

Installation Manual



TCCW Foundation

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

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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.

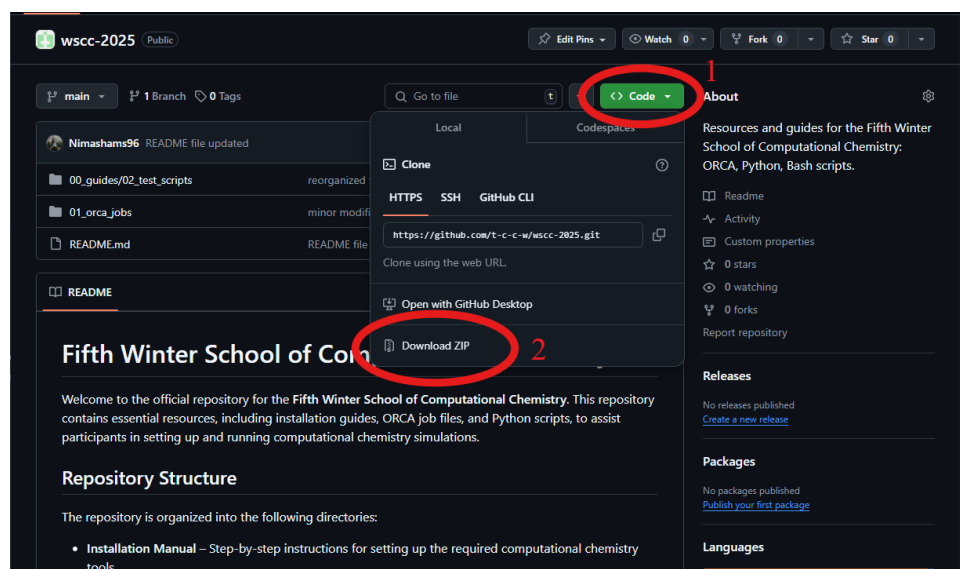
3 Github Repository

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/wsc-2025
```

2. **Manually:** Visit github.com/t-c-c-w/wsc-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 Installing 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:

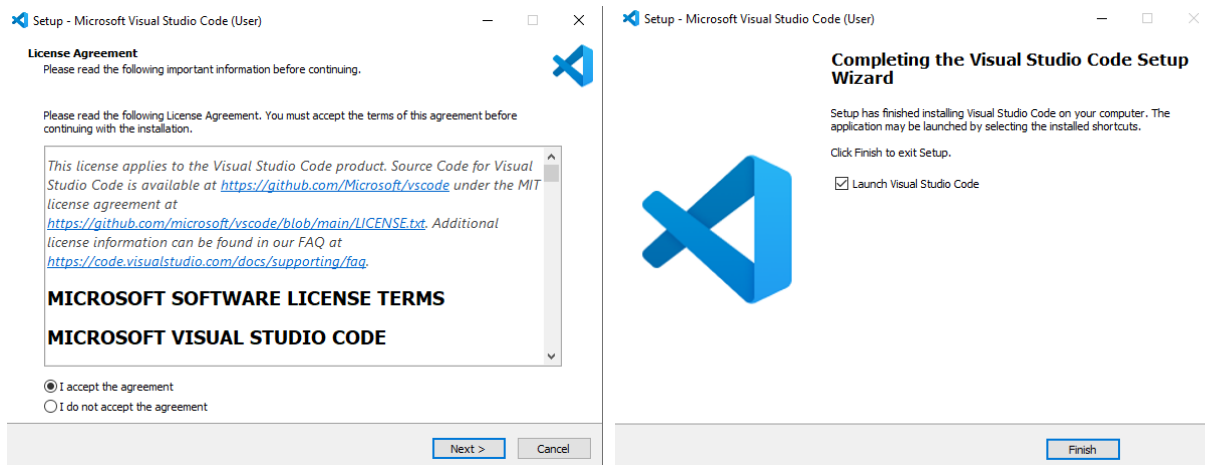
```
sudo dpkg -i <full path of the ".deb" file,  
e.g.: /home/ubuntu/Downloads/code_1.97.deb >
```

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
```

