

## FAQs

Frequently asked questions about usage of computers.

### FAQs:

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### [What will happen if the resource usage exceeds the limit](#)

New jobs won't be accepted. Please be careful not only on the CPU usage but also on the disk usage. In case group CPU points run out, jobs of that group will be removed after 24+ hours of that points exceedance.

### [How to build/debug software in RCCS?](#)

We don't have interactive or debug queue.

You can build and test software on the frontend nodes (ccfep\*, ccgpup, ccgpuv), where parallel make (e.g. make -j 12) or MPI program run (e.g. mpirun -np 12 ...) is allowed.

However, there are some performance limitations, which are intentionally employed, on those frontend nodes.

Please don't try production runs or long benchmark jobs on the frontend nodes.

CPU points will be used on ccfep\* and ccgpuv according to the actual CPU usage. (If you just login and do nothing, virtually CPU points won't be consumed.)

To login to GPU equipped frontend nodes (ccgpup or ccgpuv), you first login to ccfep\* and then "ssh" to ccgpup/ccgpuv.

No additional settings are required if you can login to ccfep\*.

### [How to know limitation on CPU/GPU usage?](#)

CPU/GPU limitation is basically determined from the initially assigned points. [The actual values can be found in this table \(right columns\).](#)

Current limitation can be shown by "jobinfo -q PN -c" command (do not add -l options in this case).

Here are the example. Blue- and red-colored "\*\*\*\*\*" parts in "RunLim" row will show the max available CPUs/GPUs for you and your group, respectively.

```
[user@ccfep* ~]$ jobinfo -q PN -c
-----+-----+-----+-----+-----+
Queue|Job  |User(***)|Group(***)|Total
Name |Status|CPUs,GPU|Jobs CPU,GPU|Jobs| CPUs,GPU|Jobs(Usr,Grp)
-----+-----+-----+-----+-----+
PN   |RunLim|*****|**/-  ****, **/- |xxxxx,xxx/- ( -, -)
|Run  | x, x/x  x, x/x  |xxxxx, xxx/xxxx(xxx,xxx)
|Queue| x, x/x  x, x/x  |xxxxx, xxx/xxxx(xxx,xxx)
|Hold | x, x/x  x, x/x  |xxxxx, xxx/xxxx(xxx,xxx)
|Exit | x, x/x  x, x/x  | x, x/x ( x, x)
|Total| x, x/x  x, x/x  |xxxxxx,xxxxx/xxxx(xxx,xxx)
-----+-----+-----+-----+-----+
```

There are two types of limitations; user and group limitations.

Per user limitation can be assigned by the representative of the group at [resource limit page](#).

### [Cannot login via SSH / Login from outside Japan during Bussiness Trip](#)

If you have trouble in accessing from Japan, please check "SSH Connction Error messages" entry in this page (need to login) and documents in [quick start guide](#) page.

If you want to login from outside Japan, you need to submit an application form available in [this page](#).

The applicants are basically required to have a valid academic affiliation in Japan and an account of RCCS; login of oversea collaborators to RCCS is generally not allowed.

### [How to change login shell?](#)

You can use csh (tcsh), bash, or zsh as a login shell. This setting can be modified only via the center web page. To modify the setting, click " [My account](#)" item in the left pane first. (That item won't be shown if you are not logged in.) Then, click "Edit" tab in that page. You can choose your login shell using the combobox in that page. After the choice of the login shell, make sure to click "Save" button located below to save the modified setting.

It might take a time to untill the new setting becomes active. If the modification is not applied for more than a day, please contact us.



Output example:

```
Entering Gaussian System, Link 0=/local/apl/lx/g16/g16/._g16
Initial command:
/local/apl/lx/g16/g16/l1.exe "/work/users/*****/cccms1/Gau-66921.inp" -
screddir="/work/users/*****/cccms1/"
sh: /local/apl/lx/g16/g16/l1.exe: Permission denied
```

Typically, this happens when configuration files are loaded both in the default setting files (such as `.cshrc` or `.bashrc`) and in the job script. You may need to modify either of default setting file or job script to solve this problem.

On the other hand, a single setting file can be loaded safely multiple times.

