December 23, 2022

Call for proposals in FY2023

Multidisciplinary Cooperative Research Program (MCRP-2023)

APPLICATION GUIDELINES

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

- 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 started operation from May 2019.
- Pegasus: 6.1 PFLOPS or more (double precision floating-point operation). 51 TFLOPS or more per node. Supercomputer equipped with GPU (NVIDIA H100) and big memory. It is going to start operation from the beginning of 2023.

Operation of the supercomputer with many-core processors, Oakforest-PACS (OFP), will be terminated in March 2022. In MCRP2023, the simulation nodes group “Odyssey” of Wisteria/BDEC-01 (Wisteria-O) can be used through CCS. Wisteria-O is operated by the Information Technology Center, The University of Tokyo.

CCS provides about 50 % of the total resources of Cygnus, and about 10 % of the total resources of Wisteria-O to this program, MCRP2023.

Schedule

Application period:	December 23, 2022 ~ January 23, 2023 (24:00 JST)
	Member registration is open till January 31, 2022 (24:00 JST).
Notice of selection:	March 23, 2023
Period of usage:	April 1st, 2023 ~ March 31st, 2024
Submission of progress report:	April, 2024
Progress report presentation:	Autumn, 2024

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 FY2023, 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 symposium after the MCRP2023 project :

CCS International symposium “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”

It is normally held in Autumn every year.

3 Fee

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

4 Available computational resources and scales

4.1 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.

4.1.1 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.

4.1.2 Available computational resources

At maximum, 78 nodes are available. The present MCRP calls for projects of 320,000 nodes*hours in total in fiscal year 2023 (2023.4 – 2024.3). Cygnus has 78 nodes, and each node has both CPU and GPU. 32 nodes among these 78 nodes are equipped with FPGA. Project proposals utilizing the FPGA are called in another category (FPGA).

4.1.3 Computation time

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.

It is possible to transfer the budget between Cygnus and Pegasus. Note that the budget value is reduced to 1/2 when the budget is transferred from Cygnus to Pegasus. On the other hand, it increases twice moving from Pegasus to Cygnus. For instance, the budget on Cygnus "10,000", which enables us to utilize Cygnus for 10,000 node-hours, turns into "5,000" on Pegasus, which enables us to utilize Pegasus for 5,000 node-hours, if it is transferred to Pegasus. Conversely, the budget on Pegasus "10,000" is going to be "20,000" on Cygnus when it is transferred to Cygnus.

This transferring ratio may be changed during MCRP2023, in order to maximize usage efficiency of supercomputers, Cygnus and Pegasus.

4.1.4 Disk allocation

Standard allocation of the storage disk for each project differs depending on approved classes, 20 TB (MCRP-L), 10 TB (MCRP-M/MCRP-FPGA), and 5 TB (MCRP-S). 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.

4.1.5 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.

4.2 Pegasus

Pegasus is a supercomputer equipped with GPU and big memory, operated by Center for Computational Sciences, University of Tsukuba. Center for Computational Sciences provides about 50% of the total resources of Pegasus to the MCRP.

System summary and hardware specifications of Pegasus can be found at
URL: https://www.ccs.tsukuba.ac.jp/eng/supercomputers/#Pegasus
To know how to use Pegasus 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 Pegasus 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

At maximum, 78 nodes are available. The present MCRP calls for projects of 500,000 nodes*hours in total in fiscal year 2023 (2023.4 – 2024.3). Pegasus has 120 nodes, and each node has both CPU and GPU.

4.2.3 Computation time

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.

It is possible to transfer the budget between Cygnus and Pegasus. Note that the budget value is changed when you transfer the budget. See 4.1.3 for details.

4.2.4 Disk allocation

Standard allocation of the storage disk for each project differs depending on approved classes, 20 TB (MCRP-L), 10 TB (MCRP-M/MCRP-FPGA), and 5 TB (MCRP-S). 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.

4.3 Wisteria/BDEC-01 Odyssey (Wisteria-O)

The Wisteria/BDEC-01 is a supercomputer system operated by the Information Technology Center, The University of Tokyo. The simulation nodes group (Odyssey), which is called “Wisteria-O” hereafter, consists of 7,680 compute nodes equipped with Fujitsu Limited's FUJITSU Processor A64FX, same CPU as the world's most powerful supercomputer, Fugaku. Center for Computational Sciences, University of Tsukuba provides about 10% of the total resources of Wisteria-O to the MCRP.