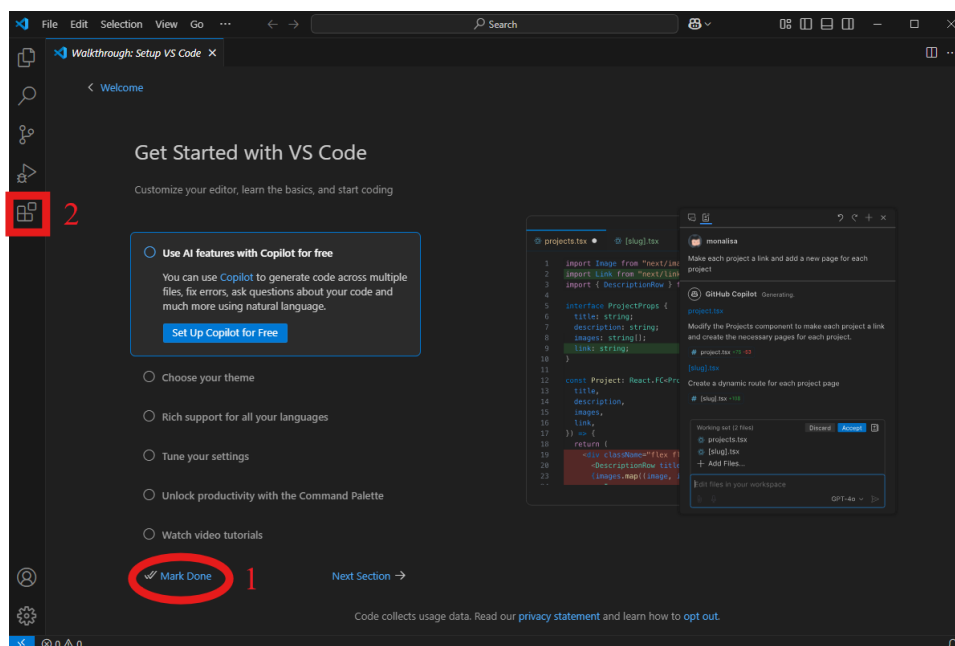
4.2.2 Windows

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

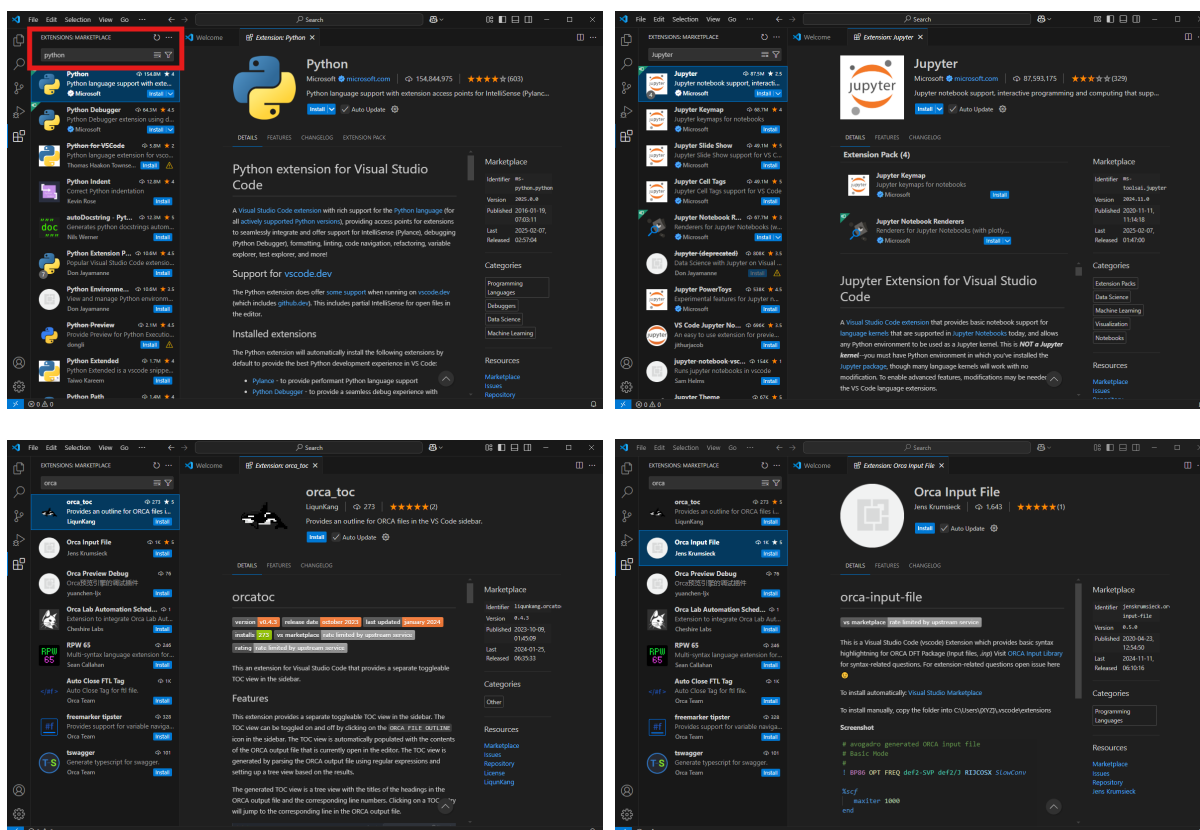


4.3 Installing the Extensions

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.

