Visualization With VMD

Spoken Tutorial Project
https://spoken-tutorial.org
National Mission on Education through ICT
http://sakshat.ac.in

Rani Parvathy
IIT Bombay

12 November 2021

Learning Objectives

Learning Objectives

- **Open a `Gromacs` generated trajectory file**

Learning Objectives

- **Open a `Gromacs` generated trajectory file**
- **Play and view the frames in the trajectory**

Learning Objectives

- **Open a Gromacs generated trajectory file**
- **Play and view the frames in the trajectory**
- **Color and display selected frames**

Learning Objectives

Learning Objectives

- **Create a movie from the trajectory**

Learning Objectives

- **Create a movie from the trajectory**
- **Align structures from two different states of the protein**

System Requirements

System Requirements

- **Ubuntu Linux v20.04 OS**

System Requirements

- **Ubuntu Linux v20.04 OS**
- **VMD 1.9.3**

System Requirements

- **Ubuntu Linux v20.04 OS**
- **VMD 1.9.3**
- **VLC media player 3.0.8**

Pre-requisites

Pre-requisites

To follow this tutorial,

Pre-requisites

To follow this tutorial,

- **Learner must be familiar with basics of VMD**

Pre-requisites

To follow this tutorial,

- **Learner must be familiar with basics of VMD**
- **For pre-requisite tutorials please visit this site https://www.spoken-tutorial.org**

Code Files

Code Files

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

Code Files

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

Summary

- **Loaded a trajectory file**
- **Played and viewed frames from the trajectory**
- **Created a movie using the frames in the trajectory**

Summary

- **Changed color and viewed selected frames**
- **Aligned the starting and equilibrated structures of the protein**

Assignment

Assignment

- **Can `1AKI.pdb` be aligned with `npt.gro` with the `mesure fit` command?**
- **Explain the reasoning and demonstrate it**

Assignment

Assignment

- **Create a new representation for** `npt.gro` **molecule**
- **In** `Selected atoms`**, enter,** `water and within 2 of protein`
- **This displays water molecules present only within 2Å of protein**

Assignment

Assignment

- **Play the trajectory and notice the movement of water molecules**

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**

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**
- **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

Spoken Tutorial Project is supported by

- **National Mission on Education through ICT (NMEICT)**
- **Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching (PMMMNMTT)**

MoE, Government of India