December 28th, 2018

Call for proposals in FY2019

Multidisciplinary Cooperative Research Program (MCRP-2019)

Center for Computational Sciences (CCS), University of Tsukuba, is operating the following supercomputers.

- Oakforest-PACS (OFP): 25 PFLOPS. Supercomputer with many-core processors (Knights Landing architecture), operated under collaboration between University of Tokyo and University of Tsukuba, since April 2017. In the following, this is called "OFP".
- Cygnus: 2.4 PFLOPS (double precision floating-point operation). Supercomputer equipped with GPU (NVIDIA V100) and FPGA (Intel Stratix10). It has high-performance operation nodes of 30 TFLOPS per node, and is planned to start operation from May 2019.

CCS provides about 30 % of the resources of OFP owned by University of Tsukuba (about 10 % of the total resources), and 50 % of the total resources of Cygnus to this program, MCRP-2019.

Schedule

Application period:	January 5, 2019 ~ February 3, 2019 (24:00 JST)
	Member registration is open till February 7, 2019 (24:00 JST).
Notice of selection:	March 22, 2019
Period of usage:	April 1st, 2019 ~ March 31st, 2020
Progress/Interim presentation:	Autumn, 2019
Submission of progress report:	April, 2020

1 Multidisciplinary Cooperative Research Program

The Multidisciplinary Cooperative Research Program (MCRP) in Center for Computational Sciences (CCS) calls proposals for innovative research projects that require large-scale computation, projects promoting cooperation among different fields, and projects performed under collaboration with staff members in CCS. For FY2019, we call proposals in the following research fields: Science (Particle physics, Astrophysics, Nuclear physics, Material Science, Life science, Environmental science, Biology, Chemistry) and Computer science (High-performance computing systems, Computational informatics, Numerical analysis).

2 Report meeting

It is compulsory for approved projects to report at the following meetings:

Interim report meeting: Autumn, 2019

Progress report meeting: Autumn 2020

These will be held together with CCS International symposium “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”.

3 Fee

The computer usage in the Multidisciplinary Cooperative Research Program (MCRP) is free of charge.

4 Available computational resources and scales

4.1 Oakforest-PACS (OFP)

Oakforest-PACS (OFP) is a massively parallel many-core architecture cluster operated by Joint Center for Advanced High Performance Computing (JCAHPC) which is cooperated by University of Tsukuba and University of Tokyo. While OFP is shared by these two universities, Center for Computational Sciences, University of Tsukuba provides about 10% of the total resources of OFP to the MCRP.

System summary and hardware specifications of OFP can be found at
URL: https://www.ccs.tsukuba.ac.jp/eng/supercomputers/

To know how to use OFP in details, a users' guide will be provided after the approval of the project.

4.2.1 Accessibility of MCRP users

A unit of usage for OFP is a computation node, thus, only a single job can run on each node without job mixing with other jobs. In other words, each job occupies all the resources in the allocated nodes. The parallel computing with MPI is recommended for use of more than one node. It is possible to simultaneously perform many tasks, each of which runs in a single node. Consumption of the allocated budget is calculated in terms of the number of utilized nodes and computation time (wall clock).

In each project, the maximum number of nodes per job and the total computational time (node*hour) are determined with the MCRP proposals reviewed by the Cooperative Research Committee. There is also a restriction in capacity of the file system. Although the usage period ends at March, users' login and access to the file system are allowed till the end of April. Every user must download all the files during this one month, after that, all the files of finished projects will be deleted.

4.2.2 Available computational resources

Hereafter, the scale of performing parallel jobs is called "parallel environment (PE)". According to the category of application (L/M/S), we set a different maximum number of nodes used for calculations. At maximum, the PE with 2,048 nodes is available. The present MCRP calls for projects of 7,000,000 nodes*hours in total in fiscal year 2019 (2019.4 – 2020.3). OFP can perform large-scale calculations with up to 8,208 nodes which are, however, not treated in the MCRP.

4.2.3 Computation time

The maximum time duration of each job is 24 hours, irrespective of the number of nodes used. It is not the CPU time (user time), but the wall clock time (elapsed time) including synchronization and communication time, time necessary for file access, etc.

