1 Outline

1.1 Supercomputer System

In SY2016, the ISSP supercomputer center provided users with two types of systems:

System B - SGI ICE XA/UV hybrid system 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.

System C - FUJITSU PRIMEHPC FX10 has been in service since April, 2013. It is highly compatible with K computer in Kobe. System C consists of 384 nodes, and each node has 1 SPARC64TM IXfx CPU (16 cores) and 32 GB of memory. The total system achieves 90.8 TFlops theoretical peak performance.

SY2016 was the second year of the operation of the current System B and the last year of 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.

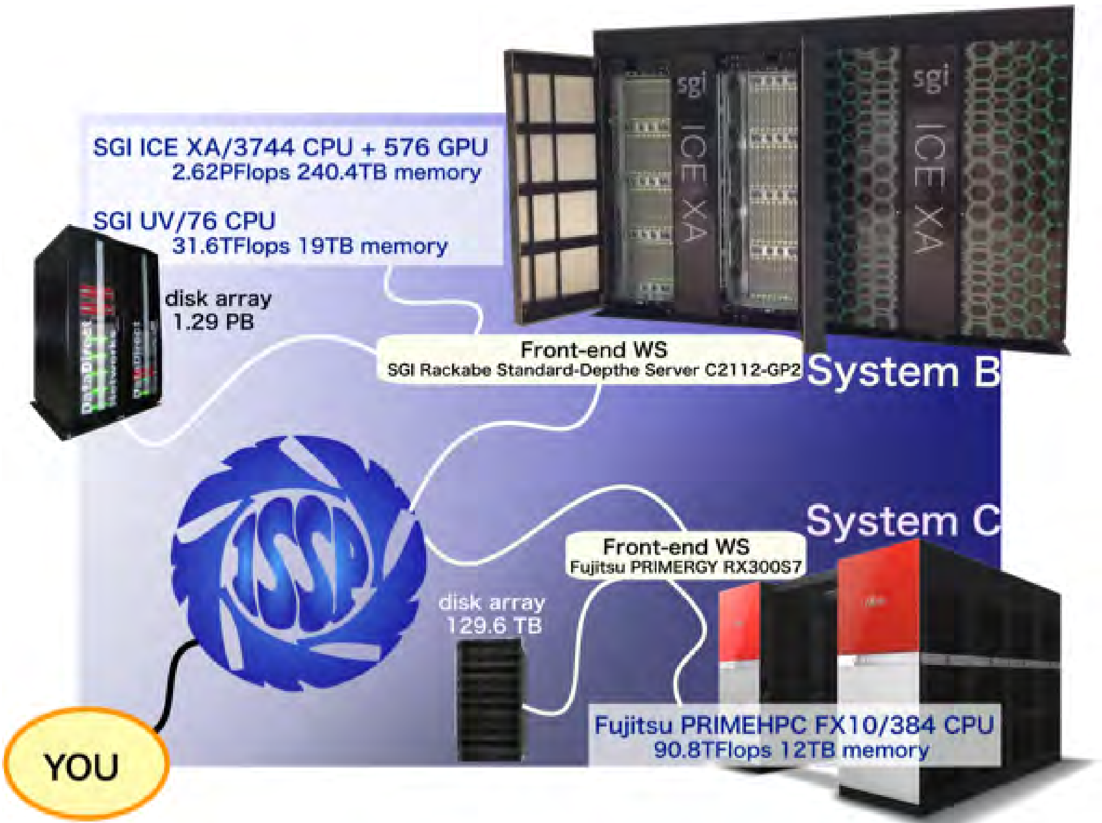


Figure 1: Supercomputer System at the SCC-ISSP

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 2016. 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.

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

Table 1: Classes of research projects in SY 2016

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	9	0.9k	0.9k	0.9k	0.9k
B	1k	500	twice a year	50	41.7k	8.2k	29.1k	7.2k
C	10k	2.5k	twice a year	166	1387.8k	164.7k	679k	126.7k
D	10k	2.5k	any time	7	59k	5k	33.3k	3k
E	30k	2.5k	twice a year	12	350k	30k	219.5k	26.5k
S	–	–	twice a year	0	0	0	0	0
SCCMS				32	218.9k	103.5k	218.9k	103.5k
Total				276	2058.3k	312.3k	1180.7k	267.8k

- 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 SY 2016 were as follows:

Steering Committee of the MDCL

HIROI, Zenji	ISSP (Chair person)
KATO, Takeo	ISSP
KAWASHIMA, Naoki	ISSP
MORI, Hatsumi	ISSP
NAKATSUJI, Satoru	ISSP
NOGUCHI, Hiroshi	ISSP
SUGINO, Osamu	ISSP
KIMURA, Kaoru	Univ. of Tokyo
YOSHIMOTO, Yoshihide	Univ. of Tokyo
SAWA, Hiroshi	Nagoya Univ.
KAGEYAMA, Hiroshi	Kyoto Univ.
MORIKAWA, Yoshitada	Osaka Univ.
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
SUGINO, Osamu	ISSP
TSUNETSUGU, Hirokazu	ISSP
KATO, Takeo	ISSP
MASUDA, Takatsugu	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
MOHRI, Tetsuo	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
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.
MOHRI, Tetsuo	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.
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.
OKAMOTO, Yuko	Nagoya Univ.
SHIRAISHI, Kenji	Nagoya Univ.
TANAKA, Yukio	Nagoya Univ.
KAWAKAMI, Norio	Kyoto Univ.
KAWAMURA, Hikaru	Osaka Univ.
KUROKI, Kazuhiko	Osaka Univ.
KUSAKABE, Koichi	Osaka Univ.
MORIKAWA, Yoshitada	Osaka Univ.
OGUCHI, Tamio	Osaka Univ.
SHIRAI, Koun	Osaka Univ.
YOSHIDA, Hiroshi	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
SUGINO, Osamu	Associate Professor
WATANABE, Hiroshi	Research Associate

KASAMATSU, Shusuke	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 2016)

2.1 System and User Statistics

In the following, we present statistics for operation time taken in the period from April 2016 to March 2017 (SY 2016). In Table 2, we show general statistics of the supercomputer system in SY 2016. The total number of compute nodes in System B, and C is 1891 and 384 respectively. Consumed disk points amount to about 2% and 3% of the total consumed points in System B and C respectively. Roughly 20% of the total points in System B and 40% of that in System C 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 each system are plotted for each month. Throughout the school year, the utilization rates were very high. Especially in System B, they were 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 each system is around 250, and 60 for System B and C 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 System B and C in SY 2016 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. 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

Table 2: Overall statistics of SY 2016

	System-B	System-C
total service time ($\times 10^3$ node·hours)	16035	3327.0
number of executed jobs	397032	19461
total consumed points ($\times 10^3$ point)	642.2	82.4
CPU points ($\times 10^3$ point)	630.8	79.6
disk points ($\times 10^3$ point)	11.3	2.8
total exec. time ($\times 10^3$ node·hours)	14598.4	1860.3
availability	97.2%	97.3%
utilization rate	91.0%	57.5%

30 minutes. The number following "F", "L", or "i" correspond to the number of nodes that can be used by one user job.

In System C, the "F" and "L" queues are set up similarly to System B. In addition, a debug queue is set up for short debugging jobs utilizing 1 to 4 CPUs, and an interactive queue that can use 1 to 4 CPUs is also available.

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.

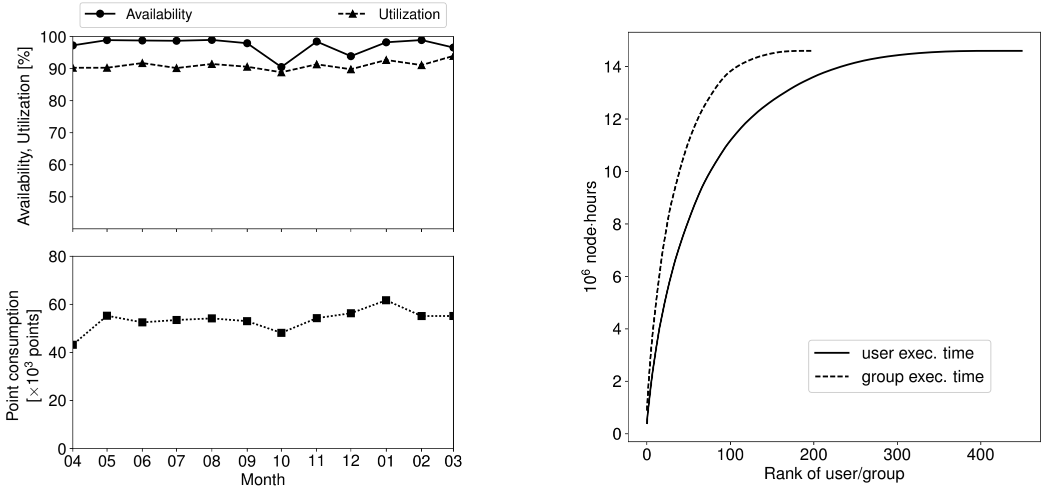
Although we do not mention here in detail, to promote utilization of the massively parallel supercomputer, background queues ("B4cpu", "B36cpu", "B144cpu", "B18acc", "B72acc", and "B2fat") which charge no points for the jobs have also been open in System B.