The image is a screenshot of the ORCA Forum website. The page has a blue header with the 'phpBB ORCA Forum' logo. Below the header, there is a navigation bar with links for 'Downloads', 'Portal', and 'Board index'. The main content area features a welcome message and two announcements: 'ORCA 6.0.1 has been released!' dated Nov 5th, 2024, and 'ORCA 6.0 has been released!' dated July 25th and 26th, 2024. Below these announcements is a section titled 'Excerpt of new features' with a bulleted list of features. On the right side of the page, there is a 'USER MENU' panel with a red circle around the login fields. The login fields include 'Username:', 'Password:', and a 'Remember me' checkbox. Below these fields are links for 'Register now!' and 'Login'. To the right of the login panel is a 'STATISTICS' panel showing various forum statistics.

3. Navigate to the “Downloads” section.


The screenshot shows the phpBB ORCA Forum homepage. The top navigation bar includes links for 'Quick links', 'FAQ', and 'Downloads'. The 'Downloads' link is circled in red. Below the navigation bar, there is a 'Board index' link and a status bar indicating the current time and date. The main content area displays a list of forum topics with columns for 'FORUM', 'TOPICS', 'POSTS', and 'LAST POST'. The topics listed include ORCA FAQ, Common Discussions, Installation, Feature Request, Compound Scripts, Bugs, ORCA Publications, Release Notes, ORCA User Meeting 2022, ORCA User Meeting 2021, and ORCA User Meeting 2020. At the bottom, there is a section for 'WHO IS ONLINE' showing the number of users online and a list of registered users.

4. Select ORCA version 5.0.4.

The screenshot shows the 'Downloads - Categories' page on the phpBB ORCA Forum. The page has a search bar and a 'Search download' button. Below the search bar, there is a table with columns for 'CATEGORY / DESCRIPTION', 'FILES', and 'LATEST DOWNLOAD'. The table lists various ORCA versions and manuals. The 'ORCA 5.0.4' category is circled in red. The table also includes links to download the files and information about the latest download.

CATEGORY / DESCRIPTION	FILES	LATEST DOWNLOAD
ORCA 6 Release Event	14	Energy decomposition and wavefunction analysis with ORCA orcaadm Thu Aug 01, 2024 4:36 pm
ORCA 6.0.1	11	ORCA 6.0.1, MacOS X, Intel, tar.bz2 Archive bugchucker Wed Jan 29, 2025 11:45 am
ORCA Manuals	12	ORCA 6.0.1 Manual bugchucker Tue Nov 05, 2024 3:59 pm
ORCA 6.0.0	11	ORCA 6.0.0, MacOS X, Intel, tar.bz2 Archive bugchucker Mon Jul 29, 2024 12:57 pm
ORCA 5.0.4	13	ORCA 5.0.4, MacOS X 10.7 up, Intel (Accelerate), tar.xz Archive (SERIAL only) bugchucker Thu Aug 17, 2023 3:36 pm
ORCA 5.0.3	10	ORCA 5.0.3, MacOS X, Arm64, tar.xz Archive bugchucker Mon Apr 25, 2022 3:43 pm
ORCA 5.0.2	9	ORCA 5.0.2, Windows, 64bit, zip Archive, Part 3/3 bugchucker Wed Dec 08, 2021 4:31 pm
ORCA 5.0.1	9	ORCA 5.0.1, Linux, x86-64, tar.xz Archive, Part 4/4 bugchucker Fri Jul 23, 2021 6:39 pm
ORCA 5.0.0	13	ORCA 5.0.0, MacOS X, arm64, tar.xz Archive bugchucker Mon Jul 12, 2021 1:05 pm
ORCA 5.x End User License Agreement (EULA)	1	ORCA 5.x software EULA bugchucker Thu Jul 01, 2021 12:35 pm
ORCA 4.x End User License Agreement (EULA)	1	ORCA 4.x software EULA bugchucker Fri Feb 08, 2019 4:17 pm
ORCA 4.2.1	13	ORCA 4.2.1, Windows, 64bit, zip Archive bugchucker Fri Dec 06, 2019 6:15 pm
ORCA 4.2.0	13	ORCA 4.2.0, Windows, 64bit, zip Archive bugchucker Fri Aug 09, 2019 4:07 pm
ORCA 4.1.2	11	ORCA 4.1.2, Linux, x86-64, shared- bugchucker Thu Aug 01, 2019 4:07 pm

5. Download the appropriate version for your operating system.



ORCA Forum














[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	CLOCKS 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 orca_5_0_4_linux_x86-64_openmpi411_part3.tar.xz	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	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_msmmpi10_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_msmmpi10_part2_update1.zip	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_msmmpi10_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	

Linux users

Windows users

5.2 Installing the Softwares

5.2.1 Linux

5.2.2 Windows

5.3 Verifying the Installation

6 Parallelization Packages (Optional)

6.1 Downloading the Softwares

6.2 Installing the Softwares

6.2.1 Linux

6.2.2 Windows

6.3 Verifying the Installation

7 Python

7.1 Downloading the Softwares

7.2 Installing the Softwares

7.2.1 Linux

7.2.2 Windows

7.3 Verifying the Installation

8 Support and Contact Information

Provide details for contacting support.