4th Winter School of Computational Chemistry

Sharif University of Technology

ORCA Installation Guide

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1. Introduction

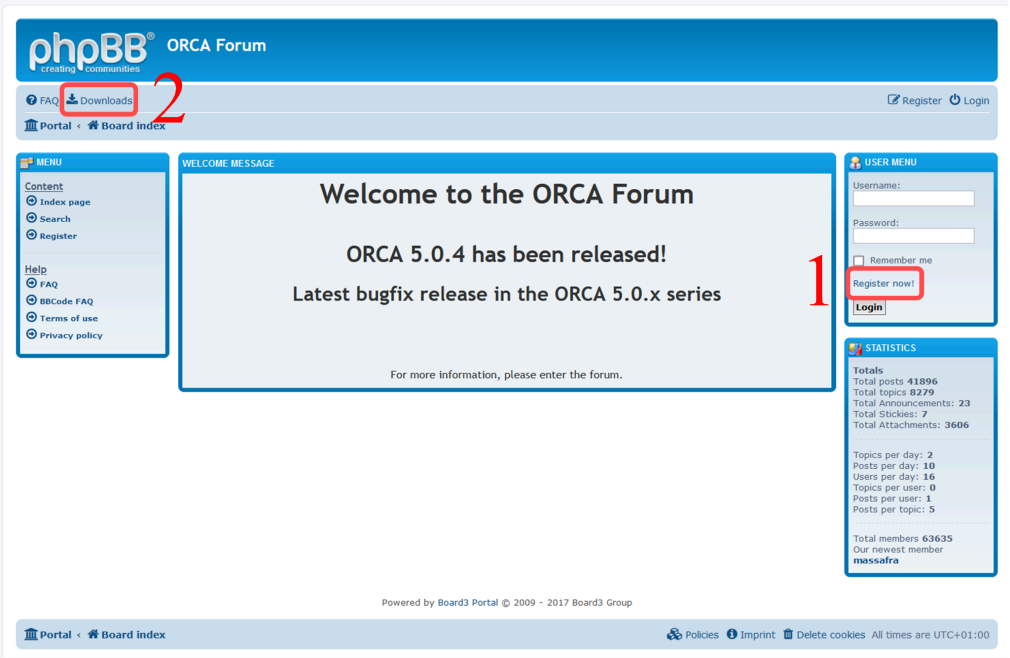
ORCA is an ab initio quantum chemistry program package developed by Prof. Frank Neese and his research group, offering a wide range of modern electronic structure methods, including density functional theory, many-body perturbation, coupled cluster, and semi-empirical quantum chemistry methods. It is designed for the study of larger molecules, transition metal complexes, and their spectroscopic properties, making it a valuable tool for computational chemists, as well as chemists, physicists, and biologists interested in the full information content of their systems. The program is available for various operating systems, including Linux, Microsoft Windows, and macOS, and the free version is accessible for academic use at academic institutions. ORCA is known for its user-friendly nature and is considered to be an efficient and flexible tool for quantum chemistry simulations, with a specific emphasis on the spectroscopic properties of open-shell systems.

2. Downloading Materials

Before you begin installing ORCA, download the version compatible with your operating system. Also, if you want to run your jobs in parallel, you need to download the dedicated message-passing interface library. This library allows ORCA to distribute tasks across multiple processors, which can significantly speed up your calculations. You may also want to add computational chemistry visualization software to your arsenal. This will help you to visualize the results of your calculations. Finally, make sure to download the ORCA manual. It is an essential resource for learning how to use the software effectively.

2.1 ORCA Software

To download ORCA from its official website you need to go to [ORCA Forum website]:

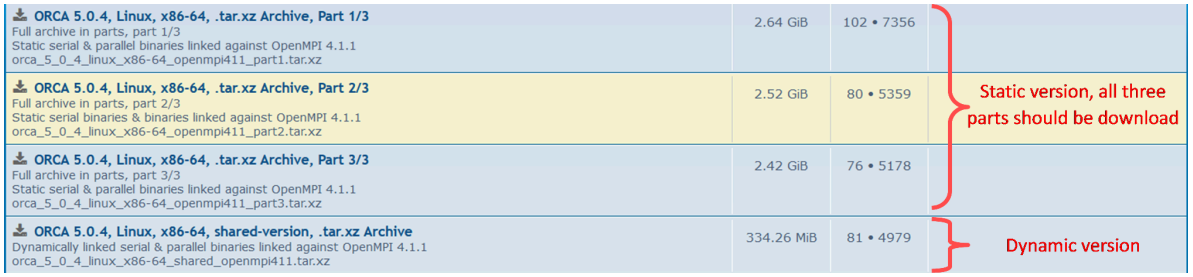


1. First, you need to register on the site

2. After registering and activating your account, head to the download section. This section includes different versions of the ORCA software, manuals, tutorials, and visualization packages. It's a great resource for learning more about ORCA and computational chemistry in general.
3. For the sake of this winter school, please download the ORCA 5.0.4.