The computation time (node*hour product) allocated for each project is called "budget". When a job finishes, the used node*hour product is subtracted from the budget of the project. When the budget vanishes, no more job is allowed to be submitted. The project budget is shared by the users belonging to the project, thus, the budget decreases after the usage of any user of the project. If the submitted job is interrupted due to important system failure, the amount of consumed budget is returned to the project budget.

It is possible to submit a job using nodes more than the maximum allowance in the category MCRP-M and MCRP-S (up to 2,048). In such cases, the budget is consumed double for the usage beyond the limitation. For instance, a project with the maximum 256 nodes consumed 2,560 node*hours for a 10-hour job using 256 nodes, while if it uses 512 nodes for 5 hours, it consumes [256+(512-256) x 2] x 5=3,840 node*hours.

4.2.4 Disk allocation

Standard allocation of the storage disk for each project is 20 TB. If the project needs larger

capacity of storage due to special requirements of the project, the applicants should describe the size and reason on the proposal. The renewal project from the last year is able to use the same disk capacity as the previous year. In this case, the applicant must describe on the proposal that the oversized disk usage has been approved. The storage size is determined by evaluation of the Cooperative Research Committee and may be reduced from the requested size.

4.2 Cygnus

Cygnus is a supercomputer equipped with GPU and FPGA in a single node, operated by Center for Computational Sciences, University of Tsukuba. Center for Computational Sciences provides about 50% of the total resources of Cygnus to the MCRP.

System summary and hardware specifications of Cygnus can be found at
URL: https://www.ccs.tsukuba.ac.jp/eng/supercomputers/#Cygnus
To know how to use Cygnus in details, a users' guide will be provided after the approval of the project.

4.2.1 Accessibility of MCRP users

A unit of usage for Cygnus is a computation node, thus, only a single job can run on each node without job mixing with other jobs. In other words, each job occupies all the resources in the allocated nodes. The parallel computing with MPI is recommended for use of more than one node. It is possible to simultaneously perform many tasks, each of which runs in a single node. Consumption of the allocated budget is calculated in terms of the number of utilized nodes and computation time (wall clock).

In each project, the maximum number of nodes per job and the total computational time (node*hour) are determined with the MCRP proposals reviewed by the Cooperative Research Committee. There is also a restriction in capacity of the file system. Although the usage period ends at March, users' login and access to the file system are allowed till the end of April. Every user must download all the files during this one month, after that, all the files of finished projects will be deleted.

4.2.2 Available computational resources

According to the category of application (L/M/S), we set a different maximum number of nodes used for calculations. At maximum, the PE with 32 nodes is available. The present MCRP calls for projects of 320,000 nodes*hours in total in fiscal year 2019 (2019.4 – 2020.3). Cygnus has 80 nodes, and each node has both CPU and GPU. 32 nodes among these 80 nodes are equipped with FPGA. Project proposals utilizing the FPGA are called in another category (FPGA).

4.2.3 Computation time

The maximum time duration of each job is 24 hours, irrespective of the number of nodes used. It is not the CPU time (user time), but the wall clock time (elapsed time) including synchronization and communication time, time necessary for file access, etc.

The computation time (node*hour product) allocated for each project is called "budget". When a

job finishes, the used node*hour product is subtracted from the budget of the project. When the budget vanishes, no more job is allowed to be submitted. The project budget is shared by the users belonging to the project, thus, the budget decreases after the usage of any user of the project. If the submitted job is interrupted due to important system failure, the amount of consumed budget is returned to the project budget.

4.2.4 Disk allocation

Standard allocation of the storage disk for each project is 15 TB. If the project needs larger capacity of storage due to special requirements of the project, the applicants should describe the size and reason on the proposal. The storage size is determined by evaluation of the Cooperative Research Committee and may be reduced from the requested size.

4.2.5 Usage of Cygnus-FPGA part

Projects utilizing the FPGA part of Cygnus must be performed in collaboration with Division of High Performance Computing Systems (HPCS) in Center for Computational Sciences, University of Tsukuba. This collaborative research must include, at least, one faculty staff of Division of HPCS as either the project leader or the project members. The project leader needs to have a close consultation with the faculty staff and to indicate his/her roles on the proposal.

