Materials Design and Characterization Laboratory (MDCL)

The MDCL was established as the third research facility of the Institute for Solid State Physics (ISSP) when the latter was reorganized in May 1996. Its aim is to promote material science with an emphasis on the "DSC cycle", where DSC stands for design, synthesis and characterization, three processes for developing new materials.

The MDCL consists of two sections, Materials Design (MD) section and Materials Synthesis and Characterization (MSC) section. The Supercomputer Center of the ISSP (SCC-ISSP) is placed in the MD section, while in the MSC section there are seven laboratories for joint use; Materials Synthesis Laboratory, Chemical Analysis Laboratory, X-ray Diffraction Laboratory, Electron Microscope Laboratory, Electromagnetic Measurement Laboratory, Spectroscopy Laboratory, and High-Pressure Synthesis Laboratory.

Almost all the facilities of the MDCL are open to scientists in Japan through the User Programs conducted by two steering committees of the MDCL. One is the steering committee of the SCC-ISSP, under which the Supercomputer Project Advisory Committee is placed for reviewing proposals. The other is the steering committee of the MSC facilities. More than half of the members of these committees are from the outside of ISSP.

COVER FIGURE

Karman Vortex with cavilation

See Y. Asano et al. Page 36–46, "Large-Scale Molecular Dynamics Simulations of Karman Vortex and Sound Wave: Cavitation and Polymer Effects".

PREFACE

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 replaced recently (Oct. 2020), is intended for larger total computational power and has more nodes with relatively loose connections. 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 (enaga, installed in Jan. 2018) consists of 252 nodes of HPE SGI 8600 with 0.77 PFLOPS. Replacement of the System C is scheduled in Spring 2022.

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. Three target programs were selected in fiscal year 2020 and developed or enhanced the ustablity of software were released as (1) PHYSBO (proposal made by R. Tamura (NIMS)), (2) 2DMAT (proposal made by T. Hoshi (Tottori Univ.)), and (3) MateriApps Installer (proposal made by S. Todo (Univ. of Tokyo)). In 2021, we also started the data repository service.

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 2020, totally 387 projects were approved. The total points applied and approved are listed on Table. 1 below. Additionally, we supported FUGAKU and other computational materials science projects through Supercomputing Consortium for Computational Materials Science (SCCMS).

The research projects are roughly classified into the following three (the number of projects approved):

First-Principles Calculation of Materials Properties (189)
Strongly Correlated Quantum Systems (40)
Cooperative Phenomena in Complex, Macroscopic Systems (137)

In all the three categories, most proposals involve both methodology and applications. The results of the projects are reported in 'Activity Report 2020' of the SCC. Every year 3-4 projects are selected for “invited papers” and published at the beginning of the Activity Report. In the Activity Report 2020, the following three invited papers are included:

"Some Recent Developments in ab initio Thermodynamics of Ion Disorder in Solids",
Shusuke KASAMATSU (Yamagata Univ.)

"High precision study of the Anderson transition”,
Tomi OHTSUKI (Sophia Univ.) and Keith SLEVIN (Osaka Univ.)

"Large-Scale Molecular Dynamics Simulations of Karman Vortex and Sound Wave: Cavitation and Polymer Effects",
Yuta ASANO (ISSP), Hiroshi WATANABE (Keio Univ.) and Hiroshi NOGUCHI (ISSP)

June 1, 2021

Naoki Kawashima
(Chairman of the steering committee, SCC, ISSP)

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