

ORCA 4.2.1 available

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How to use ORCA in 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 add your RCCS account ID in the mail. We can confirm registration status from that e-mail. Please tell us if you lost that e-mail.

Use

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

Currently, shared version of 4.2.1 is available in our system. (Note: we avoid static version simply because it was too slow.)

Installation directory:

- ▶ /local/apl/lx/orca421
 - ▶ orca/ : ORCA 4.2.1
 - ▶ openmpi-3.1.4/ : corresponding version of OpenMPI
 - ▶ samples/ : sample input is available here