Fugaku Commercial Software
Gaussian
User's Guide

October, 2022

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Table of Contents

1. Preface

Purpose of This Document

This manual explains how to use Gaussian that the RIKEN Center for Computational Science (R-CCS) installed for the supercomputer Fugaku.

- For the general usage of Fugaku, refer to the manuals in the Fugaku Portal Site.
- For the general usage of Gaussian, refer to the manual of Gaussian (https://gaussian.com/man/).
- This manual deals with Gaussian that R-CCS installed.

Premises

It is assumed that you complete the procedure described in "Gaussian - Application Information" and receive the completion notice of the account configuration for Gaussian.

Please note that the details of your inquiries about Gaussian could be shared among R-CCS, its cooperating organizations, and the software vendor to investigate them.

2. Executing Gaussian

You can execute Gaussian on the compute node. Note that Gaussian on Fugaku can be run on single node but cannot on multiple nodes.

To execute Gaussian on the compute node, use a job script. Below is an example, which you should modify for your environment. The red lines in the script are explained below. The job is submitted to be executed on the compute node.

```
#!/bin/bash
#PJM -L "rscgrp=small"
#PJM -L "node=1"
#PJM -L "freq=2200,eco_state=2"
#PJM -L "elapse=00:01:00"
#PJM -g <groupname>
#PJM -x PJM_LLIO_GFSCACHE=/vol0004
#PJM -S

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

. $g16root/g16/bsd/g16.profile
g16 < InputFile >& OutputFile
```

It is assumed that the job is submitted in the same directory where the input file exists.

2.1. Settings in Input File

The recommended setting of the options specified in the input file for executing Gaussian on Fugaku is as follows. For details on the meaning and format of each option, please refer to the manual of Gaussian (https://gaussian.com/man/).

- memory size

  This setting could improve the performance of parallel execution.

  ```
  %mem=16GB
  ```

- detailed logging

  This setting enables detailed logging, which is not needed on normal runs but recommended when you request support to the Fugaku support site.

  ```
  Replace a prefix # with #p
  e.g.: # rhf/sto-3g → #p rhf/sto-3g
  ```

2.2. Settings for Gaussian in Job Script

- #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/operation/20220701_01

- #PJM -x PJM_LLIO_GFSCACHE=/vol0004

  The environment variable PJM_LLIO_GFSCACHE must be set to /vol0004.

- module command

  sets environment variables.

- module use

  specifies the location of the modulefiles. Don't change this.

- module load *modulefile*

  sets environment variables defined in *modulefile*.

```
module load Gaussian
```

The command above is for using the latest version available on Fugaku.

Note: the “module load” command sets some environment variables which include parameters for Gaussian; the “module load” command should be followed in job scripts by the setting of the runtime parameters if any.

To use a specific version of Gaussian, select a specific *modulefile.*

```
e.g.: to use version g16c01
  module load Gaussian/g16c01
```

The commands below list all the available modulefiles which can be specified as *modulefile*.

```
module use /vol0004/apps/isv/Gaussian/modulefiles
module avail Gaussian
```

The commands below display the settings applied by the modulefile.

```
module use /vol0004/apps/isv/Gaussian/modulefiles
module show modulefile
```

2.3. Settings for execution performance on Fugaku

- Environment variable for paging method

  The following change of the dynamic memory allocation area to demand is expected to improve Gaussian's execution performance on Fugaku.

```
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand
```

  For more information about the paging method, see Users Guide and Programming Guide (Programming common part).

3. Using GaussView

Below is an example of the commands to execute GaussView, which you should modify for your environment. The red lines are explained below. GaussView is available on the pre/post environment, which is described in Pre/Post Environment Users Guide on the Fugaku portal site.

```
[PrePost]$  module use /vol0004/apps/isv/Gaussian/modulefiles
[PrePost]$  module load GaussView
[PrePost]$ . $g16root/g16/bsd/g16.profile
[PrePost]$ gv
```

Note: the prefix "[PrePost]$" implies the command to be executed on the pre/post environment.

・[Note] If you have any graphical trouble with GaussView, the setting below might resolve it.

```
[PrePost]$ export USE_MESAGL=1
```

After this setting applied , execute gv again.

3.1. Settings for GaussView

- module command

  sets environment variables.

- module use

  specifies the location of the modulefiles. Don't change this.

- module load *modulefile*

  sets environment variables defined in *modulefile*.

```
module load GaussView
```

  The command above is for using the latest version available on Fugaku.

Note: the “module load” command sets some environment variables which include parameters for GaussView; the “module load” command should be followed by the setting of the runtime parameters if any.

To use a specific version of GaussView, select a specific *modulefile.*

```
e.g. to use version 6.1.1
  module load GaussView/6.1.1
```

The commands below list all the available modulefiles which can be specified as *modulefile*.

```
  module use /vol0004/apps/isv/Gaussian/modulefiles
  module avail GaussView
```

The commands below display the settings applied by the modulefile.

```
  module use /vol0004/apps/isv/Gaussian/modulefiles
  module show modulefile
```

4. Change of Gaussian Environment

When the environment of Gaussian is changed, the details and date are posted in the Fugaku portal site. Please deal with the change as follows if necessary.

- **Update**

  If you run the “module load Gaussian” command to use the latest version of Gaussian, it will be changed to another version after the update. To keep using the current one, specify its version explicitly in *modulefile.*

- **Removal of specific versions**

  If you use any of the versions by specifying explicitly it in the “module load” command, it will not work after the removal. Change *modulefile* to use any of existing versions.

5. Support

You can request supports about Gaussian on Fugaku via Fugaku support site (see below). For general usage of Gaussian, please refer to the manual of Gaussian (https://gaussian.com/man/).

5.1. Contact Form in Fugaku Support Site

Please access the Fugaku support site (https://fugaku.zendesk.com/hc/en/requests/new) and request supports in the following way.

- "Please select the issue from the following options.": select "Application Software" from the drop-down list.
- "Project ID": select your project ID from the drop-down list.
- "Inquiry type": select "Commercial Software" from the drop-down list.
- "Subject": fill in the subject of your inquiry.
- "User name": fill in you name.
- "Account name": fill in your account.
- "Application name": fill in "Gaussian".
- "Inquiry details": fill in the detail of your inquiry.
- "Attachments": we could answer your inquiries about Gaussian more quickly if you provide the output file, which is specified in the example job script in "2. Executing Gaussian." For the settings about this output file, refer to "detailed logging" in the section 2.1.