ORCA 4.x or later 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 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, ORCA 6.1.0, 6.0.1, 5.0.4, 5.0.3, 4.2.1 are available in RCCS.

You can run ORCA jobs with osub command. You only need to prepare input file of ORCA.

If you want to submit ORCA job with jsub command, sample input and scripts can be found in /apl/orca/(version)/samples directory.