1 OUTLINE

1.1 Supercomputer System

In School year 2021 (SY 2021), the ISSP supercomputer center provided users with System B - Dell PowerEdge C6525/R940 system named "ohtaka" and System C - HPE SGI 8600 system named "enaga". System B is a massively-parallel supercomputer with two types of compute nodes: 8 "Fat" nodes and 1680 "CPU" nodes. "Fat" nodes are each comprised of four Intel Xeon Platinum 8280 CPUs (28 cores/CPU) and 3 TB of memory per node. "CPU" nodes have two AMD EPYC 7702 CPUs (64 cores/CPU) and 256 GB of memory per node. System B achieves about 6.881 PFLOPS in theoretical peak performance with high power efficiency. The subsystem comprised of only CPU nodes ranks 87st in the Nov. 2020 Top 500 List, which is a ranking based on total performance measured by the HPL benchmark. The compute nodes communicate to each other through HDR100 Infiniband and are connected in fat tree topology. SY 2021 was the second year of the operation of the current System B. System C is a massively-parallel supercomputer with 252 "CPU" nodes, which have two Intel Xeon Gold 6148 CPUs (20 cores/CPU) and 192 GB of memory. System C achieves 774 TFLOPS in theoretical peak performance. SY 2021 was the last year of the operation of the current System C. For further details, please contact ISSP Supercomputer Center (SCC-ISSP).

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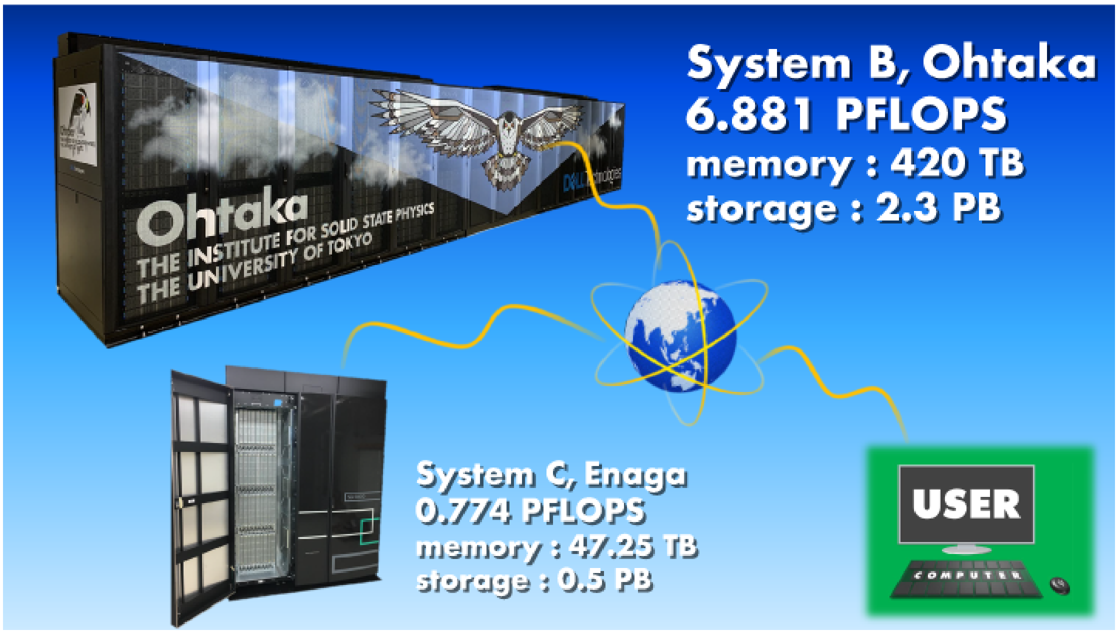

Figure 1: Supercomputer System at the SCC-ISSP

1.2 Project Proposals

The ISSP supercomputer system provides computation resources for scientists working on condensed matter sciences in Japan. All scientific staff members (including post-docs) at universities or public research institutes in Japan can submit proposals for projects related to research activities on materials and condensed matter sciences. These proposals are peer-reviewed by the Advisory Committee members (see Sec. 1.3), and then the computation resources are allocated based on the review reports. The leader of an approved project can set up user accounts for collaborators. Other types of scientists, including graduate students, may also be added. Proposal submissions, peer-review processes, and user registration are all managed via a web system.