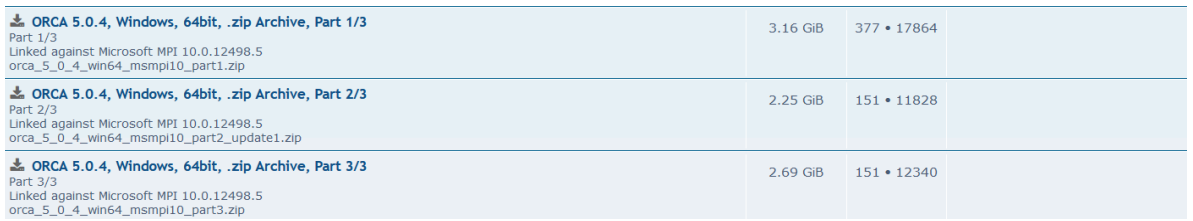
a. Linux

For Linux, two download options differ in their code architecture. The static version includes all necessary libraries, making it larger. The dynamic version relies on system libraries and is significantly smaller. Both versions function identically in terms of usage and application. We recommend starting with the dynamic version (lighter) and switching to the static version (heavy) only if you encounter issues.



b. Windows

For Windows, there are three zip files that need to be downloaded.



c. Mac OS

On macOS, you have several download options for ORCA 5.0.4, regardless of your CPU architecture, each option is a single file. However, keep in mind that some options are limited to running jobs only in a serial fashion (using single CPU).

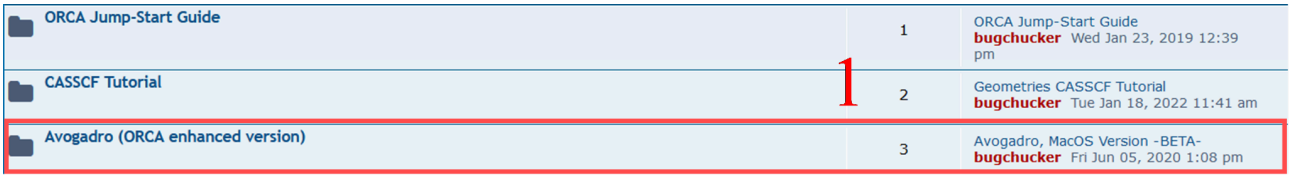
ORCA 5.0.4, MacOS X, Arm64 (Accelerate), .tar.xz Archive Linked against OpenMPI 4.1.1 orca_5_0_4_macosx_arm64_openmpi411.tar.xz Linked against Apple Accelerate Framework. Minimum OS requirement: MacOS 12.3	202.1 MiB	22 • 1284
ORCA 5.0.4, MacOS X, Arm64 (OpenBLAS), .tar.xz Archive Linked against OpenMPI 4.1.1 orca_5_0_4_macosx_arm64_openblas_openmpi411.tar.xz Linked against OpenBLAS Minimum OS requirement: MacOS 12.3	214.79 MiB	4 • 280
ORCA 5.0.4, MacOS X 11.0 up, Arm64 (Accelerate), .tar.xz Archive (SERIAL only!) orca_5_0_4_macosx11.0_arm64.tar.xz Compatibility version for MacOS X, linked against Apple Accelerate Framework. Minimum OS requirement: MacOS 11.0 Does only contain the serial version!	120.86 MiB	2 • 78
ORCA 5.0.4, MacOS X, Intel, .tar.xz Archive Linked against OpenMPI 4.1.1 orca_5_0_4_macosx_intel_openmpi411.tar.xz Linked against Apple Accelerate Framework. Minimum OS requirement: MacOS 12.3	243.94 MiB	8 • 634
ORCA 5.0.4, MacOS X 10.7 up, Intel (Accelerate), .tar.xz Archive (SERIAL only!) orca_5_0_4_macosx10.7_intel.tar.xz Compatibility version for MacOS X, linked against Apple Accelerate Framework. Minimum OS requirement: MacOS 10.7 Does only contain the serial version!	140.55 MiB	15 • 449

Note that in each download section, you will find complementary information listed below the software name, version, and operating system, regardless of the MPI library you choose.

