

# Solvate and Grompp Commands

**Spoken Tutorial Project**

**<https://spoken-tutorial.org>**

**National Mission on Education through ICT**

**<http://sakshat.ac.in>**

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# Learning Objectives



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- ▶ **Solvent input files with coordinates**



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- ▶ Solvent input files with coordinates
- ▶ Add solvent molecules to the system with `solvate` command



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- ▶ Add solvent molecules to the system with `solvate` command
- ▶ Open the solvated gro file in **VMD**



# Learning Objectives



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## ► About mdp file



# Learning Objectives

- ▶ **About** `mdp` file
- ▶ **Generate** `tpr` file with the `grompp` command





# System Requirements



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► **Ubuntu Linux v20.04 OS**



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- ▶ **Gromacs v2021.2**



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- ▶ **VMD 1.9.3**



# Pre-requisites



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



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To follow this tutorial,

- ▶ Learner must be familiar with basic computer skills
- ▶ For pre-requisite tutorials please visit this site

<https://www.spoken-tutorial.org>



# Code Files



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- ▶ The files used in this tutorial are provided in the **Code files** link



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- ▶ Make a copy and then use them while practising



# Summary

- ▶ Solvent input files containing coordinates
- ▶ Added solvent molecules with `solvate` command
- ▶ About `mdp` file



# Summary

- ▶ Opened the solvated `gro` file in `VMD`
- ▶ Generated a `tpr` file with the `grompp` command
- ▶ About `dump` command
- ▶ Added ions with the `genion` command





# Assignment



# Assignment

- ▶ **Use a PDB ID of another protein of your choice**
- ▶ **Practice the commands learnt in this tutorial**



# Assignment



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- ▶ From the [Gromacs](#) manual , read on the following file extensions
  - ▶ [top](#), [gro](#), [mdp](#), [tpr](#) and [itr](#)
- ▶ Create a table to keep track of which file gets generated in which step



# About the Spoken Tutorial Project

- ▶ Watch the video available at [https://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](https://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- ▶ It summarises the Spoken Tutorial project



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- ▶ It summarises the Spoken Tutorial project
- ▶ 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](mailto: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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