The computation resources are distributed in a unit called "point", determined as a function of available CPU utilization time and consumed disk resources. There were calls for six classes of research projects in SY 2021. The number of projects and the total number of points that were applied for and approved in this school year are listed in Table 1.

- Class A is for trial use by new users; proposals for Class A projects are accepted throughout the year.
- Proposals for projects in Classes B (small), C (mid-size), E (large-scale), and S (exceptional) can be submitted twice a year. Approved projects in Classes A, B, C, and E continue to the end of the school year.
- In Class D, projects can be proposed on rapidly-developing studies that need to perform urgent and relatively large calculations. An approved project continues for 6 months from its approval.
- Class S is for projects that are considered extremely important for the field of condensed matter physics and requires extremely large-scale computation. The project may be carried out either by one research group or cooperatively by several investigators at different institutions. A project of this class should be applied with at least 10,000 points; there is no maximum. We require group leaders applying for Class S to give a presentation on the proposal to the Steering Committee of the SCC-ISSP. Class S projects are carried out within one year from its approval.
- Project leaders can apply for points so that the points for each system do not exceed the maximum point shown in this table.

In addition, from SY 2016, ISSP Supercomputer has been providing 20% of its computational resources for Supercomputing Consortium for Computational Materials Science (SCCMS), which aims at advancing parallel computations in condensed matter, molecular, and materials sciences on the 10-PFlops K Computer and the exascale post-K project. From SY 2020, about 10% of the computational resources have been provided for SCCMS. Computational resources have also been allotted to Computational Materials Design (CMD) workshops, as well as CCMS hands-on workshops.

Table 1: Classes of research projects in SY 2021. Total points listed in this table are rounded. In Class D, we collect information about the projects ended in each semester. Note that the maximum points of Classes A and D in the first semester had been changed to those listed in the second semester since May 2021.

First semester (Apr.-Sep.)

Class	Maximum Points		Application	# of Proj.	Total points			
					Applied		Approved	
	Sys–B	Sys–C			Sys–B	Sys–C	Sys–B	Sys–C
A	100	50	any time	12	1.2k	0.5k	1.2k	0.5k
B	800	100	twice a year	58	40.9k	4.5k	23.2k	3.4k
C	8k	1k	twice a year	116	725.7k	71.1k	372.6k	50.8k
D	10k	1k	any time	0	0	0	0	0
E	24k	3k	twice a year	8	187.0k	24.0k	110.0k	17.3k
S	–	–	twice a year	0	0	0	0	0
SCCMS				11	26.1k	5.0k	26.1k	5.0k
Total				205	980.9k	105.1k	533.1k	77.0k

Second semester (Oct.-Mar.)

Class	Maximum Points		Application	# of Proj.	Total points			
					Applied		Approved	
	Sys–B	Sys–C			Sys–B	Sys–C	Sys–B	Sys–C
A	100	40	any time	5	0.5k	0.2k	0.5k	0.2k
B	800	40	twice a year	38	27.2k	0.8k	14.7k	0.7k
C	8k	400	twice a year	53	327.6k	8.5k	159.8k	6.6k
D	10k	400	any time	3	16.0k	0	13.5k	0
E	24k	1.2k	twice a year	6	136.0k	7.2k	83.0k	5.5k
S	–	–	twice a year	0	0	0	0	0
SCCMS				11	28.0k	2.4k	28.0k	2.4k
Total				116	535.2k	19.1k	299.5k	15.3k

1.3 Committees

In order to fairly manage the projects and to smoothly determine the system operation policies, the Materials Design and Characterization Laboratory (MDCL) of the ISSP has organized the Steering Committee of the MDCL and the Steering Committee of the SCC-ISSP, under which the Supercomputer Project Advisory Committee (SPAC) is formed to review proposals. The members of the committees in SY 2021 were as follows:

Steering Committee of the MDCL

KAWASHIMA, Naoki	ISSP (Chair person)
HIROI, Zenji	ISSP
OZAKI, Taisuke	ISSP
NOGUCHI, Hiroshi	ISSP
UWATOKO, Yoshiya	ISSP
SUGINO, Osamu	ISSP
KUBO, Momoji	Tohoku Univ.
ONO, Tomoya	Kobe Univ.
YAMAURA, Jun-ichi	Tokyo Tech.
TAKAHASHI, Hiroki	Nihon Univ.
MOTOME, Yukitoshi	Univ. of Tokyo
HOSHI, Takeo	Tottori Univ.
ISHIWATA, Shintaro	Osaka Univ.
HASEGAWA, Masashi	Nagoya Univ.
NAKATSUJI, Satoru	ISSP

