1 Outline

1.1 Supercomputer System

In SY2017, the ISSP supercomputer center provided users with System B - SGI ICE XA/UV hybrid system, which is a massively-parallel supercomputer with three types of compute nodes: 19 “Fat” nodes, 1584 “CPU” nodes, and 288 “ACC” nodes. “Fat” nodes are each comprised of four Intel Xeon E5-4627v3 CPUs (10 cores/CPU) and 1 TB of memory. “CPU” nodes have two Intel Xeon E5-2680v3 CPUs (12 cores/CPU) and 128 GB of memory. “ACC” nodes have two nVIDIA Tesla K40 GPUs in additon to two Xeon E5-2680v3 CPUs and 128 GB of memory. System B achieves 2.6 PFLOPS in theoretical peak performance with high power efficiency. The subsystem comprised of only CPU nodes ranks 61st on the November 2015 Top 500 List, which is a ranking based on total performance measured by the HPL benchmark. The subsystem of ACC nodes ranks 104th on the Top 500 List, and it also ranks 23rd on the Green 500 List, which is a ranking based on performance per watt of electrical power consumption. The compute nodes communicate to each other through FDR Infiniband. The Fat nodes are interconnected in fat tree topology, while the CPU and ACC nodes are connected in enhanced hypercube topology. System B entered official operation on Aug. 21, 2015.

The previous System C - FUJITSU PRIMEHPC FX10 ceased operation at the end of the previous school year. It has been replaced by the new System C - HPE SGI 8600 system, which entered official operation in April, 2018.

SY2017 was the third year of the operation of the current System B. 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 were calls for six classes of research projects in SY 2017. 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.

Table 1: Classes of research projects in SY 2017

Class	Maximum Points		Application	# of Proj.	Total points			
					Applied		Approved	
	Sys–B	Sys–C			Sys–B	Sys–C	Sys–B	Sys–C
A	100	100	any time	12	1.2k	–	1.2k	–
B	1k	500	twice a year	62	56.9k	–	40.0k	–
C	10k	2.5k	twice a year	171	1433.8k	–	633.0k	–
D	10k	2.5k	any time	6	26.5k	–	24.5k	–
E	30k	2.5k	twice a year	16	474.0k	–	258.0k	–
S	–	–	twice a year	0	0	–	0	–
SCCMS				35	271.5k	–	271.5k	–
Total				302	2263.9k	–	1228.2k	–

- 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.

- There was no official System C operation in SY2017.

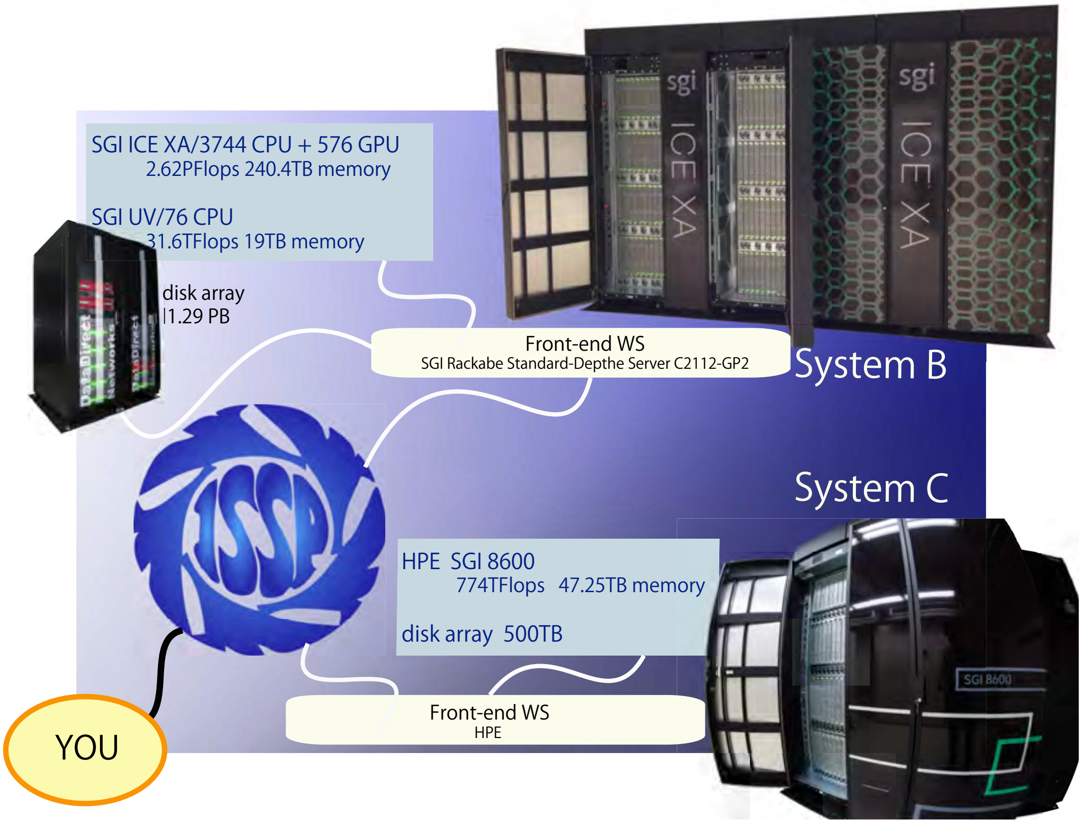

Figure 1: Supercomputer System at the SCC-ISSP

In addition, from SY 2016, ISSP Supercomputer is 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. Computer time has also been alloted to Computational Materials Design (CMD) workshops, as well as for Science Camps held in ISSP for undergraduate students.

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 2016 were as follows:

Steering Committee of the MDCL

HIROI, Zenji	ISSP (Chair person)

KATO, Takeo	ISSP
KAWASHIMA, Naoki	ISSP
NOGUCHI, Hiroshi	ISSP
SUGINO, Osamu	ISSP
UWATOKO, Yoshiya	ISSP
KIMURA, Kaoru	Univ. of Tokyo
YOSHIMOTO, Yoshihide	Univ. of Tokyo
SAWA, Hiroshi	Nagoya Univ.
KAGEYAMA, Hiroshi	Kyoto Univ.
SUZUKI, Takafumi	Univ. of Hyogo
OKUMURA, Hisashi	NINS-RSCS
OTSUKI, Tomi	Sophia Univ.
TAKEDA Mahoto	Yokohama Natl. Univ.

Steering Committee of the SCC-ISSP

NOGUCHI, Hiroshi	ISSP (Chair person)
KAWASHIMA, Naoki	ISSP
OZAKI, Taisuke	ISSP
SUGINO, Osamu	ISSP
TSUNETSUGU, Hirokazu	ISSP
KATO, Takeo	ISSP
MASUDA, Takatsugu	ISSP
HIGUCHI, Yuji	ISSP
KASAMATSU, Shusuke	ISSP
MORITA, Satoshi	ISSP
WATANABE, Hiroshi	ISSP
HATANO, Naomichi	Univ. of Tokyo
IMADA, Masatoshi	Univ. of Tokyo
NAKAJIMA, Kengo	Univ. of Tokyo
TSUNEYUKI, Shinji	Univ. of Tokyo
YOSHIMOTO, Yoshihide	Univ. of Tokyo
KUBO, Momoji	Tohoku Univ.
MORIKAWA, Yoshitada	Osaka Univ.
OTSUKI, Tomi	Sophia Univ.
OKUMURA, Hisashi	NINS-RSCS
HOSHI, Takeo	Tottori Univ.
SUZUKI, Takafumi	Univ. of Hyogo
YATA, Hiroyuki	ISSP
FUKUDA, Takaki	ISSP

