Installation Manual

TCCW Foundation

The Fifth Winter School of Computational Chemistry
Sharif University of Technology, Azadi Ave., Tehran, Iran

Tuesday 11th February, 2025

Contents

1 Introduction

This document provides a step-by-step guide for installing the software/hardware.

2 System Requirements

For the successful installation of softwares used in the Winter School, the system should meet the following minimum requirements: at least 8 GB of RAM for optimal performance, though 16 GB is recommended for handling larger systems. A modern operating system, such as Windows 10/11, macOS 10.14 or later, or a Linux distribution (Ubuntu 20.04 or higher), is necessary. Ensure that sufficient disk space is available , with at least 20 GB free for installation and dependencies. Additionally, a stable internet connection is required for downloading software packages and updates.

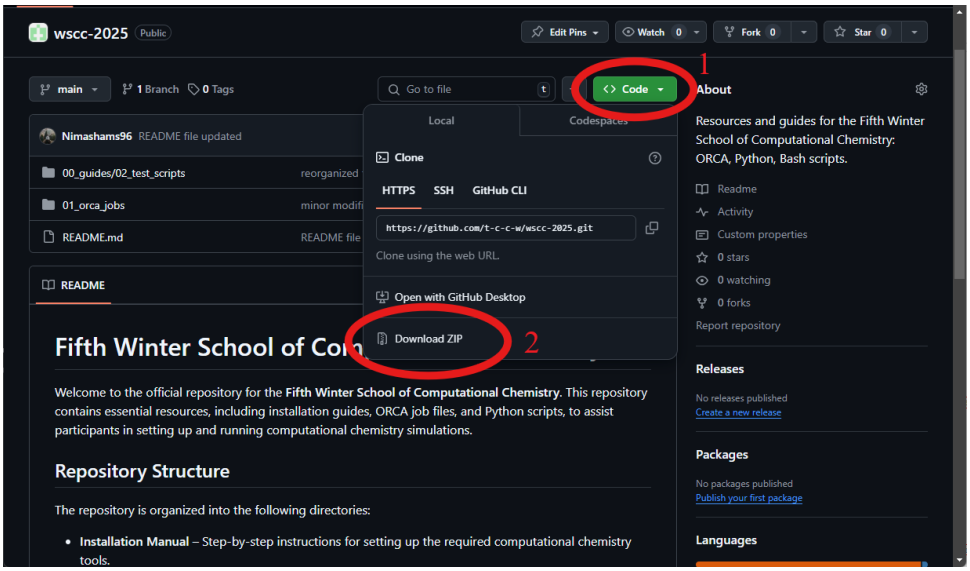
3 Github Repository

To access all materials for the Winter School, we have created a GitHub repository. You can download the materials in two ways:

1. **Using Git Bash**: Run the following command:

   ```
   git clone https://github.com/t-c-c-w/wscc-2025
   ```

2. **Manually**: Visit github.com/t-c-c-w/wscc-2025, and download the ZIP file by following the instructions in the image below:



4 VSCode

Visual Studio Code (VSCode) is a powerful and versatile integrated development environment (IDE) that supports multiple programming languages, including Python, C++, and even LaTeX for document preparation. It is widely used for tasks ranging from

software development to data analysis, making it an excellent choice for computational chemists. VSCode is free, open-source, and backed by a large community, offering extensive extensions and tools to enhance productivity. Its flexibility, lightweight design, and rich ecosystem make it a go-to editor for scientific computing and programming.

4.1 Downloading the Softwares

To download VSCode, visit the official download page: code.visualstudio.com/download Select the appropriate version for your operating system and proceed with the download.

4.2 Installating the Softwares

4.2.1 Linux

To install VSCode on Linux, specifically on Debian-based distributions, follow these steps:

