

## ORCA 4.x or later user registration

Last update: Nov 6, 2024.

## How to use ORCA at RCCS supercomputer

We cannot make ORCA freely available to all users due to its license restriction.

[Please register at the official site first](#). Moreover, you need to agree with the EULA before using ORCA.

## How to register at RCCS

Please forward account confirmation e-mail (which name maybe 'Welcome to "ORCA Forum"') to rccs-admin\_at\_ims.ac.jp (change \_at\_ to @), where please also write your RCCS account ID in the mail text. Please tell us in case you lost that e-mail.

## Use

Once the procedure above completed, access to ORCA files would be approved.

Currently, following versions are available in RCCS.

Installation directories:

- /apl/orca/6.0.1
  - orca/ : ORCA 6.0.1
  - samples/ : sample input available here
- /apl/orca/5.0.4
  - orca/ : ORCA 5.0.4
  - samples/ : sample input available here
  - testsuite/ : official test suite (input files in OutputFiles/ directory, output files in RCCS\_OutputFiles directory)
- /apl/orca/5.0.3
  - orca/ : ORCA 5.0.3
  - samples/ : sample input available
- /apl/orca/4.2.1
  - orca/ : ORCA 4.2.1
  - openmpi-3.1.4/ : OpenMPI required for orca 4.2.1
  - samples/ : sample input available here

(Note: we employ shared version simply because it shows better performance than static linked version.)