FAQ (Molecular Science)

(Last Update: Oct 7, 2025)

Frequently asked questions about molecular science applications.
Please check this page for general questions about RCCS system.

FAQ

How to run applications installed by RCCS

For molecular science applications installed on RCCS system, sample jobs are provided. You can copy the sample files to your own directory and run them, or modify the samples to create your own input files. Typically, job scripts are provided with names like "sample.sh" (the name may vary, though), and can be submitted using a command like "jsub sample.sh".

The path of the sample jobs are listed in Package Programs List page. Or, you can directly access typical sample directory /apl/(application name)/(version)/sample.

- ref: Sample Jobs

Cannot use formchk (Gaussian checkpoint file converter)?

You need to load setting file before running formchk. If you want to convert checkpoint file, you need to run the following command. Please note that the setting file name depends on your login shell.

bash or zsh:

```
$ source /apl/gaussian/16c02/g16/bsd/g16.profile
```

csh (tcsh):

```
$ source /apl/gaussian/16c02/g16/bsd/g16.login
```

(You can ignore "PYTHONPATH: Undefined variable." message. Setting is correctly loaded and formchk is available in this case.) If you are using different version of Gaussian or queue, please replace the directory names above to the corresponding ones. If you load one of gaussian modules (environment modules), corresponding version of formchk becomes available.

formchk failed with insufficient memory error

If not enough memory is available for formchk, it will fail with the error message like below.

```
Out-of-memory error in routine WrCIDn-* (IEnd= ******** MxCore= **********)
Use %mem=***MW to provide the minimum amount of memory required to complete this step.
Error termination via Lnk1e at (***date***).
```

The memory amount of formchk can be modified via GAUSS_MEMDEF environment variable. Please set enough value according to the error message above, and then run formchk again.

- bash/zsh:

```
export GAUSS_MEMDEF=400MW
```

- csh:

```
setenv GAUSS_MEMDEF 400MW
```

In this example, 400MW (=3200MB) of memory is specified. It can also be specified in bytes like "export GAUSS_MEMDEF=3200MB".

Restricted Software (ORCA, GRRM23, Open OnDemand, Crystal, AlphaFold3)

Following applications require an application for use or registration.

- ORCA => User registration on the official site and e-mail to RCCS required.
- GRRM23 => An application for use required.
- Open OnDemand => You need to register a password on this website.
- Crystal => An application for use required (see the bottom of the page).
- AlphaFold3 => Model parameters required.

How to run GUI applications (such as GaussView or VMD)?

You can use GUI applications on login node using X11 forwarding or Open OnDemand.Please check this general FAQ item.

The actual command name of GUI applications are listed inPackage Programs List page (e.g., "gview6" for GaussView6). If applications such as VMD do no work with X11 forwarding, please try Open OnDemand.

Request installation of software

Please fill the following items and send it torccs-admin[at]ims.ac.jp (please replace [at] by @).

- Software name and version that you want to use
- Overview of the software and its feature
- Why that software is necessary in RCCS supercomputer
- URL of the official website

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