2.2 Visualization Software

In order to visualize ORCA 5 outputs you will need to download the Avogadro enhanced version from ORCA Forum.

1. In the download section head to “Avogadro (ORCA enhanced version)”.



2. Enhanced Avogadro currently only has versions for Windows and macOS. However, you might be able to run the Windows version on your Linux machine using the Wine package. Documentation for installing Wine on Linux can be found on this page. Windows users must download the version with the “BETA” tag.

Avogadro, Windows Version -BETA- ORCA enhanced Avogadro version, able to read newer ORCA output files This version should be considered BETA status	17.21 MiB	92 • 16098
Avogadro, MacOS Version -BETA- ORCA enhanced Avogadro version, able to read newer ORCA output files This version should be considered BETA status	51.55 MiB	18 • 3121
Avogadro, Windows Version Enhanced Avogadro version, able to process ORCA 4.1 ouput files	10.11 MiB	21 • 9333

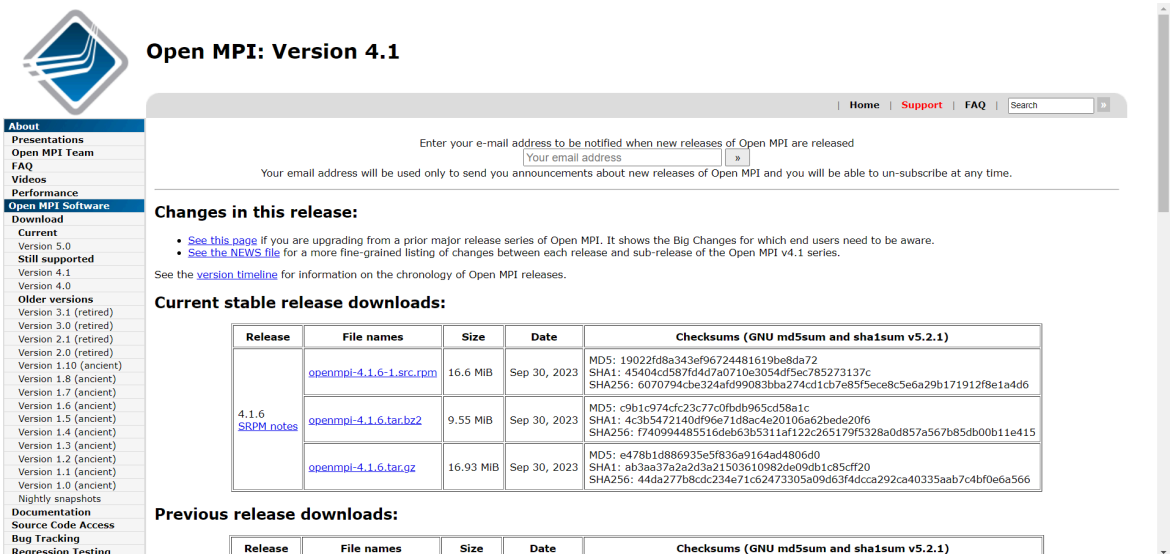
2.3 MPI Library

Heavy calculations in computational chemistry often require parallel processing to reduce time and maximize software efficiency. Unlike many commercial programs, ORCA has no limit on the number of CPUs for parallel jobs. Linux and macOS versions of ORCA work with the OpenMPI

library, while Windows requires Microsoft MPI. As mentioned earlier, each ORCA version is compatible with specific MPI library versions. This information is provided below the download section for each ORCA version. Here you will find download links for appropriate MPI packages depending on your operating system for ORCA 5.0.4.

a. OpenMPI

1. ORCA 5.0.4 in Linux and MacOS use OpenMPI 4.1.1. To download it first, head to the OpenMPI. Version 4.1 website.



Open MPI: Version 4.1

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Version 1.8 (ancient)
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Version 1.6 (ancient)
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Version 1.0 (ancient)
Nightly snapshots
Documentation
Source Code Access
Bug Tracking
Regression Testing

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Enter your e-mail address to be notified when new releases of Open MPI are released
Your email address »
Your email address will be used only to send you announcements about new releases of Open MPI and you will be able to un-subscribe at any time.