Steering Committee of the SCC-ISSP

KAWASHIMA, Naoki	ISSP (Chair person)
NOGUCHI, Hiroshi	ISSP
OZAKI, Taisuke	ISSP
SUGINO, Osamu	ISSP
TSUNETSUGU, Hirokazu	ISSP
KATO, Takeo	ISSP
YAMASHITA, Minoru	ISSP
MORITA, Satoshi	ISSP
HIGUCHI, Yuji	ISSP
FUKUDA, Masahiro	ISSP
IDO, Kota	ISSP
KAWAMURA, Mitsuaki	ISSP
NAKAJIMA, Kengo	Univ. of Tokyo
HATANO, Naomichi	Univ. of Tokyo
MOTOME, Yukitoshi	Univ. of Tokyo
ONO, Tomoya	Kobe Univ.

TODO, Synge	Univ. of Tokyo
KUBO, Momoji	Tohoku Univ.
OBA, Fumiyasu	Tokyo Tech.
WATANABE, Hiroshi	Keio Univ.
YOSHINO, Hajime	Osaka Univ.
OKUMURA, Hisashi	NINS-RSCS
HOSHI, Takeo	Tottori Univ.
YOSHIMI, Kazuyoshi	ISSP
YATA, Hiroyuki	ISSP
FUKUDA, Takaki	ISSP

Supercomputer Project Advisory Committee

KAWASHIMA, Naoki	ISSP (Chair person)
OZAKI, Taisuke	ISSP
NOGUCHI, Hiroshi	ISSP
SUGINO, Osamu	ISSP
TSUNETSUGU, Hirokazu	ISSP
YAMASHITA, Minoru	ISSP
KATO, Takeo	ISSP
MORITA, Satoshi	ISSP
HIGUCHI, Yuji	ISSP
FUKUDA, Masahiro	ISSP
IDO, Kota	ISSP
KAWAMURA, Mitsuaki	ISSP
NAKAJIMA, Kengo	Univ. of Tokyo
HATANO, Naomichi	Univ. of Tokyo
MOTOME, Yukitoshi	Univ. of Tokyo
ONO, Tomoya	Univ. of Tsukuba
TODO, Synge	Univ. of Tokyo
KUBO, Momoji	Tohoku Univ.
OBA, Fumiyasu	Tokyo Tech.
WATANABE, Hiroshi	Keio Univ.
YOSHINO, Hajime	Osaka Univ.
OKUMURA, Hisashi	NINS-RSCS
HOSHI, Takeo	Tottori Univ.
TSUNEYUKI, Shinji	Univ. of Tokyo
SUZUKI, Takafumi	Univ. of Hyogo
YOSHIMOTO, Yoshihide	Univ. of Tokyo
TOHYAMA, Takami	Tokyo Univ. of Sci.
KITAO, Akio	Tokyo Tech.
ARITA, Ryotaro	Univ. of Tokyo
IKUHARA, Yuichi	Univ. of Tokyo
SHIBATA, Naokazu	Tohoku Univ.
AKAGI, Kazuto	Tohoku Univ.