1. Open a terminal.
2. Run the following command to install the VSCode `.deb` package:

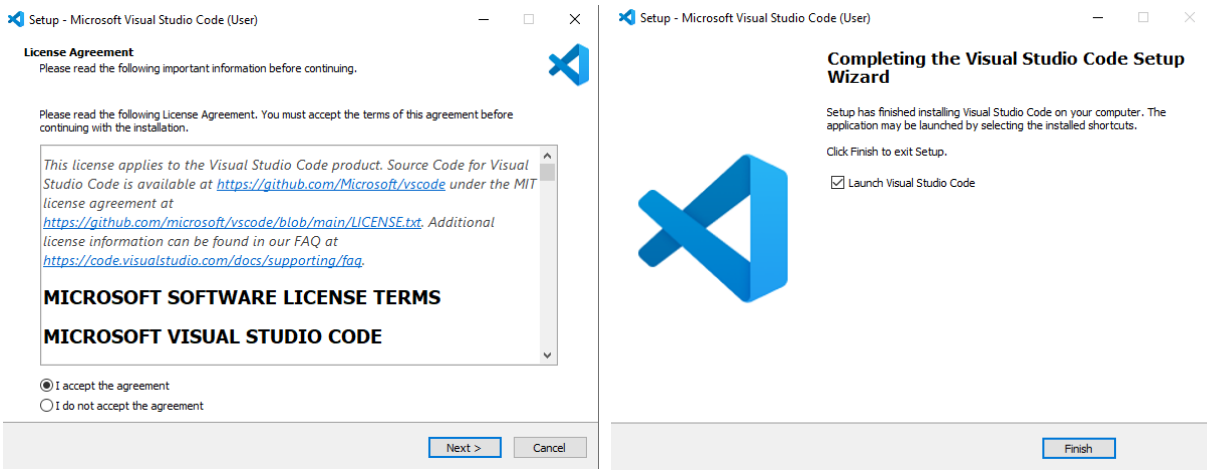
```
sudo dpkg -i <full path of the ".deb" file,
    e.g.: /home/ubuntu/Downloads/code_1.97.deb >
```

3. If you are using Ubuntu 20.04 or later, the installation should proceed without issues.
4. For older Ubuntu versions, you may need to install an older VSCode version. Install VSCode using Snap:

```
sudo snap install --classic code
```

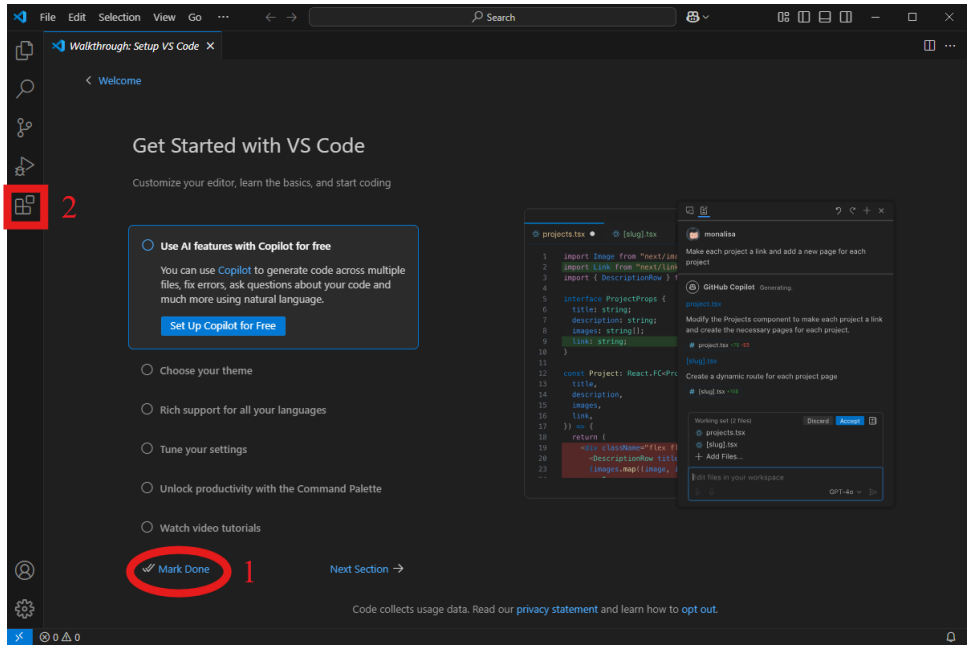
4.2.2 Windows

To install VSCode on Windows, run the setup file and follow the standard installation procedure.

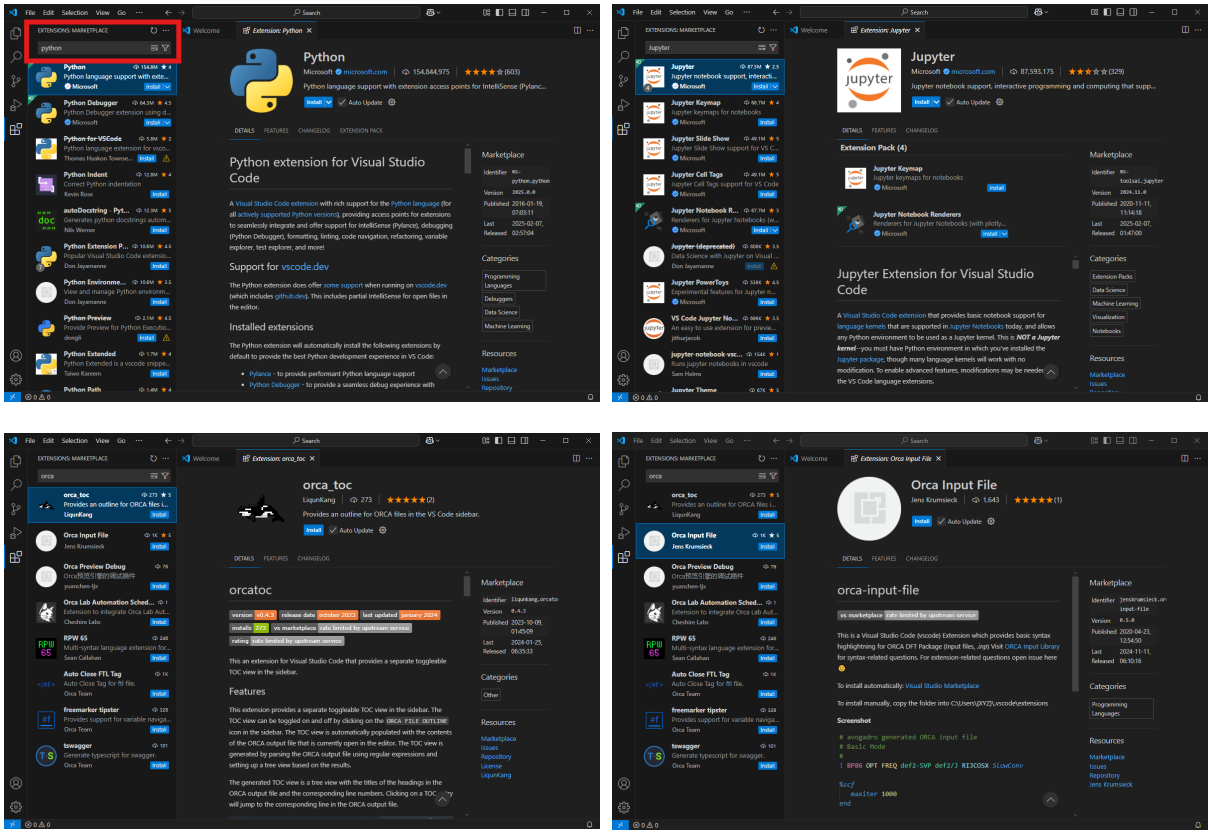


4.3 Installating the Extensions

After installing the VSCode successfully open the software, and follow the setps like the picture below to open "Extensions" store.



In the search box you can search for your desired extensions, for the sake of this winter school you need to search and install these four extensions: "Python", "Jupyter", "orca_toc", and "Orca Input File".

