

Application Guidelines on Collaborative Research, Center for Computational Materials Science

1. Application Guidelines

The potential properties of materials are infinite. They show a wide variety of behaviors, which depend on their constituent elements and forms. The discovery of new materials is due to the development of new basic science. As their usefulness is clarified, these materials will become research objects and contribute to the society directly. Current materials science research is required to design and develop more advanced materials. One method with great potential is computer simulations. At the Center for Computational Materials Science (hereinafter referred to as “CCMS”), we strive to optimize the use of supercomputers for a wide range of materials, searching for and designing innovative materials through ultra-large-scale simulations. We provide our computer resources to researchers. For details of CCMS, please refer to the following website.

Center for Computational Materials Science website
<https://www.sc.imr.tohoku.ac.jp/eng/index.html>

- Supercomputing system configuration

The main configuration is as follows.

1. Supercomputers: Cray XC50-LC and Cray CS-Storm 500GT
2. Parallel computing / Informatics server: HPE ProLiant DL360 Gen 10
3. Storage systems: DDN EXAScaler and DDN GRIDScaler

For details, refer to “System Overview” page below:

<https://www.sc.imr.tohoku.ac.jp/eng/center/system.html>

2. Applicant qualifications

(1) Full-time researchers of national/public/private universities, technical colleges, incorporated administrative agencies, national research and development corporations, and public corporations (collectively referred to as “universities”) may apply as research representatives.

(2) As part of the research organization, faculty members other than full-time researchers, graduate students, undergraduates (for technical colleges, major college students and academic advisors shall be specified), and researchers belonging to foreign organizations* can be included as collaborators. In addition, those who have been approved by the director can be collaborators.

(3) For organizations with a large number of collaborators, we may ask the principal investigator to explain each member's contribution and responsibilities. In the report, we may also ask for clarification of the relationship between the use situation of the representative and collaborators and the outcome.

(4) If researchers belonging to foreign organizations are involved as collaborator, please assign one of them as co-principal investigator. The main principal investigator must belong to domestic institute for technical reasons related to the Export control.

(5) When researchers belonging to foreign organizations use supercomputers, security export control procedures are required. (See “9. Security Export Control”)

3. Application procedure

(1) Please submit at GIMRT user system. An applicant not belonging to the Institute, should consult with the faculty of the Institute about collaborative research in advance. We request you to assign one of IMR faculty to be a local contact.

GIMRT user system

<https://imr-kyodo.imr.tohoku.ac.jp/?lang=en>

(2) Application deadline

1. Proposal application deadline: **20 December 2018 (Thursday)** for this round.
2. For accepted proposal, Collaborative Research Agreement (Attachment) is required before you start your research. : Details will be informed later when the proposal is accepted.

(3) Points of Attention

1. When using supercomputers, a **user registration to CCMS is required in addition to the acceptance of scientific proposal.** For details, refer to CCMS website.

Center for Computational Materials Science

<https://www.sc.imr.tohoku.ac.jp/eng/index.html>

2. Applications should be written either by Japanese or English.
3. We allocate the time-node amount of each project from the viewpoint maximizing the number of users of our limited computer resources. We try to make effective use of the allocated time-node amount. With respect to the allocation of time-node amount to each project, considering “5. Application results”, CCMS Steering Committee makes the final decision. Allocation may be changed depending on the application status and the operation status of CCMS. The upper limit is 200,000 time-node amount per project.
4. GIMRT opens proposal call for every quarter of the year. However, CCMS call may not be open for all of them depending on the available resources. Since FY **2016**, the time-node amount is allocated in advance to each project. Hence allocation of time-node amount may be limited and we accept mainly urgent proposals. Be sure to state the reason for urgent application in the proposal. Please consult with CCMS administration office or the corresponding faculty in advance. The information of application is open 4 times in year at GIMRT web site.

4. Research Period

The research period is from **1 April 2019 to 31 March 2020**. If you continue with the same proposal, the extension is acceptable up to three times (including initial one). However, progress should be reported and explained.

5. Application results

Each proposal is reviewed by three referees, and decision is made by the corresponding proposal committee based on the review results. In the review of the continuing proposal, the progress and registered research results (published journal paper etc.) are considered. Please be sure to register the research results on the GIMRT user system. (Results registration is possible and requested even after the adoption period.) Also, for applying new research projects, please be sure to fill out “Previous Research Results” column.

Applicants will be notified the review result around the end of March **2019**.

6. Publication

- The results obtained by this collaborative research shall be published as a paper.
- Please be sure to describe CCMS in the Acknowledgments section of the paper. Please state that research “used supercomputers of the Center for Computational Materials Science.”

Name of CCMS: Center for Computational Materials Science

Example 1:

This work was performed under the GIMRT program of the Center for Computational Materials Science, Institute for Materials Research, Tohoku University (Proposal No. **S****)

Example 2:

The authors would like to express their sincere gratitude to the staff of the Center for Computational Materials Science, Institute for Materials Research, Tohoku University for their continuous support of the supercomputing facilities.

7. Research Report

The principal investigator shall submit “Research Report” via the Institute’s website by **10 April 2020 (Friday)**.

When summarizing the research results, the principal investigator shall submit the Research Report, as well as reprints of published papers of all collaborators (electronic one is acceptable).

8. Handling of Intellectual Property Rights

Intellectual property rights generated as a result of research shall conform to the Tohoku University Joint Research Regulations.

9. Security Export Control

As of FY 2014, applicants for the use of supercomputers who are of foreign nationality or belong to a foreign organization must demonstrate necessity. Such applicants must submit a permission application to the Ministry of Economy, Trade and Industry of Japan through the Security Export Control Office of Tohoku University. Note that the applicants cannot use the supercomputers until the application is approved. Upon approval, we may ask such applicants to submit additional documents such as certificate of enrollment.

10. Miscellaneous

Note that due to unavoidable circumstances, restrictions may be placed on the use if the steady operations of the supercomputers become difficult.

■ Contact for the Application Guidelines

GIMRT office, Research Collaboration Division, General Affairs Section, Institute for Materials Research, Tohoku University

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Attachment 1 (one can download this form GIMRT user system after the notice of acceptance)

Collaborative Research Agreement

To Director of Institute for Materials Research, Tohoku University

Project Number:
Research Project:

Name	Job Title	Home Organization

We acknowledge that the above persons will become collaborators.

Day Month Year

Director of Research Institution
Affiliation/Title /Name

Personal Seal or Signature

I acknowledge that the undergraduate students (or students in advanced courses in national institutes of technology) among the aforementioned persons will become collaborators in this research.

Supervisor:

Personal Seal or Signature

Notes

1. "Director of Research Institution" is the head of the home institution: such as president, dean, director of the department, head of center, or person in the equivalent position who has the responsibility for this agreement.
2. If an undergraduate (major student of a technology college) is included as a collaborator, the supervisor must acknowledge the student.