1 OUTLINE

1.1 Supercomputer System

In SY2018, the ISSP supercomputer center provided users with System B - SGI ICE XA/UV hybrid system and System C - HPE SGI 8600 system. System B 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. SY2018 was the fourth 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. System C entered official operation in April, 2018. SY2018 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 were calls for six classes of research projects in SY 2018. The number of projects

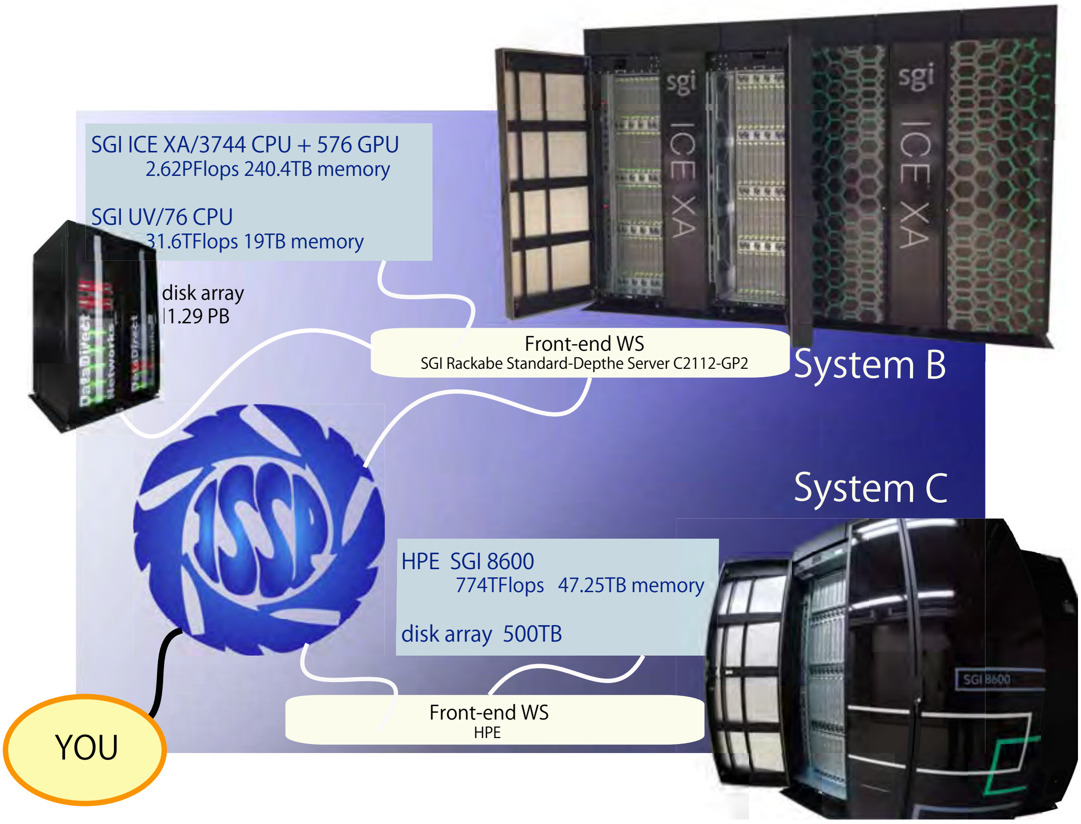


Figure 1: Supercomputer System at the SCC-ISSP

and the total number of points that were applied for and approved in this school year are listed in Table 1.

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. Computational resources have 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 2018 were as follows:

Table 1: Classes of research projects in SY 2018

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	20	2.0k	1.0k	2.0k	1.0k
B	1k	500	twice a year	70	64.2k	3.5k	42.6k	2.9k
C	10k	2.5k	twice a year	168	1,395.3k	77.2k	620.0k	62.0k
D	10k	2.5k	any time	8	42.3k	3.0k	30.0k	2.5k
E	30k	2.5k	twice a year	17	490.0k	46.0k	279.5k	39.8k
S	–	–	twice a year	0	0	0	0	0
SCCMS				25	235.5k	19.1k	235.5k	19.1k
Total				308	2229.3k	149.7k	1209.6k	127.28k

- 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.