Supercomputer Project Advisory Committee

NOGUCHI, Hiroshi	ISSP (Chair person)
KATO, Takeo	ISSP

KAWASHIMA, Naoki	ISSP
OZAKI, Taisuke	ISSP
SUGINO, Osamu	ISSP
TSUNETSUGU, Hirokazu	ISSP
MASUDA, Takatsugu	ISSP
HIGUCHI, Yuji	ISSP
KASAMATSU, Shusuke	ISSP
MORITA, Satoshi	ISSP
WATANABE, Hiroshi	ISSP
HATANO, Naomichi	Univ. of Tokyo
HUKUSHIMA, Koji	Univ. of Tokyo
IKUHARA, Yuichi	Univ. of Tokyo
IMADA, Masatoshi	Univ. of Tokyo
IWATA, Jun-Ichi	Univ. of Tokyo
MIYASHITA, Seiji	Univ. of Tokyo
MOTOME, Yukitoshi	Univ. of Tokyo
NAKAJIMA, Kengo	Univ. of Tokyo
OGATA, Masao	Univ. of Tokyo
OSHIYAMA, Atsushi	Univ. of Tokyo
TODO, Synge	Univ. of Tokyo
TSUNEYUKI, Shinji	Univ. of Tokyo
WATANABE, Satoshi	Univ. of Tokyo
YOSHIMOTO, Yoshihide	Univ. of Tokyo
ARITA, Ryotaro	RIKEN-CEMS
NEMOTO, Koji	Hokkaido Univ.
AKAGI, Kazuto	Tohoku Univ.
KAWAKATSU, Toshihiro	Tohoku Univ.
KUBO, Momoji	Tohoku Univ.
SHIBATA, Naokazu	Tohoku Univ.
YANASE, Yoichi	Niigata Univ.
ISHIBASHI, Shoji	AIST
OTANI, Minoru	AIST
KOBAYASHI, Kazuaki	NIMS
TATEYAMA, Yoshitaka	NIMS
HATSUGAI, Yasuhiro	Univ. of Tsukuba
KOBAYASHI, Nobuhiko	Univ. of Tsukuba
OKADA, Susumu	Univ. of Tsukuba
ONO, Tomoya	Univ. of Tsukuba
YABANA, Kazuhiro	Univ. of Tsukuba
ODA, Tatsuki	Kanazawa Univ.
SAITO, Mineo	Kanazawa Univ.
HIDA, Kazuo	Saitama Univ.
NAKAYAMA, Takashi	Chiba Univ.
FURUKAWA, Nobuo	Aoyama Gakuin Univ.
MATSUKAWA, Hiroshi	Aoyama Gakuin Univ.

TAKANO, Hiroshi	Keio Univ.
YAMAUCHI, Jun	Keio Univ.
YASUOKA, Kenji	Keio Univ.
TOMITA, Yusuke	Shibaura Inst. Tech.
OTSUKI, Tomi	Sophia Univ.
OBATA, Shuji	Tokyo Denki Univ.
KITAO, Akio	Tokyo Tech.
TADA, Tomofumi	Tokyo Tech.
HOTTA, Takashi	Tokyo Metropolitan Univ.
TOHYAMA, Takami	Tokyo Univ. of Sci.
WATANABE, Kazuyuki	Tokyo Univ. of Sci.
HAGITA, Katsumi	National Defense Academy
KONTANI, Hiroshi	Nagoya Univ.
MASUBUCHI, Yuichi	Nagoya Univ.
SHIRAISHI, Kenji	Nagoya Univ.
TANAKA, Yukio	Nagoya Univ.
KAWAKAMI, Norio	Kyoto Univ.
KAWAMURA, Hikaru	Osaka Univ.
KIM, Kang	Osaka Univ.
KUROKI, Kazuhiko	Osaka Univ.
KUSAKABE, Koichi	Osaka Univ.
MORIKAWA, Yoshitada	Osaka Univ.
OGUCHI, Tamio	Osaka Univ.
SHIRAI, Koun	Osaka Univ.
YOSHINO, Hajime	Osaka Univ.
YUKAWA, Satoshi	Osaka Univ.
SAKAI, Toru	JAEA
SUGA, Seiichiro	Univ. of Hyogo
SUZUKI, Takafumi	Univ. of Hyogo
TATENO, Masaru	Univ. of Hyogo
HOSHI, Takeo	Tottori Univ.
YASUDA, Chitoshi	Univ. of the Ryukyus
OKUMURA, Hisashi	NINS-RSCS

1.4 Staff

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

NOGUCHI, Hiroshi	Associate Professor (Chair person)
KAWASHIMA, Naoki	Professor
OZAKI, Taisuke	Professor
SUGINO, Osamu	Associate Professor
WATANABE, Hiroshi	Research Associate
KASAMATSU, Shusuke	Research Associate

