

ORCA 4.x/5.x user registration

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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 and 5.0.3 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.)