YANASE, Yoichi	Kyoto Univ.
HATSUGAI, Yasuhiro	Univ. of Tsukuba
OKADA, Susumu	Univ. of Tsukuba
KOBAYASHI, Nobuhiko	Univ. of Tsukuba
NAKAYAMA, Takashi	Chiba Univ.
HOTTA, Takashi	Tokyo Metropolitan Univ.
MATSUKAWA, Hiroshi	Aoyama Gakuin Univ.
YAMAUCHI, Jun	Keio Univ.
HAGITA, Katsumi	National Defense Academy
KONTANI, Hiroshi	Nagoya Univ.
SAITO, Mineo	Kanazawa Univ.
KAWAKAMI, Norio	Kyoto Univ.
YUKAWA, Satoshi	Osaka Univ.
SUGA, Seiichiro	Univ. of Hyogo
TATENO, Masaru	Univ. of Hyogo
YASUDA, Chitoshi	Univ. of the Ryukyus
OGATA, Masao	Univ. of Tokyo
WATANABE, Satoshi	Univ. of Tokyo
HUKUSHIMA, Koji	Univ. of Tokyo
NEMOTO, Koji	Hokkaido Univ.
YABANA, Kazuhiro	Univ. of Tsukuba
FURUKAWA, Nobuo	Aoyama Gakuin Univ.
KUROKI, Kazuhiko	Osaka Univ.
YASUOKA, Kenji	Keio Univ.
TANAKA, Yukio	Nagoya Univ.
MASUBUCHI, Yuichi	Nagoya Univ.
KUSAKABE, Koichi	Osaka Univ.
SHIRAI, Koun	Osaka Univ.
SAKAI, Toru	Univ. of Hyogo
ISHIBASHI, Shoji	AIST
OTANI, Minoru	AIST
TOMITA, Yusuke	Shibaura Inst. Tech.
SHIRAISHI, Kenji	Nagoya Univ.
OGUCHI, Tamio	Osaka Univ.
KAWAKATSU, Toshihiro	Tohoku Univ.
KOBAYASHI, Kazuaki	NIMS
TATEYAMA, Yoshitaka	NIMS
KIM, Kang	Osaka Univ.
OTSUKI, Tomi	Sophia Univ.
MORIKAWA, Yoshitada	Osaka Univ.
ODA, Tatsuki	Kanazawa Univ.
OTSUKI, Junya	Okayama Univ.
KOGA, Akihisa	Tokyo Tech.
SHIMOJO, Fuyuki	Kumamoto Univ.
TAKETSUGU, Tetsuya	Hokkaido Univ.

TSURUTA, Kenji	Okayama Univ.
HAMAGUCHI, Satoshi	Osaka Univ.
NISHIDATE, Kazume	Iwate Univ.
KAGESHIMA, Hiroyuki	Shimane Univ.
ISHII, Fumiyuki	Kanazawa Univ.
TATETSU, Yasutomi	Meio Univ.
YANAGISAWA, Susumu	Univ. of the Ryukyus
SHUDO, Ken-ichi	Yokohama Natl. Univ.
OHMURA, Satoshi	Hiroshima Inst. Tech.
NOGUCHI, Yoshifumi	Shizuoka Univ.
NAKAMURA, Kazuma	Kyushu Inst. Tech.
GOHDA, Yoshihiro	Tokyo Tech.
HAMADA, Ikutaro	Osaka Univ.
RAEBIGER, Hannes	Yokohama Natl. Univ.
KAWARABAYASHI, Tohru	Toho Univ.
KATO, Yusuke	Univ. of Tokyo
NASU, Joji	Tohoku Univ.
HOTTA, Chisa	Univ. of Tokyo
ISOBE, Masaharu	Nagoya Inst. Tech.
HARADA, Ryuhei	Univ. of Tsukuba
TAMURA, Ryo	NIMS
TANAKA, Shu	Keio Univ.
TADA, Tomofumi	Kyushu Univ.

1.4 Staff

The following staff members of the SCC-ISSP usually administrate the ISSP Supercomputer.

KAWASHIMA, Naoki	Professor (Chair person)
NOGUCHI, Hiroshi	Associate Professor
OZAKI, Taisuke	Professor
SUGINO, Osamu	Professor
IDO, Kota	Research Associate
FUKUDA, Masahiro	Research Associate
HIGUCHI, Yuji	Research Associate
KAWAMURA, Mitsuaki	Research Associate
MORITA, Satoshi	Research Associate
YOSHIMI, Kazuyoshi	Project Researcher
MOTOYAMA, Yuichi	Project Researcher
YATA, Hiroyuki	Technical Specialist
FUKUDA, Takaki	Technical Specialist
ARAKI, Shigeyuki	Project Academic Specialist

2 STATISTICS (SCHOOL YEAR 2021)

2.1 System and User Statistics

In the following, we present statistics for operation time taken in the period from April 2021 to March 2022 (SY 2021). In Table 2, we show general statistics of the supercomputer system in SY 2021. The total numbers of compute nodes in System B “ohtaka” and System C “enaga” are 1688 and 252, respectively. Consumed disk points amount to about a few percent of the total consumed points in both System B and System C.