HIGUCHI, Yuji	Research Associate
NOGUCHI, Yoshifumi	Research Associate
MORITA, Satoshi	Research Associate
YATA, Hiroyuki	Technical Associate
FUKUDA, Takaki	Technical Associate
ARAKI, Shigeyuki	Technical Associate

2 Statistics (School Year 2017)

2.1 System and User Statistics

In the following, we present statistics for operation time taken in the period from April 2017 to March 2018 (SY 2017). In Table 2, we show general statistics of the supercomputer system in SY 2017. The total number of compute nodes in System B is 1891. Consumed disk points amount to about 3% of the total consumed points in System B. Roughly 20% of the total points in System B were consumed by SCCMS projects. This means that about 20% of the total computational resources in this school year were actually used by SCCMS projects.

In the left column of Fig. 2, availabilities, utilization rates, and consumed points in System B are plotted for each month. Throughout the school year, the utilization rates were very high. exceeding 90% throughout most of the year.

The user statistics are shown in the right column of Fig. 2. 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 number of "active" users of System B is around 300. 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 2017

	System B
total service time ($\times 10^3$ node·hours)	15814
number of executed jobs	665306
total consumed points ($\times 10^3$ point)	629
CPU points ($\times 10^3$ point)	613
disk points ($\times 10^3$ point)	16
total exec. time ($\times 10^3$ node·hours)	14399
availability	95.9%
utilization rate	91.1%

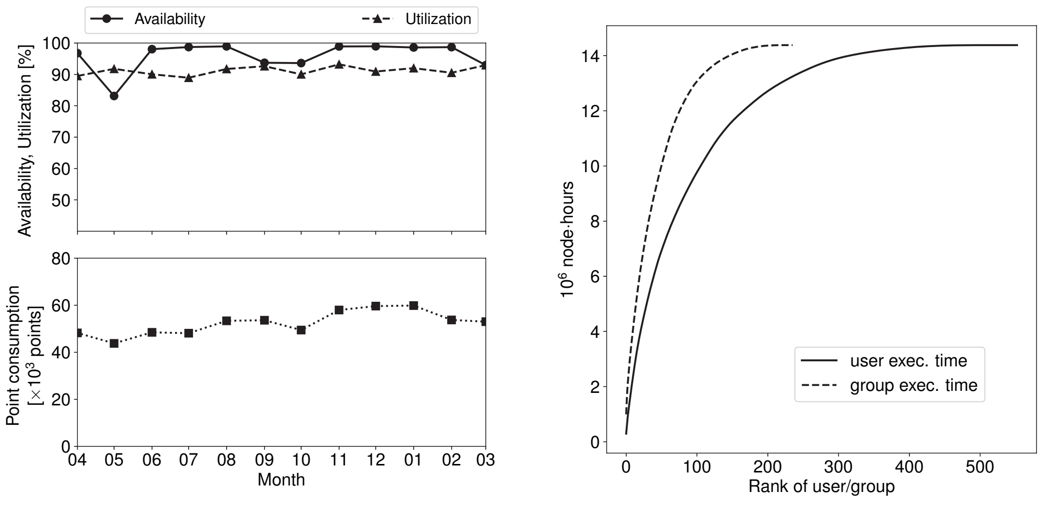

Figure 2: Left: Availabilities, utilization rates and point consumptions of each month during SY 2017. Right: User statistics. The horizontal axis shows the rank of the user/group arranged in the descending order of the execution time (hour×nodes). The vertical axis shows the sum of the execution time up to the rank.

2.2 Queue and Job Statistics

Queue structure of System B in SY2017 is shown in Table 3. In System B, users can choose from three types of compute nodes; jobs submitted to queues with “cpu”, “acc”, and “fat” at the end of their queue names are submitted to CPU, ACC, and Fat nodes, respectively. 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.

To prevent overuse of the storage, points are charged also for usage of disk quota in the three systems, as shown in Table 4. Disk points are revised often for optimal usage of the resources by examining usage tendencies each year.

Although we do not mention here in detail, to promote utilization of the massively parallel supercomputer, background queues (“B4cpu”, “B36cpu”, “B144cpu”, “B18acc”, “B72acc”, and “B2fat”) which charge no points for the jobs have also been open in System B.

