1 OUTLINE

1.1 Supercomputer System

In School year 2022 (SY 2022), the ISSP supercomputer center provided users with System B - Dell PowerEdge C6525/R940 system named "ohtaka" and System C - HPE Apollo 2000 Gen10 Plus/HPE Apollo 6500 Gen10 Plus system named "kugui". 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 2022 was the third year of the operation of the current System B. In June 2022, "kugui" was introduced as System C, which will be operated for the next six years. System C is a massively-parallel supercomputer with two types of compute nodes: 128 "CPU" nodes and 8 "ACC" nodes. "CPU" nodes are each comprised of two AMD EPYC 7763 CPUs (64 cores/CPU) and 256 GB of memory. The compute nodes communicate to each other through HDR200 Infiniband and are connected in fat tree topology. "ACC" nodes are each comprised of one AMD EPYC 7763 CPUs (64 cores/CPU), four NVIDIA A100 40GB for HGX GPUs and 256 GB of memory. System C achieves 973 TFLOPS in theoretical peak performance. System C entered official operation in June 14th, 2022. Trial operation of System C continued until July 18th, 2022. SY 2022 was the first year of the operation of the current System C. For further details, please contact ISSP Supercomputer Center (SCC-ISSP).

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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

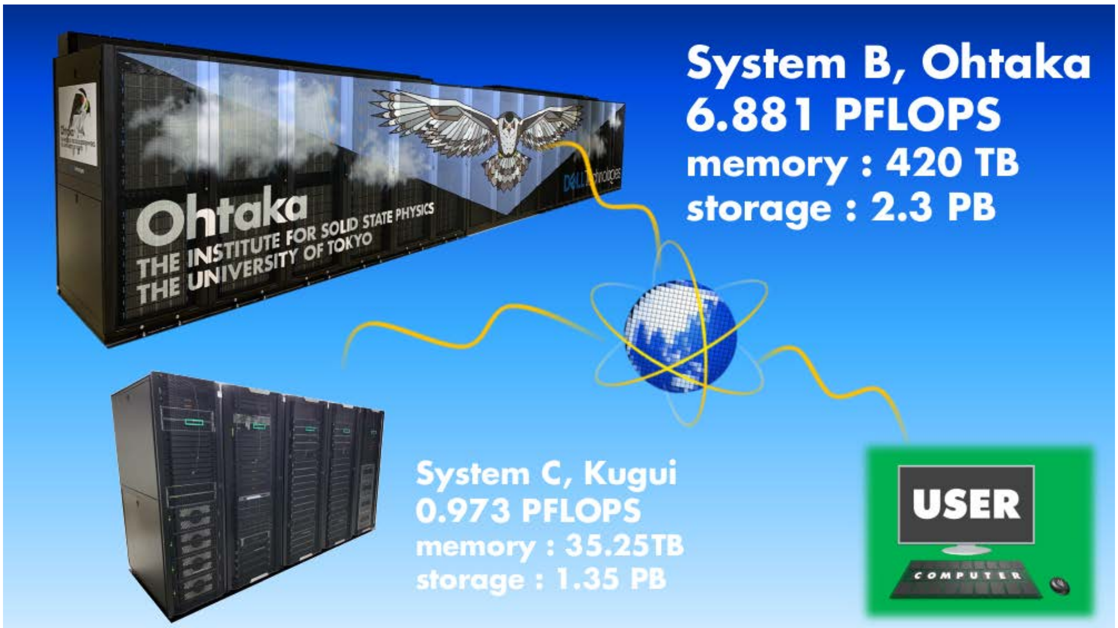

Figure 1: Supercomputer System at the SCC-ISSP

were calls for six classes of research projects in SY 2022. 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.

Table 1: Classes of research projects in SY 2022. Total points listed in this table are rounded. In Class D, we collect information about the projects ended in each semester.

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	28	2.8k	1.4k	2.8k	1.4k
B	800	100	twice a year	94	65.9k	6.7k	38.6k	5.5k
C	8k	500	twice a year	176	1092.9k	47.4k	566.8k	35.7k
D	10k	500	any time	6	28.5k	1.2k	23.0k	1.0k
E	24k	1.5k	twice a year	13	273.0k	18.0k	185.5k	14.4k
S	–	–	twice a year	0	0	0	0	0
SCCMS				20	52.3k	5.2k	52.3k	5.2k
Total				337	1515.4k	79.9k	869.0k	63.2k

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, up to 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.