The number of jobs, average waiting time, and total execution time in each queue are shown in Table 5. In both System 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 "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 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

System B



System C

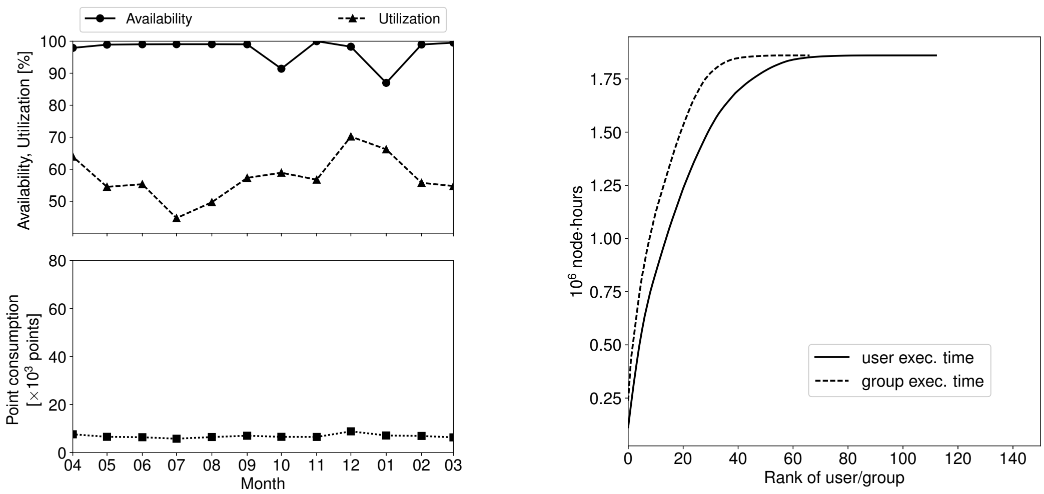


Figure 2: Left: Availabilities, utilization rates and point consumptions of each month during SY 2016. Right: User statistics. The horizontal axis shows the rank of the user/group arranged in the descending order of the execution time (hour×nodes). The vertical axis shows the sum of the execution time up to the rank.

Table 3: Queue structures in SY 2016

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	108	120/node	2
L18acc	120	1–18	54	120/node	2
F72acc	24	19–72	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

System–C

queue name	Elapsed time limit (hr)	# of nodes /Job	# of nodes /queue	job points /(node·day)
debug	0.5	1-4	24	1
interactive	0.5	1-4	24	1
F12	24	2-12	60	1
F96	24	2-12	288	1
L12	120	24-96	24	1
L96	120	24-96	192	1

* The available memory size is limited to 28 GB per one CPU.

Table 4: Disk points of System B and C

		point/day
System B	`/home`	$0.001 \times \theta(q-300)$
	`/work`	$0.0001 \times \theta(q-3000)$
System C	`/home`	$0.05 \times \theta(q-10)$
	`/work`	$0.005 \times \theta(q-100)$

* 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	179051	33.32	1227.13	1.59
L4cpu	8018	44.28	541.52	1.91
F36cpu	21986	24.71	1424.16	13.63
L36cpu	1266	79.09	770.36	16.49
F144cpu	11256	28.61	7040.09	87.93
L144cpu	273	170.56	951.20	112.62
i18cpu	55870	0.60	104.88	8.98
F18acc	36569	9.20	499.59	1.80
L18acc	2616	11.09	174.25	1.78
F72acc	2034	30.72	712.90	51.96
i9acc	8346	0.15	3.49	3.41
F2fat	6539	35.34	76.03	1.05
L2fat	394	25.49	23.76	1.24
i1fat	4943	0.09	0.82	1.00

System-C

queue	# of Jobs	Waiting Time (hour)	Exec. Time ($\times 10^3$ node·hour)	# of nodes
F12	8628	2.43	266.62	5.71
L12	181	18.74	40.39	8.35
F96	4677	7.64	1399.77	42.67
L96	78	31.00	141.65	63.58
debug	4826	0.07	2.74	3.22
interactive	705	0.00	0.18	1.62

Table 6: List of Project for advancement of software usability in materials science for SY 2016.

Software	Project Proposer
Novel numerical solvers for large-scale material computations with shifted Krylov-subspace theory	Takeo Hoshi Tottori University
Development of open-source software for many-variable variational Monte Carlo method	Takahiro Misawa The University of Tokyo

of SCC. The projects are carried out by the software development team composed of three members in ISSP. In SY 2016, two projects are 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 vender suppling 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 2016, 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.

Table 7: List of supported software and project proposers for the GPGPU support service for SY 2016.

Software	Project Proposer
Acceleration of molecular dynamics calculation codes based on fast multipole method by GPGPU	Yoshimichi Andoh Nagoya University
GPU Implementation of Car-Parrinello Molecular Dynamics using Real-space DFT (RS-CPMD)	Yasuteru Shigeta University of Tsukuba
GPGPU implementation of many-variable variational Monte Carlo method	Takahiro Misawa The University of Tokyo