Changes in this release:

- See this page if you are upgrading from a prior major release series of Open MPI. It shows the Big Changes for which end users need to be aware.
- See the NEWS file for a more fine-grained listing of changes between each release and sub-release of the Open MPI v4.1 series.

See the version timeline for information on the chronology of Open MPI releases.

Current stable release downloads:

Release	File names	Size	Date	Checksums (GNU md5sum and sha1sum v5.2.1)
4.1.6 SRPM notes	openmpi-4.1.6-1.src.rpm	16.6 MiB	Sep 30, 2023	MD5: 19022fd8a343ef96724481619be8da72 SHA1: 45404cd587fd4d7a0710e3054df5ec785273137c SHA256: 6070794cbe324afd99083bba274cd1cb7e85f5ece8c5e6a29b171912f8e1a4d6
	openmpi-4.1.6.tar.bz2	9.55 MiB	Sep 30, 2023	MD5: c9b1c974cfc23c77c0fbdb965cd58a1c SHA1: 4c3b5472140df96e71d8ac4e20106a62bede20f6 SHA256: f740994485516deb63b5311af122c265179f5328a0d857a567b85db00b11e415
	openmpi-4.1.6.tar.gz	16.93 MiB	Sep 30, 2023	MD5: e478b1d886935e5f836a9164ad4806d0 SHA1: ab3aa37a2a2d3a21503610982de09db1c85cff20 SHA256: 44da277b8cdc234e71c62473305a09d63f4dcca292ca40335aab7c4bf0e6a566

Previous release downloads:

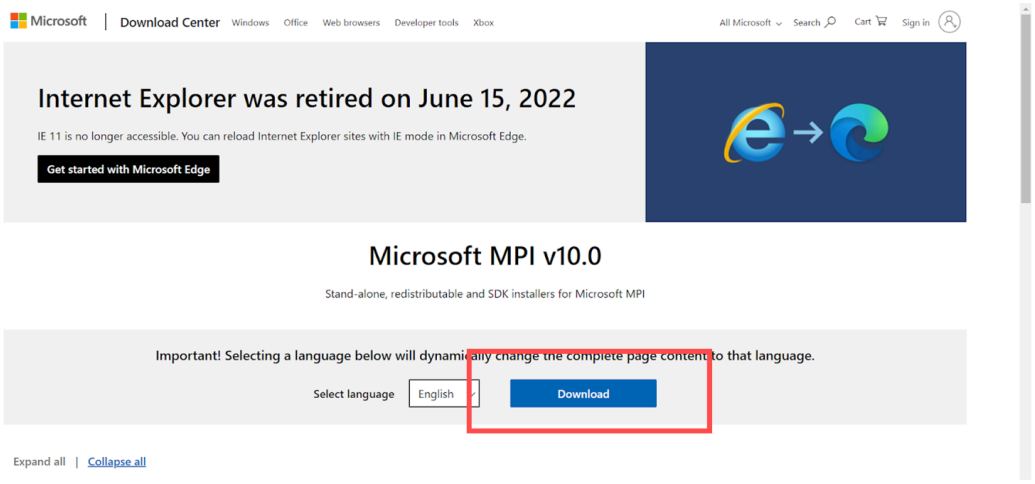
Release	File names	Size	Date	Checksums (GNU md5sum and sha1sum v5.2.1)

2. Scroll down until you find the 4.1.1 release. The version has no difference but their compression algorithm. For the sake of this installation guide please download the ".tar.gz" file.

4.1.1 SRPM notes	openmpi-4.1.1-1.src.rpm	16.49 MiB	Apr 24, 2021	MD5: 942596a08a6d8a986caacb118add584b SHA1: 5014439072c0fadba77e7fb83c375311f83d68dd SHA256: 86adb74195421eec32a1694e1f56b1071402d676c1517a4da5f62bdafc8e955c
	openmpi-4.1.1.tar.bz2	9.59 MiB	Apr 24, 2021	MD5: 9aa7cb64a8b1a773cac719e700d5bb2a SHA1: fa4dc97da18c8c26d5aadb85262a0f2d52b1aa90 SHA256: e24f7a778bd11a71ad0c14587a7f5b00e68a71aa5623e2157bafee3d44c07cda
	openmpi-4.1.1.tar.gz	16.85 MiB	Apr 24, 2021	MD5: 8239df775478285fb14edf37d02f5bfa SHA1: eb6b60162f777a5149ac3724acb2cb0c8e073e2a SHA256: d80b9219e80ea1f8bcfe5ad921bd9014285c4948c5965f4156a3831e60776444

b. Microsoft MPI

For parallel calculations on Windows, ORCA 5.0.4 needs Microsoft MPI 10.0.1. You can get the installer from the Microsoft webpage.