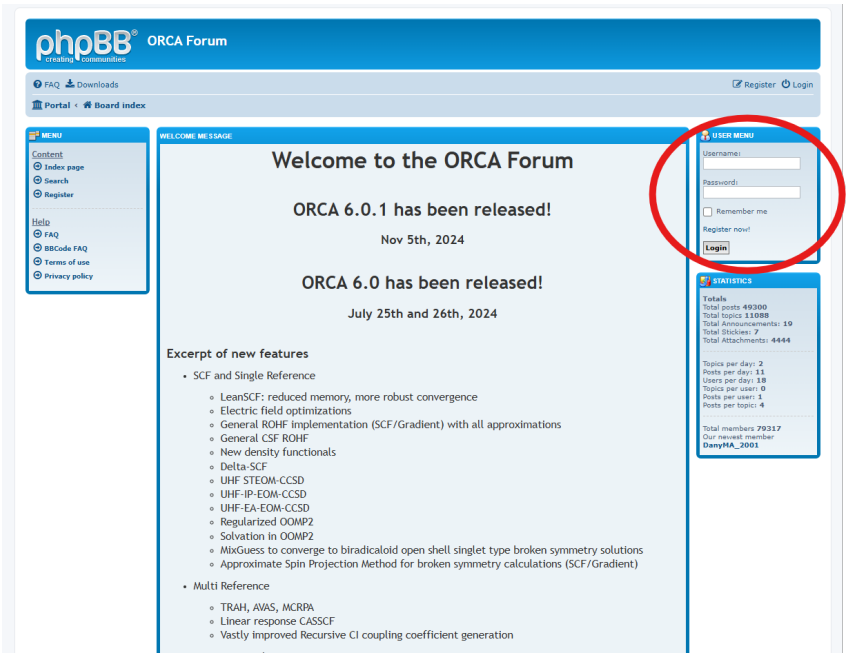


5 Orca

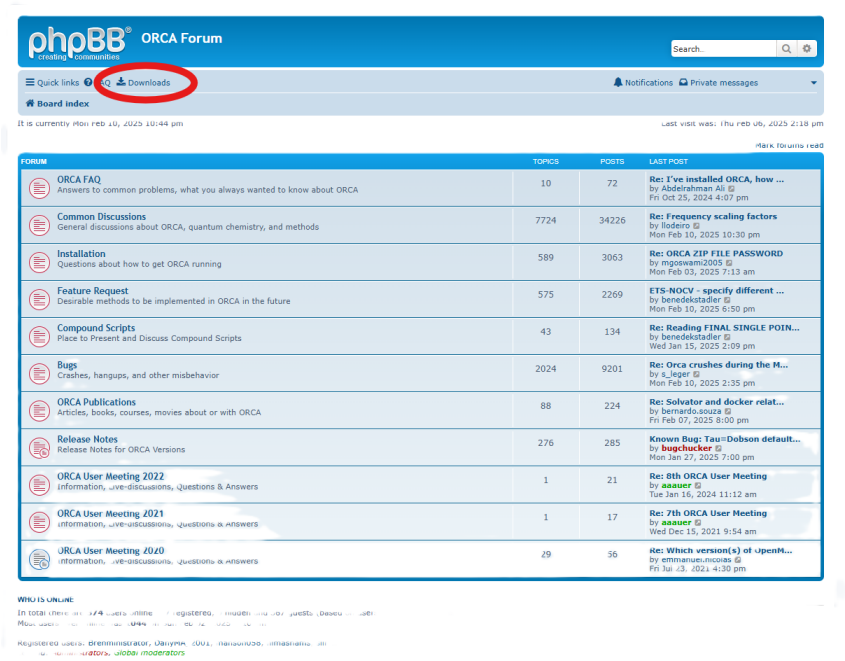
5.1 Downloading the Softwares

To download ORCA, follow these steps:

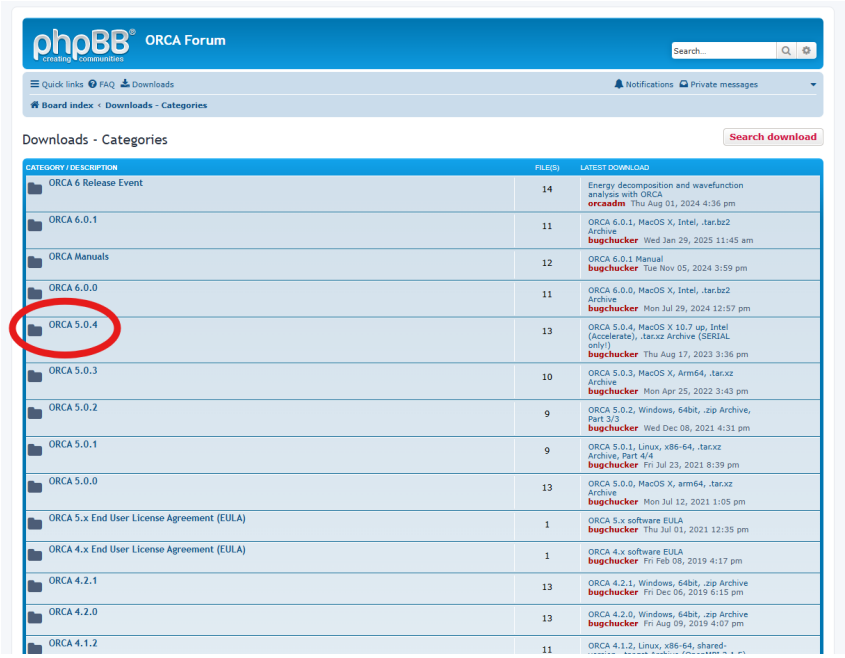
1. Visit the ORCA forum webpage: orcaforum.kofo.mpg.de.
2. Use the panel on the right side to log in to your account. If you have not registered before, create an account and then sign in.