5 Requirements of application and usage

5.1 Qualification of application

Project leaders (representatives) must correspond to one of the following:

1. Employees, students (including auditor students, Research Students, Exchange Students, Exchange Research Students), researchers, joint research fellows of University of Tsukuba.
2. Teaching staff and students affiliated in universities in Japan (including graduate universities and junior colleges), technical colleges, and universities in the following countries listed below[*1)].
3. Researchers who belong to institutes aiming at academic researches and promotion operated by national and local governments (including those in the following countries listed below[1)]).
4. Persons who are exceptionally approved by Director of Center for Computational Sciences.

5.2 Qualification of usage of computers

In addition to those of 1. to 4. in section 5.1, researchers in industries are able to be a member of the MCRP project under the condition that the achievements must be open to the public. The project leaders must take a firm promise of publishing the results from the industrial researchers if they include them as project members.

Researchers affiliated in institutes in the following countries[*1)] are approved for the usage after prescribed procedure. The procedure will be given by the Cooperative Operational Committee.

*1) Countries eligible for application and usage

Argentina, Australia, Austria, Belgium, Bulgaria, Canada, Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Republic of Korea, Luxembourg, Netherlands, New Zealand, Norway, Poland, Portugal, Spain, Sweden, Switzerland, United Kingdom of Great Britain and Northern Ireland, and United States of America

(NB: According to the export regulation "Export Trade Control Order", we have to restrict the users' affiliations to institutes in the listed countries only.)

5.3 Applicants through HPCI

OFP and Cygnus can be utilized through applications to HPCI. Center for Computational Sciences, University of Tsukuba is aiming at efficient supply of resources. In this respect, we might give some incentive to projects applying for both MCRP and HPCI, such as additional allocation of budget, under the condition that the project leader of MCRP is either a representative or vice representative of the HPCI application for the usage of OFP and/or Cygnus.

The application procedure through HPCI can be found at
URL: http://www.hpci-office.jp

6 Application

6.1 Call for proposals, period of submission and project

The online submission opens on January 5, 2019 and closes at 24:00 on February 3, 2019. The announcement of the selection and the awards is scheduled to be given by March 22, 2019. The project period is from April 1, 2019 to March 31, 2020.

6.2 Categories and forms of application

There are three categories of application of projects for OFP and those utilizing only the GPU part of Cygnus (Cygnus-GPU), according to the project size (L/M/S). The product run must be a main aim of the project for the case of MCRP-L, while the program development can be the main aim for MCRP-M/S. Projects using both OFP and Cygnus-GPU should write both contents in a single form, thus, do not need to submit two proposals. The product run must be a main aim of the project for the case of MCRP-L. A project using the FPGA part of Cygnus (Cygnus-FPGA) should be submitted as an individual proposal. The proposals of Cygnus-FPGA should be written in a form of "MCRP-FPGA", since they are performed as "Cooperative Research Program" with Center for Computational Sciences, University of Tsukuba.

(1) MCRP-L (Large), Language of proposals: English only
OFP: The maximum node-hour product: 1,000,000
The maximum number of nodes: 2,048
Cygnus: The maximum node-hour product: 100,000
The maximum number of nodes: 78

(2) MCRP-M (Medium), Language of proposals: English or Japanese
OFP: The maximum node-hour product: 300,000
The maximum number of nodes: 1,024

Cygnus: The maximum node-hour product: 50,000
The maximum number of nodes: 32

(3) MCRP-S (Small), Language of proposals: English or Japanese
OFP: The maximum node-hour product: 50,000
The maximum number of nodes: 1,024
Cygnus: The maximum node-hour product: 5,000
The maximum number of nodes: 16

(4) MCRP-FPGA (Cygnus-FPGA) , Language of proposals: English or Japanese
Cygnus: The maximum node-hour product: 10,000
The maximum number of nodes: 32

6.3 Project submission

Submission is available only by online. Every applicant must carefully read the guidance of submission. The application form is different according to the categories in section 6.2.

