

Guideline (Version 1.1) – Updated 20 October 2022

Project Name		
Project Representative	Affiliation*:	Name:

*Affiliation refers to the organization or institute that you belong to.

1. Significance and Purpose the Research

- Describe a concrete plan and methods for achieving goals in the Project or for preparation for the fullfledged research on Fugaku (software verification, porting, tuning, test runs before production runs etc.).
- For each application program to be used, describe target fields and calculation methods (calculation models, analysis methods, parallelization techniques, etc.). If you use more than one program, descriptions are needed for each of them.

2. Utilization Plan of Computational Resources

Program Information

Program Name	Maximum Number of Nodes	Utilization History (computational target, system used in the past)
Molecular dynamics software "AAA" Ver. 16	X nodes	Executed with max. X nodes on the system O using data A.
Quantum chemistry software "BBB" Rev.8	X nodes	Executed with max. X nodes on the system O using data B

- If commercial software is to be used, the license which is valid for the requesting computational resources. In case of commercial software, state if you already have or will purchase the license valid during the project execution period.
- Program name: name and version of program (application software) to be used.
- Maximum Number of Nodes: Maximum number of nodes to be executed.
- Utilization history: provide usage record of the program including target data, name of the system, number of executing nodes, and performance information. If the program has not been used in Fugaku, state so (e.g., "No utilization history in Fugaku").

Requesting Resources

Provider Name/ Computational Resource Name	Amount of Resources to Request	
RIKEN R-CCS / Supercomputer Fugaku		X NH
	Local Storage	Y GB

* The node-hours above must be consistent with the online application system. If an inconsistency is found, the input in the online application system will be adopted.

* It is not necessary to input the request for the local storage of Fugaku in the HPCI Application System. 5TB is allocated by default, and it can be increased per request.

You may refer to the following links for more information on the performances of open-sourced software on Fugaku to help in the estimation of resources required.

- a) GROMACS (Simulation of Molecular Dynamics)
https://www.hpci-office.jp/documents/appli_software/Fugaku_Gromacs_performance.pdf
- b) LAMMPS (Simulation of Molecular Dynamics)
https://www.hpci-office.jp/documents/appli_software/Fugaku_LAMMPS_performance.pdf
- c) OpenFOAM (Simulation of Fluid Dynamics)
https://www.hpci-office.jp/documents/appli_software/Fugaku_OpenFOAM_performance.pdf
- d) Quantum Espresso (Simulation of Solid-State Physics)
https://www.hpci-office.jp/documents/appli_software/Fugaku_QE_performance.pdf
- e) FDS (Simulation of Fire Dynamics)
https://www.hpci-office.jp/documents/appli_software/Fugaku_FDS_performance.pdf
- f) Other applications
https://www.hpci-office.jp/en/using_hpci/hardware_software_software?expand=1&select=rsc0000089

Basis of Request for Computational Resources

Describe basis of request in a way that program and target of calculation (data etc.) can easily be understood.

(Example)

Molecular dynamics software "AAA"

Calculate the AAA status

YYYY nodes x YY hours x YY cases = A NH

Quantum chemistry software "BBB"

Calculate the BBB status

ZZZZ nodes x ZZ hours x ZZ cases = B NH

Total: A NH + B NH = X NH

Basis of Request for Local Storage

Estimation of the local storage space that is needed during the Project.

(Example)

Molecular dynamics software "AAA"

AA GB per case x AA cases = AA GB

Quantum chemistry software "BBB"

BB GB per case x BB cases = BB GB

Total: AA GB + BB GB = Y GB

3. HPCI Shared Storage (Fill out only if you request it)

HPCI shared storage: GB

Basis of the estimate:

4. Research Structure

Project Member	Affiliation	Expertise	Whether to use the resource	Roles/ Experience and Background
Researcher A	E University	Molecular biology	use	Project Representative, problem definition, Verification of results, Analysis
Researcher B	F University	Immunology, Bioinformatics	no use	Advisor Scientific background about zz
Collaborator C	G Research Institute	High performance computing	use	Program porting, production run, she has X years of experience in executing of CC jobs

- Describe research structure to carry out the research plan with project member's affiliation, name, expertise, whether to use the resources, and roles/experience and background.
- Accounts of computational resources are issued for the members who are listed on the Online Application System. Except for members who will be added during the project period, make sure that the input on the Online Application System is consistent with the persons for whom "use" is written in the "Whether to use the resource" field of the Table above.
- In principle, all the project members must be listed in the application form. If it is not possible to list names, the reason needs to be stated in the form. (e.g. a new member is expected to be assigned but his/her name is unknown, some tasks are planned to be outsourced to a vendor of application software, etc.)

5. Ongoing Project

- Ongoing project ID:
- Ongoing project name:
- Status of the ongoing project (goal achievement status, etc.)

6. Validity to Perform the Project

- Is this a small-scale project which conducts research or preparatory work on Fugaku, such as implementation, performance evaluation, or execution of software? Yes No
 - Are project implementation and utilization of the results limited to non-military purposes? Is this project appropriate in terms of societal benefits and values? Yes No
- (If the answers are "No", the project will not be allowed to use Fugaku.)

7. Experience with NSCC or Fugaku

- Have you made use of NSCC before? Yes No
 - If yes, please indicate your past project IDs:
- Have you made use of Fugaku before? Yes No
 - If yes, please indicate your past project IDs: