FAQ (general & Molecular Science)

(Last update: Feb 20, 2025)

Frequently asked questions about usage of computers.

FAQ

Failed to reset password / three-character user id?

Only the registered Email address is necessary to reset password or/and register public keys on this website. The three-character user id is required when you modify your information on this website after the first login or when you login to the supercomputer system.

When you failed to receive password reset Email, there may be something wrong with the entered or registered address. Please contact us if you can't receive the email. For the initially registered Email addresses of group members, the representative person can see them on the "Members" tab ("組織表ダウンロード" button; sorry, English UI is not yet available for this part...) in the page of your application on NOUS.

Alternatively, if there are already logged in users in the group, they can see the three-character account names of the group members at "List group members" page on this website (login required). You may also be able to check whether you are registered in the correct group.

If you are the representative person of the group, you can find the list of user accounts in the "Members" tab in your application page at NOUS. Even when the user account field was left blank when you submitted the application, the member's correct user accounts should be added.

I want to change my Email address during use

It is not possible to change your email address on this website after the submission of your application for this FY. Please enter your new Email address in the form available in "Member Management" page and then send us in the manner indicated on that page.

For the Email addresses of group members registered upon submission, the representative person can see them on the "Members" tab ("組織表ダウンロード" button) in the page of your application on NOUS.

Cannot login / Login from outside Japan during Bussiness Trip

If you want to login from outside Japan, you need to submit an application. The template file can be downloaded from this page. The applicants are required to have a valid academic affiliation in Japan and an account of RCCS; login of oversea collaborators to RCCS is generally not allowed.

If you have trouble in accessing from Japan, please check documents in quick start guide page.

■ Remote host name and user name

The host name is "ccfep.ims.ac.jp". The user name is a 3-character account (English letters only or English letters + numbers) assigned by RCCS.

■ Registration of public key(s)

You need to register your public key on this website. Please check this page for information on how to register.

■ In case permissions of ssh related files/directories are wrong

In case you accidentally change the permissions of your home directory or ~/.ssh, ~/.ssh/authorized_keys, you can no longer login. If a login session remains, please fix the permissions using that. If you have already logged out, please contact us. We will fix the permissions.

■ Connection closed immediately / Connection timed out

This situation may occur during system troubles. Please check the information on the top page of our website first. Also, you will not be able to login during maintenance. Please wait until the maintenance is finished.

If you receive a "Permission denied" message, your public key or user name may not be correct. Please review your settings by referring to the Quick Start Guide.

If you are waiting for a long time without any response, or if a message such as "Connection timed out" or "Connection closed" is displayed

immediately, network connection might be blocked by something like firewall. In this case, please contact the person in charge of your network environment.

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.

It will take up to 10 minutes before the system updates the usage status (i.e. before the update of showlim command output). For example, suppose you notice that you have exceeded your disk usage and immediately delete the file. Still you need to wait up to 10 minutes before the your new submission is allowed.

How are CPU points for a job calculated?

CPU points of a job are calculated from the elapsed time (execution time) of the job. For example, if the job's time limit (walltime) is 24 hours and the elapsed time is 1 hour, CPU points for 1 hour will be used.

Available memory amount for a job

The amount of available memory for a job is proportional to the number of the CPU cores allocated to that job. For largemem jobs, you can use about 8 GB (~7.45 GiB) per core. For other types of jobs, you can use about 2 GB (~1.86 GiB) per core.

When you employ 64 CPU cores (ncpus=64), you can use ~512 GB for jobtype=largemem jobs and ~128 GB for other jobs, respectively. If a large amount of memory is needed but not so many CPU cores, it is still necessary to employ many CPU cores.

How to add/remove members?

Please check this page.

How to build/debug software in RCCS?

You can build and test software on the login servers (ccfep*).Parallelized build of programs (e.g. make -j 12) and MPI program tests (e.g. mpirun -np 12 ...) are also allowed. For GPU software, please use ccgpu (do "ssh ccgpu" on ccfep to login).

However, there are some performance limitations, which are intentionally employed, on those login servers. Please don't try production runs or long benchmark jobs. CPU points will be used on ccfep* according to the actual CPU usage. (If you are just logged in and do nothing, CPU points won't be consumed.)

Interactive jobs are not available to all the users for now. If you want to use interactive jobsplease ask us. Please note that there are some additional restrictions (walltime, number of CPUs/GPUs for example) in interactive jobs.

How to know limitation on CPU/GPU usage?

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

Current limitation can be shown by "jobinfo -s" command. (See "User/Group Stat" part in the beginning.)
Here are the example. Red- and blue-colored "****" parts ("RunLim" column) will show the max available CPUs/GPUs for you and your group, respectively.

```
[user@ccfep* ~]$ jobinfo -s

User/Group Stat:
-------------------------------------------------------------------------------
 queue: H                    | user               | group
-------------------------------------------------------------------------------
   NJob (Run/Queue/Hold/RunLim) |    x/    x/    x/-    |    x/    x/    x/****
   CPUs (Run/Queue/Hold/RunLim) |    x/    x/    x/**** |    x/    x/    x/****
   GPUs (Run/Queue/Hold/RunLim) |    x/    x/    x/**** |    x/    x/    x/****
   core (Run/Queue/Hold/RunLim) |    x/    x/    x/**** |    x/    x/    x/****
   lmem (Run/Queue/Hold/RunLim) |    x/    x/    x/-    |    x/    x/    x/***
 sncore (Run/Queue/Hold/RunLim) |    x/    x/    x/-    |    x/    x/    x/***
-------------------------------------------------------------------------------
note: "core" limit is for per-core assignment jobs (jobtype=core/gpu*)
note: "lem" limit is for jobtype=largemem
note: "sncore" limit is for 64 or 128 cores jobs

Queue Status (H):
(skipped)
```

There are two types of limitations; user and group limitations. Per user limitation can be assigned by the representative of the group atesource limit page.

We need extra CPU points / disk space

You can apply for additional CPU points or/and disk space.Details can be found at this page.Please be careful about limitations.

How to change login shell?

You can use csh (tcsh), bash, or zsh as a login shell. This setting can be modified only at this RCCS web site. To modify the setting, click"My account" item at the top pf page. (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 combo box. After the choice of the login shell, make sure to click "Save" button at the bottom of the page.

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

My jobs have been waiting for very long time

Major reasons why your jobs won't run are listed below. If you meet exceptional/unknown cases, feel free to contact us.

■ Not enough resources (CPU, GPU) available

You can check the status of available resources in this website. Once login to this site and go to the top page, you will find the status on the right column of the page. There can be enough space for other types of jobs. Switching jobtype (if it is possible) might be a good idea in this case.

■ My job won't run even though enough computational resources are available.

First, run jobinfo command to check the reason why your jobs won't run. You can find the reason at the rightmost column of the output. Major reasons are:

- (cpu), (gpu): not enough cpu/gpu available
- (group): due to the group limit
- (long): walltime too long (once a job began to run, that must be finished before the next maintenance)
- (other): scheduler of the system not yet tried to run your job (or other unknown reason)
    - in some case of (other), "jobinfo -c" can't show the correct reason due to the insufficient information from the queuing system. Please try without "-c" option.

In case of (group), you or members of your group are using large amount of resources. Please ask corresponding person to do something. FYI, representative person can limit the resource usage of each member at the resource limit page.

On the other hand, in case of (long), you may need to shorten the walltime of your job or wait until the end of next maintenance. (NOTE: queued jobs won't be deleted upon monthly maintenance.)

■ My jobtype=core jobs won't run even though enough computational resources are available.

Multinode jobs are not allowed for jobtype=core jobs; a job must reside on single node. Even when there are so many free CPU cores for jobtype=core in total, those free cores are often scattered among nodes and there may be not enough space for your large jobtype=core jobs. You might want to use 64 cores (jobtype=vnode) in some cases; jobtype=vnode may have room for your job. Also, for ncpus=46-63 jobs, switching to ncpus=64 is more advantageous in terms of CPU points (64 cores => 45 points/hour, 46 cores => 46 points / hour, 63 cores => 63 points / hour).

"Cgroup mem limit exceeded" message

In case used memory amount exceeds the limit, the job would exit with the error message like below.

```
Cgroup mem limit exceeded: oom-kill:constraint=CONSTRAINT_MEMCG,nodemask=
(null),cpuset=*******.ccpbs1,mems_allowed=*,oom_memcg=/pbs_jobs.service/jobid/*******.ccpbs1,task_memcg=/pbs_jobs.service/jobid/*******.ccpbs1,task=molpro.exe,pid=******,uid=******

[Wed Feb  1 **:**:** 2023] memory: usage ********kB, limit ********kB, failcnt ********
[Wed Feb  1 **:**:** 2023] memory+swap: usage *********kB, limit *****************kB, failcnt 0
[Wed Feb  1 **:**:** 2023] kmem: usage ******kB, limit *****************kB, failcnt 0
[Wed Feb  1 **:**:** 2023] Memory cgroup stats for /pbs_jobs.service/jobid/*******.ccpbs1:
```

You need to reduce amount of memory usage or use jobtype=largemem where large amount of memory available. For jobtype=core, please note that the amount of available memory is proportional to "ncpus" value in job header. In some case, you may need to specify ncpus=8 in the header, while you actually use only 4 cpu cores (e.g. mpirun -np 4).

In case memory is over-allocated but not used, the job would run normally even though "Cgroup mem limit exceeded" appears in stderr output. Anyways, you should reduce the memory amount in your input file to avoid potential errors.

"No space left on device" error

You may have exceeded the size limit of local scratch space for the job (/lwork/users/(username)/(job id)). The size limit of local scratch is 11.9 GB * ncpus (where ncpus is available cores in that node; not a total number of ncpus of the job). Therefore, you can avoid those errors by increasing "ncpus" of your job. Or, you can use global scratch space (/gwork/users/(username)) instead of the local scratch. Please note that /gwork is huge but slower than /lwork.

For g16sub and g09sub, they use /lwork/users/(username)/(jobid) in the default setting. You can switch scratch space to /gwork by adding "-N" option.

Got an email titled "[RCCS] 障害発生と影響を受けたジョブに関するお知らせ"

In case computation node, network switch, or storage fails, this email would be sent to the owners of jobs which are affected by the trouble. (English version of this email is not yet available, sorry.)

```
(uid)様

2020年**月**日**時**分頃、****において
障害(***************)が発生しました。

影響を受けたジョブの一覧をお知らせします。
--------+--------+--------+--------------+-----+-----------------
Job ID   Jobtype  User     Job Name       #Core Treatment
--------+--------+--------+--------------+-----+-----------------
 (jobid) *****    (uid)    (jobname)      (num)XXX
--------+--------+--------+--------------+-----+-----------------
```

In this email, you should check the action for that aborted job (Treatment column, colored with red in above sample).

- 異常終了(Abort) => Job was aborted (including the where a job failed to rerun). CPU points for that job will be paid back (later).
- リラン(Rerun) => Job reran from the beginning. CPU points spent for the aborted run will be ignored.

In the default setting, aborted job would rerun. However, in case of system troubles, the job system might fail to recognize the job status and the job might abort. You need to submit the job again in this case. If you want to disable rerun of jobs, please add "#PBS -r n" in your job script.

Can't connect via sftp (including WinSCP etc.) with "Received message too long" error

This error will happen when output of .bashrc is large. For example, if setvars.sh of Intel oneAPI is loaded in .bashrc, this message may appear. There are some ways to avoid this error.

- discard output to /dev/null
- allow output only if $PS1 exists (interactive case)
- move the corresponding lines to ~/.bash_profile

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 WrClDn-* (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 800MW
```

- bash/zsh:

```
export GAUSS_MEMDEF=800MW
```

In this example, 800MW (=6400MB) of memory is specified. It can also be specified in bytes like "export GAUSS_MEMDEF=6400MB".

Python environment (version, libraries) construction

Some python versions and libraries are available via yum.Please ask us if you need them. Or you can install packages by yourself using pip3 command with --user option (see example below). Packages will be installed in your home directory (probably under ~/.local).

```
$ pip3 install numpy --user
```

You can also use pyenv or/and miniforge. Anaconda is also a very good solution if there is no problem about license. If you are planning to use GPUs, we recommend to use conda environment such as miniforge. Runtime library for GPUs (cudatoolkit) can be installed easily with conda.

Miniforge environments prepared by RCCS are also available. You can load them by sourcing /apl/conda/(date)/conda_init.sh or /apl/conda/(date)/conda_init.csh.

Intel Compilers (ifort, icc, icpc) not available

In the current system, we don't provide Intel Compilers to users. If you need them, please install Intel oneAPI Base Toolkit and HPC Toolkit into your directory.
https://www.intel.com/content/www/us/en/developer/tools/oneapi/base-toolkit.html (Base Toolkit)
https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit.html (HPC Toolkit)
(These toolkits can be installed free of charge. However, there are restrictions upon redistribution.)

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.

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 (/apl/(name)/(version)/samples) may also be worth to check.

Request installation of software

Please fill the following items and send it to rccs-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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