System summary and hardware specifications of Wisteria-O can be found at
URL: https://www.cc.u-tokyo.ac.jp/en/supercomputer/wisteria/system.php
To know how to use Wisteria-O in details, User Support Portal site is available (User account, provided after the approval of the project, is necessary.)
URL: https://wisteria-www.cc.u-tokyo.ac.jp/cgi-bin/hpcportal.en/index.cgi

4.3.1 Accessibility of MCRP users

A unit of usage for Wisteria-O 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.

In each project, the total computational time (node*hour) are determined, based on the MCRP proposals reviewed by the Cooperative Research Committee. There is also a restriction in capacity of the file system. The usage period ends at March, after that, all the files of projects will be deleted.

4.3.2 Available computational resources

At maximum, 2,304 nodes are available. The present MCRP calls for projects of about 6,000,000 nodes*hours in total in fiscal year 2023 (2023.4 – 2024.3).

4.3.3 Computation time

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.

4.3.4 Disk allocation

Standard allocation of the storage disk for each project differs depending on approved classes, 30

TB (MCRP-L), 15 TB (MCRP-M), and 5 TB (MCRP-S). 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.

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 (including graduate universities and junior colleges), and technical colleges, in Japan.
3. Researchers who belong to institutes aiming at academic researches and promotion operated by national and local governments in Japan.
4. Persons who are exceptionally approved by Director of Center for Computational Sciences.

For projects to use Cygnus and Pegasus, project leaders living overseas, who are affiliated in universities or academic institutes operated by national and local government in the following countries listed below[*1)], are eligible to apply for MCRP.

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. For usage of Wisteria-O, researchers in industries are required to submit “Copy of Joint Collaboration Agreement”, or “Copy of Contract” and “Written Pledge”.

Non-resident researchers living in overseas countries are required to submit several documents before starting to use the computers. The procedure will be given by the Supporting Committee (See 12 for Contact information). It may take time for non-resident researchers to be approved for the usage.

*1) Countries eligible for project leaders (Cygnus & Pegasus) are listed in footnote 9 of page 15 of the following document:
https://www.meti.go.jp/policy/anpo/law_document/tutatu/t07sonota/t07sonota_jishukanri03_eng.pdf
In November2022, the following countries are eligible. Note that the list may be changed in future.

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

5.3 Applicants through HPCI

Cygnus and Wisteria-O 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 Cygnus, Pegasus, and Wisteria-O.

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 December 23, 2022 and closes at 24:00 on January 23, 2023. The announcement of the selection and the awards is scheduled to be given by March 23, 2023. The project period is from April 1, 2023 to March 31, 2024. Under various circumstances, the start (end) of the project may be delayed (advanced) from April 1 (March 31).

6.2 Classes and forms of application

There are three classes (L/M/S) of project applications, according to the project size. 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. Since the budget can be transferred between Cygnus and Pegasus, **the maximum budget values listed below should be regarded as the values assuming that all the budget is consumed on Cygnus. Thus, it is "(node*hour product on Cygnus)+(node*hour product on Pegasus)× 2".** Projects using both Wisteria-O and Cygnus/Pegasus-GPU should write both contents in a single form, thus, do not need to submit two proposals. 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
Cygnus: The maximum node-hour product: 120,000, Disk capacity: 20 TB
Wisteria-O: The maximum node-hour product: 550,000, Disk capacity: 30 TB

(2) MCRP-M (Medium), Language of proposals: English or Japanese
Cygnus: The maximum node-hour product: 40,000, Disk capacity: 10 TB
Wisteria-O: The maximum node-hour product: 200,000, Disk capacity: 15 TB

(3) MCRP-S (Small), Language of proposals: English or Japanese
Cygnus: The maximum node-hour product: 10,000, Disk capacity: 5 TB
Wisteria-O: The maximum node-hour product: 50,000, Disk capacity: 5 TB

(4) MCRP-FPGA (Cygnus-FPGA) , Language of proposals: English or Japanese
Cygnus: The maximum node-hour product: 10,000, Disk capacity: 10 TB

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 class 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 Wisteria-O and Cygnus/Pegasus 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.

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	3	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 Publication of research achievements and reporting requirements

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 Cygnus and Pegasus, 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. For Wisteria-O, “group id” and “user id” are automatically determined.
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 for Cygnus and Pegasus 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. On the other hand, those for Wisteria-O will be terminated and deleted immediately after the project

finishes.

11 Notes

- Titles and leaders' names of approved projects, and project reports will be publicized in the MCRP web site. Names and affiliations of project members are also open to public as needed, such as the reviewing, etc.
- 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).

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