Table 2: Overall statistics of SY 2021

	System B ohtaka	System C enaga
total service time ($\times 10^3$ node·hours)	14396	1601
number of executed jobs	456984	46166
total consumed points ($\times 10^3$ point)	498	30
CPU points ($\times 10^3$ point)	480	29
disk points ($\times 10^3$ point)	18	2
total exec. time ($\times 10^3$ node·hours)	12980	1367
availability	97.34%	96.23%
utilization rate	90.14%	85.47%

In Fig. 2, availabilities, utilization rates, and consumed points in Systems B and C are plotted for each month. Throughout the school year, the availability and the utilization rates were very high : the availability and the utilization rates exceed about 90% and 80% throughout most of the year, respectively.

The user statistics are shown in Fig. 3. The horizontal axis shows the rank of the user/group arranged in the descending order of the execution time (hour×nodes). The execution time of the user/group of the first rank is the longest. The vertical axis shows the sum of the execution time up to the rank. From the saturation points of the graphs, the numbers of “active” users of Systems B and C are around 400 and 100, respectively. The maximum ranks in the graphs correspond to the number of the users/groups that submitted at least one job.

2.2 Queue and Job Statistics

Queue structures of Systems B and C in SY2021 are shown in Tables 3 and 4, respectively. In System B “ohtaka”, users can choose from two types of compute nodes; jobs submitted to queues with “cpu” and “fat” at the end of their queue names are submitted to CPU and Fat nodes, respectively, while only CPU nodes are available in System C “enaga”. See Sec. 1.1 for a description of each type of compute node. The user then has to choose the queue according to the number

Table 3: Queue structures of System B in SY 2021

System B, ohtaka

queue name	Elapsed time limit (hr)	# of nodes /job	# of nodes /queue	Memory limit (GB)	job points /(node·day)
F1cpu	24	1	600	230/node	1
L1cpu	120	1	300	230/node	1
F4cpu	24	2–4	216	230/node	1
L4cpu	120	2–4	108	230/node	1
F16cpu	24	5–16	288	230/node	1
L16cpu	120	5–16	144	230/node	1
F36cpu	24	17–36	72	230/node	1
L36cpu	120	17–36	36	230/node	1
F72cpu	24	72	576	230/node	1
L72cpu	120	72	288	230/node	1
F144cpu	24	144	432	230/node	1
L144cpu	120	144	144	230/node	1
i8cpu	0.5	1–8	72	230/node	1
F2fat	24	1–2	7	2900/node	4
L2fat	120	1–2	3	2900/node	4
i1fat	0.5	1	1	2900/node	4

of nodes to use and the duration of their calculation jobs. Queue names starting with "F" are for jobs taking 24 hours or less, while those starting with "L" can run much longer up to 120 hours. More nodes are allotted to "F" queues in order to maximize the turnaround time of user jobs. The queue names starting with "i" are used for interactive debugging of user programs and the elapsed time limit is 30 minutes. The number following "F", "L", or "i" correspond to the number of nodes that can be used by one user job. Although we do not mention here in detail, to promote utilization of the massively parallel supercomputer, background queues (queue name starting with "B") for Systems B and C which charge no points for the jobs have also been open.

To prevent overuse of the storage, points are charged also for usage of disk quota in the three systems, as shown in Table 5. Disk points are revised often for optimal usage of the resources by examining usage tendencies each year.

The number of jobs, average waiting time, and total execution time in each queue are shown in Tables 6 and 7. In System B, a large portion of jobs have been executed in "F" queues. The largest amount of the execution time has been consumed in the large-scale "F72cpu" queues for ohtaka, respectively. However, substantial number of jobs were run in every queue, suggesting that a wide variety of user needs are met by this queuing scheme. In most of these queues, the queue settings meet the user's tendencies in that the waiting times are on the order of the elapsed-time limit.

