Call for proposals in FY2025

Multidisciplinary Cooperative Research Program (MCRP-2025)

APPLICATION GUIDELINES

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

- Pegasus: 8.1 PFLOPS (double precision floating-point operation). 54 TFLOPS per node. Supercomputer equipped with GPU (NVIDIA H100) and big memory. It has started operation since 2023.
- Miyabi: 80.1 PFLOPS (double precision floating-point operation). Supercomputer equipped with NVIDIA GH200 Grace-Hopper Superchip (Miyabi-G) and Xeon Max 9480 (Miyabi-C). It is operated by JCAHPC under collaboration between University of Tokyo and University of Tsukuba. The operation is planned to start from January 2025.

CCS provides about 50 % of the total resources of Pegasus, and about 17 % of the total resources of Miyabi to this program, MCRP2025.

Schedule

Application period:	December 20, 2024 ~ January 23, 2025 (24:00 JST)					
	Member registration is open till January 31, 2025 (24:00 JST					
Notice of selection:	March 23, 2025					
Period of usage:	April 1st, 2025 ~ March 31st, 2026					
Submission of progress report:	: April, 2026					
Progress report presentation:	Autumn, 2026					

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 FY2025, 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 MCRP2025 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 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: <u>https://www.ccs.tsukuba.ac.jp/eng/supercomputers/#Pegasus</u> To know how to use Pegasus 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 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 available for use of more than one node.

4.1.2 Available computational resources

At maximum, 150 nodes are available. The present MCRP calls for projects of 650,000 nodes*hours in total in fiscal year 2025 (2025.4 – 2026.3). Pegasus has 150 nodes, and each node has both CPU and GPU.

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.

4.1.4 Disk allocation

Standard allocation of the storage disk for each project differs depending on approved classes. The storage size is determined by evaluation of the Cooperative Research Committee and may be reduced from the requested size.

4.2 Miyabi

Miyaba is a massively parallel cluster supercomputer operated by Joint Center for Advanced High-Performance Computing (JCAHPC) which is cooperated by University of Tsukuba and University of Tokyo. The system is comprised of 1,120 computing nodes (Miyabi-G), equipped with GH200 Grace-Hopper Superchips connected via NVIDIA's ultra-high-speed CPU-GPU link NVLink-C2C, and 190 nodes (Miyabi-C), each of which is equipped with two Intel Xeon Max 9480s connected via InfiniBand NDR200. An 11.3 PB parallel file system that uses NVMe-SSDs is available for all the drives. While Miyabi is shared by these two universities, Center for Computational Sciences, University of Tsukuba provides about 17% of the total resources of Miyabi to the MCRP.

System summary and hardware specifications of Miyabi can be found at URL: <u>https://www.ccs.tsukuba.ac.jp/eng/supercomputers/#Miyabi</u> To know how to use Miyabi in details, see the guide for Miyabi usage, which will be announced after the approval of the project.

4.2.1 Accessibility of MCRP users

Miyabi-G allows multiple jobs to be executed on a single node. When using multiple nodes for one job, parallel programming can be performed using MPI. On Miyabi-C, only a single job can run on each node without job mixing with other jobs.

4.2.2 Available computational resources

At maximum, 256 nodes (Miyabi-G) and 64 nodes (Miyabi-C) are available for each job. The present MCRP calls for projects of about 1,600,000 nodes*hours (Miyabi-G) and 270,000 nodes*hour (Miyabi-C) in total in fiscal year 2025 (2025.4 – 2026.3).

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. On Miyabi-G, it is (planned to be) allowed to use a fractional node, such as 1/4 node.

4.2.4 Disk allocation

Standard allocation of the storage disk for each project differs depending on approved classes, Miyabi-G and Miyabi-C use the same file server. 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:

- 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 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.

*1) Countries eligible for project leaders (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 November2023, 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, 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

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.

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.

5.3 Applicants through HPCI

Pegasus, and Miyabi 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 Pegasus, and Miyabi.

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

6 Application

6.1 Call for proposals, period of submission and project

The online submission opens on December 20, 2024 and closes at 24:00 on January 23, 2025. The announcement of the selection and the awards is scheduled to be given by March 23, 2025. The project period is from April 1, 2025 to March 31, 2026. 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. Projects using both Pegasus and Miyabi should write both contents in a single form, thus, do not need to submit two proposals.

In each class, applications that exceed the maximum budget and/or the maximum disk capacity cannot be accepted. If you apply for more than the standard disk capacity (up to the maximum value), you must clearly give the reason for the need and the basis for the estimate. The amount may be reduced from the applied one by the discretion of the Cooperative Research Committee.

(1) MCRP-L (Large), Language of proposals: English only The maximum budget available for application Pegasus: 80,000, Miyabi-G: 200,000, Miyabi-C: 30,000 The maximum (standard) disk capacity Pegasus: 400 TB (25 TB), Miyabi: 140 TB (10 TB)

(2) MCRP-M (Medium), Language of proposals: English or Japanese The maximum budget available for application Pegasus: 20,000, Miyabi-G: 50,000, Miyabi-C: 8,000
The maximum (standard) disk capacity Pegasus: 100 TB (10 TB), Miyabi: 36 TB (3 TB) (3) MCRP-S (Small), Language of proposals: English or Japanese The maximum budget available for application Pegasus: 5,000, Miyabi-G: 15,000, Miyabi-C: 2,000 The maximum (standard) disk capacity Pegasus: 25 TB (3 TB), Miyabi: 9 TB (1 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 Pegasus and Miyabi in one project.

6.4.2 Continuing project

For a project continuing from the previous year, the identical project code must be given in the online application. Otherwise, it is regarded as a different project. If the approved continuing project utilizes the same computer resources as the previous year, its files on the disk remain. If the amount of the files exceeds the approved limit, the disk will be write prohibited.

6.4.3 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.

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

Members of Cooperative Research Committee

<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 may 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

- 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. Failure to report may result in disqualification from future applications.
- 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 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 Miyabi, "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.
- 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

- 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