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 2022 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
OKAMOTO, Yoshihiko	ISSP
SUGINO, Osamu	ISSP
KUBO, Momoji	Tohoku Univ.

HUKUSHIMA, Koji	Univ. of Tokyo
HONDA, Fuminori	Kyushu Univ.
SHIMAKAWA, Yuichi	Kyoto 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
KIMURA, Takashi	ISSP
MORITA, Satoshi	ISSP
FUKUDA, Masahiro	ISSP
IDO, Kota	ISSP
KAWAMURA, Mitsuaki	ISSP
NAKAJIMA, Kengo	Univ. of Tokyo
OTSUKI, Junya	Okayama Univ.
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.
HUKUSHIMA, Koji	Univ. of Tokyo
KITAO, Akio	Tokyo Tech.
HAMADA, Ikutaro	Osaka 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
KIMURA, Takashi	ISSP

KATO, Takeo	ISSP
MORITA, Satoshi	ISSP
FUKUDA, Masahiro	ISSP
IDO, Kota	ISSP
KAWAMURA, Mitsuaki	ISSP
NAKAJIMA, Kengo	Univ. of Tokyo
MOTOME, Yukitoshi	Univ. of Tokyo
TODO, Synge	Univ. of Tokyo
KUBO, Momoji	Tohoku Univ.
OBA, Fumiyasu	Tokyo Tech.
WATANABE, Hiroshi	Keio Univ.
HUKUSHIMA, Koji	Univ. of Tokyo
ONO, Tomoya	Kobe Univ.
OTSUKI, Junya	Okayama Univ.
KITAO, Akio	Tokyo Tech.
HAMADA, Ikutaro	Osaka Univ.
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.
YUKAWA, Satoshi	Osaka Univ.
SUGA, Seiichiro	Univ. of Hyogo
YASUDA, Chitoshi	Univ. of the Ryukyus
KIM, Kang	Osaka Univ.
MORIKAWA, Yoshitada	Osaka 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.
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
TANAKA, Shu	Keio Univ.
KOBAYASHI, Kazuaki	NIMS
TATEYAMA, Yoshitaka	NIMS
TAMURA, Ryo	NIMS
TADA, Tomofumi	Kyushu Univ.
HATANO, Naomichi	Univ. of Tokyo
YOSHINO, Hajime	Osaka Univ.
OKUMURA, Hisashi	NINS-ExCELLS
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.
ARITA, Ryotaro	Univ. of Tokyo
OGATA, Masao	Univ. of Tokyo
WATANABE, Satoshi	Univ. of Tokyo
YABANA, Kazuhiro	Univ. of Tsukuba
FURUKAWA, Nobuo	Aoyama Gakuin Univ.
KUROKI, Kazuhiko	Osaka Univ.
TANAKA, Yukio	Nagoya Univ.
KUSAKABE, Koichi	Univ. of Hyogo
SAKAI, Toru	Univ. of Hyogo
ISHIBASHI, Shoji	AIST
OTANI, Minoru	Univ. of Tsukuba
TOMITA, Yusuke	Shibaura Inst. Tech.
SHIRAISHI, Kenji	Nagoya Univ.
OGUCHI, Tamio	Osaka Univ.
KAWAKATSU, Toshihiro	Tohoku Univ.
OTSUKI, Tomi	Sophia Univ.
ODA, Tatsuki	Kanazawa Univ.
ARAI, Noriyoshi	Keio Univ.
UNEYAMA, Takashi	Nagoya 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
KAWAMURA, Mitsuaki	Research Associate
MORITA, Satoshi	Research Associate
NAKANO, Hiroyoshi	Research Associate
YOSHIMI, Kazuyoshi	Project Researcher
AOYAMA, Tatsumi	Project Researcher
MOTOYAMA, Yuichi	Technical Specialist
YATA, Hiroyuki	Technical Specialist
FUKUDA, Takaki	Technical Specialist
ARAKI, Shigeyuki	Project Academic Specialist

2 STATISTICS (SCHOOL YEAR 2022)

2.1 System and User Statistics

In the following, we present statistics for operation time taken in the period from April 1st 2022 to April 3rd 2023 (SY 2022). In Table 2, we show general statistics of the supercomputer system in SY 2022. The total numbers of compute nodes in System B "ohtaka" and System C "kugui" are 1688 and 136, respectively. Consumed disk points amount to about a few percent of the total consumed points in both System B and System C.

