

ORCA 4.x/5.x user registration

Last update: Jul 16, 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 in 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, shared version binaries of 4.2.1, 5.0.3, and 5.0.4 are available in RCCS.

Installation directories:

- `/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
- `/apl/orca/5.0.3`
 - `orca/` : ORCA 5.0.3
 - `samples/` : sample input available
- `/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)

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