6.4 Notes on application

6.4.1 Restriction on number of applications

Each applicant can submit only one proposal as a project leader, while he/she can be members of other projects. The maximum number of the projects he/she belongs to is three. It is possible to use both OFP and Cygnus in one project. Projects using the FPGA part in Cygnus are treated separately, thus, they are not counted for this limitation.

6.4.2 Special notice

Project proposals to MCRP-L which are not approved may be reviewed and awarded smaller resources in the category of MCRP-M/S. Although the maximum number of nodes in MCRP-M/S is 1,024, we allow applicants to submit the proposal using 2,048 nodes at maximum if the project mainly aims at the code development.

7 Review of project proposals

The Cooperative Research Committee will review the proposals, determine adoption/rejection and allocation of computational resources.

Members of Cooperative Research Committee

Fields	Part	Ast	Nucl	Mat	Life	Env	Bio	Comp
Inside CCS	1	1	1	1	1	1	1	1
Outside CCS	2	2	2	2	2	2	2	2

<Abbreviations>
CCS: Center for Computational Sciences; Part: Particle physics; Ast: Astrophysics; Nucl: Nuclear

physics; Mat: Material Science; Life: Life science, Env: Environmental science; Bio: Biology; Comp: Computer science

Proposals in the category of MCRP-S and MCRP-FPGA will be reviewed only by the committee inside CCS. If needed, we may ask domestic/foreign researchers to review the proposals.

8 Support for travel and workshop

8.1 Travel for the project research and for presentation of the results

In order to perform the project research, the project members are eligible to apply for travel expense to stay in Center for Computational Sciences, University of Tsukuba. In order to present the results obtained in the MCRP, the project members are eligible to apply for domestic/international travel expense. The presentation must contain the acknowledgement for the MCRP of CCS, University of Tsukuba.

8.2 Support for workshops

CCS-hosted workshops/conferences necessary for the project research, the project leaders are eligible to apply for the support from CCS, University of Tsukuba. To host the workshop/conference, the project leaders can apply for the support to invite researchers and hire short-term employee. If the applicant is not affiliated in CCS, a corresponding person in CCS must be assigned.

8.3 Application procedure

In case that the project leaders not affiliated in CCS request the support, they should fill in corresponding forms of application (downloadable from the CCS home page), and send by email as attached files to

Email: project-shien@ccs.tsukuba.ac.jp

at least two months prior to the travel/workshop.

9 Obligations of users

1. Users of the adopted projects must report research results and progress in symposiums hosted by CCS, and must submit an annual report every year. However, the projects, in which there are no members in Japan, may be exempted from the progress report in the symposium.
2. When users publish results obtained in the MCRP in journal articles, conferences, press release, etc., they must mention that the results are achieved with the MCRP of CCS, University of Tsukuba. Examples of the acknowledgement can be found in “How to write acknowledgement” at the following address:

   http://www.ccs.tsukuba.ac.jp/eng/use-computers/acknowledgement

10 Management of users

1. Every user is assigned “group id” for each project and “user id” for each user.
2. For OFP, “group id” and “user id” are provided by CCS. For Cygnus, the project leaders should fill in the desired names for the “group id”. After the necessary adjustment by CCS, the “group id” will be determined. “user id” will be determined on the account registration system by each user.
3. The “user id” for a single user belonging to multiple projects is unique. A user has only one home directory but the work directory is provided for each project.
4. Only the public key authentication is allowed. Every user must register his/her own public key with passphrase on the account registration system.
5. User accounts belonging to terminated projects are active for one month after the termination, but all the remaining files are deleted after two months from the termination. This will be announced to users when the project is terminated.

11 Notes

- There may be accidental incidents to cause corruption and disappearance of users’ programs and data. All the users must prepare for themselves by backing up the files.
- CCS may request users to deliver the source files for a limited purpose, in case that it is necessary (e.g., analysis of cause of system failure).

12 Technical support

Technical support about usage of the computers should be sent to Supporting Committee by email (project-support@ccs.tsukuba.ac.jp).

Administrative Committee for Cooperative Research
Center for Computational Sciences, University of Tsukuba
Tsukuba 305-8577, Japan