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IE 11 is no longer accessible. You can reload Internet Explorer sites with IE mode in Microsoft Edge.

Get started with Microsoft Edge

Microsoft MPI v10.0

Stand-alone, redistributable and SDK installers for Microsoft MPI

Important! Selecting a language below will dynamically change the complete page content to that language.

Select language English Download

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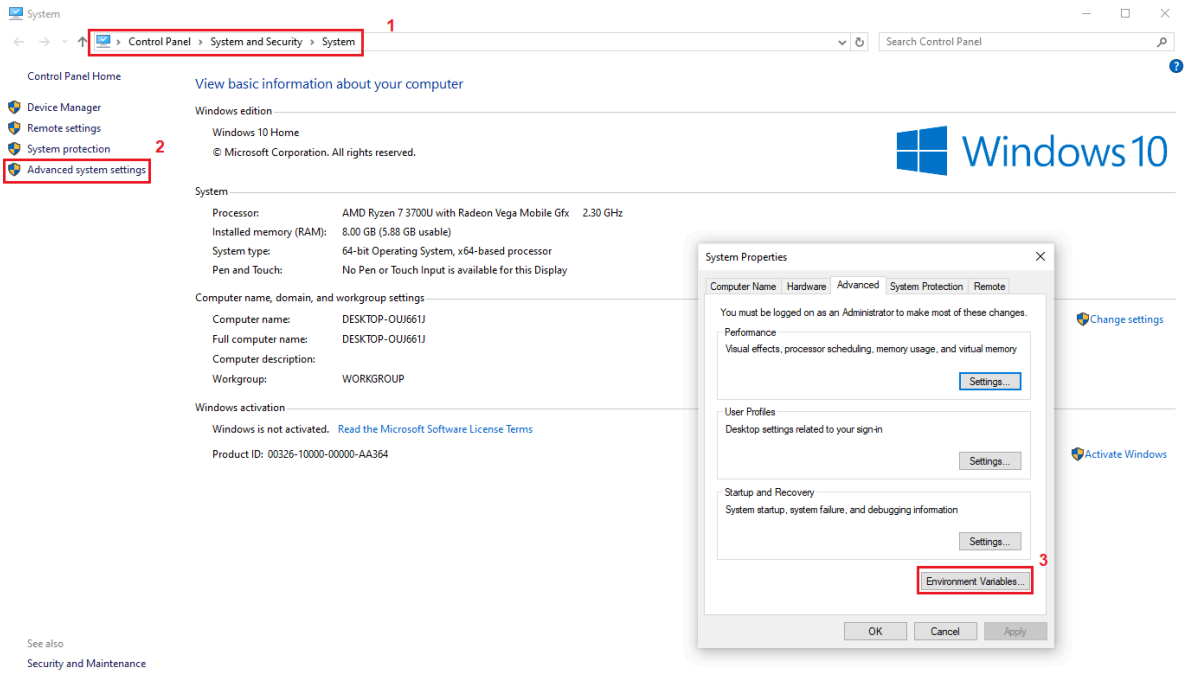
3. Installation

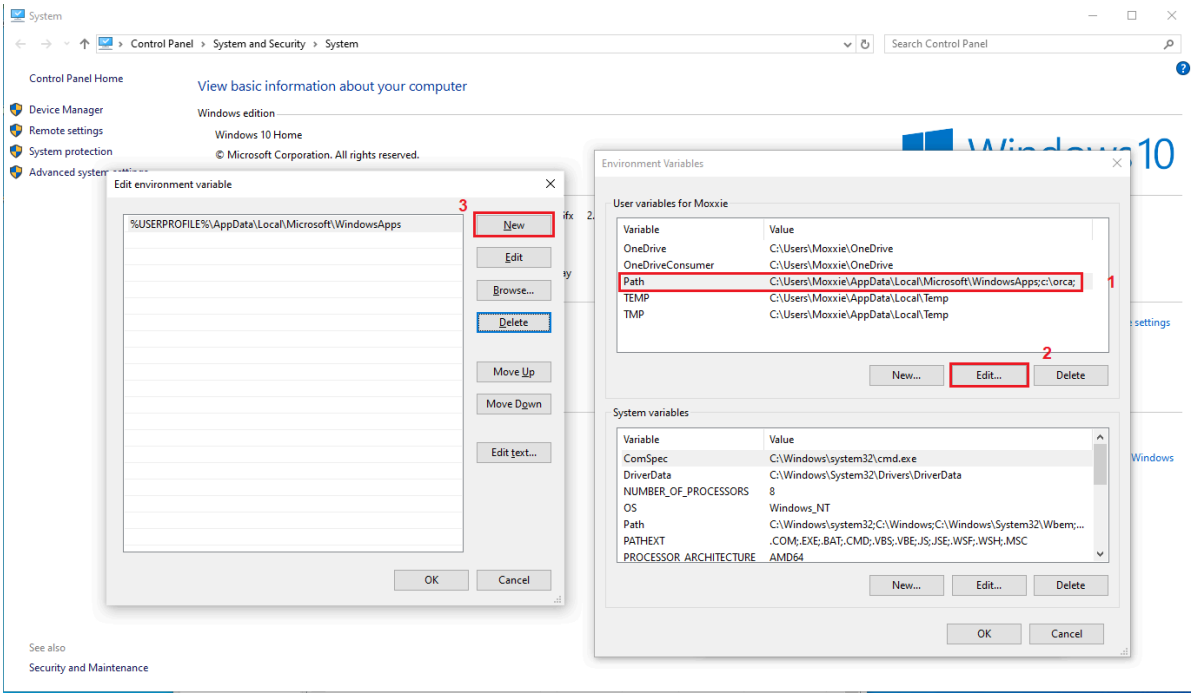
3.1 ORCA

a. Windows

1. Extract all the files into the same folder. It is better to have ORCA installed in a straightforward location rather than nested folders. The nested folder can cause problems during the installation.
2. We are going to assume that the installation will happen at the “C:\ORCA_504”. You can adjust the rest of the instructions for your desired location.
3. We need to set the PATH variable for ORCA. To do so navigate to Control Panel >System and Security>System >Advanced System Settings. Alternatively you can press Windows key and search for “Edit The System Environment Variables”.



4. In the opened menu select PATH then click on the edit button. In the new window click on the New button and type ORCA's location (in this tutorial "C:\ORCA_504") then press Ok.



5. Now your orca is installed successfully and you can access it in the terminal by just typing ORCA without specifying the full path. We will get to testing and more in the next section.

To learn more about the Windows command line you can check this webpage.

b. Linux

1. Extract the archive, rename the directory to "orca" and move to your user home folder (~).
2. Open a new Terminal window (ctrl+alt+T).
3. Paste the following text (environment variable setting) into the Terminal window and press Enter. If you use any shell interpreter other than bash, change it to your own (e.g.,~/.bashrc → ~/.zshrc):

```
echo 'export PATH="$HOME/orca:$PATH"'>> ~/.bashrc
```

```
echo 'export LD_LIBRARY_PATH= "$HOME/orca:$LD_LIBRARY_PATH"'  >> ~/.bashrc
```

```
source ~/.bashrc
```

Nothing will happen but now "orca" is available as a command in the command line. Type 'which orca' in the shell to confirm that ORCA is now available in your path. If this did not work the first time, do not repeat it but edit the ".bashrc" file manually using a text editor.

To learn more about the Linux command line you can check this webpage.

c. MacOS

1. Extract the archive, rename the directory to "orca" and move to /Applications folder. Note: ORCA can in principle be anywhere but here we choose to put it in /Applications.
2. Open the Terminal Program (under /Applications/Utilities).
    - Mac OS 10.15 (Catalina) and newer:

```
echo 'export PATH="/Applications/orca:$PATH"' >> ~/.zshrc
```

```
echo 'export LD_LIBRARY_PATH=
"/Applications/orca:$LD_LIBRARY_PATH"'  >> ~/.zshrc
```

```
source ~/.zshrc
```

    - Older Mac OS versions:

```
echo 'export PATH="/Applications/orca:$PATH"'>> ~/.bash_profile
```

```
echo 'export LD_LIBRARY_PATH=
"/Applications/orca:$LD_LIBRARY_PATH"' >> ~/.bash_profile
```

```
source ~/.bash_profile
```

3. Nothing will happen but now "orca" is available as a command in the command line.
4. New Mac OS versions have a security feature that prevents ORCA and its subprograms from running directly. To override this feature, cd to the ORCA directory in the Terminal and run the following xattr command:

```
cd /Applications/orca
```

```
xattr -d com.apple.quarantine *
```

To learn more about the MacOS command line check this webpage.

