

Installation of Gromacs on Windows 10 OS

Spoken Tutorial Project

<https://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



Learning Objectives

- ▶ Install Ubuntu 20.04 LTS app on Windows 10 OS



Learning Objectives

- ▶ **Install Ubuntu 20.04 LTS app on Windows 10 OS**
- ▶ **Install programs essential to build Gromacs**



Learning Objectives

- ▶ **Install Ubuntu 20.04 LTS app on Windows 10 OS**
- ▶ **Install programs essential to build Gromacs**
- ▶ **Download and build Gromacs 2021.2**



Learning Objectives



Learning Objectives

- ▶ Test the installation with the **help** command



Learning Objectives

- ▶ Test the installation with the **help** command
- ▶ About alternate installation method with the **sudo apt-get** command



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Installation may take few hours depending on the hardware



System and Software Requirements



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► Windows 10 OS



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- ▶ **Windows 10 OS**
- ▶ **Google Chrome v92**



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- ▶ **Google Chrome v92**
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- ▶ **Gromacs 2021.2**



System and Software Requirements

- ▶ **Windows 10 OS**
- ▶ **Google Chrome v92**
- ▶ **Ubuntu 20.04 LTS app**
- ▶ **Gromacs 2021.2**
- ▶ **A working Internet connection**



System and Software Requirements



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- ▶ **64-bit architecture and 4GB RAM or higher are must for the installation**



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- ▶ **All the Windows OS updates must be completed**
- ▶ **Sufficient disk space must be available for software build**



Pre-requisites



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- ▶ **Learner must be familiar with basic computer skills**



Download link



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- ▶ The official website of Gromacs is <http://www.gromacs.org>



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- ▶ The software is available for Linux and Windows OS



Alternate Installation Method



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- ▶ Enter the command, `sudo apt-get update`
- ▶ Enter the user `sudo` password if prompted



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Then, enter the commands

- ▶ `sudo apt-get upgrade`
- ▶ `sudo apt-get install gromacs` **to complete the installation**



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- ▶ **The latest version of the software may not get installed with this method**
- ▶ **The version in the Linux OS repository will get installed**



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Summary

- ▶ **Installed Ubuntu 20.04 LTS app**
- ▶ **Installed essential programs to build Gromacs**
- ▶ **Downloaded and built Gromacs**
- ▶ **Tested the installation**
- ▶ **About alternate installation method**



Assignment



Assignment

- ▶ Go to the Gromacs website as seen here
<https://www.gromacs.org/>
- ▶ Go through the user support and documentation
- ▶ Read research papers of your choice which use Gromacs



About the Spoken Tutorial Project

- ▶ Watch the video available at https://spoken-tutorial.org/What_is_a_Spoken_Tutorial
- ▶ It summarises the Spoken Tutorial project



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- ▶ If you do not have good bandwidth, you can download and watch it



Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to contact@spoken-tutorial.org



Forum questions

- ▶ Questions in THIS Spoken Tutorial?
- ▶ Visit <https://forums.spoken-tutorial.org>
- ▶ Choose the minute and second where you have the question
- ▶ Explain your question briefly
- ▶ The Spoken Tutorial project will ensure an answer

You will have to register to ask questions



Acknowledgements

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