

Production Run for Lysozyme

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

- ▶ **Complete 1ns production run for lysozyme**



Learning Objectives

- ▶ **Complete 1ns production run for lysozyme**
- ▶ **About timescales of motions**



Learning Objectives

- ▶ **Complete 1ns production run for lysozyme**
- ▶ **About timescales of motions**
- ▶ **Time taken for simulation**



Learning Objectives

- ▶ Complete 1ns production run for lysozyme
- ▶ About timescales of motions
- ▶ Time taken for simulation
- ▶ Load the `xtc` file for trajectory



Learning Objectives

- ▶ Complete 1ns production run for lysozyme
- ▶ About timescales of motions
- ▶ Time taken for simulation
- ▶ Load the `xtc` file for trajectory
- ▶ Calculate RMSD from trajectory



Learning Objectives



Learning Objectives

- ▶ **Save data to various output files**



Learning Objectives

- ▶ **Save data to various output files**
- ▶ **Align a frame in the trajectory with a reference molecule**



System Requirements



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- ▶ **Ubuntu Linux v20.04 OS**



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- ▶ **Gromacs v2021.2**



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- ▶ **Gromacs v2021.2**
- ▶ **VMD 1.9.3**
- ▶ **Gedit v3.36**



Pre-requisites



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To follow this tutorial,



Pre-requisites

To follow this tutorial,

- ▶ **Learner must be familiar with basics of Gromacs and VMD**



Pre-requisites

To follow this tutorial,

- ▶ Learner must be familiar with basics of Gromacs and VMD
- ▶ 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



Code Files

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- ▶ Please download and extract the files



Code Files

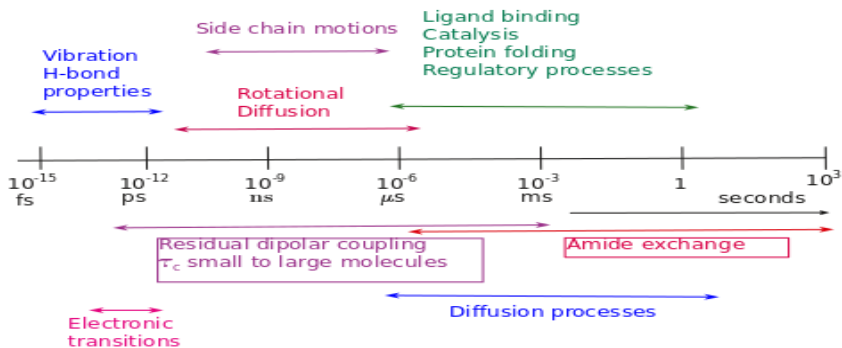
- ▶ The files used in this tutorial are provided in the **Code files** link
- ▶ Please download and extract the files
- ▶ Make a copy and then use them while practising



Timescale of Protein Motions



Timescale of Protein Motions



Timescale of Protein Motions



Timescale of Protein Motions

- ▶ In microsecond or millisecond timescale, ligand binding or folding is studied



Timescale of Protein Motions

- ▶ In microsecond or millisecond timescale, ligand binding or folding is studied
- ▶ These are computationally intensive processes



Timescale of Protein Motions



Timescale of Protein Motions

- Use a high performance computational facility or a GPU for longer calculations



Data Analysis



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Few examples of data analysis are,



Data Analysis

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▶ **Validation, visualization**



Data Analysis

Few examples of data analysis are,

- ▶ Validation, visualization
- ▶ Analysis of energetics, H-bonding



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- ▶ Analysis of energetics, H-bonding
- ▶ Secondary structure changes



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- ▶ Ligand Binding, surface analysis



Data Analysis

Few examples of data analysis are,

- ▶ Validation, visualization
- ▶ Analysis of energetics, H-bonding
- ▶ Secondary structure changes
- ▶ Ligand Binding, surface analysis
- ▶ Analysis of subset of atoms in the system



Computation Time



Computation Time

- ▶ Having more steps in MD takes longer time



Computation Time

- ▶ **Having more steps in MD takes longer time**
- ▶ **Use a computing facility to run these processes**



Computation Time

- ▶ Having more steps in MD takes longer time
- ▶ Use a computing facility to run these processes
- ▶ Take care not to overheat or burn your computer



Summary

- ▶ Completed 1ns production run for lysozyme
- ▶ About timescales of motions
- ▶ Time taken for simulation
- ▶ About output data and various types of data analysis



Summary

- ▶ Loaded the `xtc` trajectory file
- ▶ About `RMSD` trajectory tool and analysis
- ▶ Aligned a frame in the trajectory with a reference molecule



Assignment



Assignment

- ▶ Open the `log` file and go through the details
- ▶ Plot `RMSD` of `trace` (C-alpha) atoms
- ▶ Create `Ramachandran plot` of the lowest and highest energy structure



Assignment



Assignment

Using the `energy` command,



Assignment

Using the `energy` command,

- ▶ Plot solvent accessible surface area (SASA)
- ▶ Explore `gmxcheck`, and `ngmx` commands



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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