Also, you might (not always) be able to run Gaussian successfully after loading setting files of multiple Gaussian versions (g09 and g16). It is not recommended, though.

### [Cannot use formchk \(Gaussian checkpoint file converter\)?](#)

You need to load setting file before running `formchk`. If you want to convert checkpoint file from g16 output from LX queue, you need to run the following command. Please note that the setting file name depends on your login shell.

`csh` (tcsh):

```
$ source /local/apl/lx/g16/g16/bsd/g16.login
```

`bash` or `zsh`:

```
$ source /local/apl/lx/g16/g16/bsd/g16.profile
```

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` will be 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.

▶ `csh`:

```
setenv GAUSS_MEMDEF 800000000
```

▶ `bash/zsh`:

```
export GAUSS_MEMDEF=800000000
```

In this example, 800MW (=6.4GB) of memory is specified.

### [Python environment \(version, libraries\) construction](#)

If the requested version of python or the library is provided by the distribution, we can install them. However, we recommend you to build [Anaconda](#) environment in your home directory, because Anaconda covers wider area of the python applications/libraries used in academic science than the package set provided by the distribution.

We also prepared some Anaconda environments. Links to their usage page can be found at [package program list page](#).

### [Modifications to files ignored? / Not removable, not controllable file?](#)

#### ■ Modifications to files ignored?

In some rare cases upon system troubles, modifications to files would be ignored at first glance.

This is generally caused by the mishandled file cache.

If you met this unlucky event, please check it carefully according to the following procedure.

- ▶ login to other hosts (ccfepX; X=1-8)
- ▶ get checksum of the file (e.g. `md5sum`) or look directly the file (e.g. `less`)
- ▶ if the checksums of a file are different or the contents of the file is different between hosts, there maybe a cache problem.

If you find a suspicious file, please report the hostname and the file location to us: [rccs-admin@jims.ac.jp](mailto:rccs-admin@jims.ac.jp) (please replace [at] by @).

We will clear the file cache of that host. (This is because normal users cannot do this operation.)

You can fix it by yourself by file manipulation (not recommended, though).

If you try to fix, please make backup before the file manipulation.

#### ■ Not removable, not controllable file?

On the other hand, files can be broken due to a storage trouble. "ls -l" might return the following type of output in some case. (This might happen upon file creation stage. Already existing file would not experience this type of trouble.)

```
ls: cannot access (file name): No such file or directory
-???????? ? ? ? ? (file name)
```

Unfortunately, this file is completely broken. All you can do for this file is just to remove.

You may need to employ "unlink" command instead of standard "rm" command to remove this file.

### [Are there job script header samples?](#)

We prepared [some samples in this page](#).

You can find some explanations in [our manual](#). The sample scripts for each applications (/local/apl/lx/(name)/samples) may also be worth to check.

### [Request installation of software](#)

Please fill the following items and send it to [rccs-admin@lms.ac.jp](mailto:rccs-admin@lms.ac.jp) (please replace [at] by @).

- ▶ Software name and version that you want to use
- ▶ Overview of the software and its feature
- ▶ Necessity of installation to supercomputers in RCCS
- ▶ URL of the software development

### [SSH Connection Error Messages](#)

```
Permission denied (publickey)
```

```
Permission denied (publickey,hostbased).
```

Private and public keys don't match or the public key is not registered. This message may be shown if the private key is not correctly prepared or specified.

```
Permission denied (publickey,gssapi-keyex,gssapi-with-mic,hostbased).
```

This message will be shown if the private key is not correctly specified.

```
ssh:connect:Network is unreachable
```

```
ssh:connect:Host is unreachable
```

These messages will be shown if the network setting is incorrect or connection route to RCCS is not available due to some network errors.

```
ssh:connect:Connection refused
```

```
ssh:connect:Connection timed out
```

RCCS service is temporary stopped for maintenance or some troubles. Or, the connection is refused according to the rules described below.

```
ssh_exchange_identification: Connection closed by remote host  
Server unexpectedly closed network connection
```

Network failure happens or connection is refused according to the rules described below.

If the connection can't be established successfully, adding verbose option to your ssh software will give you some useful information/messages. For example, if you are using "ssh" command on the terminal (maybe on Mac and Linux), verbose messages can be enabled by adding -v option.