
Fugaku Commercial Software

Amber

User's Guide

September, 2023

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1.0		2023/09/01

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1 . Preface

Purpose of this document

This document describes how to use Amber, which is maintained by the RIKEN Center for Computational Science (R-CCS) on the supercomputer "Fugaku".

- For general information on how to use Fugaku, please refer to the manuals in the Fugaku Portal
- Please refer to the Amber manual for general Amber usage
- For information about Amber versions and features available on Fugaku, see "[Available commercial software versions](#)".

Prerequisite

The user shall have received the completion notification of the software usage environment in accordance with the "Flow to Start of Use."

When using commercial software installed on Fugaku, R-CCS and cooperating organizations cooperate to manage software licenses (operation checks) and conduct investigations when inquiring about software operation. Therefore, license information and inquiries may be shared among R-CCS and cooperating organizations. Please understand this in advance.

2. Executing Amber

The following is an example of a job script. Please modify it as appropriate for your work environment. Refer to the description below for **the red parts**. This job is submitted to the computation node. Amber20 is used as an example in this chapter.

Table 1 Sample Script

```
#!/bin/bash
#PJM -L "rscgrp=small"
#PJM -L "node=1"
#PJM -L "elapsed=00:05:00"
#PJM -L "freq=2200,eco_state=2"
#PJM -g <groupname>
#PJM -x PJM_LLIO_GFSCACHE=/vol0004
#PJM --mpi "proc=48"
#PJM -j
#PJM -S

module use /vol0004/apps/isv/Amber20/modulefiles
module load Amber20

/usr/bin/time -p mpiexec -n 48 $AMBERHOME/bin/pmemd.MPI ¥
-O -i mdin -o bench.fix.out_48 < /dev/null
```

2.1. Settings for Amber

- #PJM -L "freq=2200,eco_state=2"

This option specifies the execution mode of Fugaku. In the example above, the boost eco mode is specified. Whether or not the execution mode setting has an effect on execution performance, and how large the effect is, depends on the input data. Please select the mode which makes acceptable performance degradation and as large power reduction as possible. For more detail, please refer to:

https://www.fugaku.r-ccs.riken.jp/en/operation/20220701_01

- #PJM -x PJM_LLIO_GFSCACHE=/vol0004

When submitting jobs, be sure to specify /vol0004 in the environment variable PJM_LLIO_GFSCACHE.

- module command

Used to set environment variables.

- `module use`
Specifies where `modulefile` is stored. Change "Amber20" as appropriate version(s).
- `module load modulefile`
Sets environment variables defined in *modulefile*.

`module load Amber20`

is specified, the latest version installed on Fugaku is used.

Important: Environment variables set by the `module load` command may include runtime parameters. When specifying runtime parameters, be sure to specify them after the `module load` command.

To use a specific version, change the *modulefile*.

Example: Using Amber2021_20230802 version(*)

`module load Amber20/Amber2021_20230802`

(*)Because Amber consists of Amber and AmberTools, it defines its own modulefile for update versioning. For the information about the version to be applied when a modulefile is specified, check the messages output from the "module whatis" command.

Example: Check the messages output by Amber2021_20230802

`module use /vol0004/apps/isv/Amber20/modulefiles`

`module whatis Amber20/Amber2021_20230802`

➤ `module avail`

Displays a list of available *modulefiles*.

`module use /vol0004/apps/isv/Amber20/modulefiles`

`module avail Amber20`

➤ `module show modulefile`

Displays what is set by the module command.

Example: Show what is set when Amber20 is specified

`module use /vol0004/apps/isv/Amber20/modulefiles`

`module show Amber20`

3. Change in the environment of Amber

When environmental changes are made to Amber, the details and date of the changes will be posted on the Fugaku Portal. Please check the details of the changes and take action if necessary. The following is a list of expected changes, their impact on users, and how to deal with them. Amber20 is used as an example in this chapter.

- **Amber Version Upgrade**

If you use the latest version specified with Amber20 in module load, the software version executed after the change date will be changed to the newly latest version. If you want to keep using the currently using version, add the product version to the module load specification.

- **Amber specific version removal**

If the version to be deleted is specified in module load, the software will not be available after the change date. Please change the module load settings to switch to another available version.

4. Support

Please contact the Fugaku support (<https://fugaku.zendesk.com/hc/en-us/requests/new>) for Fugaku-specific content. For general information about Amber, visit <https://ambermd.org/Contact.php> .