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$\times$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.

Table 2: Overall statistics of SY 2022

	System B ohtaka	System C kugui
total service time ($\times 10^3$ node·hours)	14420	976
number of executed jobs	476439	108868
total consumed points ($\times 10^3$ point)	502	18
CPU points ($\times 10^3$ point)	489	18
disk points ($\times 10^3$ point)	13	1
total exec. time ($\times 10^3$ node·hours)	13293	790
availability	96.60%	97.38%
utilization rate	92.3%	80.98%

2.2 Queue and Job Statistics

Queue structures of Systems B and C in SY 2022 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. In System C, there are two types of compute nodes: CPU and ACC nodes. Jobs submitted to queues with "cpu" and "acc" at the end of their queue names are submitted to CPU and ACC nodes, respectively, If users submit a job to queues with "accs" at the end of their queue names, the job runs in the ACC node shared by other jobs of "accs" queues. 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 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 Systems B and C, 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" and "F16cpu" queues for Systems B and C, 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

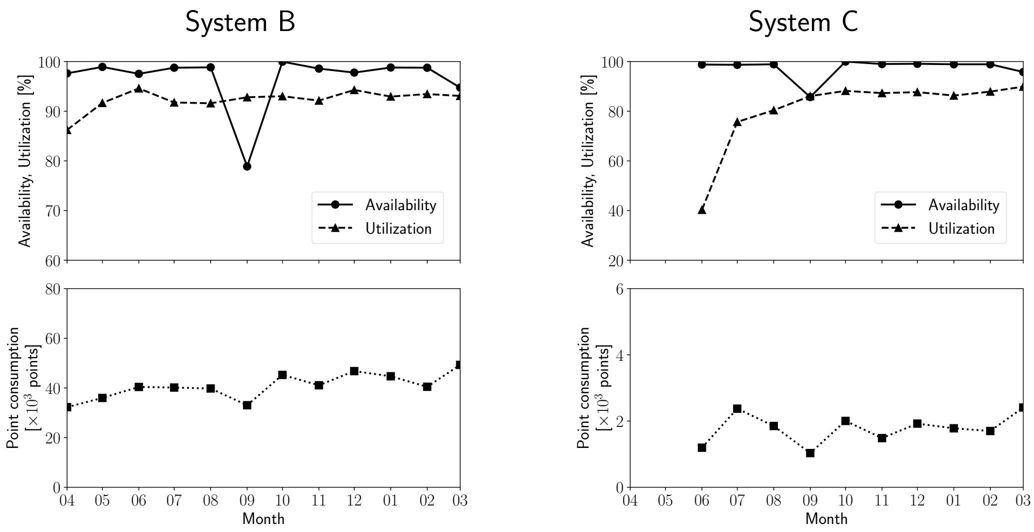

Figure 2: Availabilities, utilization rates and point consumptions of each month during SY 2022.

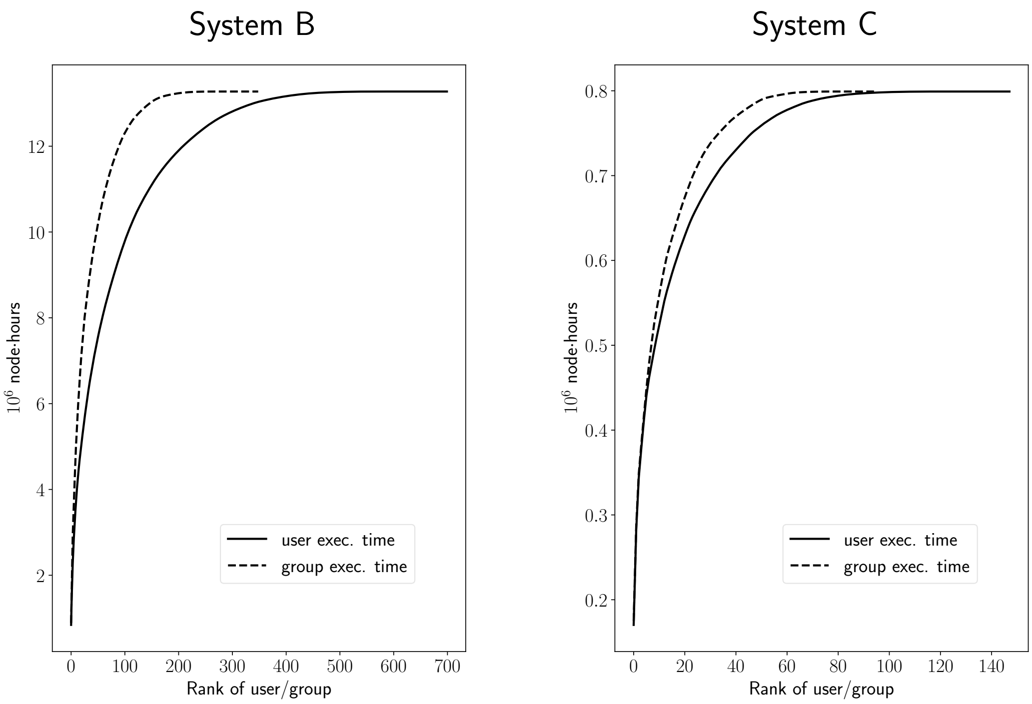

Figure 3: User statistics. The horizontal axis shows the rank of the user/group arranged in the descending order of the execution time (hour×nodes). The vertical axis shows the sum of the execution time up to the rank.

Table 3: Queue structures of System B in SY 2022

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

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.

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 2022, three projects were selected as listed in Table 8.

Table 4: Queue structures of System C in SY 2022

System C, kugui

queue name	Elapsed time limit (hr)	# of nodes /job	# of nodes /queue	Memory limit (GB)	job points /(node·day)
i2cpu	0.5	1–2	8	240/node	1
F1cpu	24	1	120	240/node	1
L1cpu	120	1	60	240/node	1
F4cpu	24	2–4	32	240/node	1
L4cpu	120	2–4	16	240/node	1
F16cpu	24	5–16	64	240/node	1
L16cpu	120	5–16	32	240/node	1
F1accs	24	1	3	$60\times N_{\mathrm{GPU}}$	1
L1accs	120	1	1	$60\times N_{\mathrm{GPU}}$	1
i1accs	0.5	1	1	$60\times N_{\mathrm{GPU}}$	1
F2acc	24	1–2	4	240/node	1
L2acc	120	1–2	2	240/node	1

* N_{GPU} in ACC queues denotes the number of occupied GPUs.

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.

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 kugui	`/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., $xH(x)$.

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	160175	31.64	290.45	1.00
L1cpu	4726	63.51	207.39	1.00
F4cpu	77846	26.01	1203.73	2.82
L4cpu	4400	58.22	493.38	2.89
F16cpu	44145	12.77	1586.63	9.23
L16cpu	1990	58.49	661.29	9.29
F36cpu	1179	52.79	311.35	28.75
L36cpu	102	69.71	115.50	22.46
F72cpu	8509	19.76	3711.88	72.00
L72cpu	101	40.95	270.27	72.00
F144cpu	3422	18.28	2090.58	144.00
L144cpu	114	257.46	581.50	144.00
i8cpu	143548	0.09	95.25	4.28
F2fat	5698	206.85	36.39	1.24
L2fat	508	60.36	17.51	1.21
i1fat	1003	0.35	0.09	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, kugui

queue	# of Jobs	Waiting Time (hour)	Exec. Time ($\times 10^3$ node·hour)	# of nodes
i2cpu	6417	0.39	0.84	1.30
F1cpu	32465	3.03	92.09	1.00
L1cpu	862	24.34	31.42	1.00
F4cpu	3780	6.13	80.44	3.31
L4cpu	374	35.69	45.22	3.44
F16cpu	1837	12.60	134.95	13.53
L16cpu	83	16.11	23.83	12.24
i1accs	3794	0.00	0.20	1.00
F1accs	2946	2.88	10.41	1.00
L1accs	418	1.16	1.57	1.00
F2acc	3225	5.96	4.16	1.04
L2acc	72	2.05	0.63	1.29

Table 8: List of Project for advancement of software usability in materials science for SY 2022.

Project Proposer	Project Name
Shusuke Kasamatsu Yamagata University	Coupling of extended ensemble sampling and first-principles solvers
Akito Kobayashi Nagoya University	Advancement of effective model solvers toward high-throughput calculations — Wavenumber based mean-field approximation and random phase approximation