two subsystems: System B, which was last replaced in Oct. 2020, is intended for larger total computational power and has more nodes with relatively loose connections whereas System C is intended for higher communication speed among nodes. System B (ohtaka) consists of 1680 CPU nodes of AMD EPYC 7702 (64 cores) and 8 FAT nodes of Intel Xeon Platinum 8280 (28 cores) with total theoretical performance of 6.881 PFlops. System C was replaced in June 2022 and the current system (kugui) consists of 128 nodes of AMD EPYC 7763 (128 cores) and 8 nodes of AMD EPYC 7763 (64 cores) with total theoretical performance of 0.973 PFLOPS.

In addition to the hardware administration, the SCC puts increasing effort on the software support. Since 2015, the SCC has been conducting “Project for advancement of software usability in materials science (PASUMS).”In this project, for enhancing the usability of the ISSP supercomputer system, we conduct several software-advancement activities: developing new application software that runs efficiently on the ISSP supercomputer system, adding new functions to existing codes, help releasing private codes for public use, creating/improving manuals for public codes, etc. Two target programs were selected for fiscal year 2023: (1) Enhancement of TeNeS for finite-temperature calculation (proposed by T. Okubo (U. Tokyo)), and (2) First-principles high-throughput computation for database generation (proposed by K. Yoshimi (ISSP)). In addition, since 2021, we have been maintaining the data repository service for secure storage and enhanced usability of results of numerical calculation.

All staff members of university faculties or public research institutes in Japan are invited to propose research projects (called User Program). The proposals are evaluated by the Steering Committee of SCC. Pre-reviewing is done by the Supercomputer Project Advisory Committee. In fiscal year 2023, totally 345 projects were approved including the ones under the framework of Supercomputing Consortium for Computational Materials Science (SCCMS), which specially supports FUGAKU and other major projects in computational materials science. The total points applied and approved are listed on Table. 1 below.

The research projects are roughly classified into the following three (the number of projects approved, not including SCCMS):

First-Principles Calculation of Materials Properties (178)

Strongly Correlated Quantum Systems (36)

Cooperative Phenomena in Complex, Macroscopic Systems (119)

In all the three categories, most proposals involve both methodology and applications. The results of the projects are reported in 'Activity Report 2023' of the SCC. Every year 3-4 projects are selected for “invited papers” and published at the beginning of the Activity Report. In the SCC Activity Report 2023, the following four invited papers are included:

1. “Density functional theory calculations of H2O adsorption monolayer on a Pt(111) surface”, Jun HARUYAMA, Osamu SUGINO (ISSP), and Toshiki SUGIMOTO (Institute for Molecular Science, JST)
2. “Theoretical studies on the spin-charge dynamics in Kondo-lattice models”, Masahito MOCHIZUKI, and Rintaro ETO (Waseda Univ.)
3. “Mixing Free Energy and Molecular Dynamics Simulations”, Naoko NAKAGAWA and Akira YOSHIDA (Ibaraki Univ.)
4. “Ab initio optical calculation by RESPACK”, Kazuma NAKAMURA (Kyutech)

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| --- | --- | --- | --- | --- |
| Class | Max Points | Application | Numberof Projects | Total Points |
| Applied | Approved |
| System B | System C | System B | System C | System B | System C |
| A | 100 | 50 | any time | 24 | 2.4k | 1.2k | 2.4k | 1.2k |
| B | 1k | 100 | twice a year | 99 | 58.1k | 7.3k | 38.5k | 6.5k |
| C | 10k | 1k | twice a year | 185 | 996.9k | 58.4k | 513.6k | 45.8k |
| D | 10k | 1k | any time | 8 | 47.5k | 2.3k | 40.6k | 1.9k |
| E | 30k | 3k | twice a year | 17 | 317.0k | 25.5k | 185.0k | 20.7k |
| S |  |  | twice a year | 0 | 0 | 0 | 0 | 0 |
| SCCMS |  |  |  | 12 | 27.0k | 2.6k | 27.0k | 2.6k |
| Total |  |  |  | 345 | 1448.9k | 97.3k | 807.1k | 78.7k |

Table 1: Research projects approved in Academic Year 2023.

The maximum points allotted to the project of each class are the sum of the points for the two systems; Computation of one node for 24 hours corresponds to one point for the CPU nodes of System B and System C. The FAT nodes require four points for a 1-node 24-hours use.