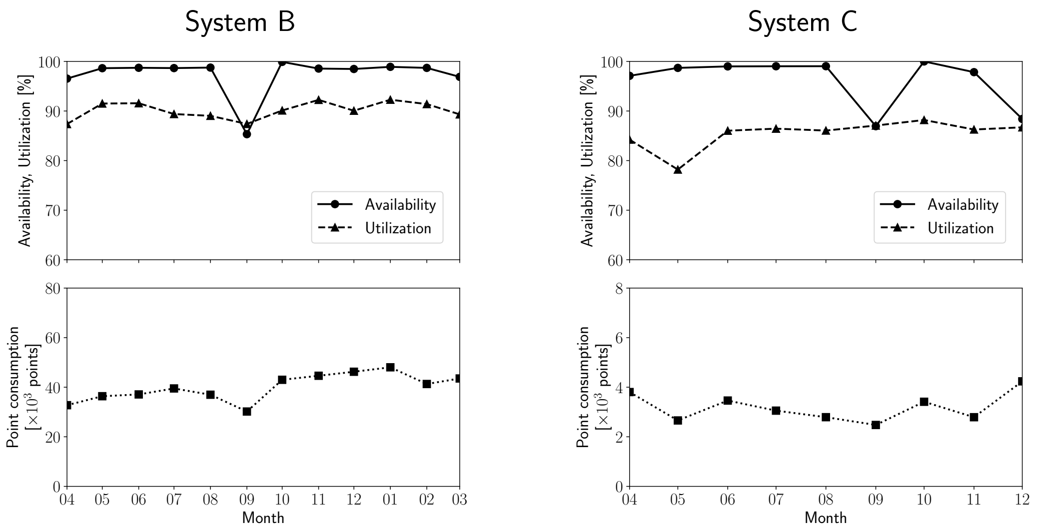

Figure 2: Availabilities, utilization rates and point consumptions of each month during SY 2021.

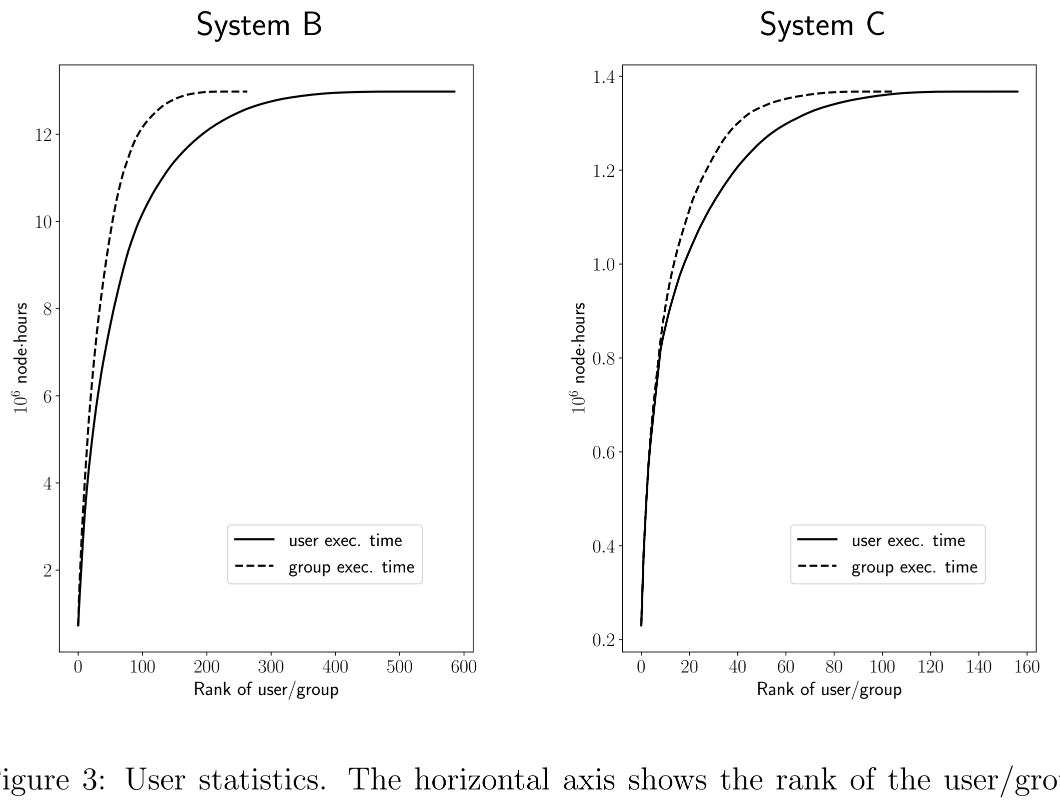

Figure 3: User statistics. The horizontal axis shows the rank of the user/group arranged in the descending order of the execution time (hour×nodes). The vertical axis shows the sum of the execution time up to the rank.