Steering Committee of the MDCL

HIROI, Zenji	ISSP (Chair person)
KAWASHIMA, Naoki	ISSP
OZAKI, Taisuke	ISSP
NOGUCHI, Hiroshi	ISSP
UWATOKO, Yoshiya	ISSP
MORI, Hatsumi	ISSP
SUGINO, Osamu	ISSP
TOHYAMA, Takami	Tokyo Univ. of Sci.
ONO, Tomoya	Univ. of Tsukuba
YAMAURA, Jun-ichi	Tokyo Tech.
TAKAHASHI, Hiroki	Nihon Univ.
YOSHIMOTO, Yoshihide	Univ. of Tokyo
TAKEDA Mahoto	Yokohama Natl. Univ.
KIMURA, Kaoru	Univ. of Tokyo
SUZUKI, Takafumi	Univ. of Hyogo

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
KONDO, Takeshi	ISSP
KASAMATSU, Shusuke	ISSP
WATANABE, Hiroshi	ISSP
MORITA, Satoshi	ISSP
HIGUCHI, Yuji	ISSP
NAKAJIMA, Kengo	Univ. of Tokyo
TSUNEYUKI, Shinji	Univ. of Tokyo
HATANO, Naomichi	Univ. of Tokyo
MOTOME, Yukitoshi	Univ. of Tokyo
ONO, Tomoya	Univ. of Tsukuba
TOHYAMA, Takami	Tokyo Univ. of Sci.
YOSHINO, Hajime	Osaka Univ.
SUZUKI, Takafumi	Univ. of Hyogo
YOSHIMOTO, Yoshihide	Univ. of Tokyo
OKUMURA, Hisashi	NINS-RSCS
HOSHI, Takeo	Tottori Univ.
YATA, Hiroyuki	ISSP
FUKUDA, Takaki	ISSP

Supercomputer Project Advisory Committee

KAWASHIMA, Naoki	ISSP (Chair person)
NOGUCHI, Hiroshi	ISSP
SUGINO, Osamu	ISSP
OZAKI, Taisuke	ISSP
TSUNETSUGU, Hirokazu	ISSP
KATO, Takeo	ISSP
KONDO, Takeshi	ISSP
KASAMATSU, Shusuke	ISSP
HIGUCHI, Yujihi	ISSP
WATANABE, Hiroshi	ISSP
MORITA, Satoshi	ISSP
NAKAJIMA, Kengo	Univ. of Tokyo
TSUNEYUKI, Shinji	Univ. of Tokyo
IMADA, Masatoshi	Univ. of Tokyo
HATANO, Naomichi	Univ. of Tokyo
SUZUKI, Takafumi	Univ. of Hyogo
YOSHIMOTO, Yoshihide	Univ. of Tokyo
OKUMURA, Hisashi	NINS-RSCS
HOSHI, Takeo	Tottori Univ.
ONO, Tomoya	Univ. of Tsukuba
YOSHINO, Hajime	Osaka Univ.
MOTOME, Yukitoshi	Univ. of Tokyo
TOHYAMA, Takami	Tokyo Univ. of Sci.
KITAO, Akio	Tokyo Tech.
ARITA, Ryotaro	RIKEN-CEMS
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
OKAMOTO, Yuko	Nagoya Univ.
HUKUSHIMA, Koji	Univ. of Tokyo
NEMOTO, Koji	Hokkaido Univ.
YABANA, Kazuhiro	Univ. of Tsukuba
HIDA, Kazuo	Saitama Univ.
WATANABE, Kazuyuki	Tokyo Univ. of Sci.
FURUKAWA, Nobuo	Aoyama Gakuin Univ.
KUROKI, Kazuhiko	Osaka Univ.
TAKANO, Hiroshi	Keio Univ.
YASUOKA, Kenji	Keio Univ.
TANAKA, Yukio	Nagoya Univ.
MASUBUCHI, Yuichi	Nagoya Univ.
KAWAMURA, Hikaru	Osaka Univ.
KUSAKABE, Koichi	Osaka Univ.
SHIRAI, Koun	Osaka Univ.
SAKAI, Toru	JAEA
ISHIBASHI, Shoji	AIST
OTANI, Minoru	AIST
TOMITA, Yusuke	Shibaura Inst. Tech.
MIYASHITA, Seiji	Univ. of Tokyo
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.
TADA, Tomofumi	Tokyo Tech.
TODO, Synge	Univ. of Tokyo