The number of jobs, average waiting time, and total execution time in each queue are shown in Table 5. In System B, a large portion of jobs have been executed

Table 3: Queue structures in SY 2017

System–B

queue name	Elapsed time limit (hr)	# of nodes /job	# of nodes /queue	Memory limit (GB)	job points /(node·day)
F4cpu	24	1–4	216	120/node	1
L4cpu	120	1–4	108	120/node	1
F36cpu	24	5–36	288	120/node	1
L36cpu	120	5–36	144	120/node	1
F144cpu	24	37–144	1008	120/node	1
L144cpu	120	37–144	144	120/node	1
i18cpu	0.5	1–18	72	120/node	1
F18acc	24	1–18	180 (108)*	120/node	2
L18acc	120	1–18	90 (54)*	120/node	2
F72acc	24	19–72	72 (144)*	120/node	2
i9acc	0.5	1–9	36	120/node	2
F2fat	24	1–2	17	1000/node	4
L2 fat	120	1–2	6	1000/node	4
i1fat	0.5	1	2	1000/node	4

* The number of nodes allocated to F18acc, L18acc, and F72acc queues were changed on Sept. 8. The number of allocated nodes before the change are given in parentheses.

in "F" queues. The largest amount of the execution time has been consumed in the large-scale "F144cpu" queue, but 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. The acc queues have relatively short waiting times, but we expect that to change as more users get accustomed to using GPGPUs.

2.3 Project for advancement of software usability in materials science

From SY 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 2017, two projects are selected as listed in Table 6.

Table 4: Disk points of System B

		point/day
System B	`/home`	$0.001 \times \theta(q-300)$
	`/work`	$0.0001 \times \theta(q-3000)$

* 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 5: Number of jobs, average waiting time, total execution time, and average number of used nodes per job in each queue.

System-B

queue	# of Jobs	Waiting Time (hour)	Exec. Time ($\times 10^3$ node·hour)	# of nodes
F4cpu	360588	36.05	1236.11	1.32
L4cpu	6087	38.66	508.93	1.76
F36cpu	25506	22.53	1425.45	12.86
L36cpu	972	91.16	731.55	16.33
F144cpu	11664	23.43	6963.52	85.27
L144cpu	176	154.74	883.50	118.64
i18cpu	82805	0.62	157.06	9.58
F18acc	39002	9.88	568.23	2.13
L18acc	2316	12.41	246.15	2.86
F72acc	1556	14.93	460.21	50.02
i9acc	8193	0.34	6.50	3.56
F2fat	7590	22.80	72.43	1.32
L2fat	546	46.75	21.91	1.20
i1fat	5238	0.19	0.85	1.00

2.4 GPGPU Support Service

As noted in Sec. 1.1, ACC nodes with graphics processing units (GPU) were introduced in System B in SY 2015. Since GPUs were introduced in the ISSP Supercomputer center for the first time, many programs developed or utilized by users of this center have not been implemented for GPU computing. To help users take advantage of GPUs, the supercomputer center has started a service for porting users' materials science software to General Purpose GPUs (GPGPU). After a call for proposals (which will usually be in December), target programs for the next school year are selected by the Steering Committee of SCC. The porting service is carried out on each program for about two months; the coding is performed by engineers from the computer vender suppling the ISSP supercomputer system, and ISSP staff oversee the progress of the project and manage necessary commu-

Table 6: List of Project for advancement of software usability in materials science for SY 2017.

Software	Project Proposer
Advancement of first-principles program based on dynamical mean-field theory for correlated electrons	Hiroshi Shinaoka Saitama University
Development of quantum lattice model simulator for integrating theoretical, experimental and data science approaches	Youhei Yamaji The University of Tokyo

Table 7: List of supported software and project proposers for the GPGPU support service for SY 2017.

Software	Project Proposer
Acceleration of large-scale coarse-grained molecular dynamics simulation by GPGPU and its application to polymers	Yuji Higuchi Tohoku University
GPGPU implementation of Fluid Particle Dynamics (FPD) method (RS-CPMD)	Kohei Takae The University of Tokyo
Implementation of GPGPU computing in full diagonalization for HΦ	Takahiro Misawa The University of Tokyo

nications with the proposer. Copyrights of the resulting software basically belong to the proposers, but the supported contents might be published under agreement with the proposer. In SY 2017, three projects are selected as listed in Table 7.

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.