Table 4: Queue structures of System C in SY 2021

System C, enaga

queue name	Elapsed time limit (hr)	# of nodes /job	# of nodes /queue	Memory limit (GB)	job points /(node·day)
F4cpu	24	1–4	54	170/node	1
L4cpu	120	1–4	18	170/node	1
i4cpu	0.5	1–4	18	170/node	1
F9cpu	24	5–9	36	170/node	1
L9cpu	120	5–9	18	170/node	1
F36cpu	24	10–36	144	170/node	18(36)/(# of nodes)*
L36cpu	120	10–36	36	170/node	18(36)/(# of nodes)*

* For F/L36cpu queue, the number of occupied node increases in increments of 18 nodes.

Table 5: Disk points of Systems B and C

		point/day
System B ohtaka	`/home`	$0.001 \times \theta(q - 600)$
	`/work`	$0.0001 \times \theta(q - 6000)$
System C enaga	`/home`	$0.001 \times \theta(q - 150)$
	`/work`	$0.0001 \times \theta(q - 1500)$

* q is denoted in unit of GB.
* $\theta(x)$ is equal to the Heaviside step function $H(x)$ multiplied by x, i.e., $xH(x)$.

2.3 Project for Advancement of Software Usability in Materials Science

From School Year 2015, the supercomputer center (SCC) has started "Project for advancement of software usability in materials science". In this project, for enhancing the usability of the supercomputer system in ISSP, we perform some software-advancement activity such as implementing a new function to an existing code, releasing a private code on Web, writing manuals. Target programs are publicly offered in December and selected in the review by the Steering Committee of SCC. The projects are carried out by the software development team composed of three members in ISSP. In SY 2021, three projects were selected as listed in Table 8.

Table 6: Number of jobs, average waiting time, total execution time, and average number of used nodes per job in each queue of System B.

System B, ohtaka

queue	# of Jobs	Waiting Time (hour)	Exec. Time ($\times 10^3$ node·hour)	# of nodes
F1cpu	211125	16.62	320.55	1.00
L1cpu	10781	60.45	289.72	1.00
F4cpu	73536	11.69	1175.58	2.87
L4cpu	5619	17.66	400.57	2.53
F16cpu	21718	15.21	1505.98	10.18
L16cpu	1621	79.48	663.18	9.93
F36cpu	1633	67.66	315.88	27.74
L36cpu	87	51.37	93.18	21.63
F72cpu	7773	33.00	3494.10	72.00
L72cpu	133	68.15	373.04	72.00
F144cpu	3023	17.02	2062.21	144.00
L144cpu	134	141.08	677.79	144.00
i8cpu	91096	0.09	42.54	3.23
F2fat	3673	28.21	24.77	1.10
L2fat	282	39.31	15.96	1.23
i1fat	522	0.50	0.06	1.00

Table 7: Number of jobs, average waiting time, total execution time, and average number of used nodes per job in each queue of System C.

System C, enaga

queue	# of Jobs	Waiting Time (hour)	Exec. Time ($\times 10^3$ node·hour)	# of nodes
F4cpu	23663	5.24	185.74	1.78
L4cpu	727	50.21	80.59	1.59
i4cpu	7775	0.05	2.64	2.33
F9cpu	1434	6.11	68.23	7.22
L9cpu	77	11.94	22.05	6.68
F36cpu	1551	8.13	301.11	29.58
L36cpu	62	10.02	28.94	20.32

Table 8: List of Project for advancement of software usability in materials science for SY 2021.

Project Proposer	Project Name
Minoru Otani AIST CD-FMat	Improvement of Quantum ESPRESSO implementing the ESM RISM method
Takeo Hoshi Tottori University	Unified platform of experiment-data analysis for 2D material structure

2.4 ISSP Data Repository

From School Year 2021, the supercomputer center (SCC) has started to operate ISSP Data Repository (ISSP-DR) for accumulating and utilizing research data in materials science. GitLab is used as the data management system, and a portal site is provided as a data registration and search system for the registered data. By using ISSP-DR, it is possible to store and publish research data used in papers and datasets useful in the field of condensed matter science. Users of ISSP Supercomputer are welcome to apply for and use ISSP-DR.

Acknowledgments

The staffs would like to thank Prof. Takafumi Suzuki (now at University of Hyogo) for developing WWW-based system (SCM: SuperComputer Management System) for management of project proposals, peer-review reports by the SPAC committee, and user accounts. We also thank Ms. Reiko Iwafune for creating and maintaining a new WWW page of the ISSP Supercomputer Center.