

Energy Minimization

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

- ▶ Unfavorable interactions in the Gromacs generated file



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- ▶ Unfavorable interactions in the `Gromacs` generated file
- ▶ Commands to set up energy minimization



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- ▶ Unfavorable interactions in the `Gromacs` generated file
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- ▶ `mdrun` command & verbose option



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- ▶ Commands to set up energy minimization
- ▶ `mdrun` command & verbose option
- ▶ About `edr` file



Learning Objectives



Learning Objectives

- ▶ **Parameters for energy minimization**



Learning Objectives

- ▶ **Parameters for energy minimization**
- ▶ **The energy command**



Learning Objectives

- ▶ **Parameters for energy minimization**
- ▶ **The `energy` command**
- ▶ **Create a file containing potentials in `xvg` format**



Learning Objectives

- ▶ Parameters for energy minimization
- ▶ The `energy` command
- ▶ Create a file containing potentials in `xvg` format
- ▶ Plot and check the output file with `Grace`



System Requirements



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► Ubuntu Linux v20.04 OS



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- ▶ **Gromacs v2021.2**



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- ▶ **Grace v5.1.25**
- ▶ **QtGrace v0.2.6 fork for Windows**



Pre-requisites



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To follow this tutorial,



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To follow this tutorial,

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



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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



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- ▶ Please download and extract the files



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- ▶ Make a copy and then use them while practising



Summary

- ▶ Unfavorable interactions in the `Gromacs` generated file
- ▶ Commands to set up energy minimization
- ▶ About `mdrun` & verbose option
- ▶ About `edr` file



Summary

- ▶ Parameters for energy minimization
- ▶ About `energy` command
- ▶ Created a file containing potentials in `xvg` format
- ▶ Plotted the `xvg` file with `Grace`



Assignment



Assignment

- ▶ Extract few more parameters from the `edr` file with the `energy` command
- ▶ Create and view the graphs with a plotting program of your choice



Assignment



Assignment

- ▶ Open the `em.gro` file in `VMD` or another program of your choice
- ▶ Ascertain the protein molecule is seen as one unit in the box



About 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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