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
WATANABE, Hiroshi	Research Associate
KASAMATSU, Shusuke	Research Associate
HIGUCHI, Yuji	Research Associate

MORITA, Satoshi	Research Associate
YATA, Hiroyuki	Technical Associate
FUKUDA, Takaki	Technical Associate
ARAKI, Shigeyuki	Technical Associate

2 STATISTICS (SCHOOL YEAR 2018)

2.1 System and User Statistics

In the following, we present statistics for operation time taken in the period from April 2018 to March 2019 (SY 2018). In Table 2, we show general statistics of the supercomputer system in SY 2018. The total numbers of compute nodes in System B and System C are 1891 and 252, respectively. Consumed disk points amount to about 3% of the total consumed points in System B.

In the left column of Fig. 2, availabilities, utilization rates, and consumed points in Systems B and C are plotted for each month. Throughout the school year, the utilization rates were very high, while the availability was reduced in August and September due to the OS update of System B and a lightning strike.

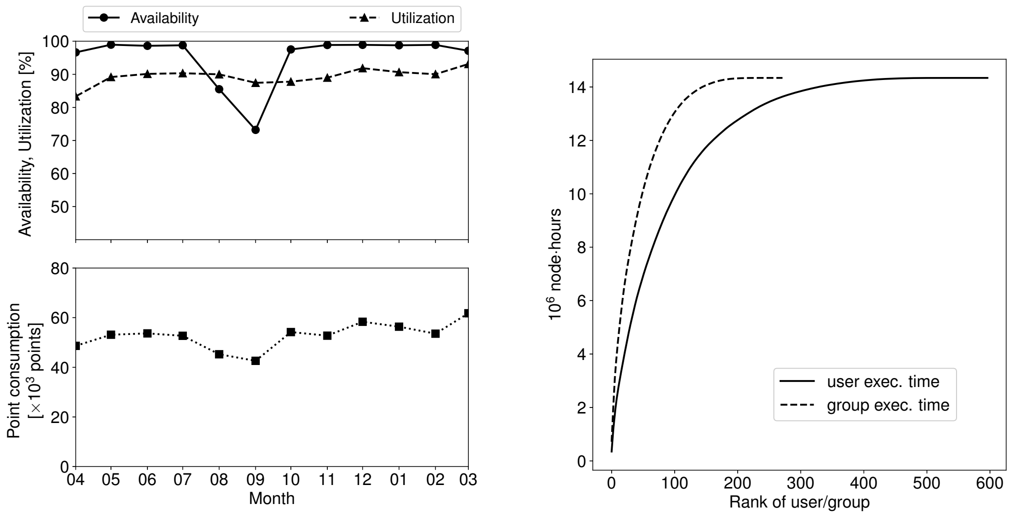
The user statistics are shown in the right column of Fig. 2. The horizontal axis shows the rank of the user/group arranged in the descending order of the execution time (hour×nodes). The execution time of the user/group of the first rank is the longest. The vertical axis shows the sum of the execution time up to the rank. From the saturation points of the graphs, the numbers of “active” users of Systems B and C are around 300 and 70, 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 SY2018 are 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, while only CPU nodes are available in System C. 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