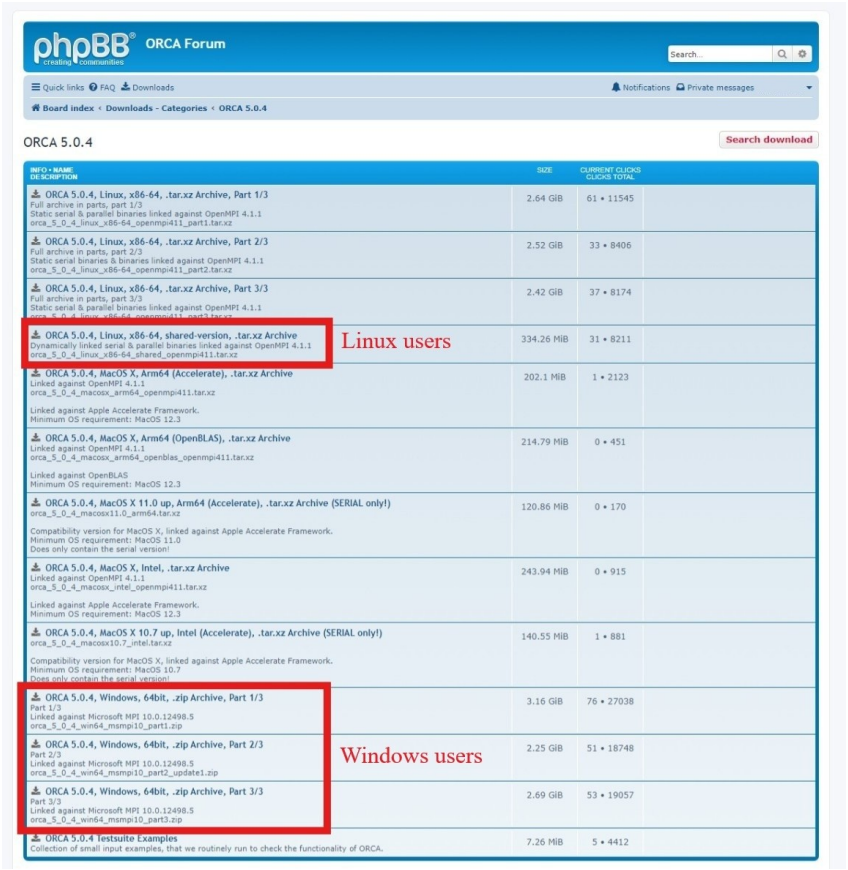
3. Navigate to the “Downloads” section.



4. Select ORCA version 5.0.4.



5. Download the appropriate version for your operating system.


phpBB creating communities
ORCA Forum
Search...
Quick links FAQ Downloads
Notifications Private messages
Board index ‹ Downloads - Categories ‹ ORCA 5.0.4
ORCA 5.0.4
Search download
INFO • NAME
DESCRIPTION
SIZE
CURRENT CLICKS
CLICKS TOTAL
ORCA 5.0.4, Linux, x86-64, .tar.xz Archive, Part 1/3
Full archive in parts, part 1/3
Static serial & parallel binaries linked against OpenMPI 4.1.1
orca_5_0_4_linux_x86-64_openmpi411_part1.tar.xz
2.64 GiB
61 • 11545
ORCA 5.0.4, Linux, x86-64, .tar.xz Archive, Part 2/3
Full archive in parts, part 2/3
Static serial binaries & binaries linked against OpenMPI 4.1.1
orca_5_0_4_linux_x86-64_openmpi411_part2.tar.xz
2.52 GiB
33 • 8406
ORCA 5.0.4, Linux, x86-64, .tar.xz Archive, Part 3/3
Full archive in parts, part 3/3
Static serial & parallel binaries linked against OpenMPI 4.1.1
2.42 GiB
37 • 8174
ORCA 5.0.4, Linux, x86-64, shared-version, .tar.xz Archive
Dynamically linked serial & parallel binaries linked against OpenMPI 4.1.1
orca_5_0_4_linux_x86-64_shared_openmpi411.tar.xz
Linux users
334.26 MiB
31 • 8211
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
1 • 2123
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
0 • 451
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
0 • 170
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
0 • 915
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
1 • 881
ORCA 5.0.4, Windows, 64bit, .zip Archive, Part 1/3
Part 1/3
Linked against Microsoft MPI 10.0.12498.5
orca_5_0_4_win64_mspi10_part1.zip
3.16 GiB
76 • 27038
ORCA 5.0.4, Windows, 64bit, .zip Archive, Part 2/3
Part 2/3
Linked against Microsoft MPI 10.0.12498.5
orca_5_0_4_win64_mspi10_part2_update1.zip
Windows users
2.25 GiB
51 • 18748
ORCA 5.0.4, Windows, 64bit, .zip Archive, Part 3/3
Part 3/3
Linked against Microsoft MPI 10.0.12498.5
orca_5_0_4_win64_mspi10_part3.zip
2.69 GiB
53 • 19057
ORCA 5.0.4 Testsuite Examples
Collection of small input examples, that we routinely run to check the functionality of ORCA.
7.26 MiB
5 • 4412

8 Support and Contact Information

Provide details for contacting support.