

Creating Input Files

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

- ▶ Flow chart to setup a MD run for a protein in a solvent box



Learning Objectives

- ▶ **Flow chart to setup a MD run for a protein in a solvent box**
- ▶ **Delete water molecules present in the starting pdb file**



Learning Objectives

- ▶ Flow chart to setup a MD run for a protein in a solvent box
- ▶ Delete water molecules present in the starting pdb file
- ▶ `pdb2gmx` command and syntax



Learning Objectives

- ▶ Flow chart to setup a MD run for a protein in a solvent box
- ▶ Delete water molecules present in the starting pdb file
- ▶ `pdb2gmx` command and syntax
- ▶ Generate `.gro` and `.top` files



Learning Objectives



Learning Objectives

► About selecting a force field



Learning Objectives

- ▶ **About selecting a force field**
- ▶ **Specify the size and shape of bounding box for MD**



Learning Objectives

- ▶ About selecting a force field
- ▶ Specify the size and shape of bounding box for MD
- ▶ `editconf` command



System Requirements



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To record this tutorial I am using,

▶ **Ubuntu Linux v20.04 OS**



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- ▶ **Firefox web browser v92**



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- ▶ **Gedit v3.36**
- ▶ **Gromacs v2021.2**



Pre-requisites



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



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- ▶ **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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- ▶ Please download and extract the files



Code Files

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- ▶ Please download and extract the files
- ▶ Make a copy and then use them while practising



File Path in Windows



File Path in Windows

- ▶ Windows users must find the path of this directory in Windows



File Path in Windows

- ▶ **Windows users must find the path of this directory in Windows**
- ▶ **Detailed instructions are provided with the tutorial**



File Path in Windows

- ▶ **Windows users must find the path of this directory in Windows**
- ▶ **Detailed instructions are provided with the tutorial**
- ▶ **Use this path when locating, opening or moving files, which are saved here**



Summary

- ▶ Steps in a MD run for a protein in a solvent box
- ▶ The `pdb2gmx` command and syntax
- ▶ About adding a force field
- ▶ Generated `.gro` and `.top` files
- ▶ About `editconf` command



Summary

- ▶ **Define the size of a bounding box**
- ▶ **Set the position of the molecule in the box**



Assignment



Assignment

- ▶ Use a PDB ID of another protein of your choice
- ▶ Practice the commands learnt in this tutorial
- ▶ Read publications of your choice which use [Gromacs](#)



Assignment



Assignment

- ▶ Go to the website seen below
<http://www.mdtutorials.com/gmx/>
- ▶ Choose a tutorial of your choice and read it



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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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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