System B



System C

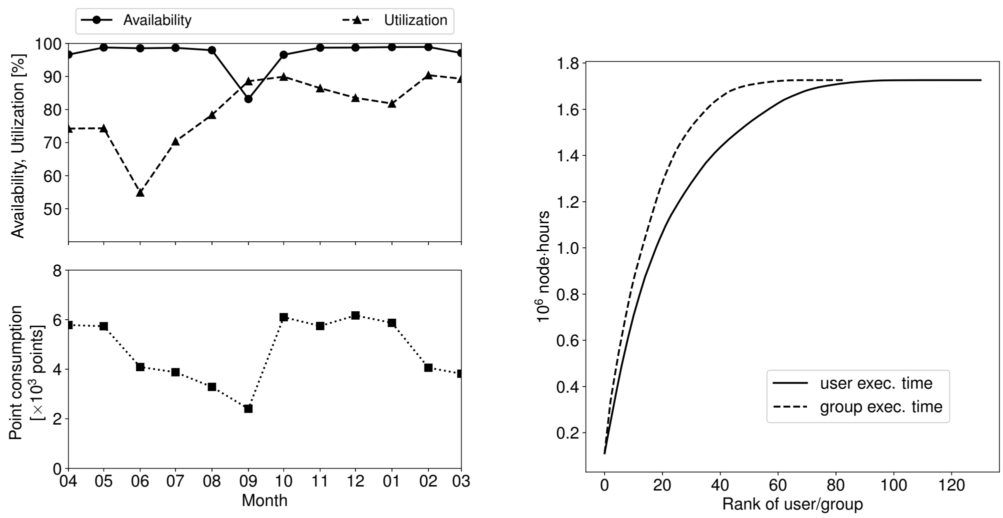


Figure 2: Left: Availabilities, utilization rates and point consumptions of each month during SY 2018. Right: User statistics. The horizontal axis shows the rank of the user/group arranged in the descending order of the execution time (hour×nodes). The vertical axis shows the sum of the execution time up to the rank.

Table 2: Overall statistics of SY 2018

	System B	System C
total service time ($\times 10^3$ node·hours)	16037	2157
number of executed jobs	728794	105
total consumed points ($\times 10^3$ point)	655	58
CPU points ($\times 10^3$ point)	633	57
disk points ($\times 10^3$ point)	22	1
total exec. time ($\times 10^3$ node·hours)	14339	1726
availability	95.14%	96.90%
utilization rate	89.40%	80.20%

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 for system B ("B4cpu", "B36cpu", "B144cpu", "B18acc", "B72acc", and "B2fat") and background queues for system C ("B4cpu", "B9cpu", "B36cpu") which charge no points for the jobs have also been open.

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 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.

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 2018, two projects were selected as listed in Table 6.

2.4 GPGPU Support Service

As noted in Sec. 1.1, ACC nodes with graphics processing units (GPU) were introduced in System B in School Year 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 programmed 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 vendor supplying the ISSP supercomputer system, and ISSP staff oversee the progress of the project and manage necessary communications 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 2018, two 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.

Table 3: Queue structures in SY 2018

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	120/node	2
L18acc	120	1–18	90	120/node	2
F72acc	24	19–72	72	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

System–C

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 4: Disk points of Systems B and C

		point/day
System B	`/home`	$0.001 \times \theta(q - 300)$
	`/work`	$0.0001 \times \theta(q - 3000)$
System C	`/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 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	235752	7.08	1153.21	1.33
L4cpu	12538	24.93	589.27	1.61
F36cpu	21578	21.71	1366.82	11.85
L36cpu	1622	73.67	765.61	14.04
F144cpu	12275	40.80	7052.94	84.86
L144cpu	374	174.22	886.26	92.21
i18cpu	74462	0.27	110.91	8.59
F18acc	34273	6.86	645.79	2.39
L18acc	5531	22.21	535.15	2.89
F72acc	2410	40.30	246.63	64.47
i9acc	8691	0.16	6.62	5.13
F2fat	7435	23.64	79.66	1.24
L2fat	813	27.46	29.55	1.33
i1fat	4903	1.67	1.01	1.00

System-C

queue	# of Jobs	Waiting Time (hour)	Exec. Time ($\times 10^3$ node·hour)	# of nodes
F4cpu	60204	3.18	246.69	1.29
L4cpu	3992	7.17	69.96	1.29
i4cpu	19973	0.05	8.63	3.54
F9cpu	3047	26.47	123.88	7.11
L9cpu	147	31.26	46.35	7.12
F36cpu	3181	22.60	749.15	26.65
L36cpu	129	34.80	122.54	28.60

Table 6: List of Project for advancement of software usability in materials science for SY 2018.

Project Proposer	Project Name
Kazuma Nakamura Kyushu Institute of Technology	Development of first-principles electronic-structure calculation software by combining effective-model derivation code (RESPACK) and model-analysis codes (HΦ/mVMC)
Masaki Akiko RIKEN	Development of a quantum Monte Carlo Solver -DSQSS- implementing nontrivial parallelization

Table 7: List of supported software and project proposers for the GPGPU support service for SY 2018.

Project Proposer	Project Name
Hiromi Nakai Waseda Univ.	Acceleration of divide-and-conquer based density-functional tight-binding molecular dynamics method by using GPGPU
Kazuyoshi Yoshimi ISSP	GPU acceleration of matrix-vector product operations in quantum lattice model solver HΦ