3.2 MPI Library

a. Windows

Install the Microsoft MPI library using the standard procedure for window “exe” programs.

b. Linux

1. Create a temporary directory for compiling OpenMPI. You can do this in a terminal by typing

```
mkdir $HOME/local/src
```

2. Move the downloaded file to the directory just created.

```
mv $HOME/Downloads/openmpi-1.4.4.tar.gz $HOME/local/src/
```

3. Extract the package using:

```
tar -xf openmpi-1.4.4.tar.gz
```

4. Go into the source directory

```
cd openmpi-1.4.4
```

5. Configure, compile, and install by executing the following commands

```
./configure --prefix=$HOME/opt/openmpi
make all
make install
```

6. Remove the temporary directories:

```
cd
rm $HOME/local/src/openmpi-1.4.4.tar.bz2
rm -r $HOME/local/src/openmpi-1.4.4
```

7. To use MPI you will have to adapt your PATH and LD_LIBRARY_PATH environment variable:

```
echo "export PATH=\$PATH:\$HOME/opt/openmpi/bin" >> $HOME/.bashrc
echo "export
LD_LIBRARY_PATH=\$LD_LIBRARY_PATH:\$HOME/opt/openmpi/lib" \>>
$HOME/.bashrc
```

c. MacOS

Installing OpenMPI for MacOS follows the same steps in the Linux system. Please see previous section.

3.3 Avogadro

a. Windows

Install the enhanced Avogadro using the standard procedure for window “exe” programs.

b. Linux

Install the Windows version using the Wine package. Note that this strategy does not work on all Linux distributions.

c. MacOS

Install the enhanced Avogadro using the standard procedure for MacOS programs.

4. Test ORCA, Hello Water!

To verify your ORCA installation is correct, follow these steps to perform a Hartree-Fock calculation on the water molecule using the def2-SVP basis set.

a. Serial run

1. Create a new folder named "H2O_S".
2. Create an input file for your ORCA job using your preferred text editor. Write the following lines:

```
!HF def2-SVP

* xyz 0 1
O    0.0000    0.0000    0.0626
H   -0.7920    0.0000   -0.4973
H    0.7920    0.0000   -0.4973
*
```

3. Save the file in “H2O_S” folder using this name: H2O.inp
4. Open your terminal, navigate to “H2O_S” folder. Run the following command:

```
orca water.inp
```

If the installation is successful, you'll see output in your terminal indicating the job is running and ends with the following lines:

```
Timings for individual modules:

Sum of individual times         ...        2.180 sec (=   0.036 min)
GTO integral calculation        ...        0.289 sec (=   0.005 min)  13.3 %

SCF iterations                  ...        1.891 sec (=   0.032 min)  86.7 %

                            ****ORCA TERMINATED NORMALLY****
TOTAL RUN TIME: 0 days 0 hours 0 minutes 2 seconds 577 msec
```

b. Parallel run

1. Create a new folder named “H2O_P”.
2. Create an input file for your ORCA job using your preferred text editor. Write the following lines:

```
!PAL2
!HF def2-SVP

* xyz 0 1
O    0.0000    0.0000    0.0626
H   -0.7920    0.0000   -0.4973
H    0.7920    0.0000   -0.4973
*
```

3. Save the file in “H2O_P” folder using this name: H2O.inp
4. Open your terminal, navigate to the “H2O_P” folder. Run the following command, Note that in parallel jobs you should provide the full path of ORCA in terminal :

```
C:\ORCA_504\orca water.inp
```

If the installation is successful, you'll see output in your terminal indicating the job is running and ends with the following lines:

```
Timings for individual modules:

Sum of individual times         ...        1.628 sec (=   0.027 min)
GTO integral calculation        ...        0.425 sec (=   0.007 min)  26.1 %
SCF iterations                  ...        1.203 sec (=   0.020 min)  73.9 %
                            ****ORCA TERMINATED NORMALLY****
TOTAL RUN TIME: 0 days 0 hours 0 minutes 2 seconds 181 msec
```